Towards an extension of the Hudson's theorem to mixed quantum states

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In this work, we make a step towards the extension of the Hudson's theorem to mixed 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, the purity of the states and the purity of Gaussian states determined by the same covariance matrix as of these states. Even though the bounds are not tight, they permit for a preliminary visualization of the space of states with positive Wigner functions and for the derivation of a bound on the purity of a state with strictly positive Wigner function and a given covariance matrix.

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I. INTRODUCTION

The Wigner representation of quantum states [1], which is realized by joint quasi-probability distributions 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 R.L. Hudson [2] and later generalized to multi-mode quantum systems by F. Soto et al [3], that the only states which have positive Wigner functions are the Gaussian ones. The question that naturally arises [2], is whether this theorem can be extended to mixed states, among which not only the Gaussian states may possess a positive Wigner function. A logical extension of the theorem would be a complete characterization of the set of such states. However, this has not been yet achieved due to the mathematical complications which emerge when one deals with convex sets of quantum states [4].

Motivated by the increasing interest and need for better understanding of de-Gaussified mixed states [5], we explore the space of states with positive Wigner functions using as a reference point the Gaussian states. We obtain a partial solution to the problem, by analytically deriving necessary conditions (bounds) on the non-Gaussianity for a state to have a positive Wigner functions. The set of conditions depend on the purity of the state and on the purity of the corresponding Gaussian state via parametric functions which can be visualized in a three dimensional space. As it is intuitively expected, the ultimate degree of non-Gaussianity is increasing with the decrease of the purity of the Gaussian reference state.

Furthermore, our derived conditions permit, in principle, the existence of non-Gaussian states less or more pure than the corresponding Gaussian ones. We present several physical examples of states less pure than the corresponding Gaussian states. This is in contrast with other measures, such as the von Neumann entropy, where the Gaussian states are extremal.

Before we derive the main results, we would like to 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,

$$\mathrm{Tr}\left(\rho\rho'\right) = 2\pi \int\int \mathrm{d}x\mathrm{d}p W_{\rho}\left(x,p\right) W_{\rho'}\left(x,p\right). \qquad (1)$$

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

Our aim is to derive bounds 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 and displacement vector. 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 [6],

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

which was especially constructed to quantify the non-Gaussian character of ρ. The domain of values for δ is $[0,\varepsilon]$, with $\varepsilon < 1$ and 0 is attained *iff* $\rho \equiv \rho_G$. For one-mode states it is conjectured in [6] that $\varepsilon = 1/2$.

II. BOUNDS ON NON-GAUSSIANITY

In a first step, we are going to derive the bounds for $\mathrm{Tr}\left(\rho\rho_G\right)$. It is then straightforward to express these bounds in terms of the distance $\delta\left[\rho,\rho_G\right]$, as $\mu[\rho_G]$ and $\mu[\rho]$ are included in the conditions of the problem.

A. Upper Bounds and ultimate distance

One can employ the expression Eq.(1) to reformulate the problem as an optimization problem that can be tackled with the method of Lagrange multipliers. More specifically we derive the desired bounds by extremizing the functional $I[W_\rho] = \mathrm{Tr}\,(\rho\rho_G)$ represented by Eq. (1) and being constrained by the condition that the Gaussian Wigner function W_{ρ_G} and the positive distribution W_ρ, are possessing the same first and second moments. In order to simplify our derivation, we apply a symplectic transformation S on the states, $S\rho S^\dagger$, $S\rho_G S^\dagger$ such that the Gaussian state becomes symmetric in x and p. Since the functional and also the purities of the states are invariant under such operations, the problem is now reduced to a simpler equivalent one with the Gaussian state being a thermal state centered in zero and of variance C. Furthermore, we claim that the function W_ρ^{ex} which extremizes the functional $I[W_\rho]$ is symmetric as well under rotation in the $x-p$ plane and we justify this assumption at the end of the derivation.

After having applied the symplectic transformation and under the assumption of symmetric solutions, the functions W_ρ and $W_{\rho_G}(r) = \frac{1}{2\pi C}\mathrm{e}^{-r/2C}$ depend only on the radius squared $r = x^2 + p^2$ and the functional $I[W_\rho]$ obtains a simpler form

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

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

1. It vanishes for $r = r_B$ and r_A, it is positive for $r_B < r < r_A$, and zero elsewhere. Below, we show that the maximum number of roots is indeed two.

2. It is normalized
$$\pi \int_{r_B}^{r_A} W_\rho(r) dr = 1. \qquad (5)$$

3. It is constrained to have the same variance as the corresponding Gaussian state, ρ_G
$$\pi \int_{r_B}^{r_A} W_\rho(r) r dr = 2C = 1/\mu\,[\rho_G]\,. \qquad (6)$$
We note here that the Heisenberg uncertainty relation is satisfied for both ρ and ϱ_G, *iff* $C \geqslant 1/2$.

4. The state ρ is of purity $\mu[\rho]$,
$$\mu[\rho] = 2\pi^2 \int_{r_B}^{r_A} W_\rho^2(r) dr. \qquad (7)$$

5. It is square integrable and continuous.

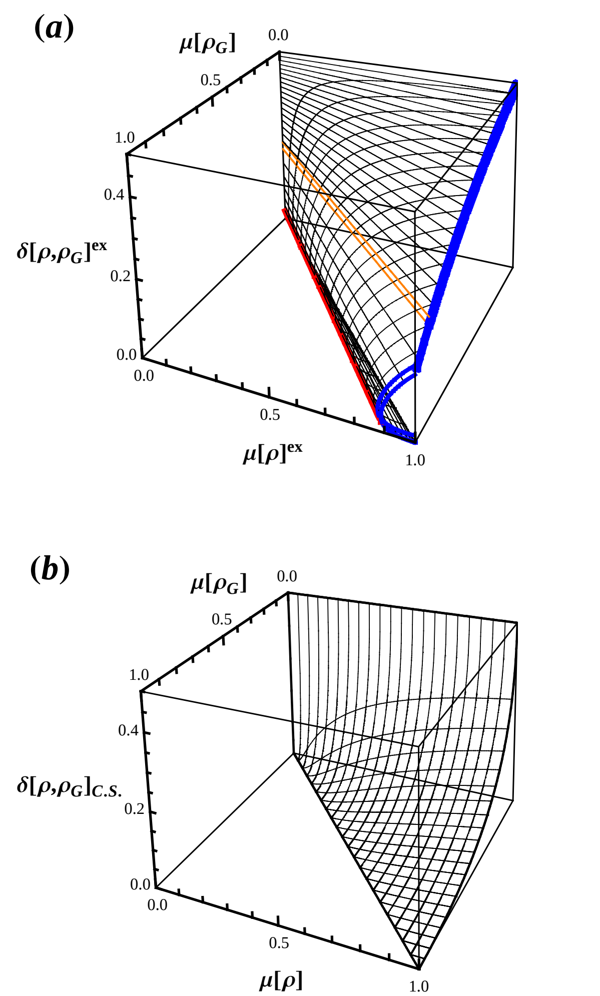

FIG. 1: *(a)* The bounds on the non-Gaussianity $\delta\,[\rho,\rho_G]^{ex}$ derived with the method of Lagrange multipliers. The *double horizontal orange* line marks the boundary between the two branches of solutions. The *blue single* line indicates the intersection with the plane $\mu\,[\rho_G] = 1$ (but also $\delta^{u.ult}$) and the *blue double* line with the plane $\mu\,[\rho_G] = 1$. The *red* line denotes the left extremity of the surface. The 'vertical' grid lines correspond to different $\mu\,[\rho_G]$ and the horizontal to parameters α and β. *(b)* The physical part of the lower bound on non-Gaussianity $\delta\,[\rho,\rho_G]_{C.S.}$ given by the Cauchy Schwarz inequality.

We would like to point out here that without the requirement of the positive definiteness of the operator ρ, the set of conditions listed above is *not sufficient* to constrain the solutions to eligible Wigner functions. To our knowledge no applicable criterion on phase-space functions does exist, ensuring that the operator ρ is physical (see [7] for an extensive discussion). On the other hand, one might be able to prove a quasi-probability distribution unphysical by using a theorem [8] which states that a square integrable and normalized function is a Wigner function, *iff* its overlap with the Wigner function of *every* pure state is positive.

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

$$W_\rho^{ex}(r) = A_1 + A_2 \frac{1}{2\pi C} \mathrm{e}^{-r/2C} + A_3 r\,, \tag{8}$$

with $A's$ to be defined by the constrains *2-4*. The condition *5* limits the class of possible $W_\rho^{ex}(r)$ functions in Eq. (8) to those that have two, one or zero roots. The latter case is the trivial one where $W_\rho^{ex}(r)$ coincides with the $W_{\rho_G}(r)$ and thus $\delta\left[\rho,\rho_G\right]$ becomes zero. We treat the two other cases separately and obtain two continuously connected branches of solutions for W_ρ^{ex}. The expressions that we obtain for $\mathrm{Tr}\left(\rho\rho_G\right)^{ex}$ and $\mu[\rho]^{ex}$ are highly non-linear so that it is not possible to derive an analytic expression that connects "directly" the two quantities. Nevertheless, we are able to express the extremum solutions in a form of parametric functions.

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

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

$$\mathrm{Tr}\left(\rho\rho_G\right)^{ex} = \mu[\rho_G] 2 Exp\left[-\frac{\alpha\left(\alpha + e^{\alpha}(2\alpha-3)+3\right)}{3\left(e^{\alpha}(\alpha-2)+\alpha+2\right)}\right]\left(e^{\alpha}-1\right)/\alpha, \tag{10}$$

where $\mu[\rho_G] \in (0,1]$. By imposing the condition $r_B > 0$ we obtain the following bounds $\alpha \in (0, x_r]$, with x_r being the root of the equation

$$e^x(x-3) + 2x + 3 = 0. \tag{11}$$

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

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

$$\mathrm{Tr}\left(\rho\rho_G\right)^{ex} = \mu[\rho_G]\frac{4(\beta(\cosh(\beta)+2) - 3\sinh(\beta))}{2e^{\beta}(\beta-3)+\beta(\beta+4)+6}, \tag{13}$$

where $\mu[\rho_G] \in (0,1]$ and $\beta = r_A\mu[\rho_G]$. The range of the parameter is $\beta \in [x_r, \infty)$.

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

$$\begin{aligned} W_\rho^{ex}(x,p) &= A_1 + A_2\frac{1}{2\pi C}\mathrm{e}^{-\left(x^2+p^2\right)/2C} \\ [2ex] &+ A_3x^2 + A_4p^2 + A_5xp, \end{aligned} \tag{14}$$

which is the analogue of Eq. (8). We can apply a symplectic rotation on the states ρ and ρ_G, to eliminate the term A_5xp in Eq. (14). Such a rotation does not affect the Gaussian state or the overlap and the resulting function has a form of an ellipsoid in the phase space. The conditions $\langle x^2\rangle = \langle p^2\rangle = C$ then can be satisfied *iff* $A_3 = A_4$. Thus, the most general solution reduces to the symmetric one, Eq.(8).

With the help of the derived bounds on the trace overlap, Eqs. (9)-(10),(12)-(13), we plot in Fig. 1(a) the corresponding bounds on the distance $\delta\left[\rho,\rho_G\right]^{ex}$. By direct inspection of the graph we conclude that the intersection of surface bound with the plane $\mu[\rho]=1$ provides us with an upper bound to the distance between a Gaussian state of purity $\mu\left[\rho_G\right]$ and any state with the same covariance matrix and positive Wigner function. We call it the *ultimate upper bound* $\delta^{u.ult}\left(\mu\left[\rho_G\right]\right)$ (see also Fig. 2 (b)) and its parametric expression can be directly derived by setting $\mu^{ex}[\rho]=1$ in Eqs. (9)-(10),(12)-(13).

Concerning the question of the physicality of the functions Eq.(8), by simply resorting to Hudson's theorem we can conclude that the intersections with the planes $\mu[\rho] = 1$ and $\mu[\rho_G] = 1$ (see Fig. 1(a)) cannot correspond to physical states. In order to arrive to more

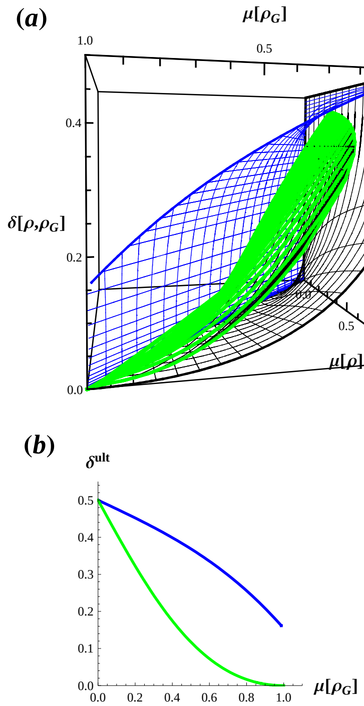

FIG. 2: *(a)* The upper (blue) and lower "Cauchy-Schwarz" (black) bounds on the non-Gaussianity of one-dimensional states with a positive Wigner function and the trial mixed state (green) Eq. (16). *(b)* The two curves,$\delta^{l.ult}$ and $\delta^{c.ult}$, limit the region where the tight ultimate bound for non-Gaussianity must be sited.

accurate conclusions we apply the theorem [8] and using the first five eigenstates of the quantum harmonic oscillator as test pure states, we prove that the functions of Eq. (8) are unphysical, hence, *our bounds are not tight.*

B. Lower Bounds

From Fig. 1(a) we observe that the bounds derived by using the method of Lagrange multipliers confine δ only from above. In order to obtain a lower bound we need to find an upper bound on the trace distance. This we can do by applying the Cauchy Schwarz inequality for the Wigner representation of the trace overlap, Eq. (1), and after recalling the definition of purity we arrive at

$$\mathrm{Tr}\left(\rho\rho_G\right) \leq \sqrt{\mu\left[\rho_G\right]\mu\left[\rho\right]} \equiv \mathrm{Tr}\left(\rho\rho_G\right)_{C.S.} \qquad (15)$$

where $C.S.$ stands for "Cauchy Schwarz".

We note here that the only property of the functions W_ρ and W_ρ^G that we have used is the non negativity. Consequently $\mathrm{Tr}\left(\rho\rho_G\right)_{C.S.}$ is not a strict bound and we expect that the requirement 3 may further constrain the upper limit in Eq. (15).

C. The Convex Set of Coherent states

The bounds Eqs. (9)-(10), (12)-(13), and (15) provide us with the necessary conditions for a one-mode mixed state to posses a positive Wigner function. The subset of convex combinations of pure Gaussian states (squeezed and displaced) is properly contained in the set of all positive Wigner functions [4]. Thus, identifying the extremities for this set could supply us with a lower estimation on the tight upper bound. Even though we have not been able to find a universal analytic solution to this optimization problem we have considered different mixtures of pure Gaussian states, such as, an optimized continuous convex combination of displaced coherent states, a "ring" of squeezed states, different discrete convex combinations of squeezed and coherent states. The visualization of the ensemble of the results is not perspicuous and therefore we have chosen to present in Fig. 2(a) only one of them, which consists of the states with the Wigner function of the form

$$W_\rho\left(x,p,q,s\right) = \alpha \mathrm{e}^{-\frac{(x-q)^2}{s}-p^2 s} + (1-\alpha)\mathrm{e}^{-\frac{(x+q)^2}{s}-p^2 s}. \qquad (16)$$

In the limit of pure states, $\mu[\rho] \to 1$, these states are the most non-Gaussian states among all different trial mixtures that we considered, achieving the highest distance $\delta^{c.ult}$. We have derived an analytic expression for it, $\delta^{c.ult}(x) = \frac{1}{2}(1 + x - 2\sqrt{2}x/\sqrt{1+x^2})$ where $x = \mu\left[\rho_G\right]$, by considering $\alpha \to 0$ and keeping the product $\alpha s q^2$ constant. The curve $\delta^{c.ult}$ (see Fig. 2(b)) gives a lower estimation on the tight upper ultimate bound. The tight bound is sited between the curves $\delta^{c.ult}$ and $\delta^{u.ult}$ in Fig. 2(b).

III. BOUNDS ON THE PURITY

One may notice in Fig. 1(a) that the left extremity of the bound (red line) is to the left of the plane $\mu[\rho_G] = \mu[\rho]$. This means that the bounds allow, in principle, the existence of states less pure than the corresponding Gaussian states. Can this possibility be realized by some physical states? Knowing about the extremality of Gaussian states [9], in particular, in terms of the von Neumann entropy, one could expect that Gaussian states are also the "least pure" states. However the answer to our question is positive and in the Appendix we demonstrate this with specific examples.

In addition, this left extremity of the surface in Fig. 1(a) limits the purity of a quantum state with positive Wigner function, for a given purity of the corresponding Gaussian state. To derive analytically this bound we employ once again the method of Lagrange multipliers but now for the functional Eq. (7) of the purity, under the constraints Eq.(5) and Eq.(6). The extremum is realized by the function,

$$W^{\mathrm{ex}}(r) = \frac{2}{3\pi}\mu[\rho_G]\left(1 - \frac{r\mu[\rho_G]}{3}\right) \qquad (17)$$

where $r \in [0, 3/\mu[\rho_G]]$ so that $W(r)$ remains everywhere positive. Positivity of second variation ensures that we have found a solution that minimizes the purity functional, and therefore a lower bound on the purity

$$\mu[\rho]^{ex} = \frac{8}{9}\mu[\rho_G]. \tag{18}$$

We plot in Fig. 3 (straight line) the difference $\mu[\rho]^{ex} - \mu[\rho_G]$ as a function of $\mu[\rho_G]$. Together, we present the function $\mu[\rho]-\mu[\rho_G]$, derived numerically or analytically, for three different examples (see Appendix) for which this function indeed attains negative values, i.e. $\mu[\rho] < \mu[\rho_G]$.

The derived limit Eq.(18) is consistent with the fact that for classical distributions the Rényi entropy is maximized by the Student distribution [10], since purity corresponds to Rényi entropy of order two and $W^{\rm ex}(r)$ realizes the Student distribution. However, this bound is unphysical for quantum state since the overlap of Eq.(17) with the Wigner function of the first number state is negative for all values of $\mu[\rho_G]$. Indeed, in Fig. 3 we see that for $\mu\left[\rho_G\right] \to 1$ all physical examples are far from our bound in agreement with Hudson's theorem. Nevertheless, in the limit of maximally mixed states $\mu\left[\rho_G\right] \to 0$ our bound Eq. (18) is asymptotically tight.

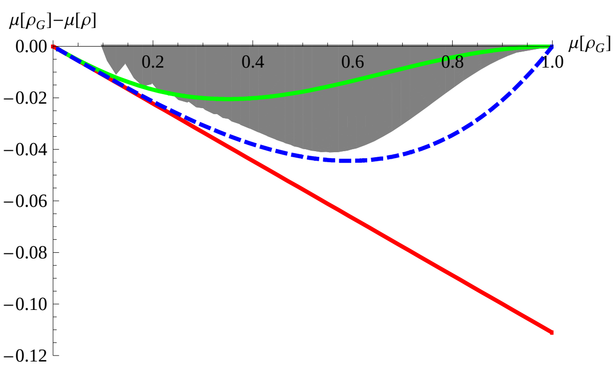

FIG. 3: Difference between the lower bounds for purity of quantum states and the purity of corresponding Gaussians. Lower *straight red* line: positive Wigner functions. *Green* line (in the grey region): optimized mixture of coherent states. *Blue dashed* line: convex combinations of number states. Grey region: "ring" of squeezed states.

IV. CONCLUSIONS

In conclusion, we have found upper and lower bounds on the non-Gaussianity of mixed states with positive Wigner function, only depending on the purity and covariance matrix of the states. In addition, we have obtained a lower bound on the purity of states with positive Wigner functions in terms of the purity of the corresponding Gaussian states. Interestingly, Gaussian states turn out not to be extremal with respect to purity. An open question remains to derive tighter bounds.

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APPENDIX: EXAMPLES OF MIXED STATES

1. Optimized mixture of coherent states

The first example we examine is a symmetric convex combination of coherent displaced states,

$$W^{\rm coh}(x,p) = \int\int \frac{{\rm d}x_0 {\rm d}p_0}{\pi} \alpha(x_0,p_0) e^{(x-x_0)^2+(p-p_0)^2}.$$

where $\alpha(x_0,p_0)$ is a classical distribution which depends only on radius of displacement $r_0 = x_0^2 + p_0^2$. The Lagrange multipliers method provides us with a lower bound for the purity of these states realized by

$$\alpha(r_0) = \frac{2}{3\pi}\frac{\mu[\rho_G]}{1-\mu[\rho_G]}\left(1 - \frac{\mu[\rho_G] r_0}{3(1-\mu[\rho_G])}\right).$$

We evaluate the purity $\mu[\rho_G]^{ex.{\rm coh}}$ numerically and plot its difference from $\mu[\rho_G]$ in Fig. 3 (the green line).

2. "Ring" of squeezed states

An example that comes closer to our bound Eq.(18) is a convex combination of Gaussian states displaced uniformly on a circle, and squeezed along the radius

$$W^{\rm sq}(x,p,r,s) = \frac{1}{2\pi^2}\int_0^{2\pi} d\theta e^{(x\cos\theta - p\sin\theta - r)^2 s + (x\sin\theta + p\cos\theta)^2/s}. \tag{19}$$

The parameter r is the displacement parameter, the radius of the "ring" and s is the squeezing parameter. The purity of this state and of the corresponding symmetric Gaussian states are

$$\begin{aligned} \mu[\rho] &= \frac{\sqrt{2}}{\pi} s \int_0^{2\pi} d\theta \frac{e^{\frac{\left(\mu_G(1+s^2)-2s\right)(1-\cos\theta)}{\mu_G(1+(s^2-1)\cos\theta+s^2)}}}{\sqrt{1+6s^2+s^4-(s^2-1)\cos 2\theta}} \\ \mu[\rho_G] &= 2s/(s^2+2sr^2+1). \end{aligned}$$

We do not perform any optimization. The gray region in Fig. 3 corresponds to the parametric plot of these equations for a representative range of the parameters r and s.

3. Mixture of number states

The last example we consider does not belong to the set of states with positive Wigner functions. This is the set of states formed by finite convex combinations of the number states,

$$\rho_N = \sum_{n=0}^{N} P_n |n\rangle\langle n|, \quad \forall n, P_n \geq 0 \quad \sum_{n=0}^{N} P_n = 1\,. \tag{20}$$

where N limits the number of photons in the number states present in this combination. The purity of such states, and the purity of the corresponding Gaussian states are

$$\sum_{n=0}^{N} P_n^2 = \mu[\rho_N]\,, \quad \sum_{n=0}^{N} P_n(n+1/2) = 1/2\mu\left[\rho_G\right]\,.$$

Assuming N large enough for the Lagrange multipliers method to be valid, we find P_n that minimizes the purity

$$\begin{aligned} P_n &= \frac{4\mu\left[\rho_G\right]}{3+\mu\left[\rho_G\right]}\left[1-\frac{2n\mu\left[\rho_G\right]}{3-\mu\left[\rho_G\right]}\right], \\ \mu\left[\rho\right]^{ex.N} &= 8\mu\left[\rho_G\right]/\left(9-\mu\left[\rho_G\right]^2\right)\,. \end{aligned} \tag{21}$$

where $n \leq \left(3-\mu\left[\rho_G\right]\right)/(2\mu\left[\rho_G\right])$. The obtained result Eq.(21) is plotted in Fig. 3 as blue dashed line.

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