Discrete Wigner distribution for two qubits: a characterization of entanglement properties

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Abstract. We study the properties of the discrete Wigner distribution for two qubits introduced by Wotters. In particular, we analyze the entanglement properties within the Wigner distribution picture by considering the negativity of the Wigner function (WF) and the correlations of the marginal distribution. We show that a state is entangled if at least one among the values assumed by the corresponding discrete WF is smaller than a certain critical (negative) value. Then, based on the Partial Transposition criterion, we establish the relation between the separability of a density matrix and the non-negativity of the WF’s relevant both to such a density matrix and to the partially transposed thereof. Finally, we derive a simple inequality –involving the covariance-matrix elements of a given WF– which appears to provide a separability criterion stronger than the one based on the Local Uncertainty Relations.

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1. Introduction

A quantum system with continuous degrees of freedom can be represented in terms of a Wigner Function \[2\] defined as a real function on the phase space. The Wigner function (WF) is similar to a probability distribution (its integration over the phase space is normalized to one) even if it can take negative values on restricted domains. There is an extensive literature on the continuous-system WF \[3\]-\[5\] due to its wide applicability in different contexts of physics. Concerning the WF of discrete systems, the literature is less extensive even if this theme has recently attracted a lot of interest mainly in view of the role that a discrete phase-space structure can play within Quantum Information Theory \[1\], \[6\]-\[14\]. In this respect paper \[7\] contains a useful list of references. Different generalizations of the WF to quantum systems with a finite-dimensional Hilbert space have been proposed in the literature such as 1) the continuous WF for spin variables \[15\] and 2) the definitions of WF based on a discrete phase space. As to the latter, early studies were made in \[16, 17\]. A discrete WF has been introduced in \[1\] and \[18\] which generalizes the \(2 \times 2\) case of \[17\] and is valid for systems having a \(N\)-dimensional Hilbert space, with \(N\) a prime or a power of a prime. More recently, an alternative definition of WF involving Galois fields \[6\]-\[8\] has allowed the study of the composite-dimensional case and evidenced several interesting tomographic properties \[6, 19\].

The present article is focused on studying the entanglement properties of a two-qubit system by using the discrete WF defined in \[1\]. It is worth noting that two-qubit (and more in general many-qubit) systems have received an increasing attention, not only within spin models, but also in the recent literature on optically trapped bosons modelled within the Bose-Hubbard picture \[20\]. The impressive experimental progress in controlling the spatial trapping of bosons makes the realization of many-qubit systems a quite realistic objective. In this paper we find some new separability criteria and recast other known criteria in terms of discrete WF’s. We check them evaluating two-qubit entanglement and show that the discrete WF describes both classical and quantum correlations better than the density-matrix approach. We note how using the WF not only improves the visualization of the system state but is also expedient experimentally: since the WF is directly related to tomographic techniques, the separability criteria coming from the WF do not require to know of all the matrix elements.

In section 2, we review the definition of discrete phase-space given in reference \[11\] –this is particularly useful for our purposes– and the corresponding discrete Wigner and Characteristic functions. We present some basic properties of these functions which provide a useful tool for studying quantum correlations. In section 3 we consider four different separability criteria in terms of the two-qubit discrete WF and of its covariance matrix. In particular, we show that 1) there is a negative value of discrete WF that allows one to discriminate between separable and entangled states, 2) the Partial Transposition criterion can be reformulated in terms of the two-qubit discrete WF, 3) there is a nontrivial link between the separability of the density matrix and the non-negativity of the WF’s corresponding both to the density matrix and to its
partial transposed matrix, 4) the Local Uncertainty Relations relevant to phase space operators can be generalized in terms of the WF covariance matrix (thus evidencing the difference between classical and quantum correlations), and 4) the Generalized Uncertainty Principle, so far studied for WF’s relevant to continuous phase space, is extended to the case of a discrete WF.

2. Discrete phase space and Wigner function

In a discrete $r$-dimensional Hilbert space, with $r$ a prime number, the phase space can be defined \[\{1\}\] as a $r \times r$ array of points. The latter can be labelled by pairs of coordinates $\alpha = (q,p)$, each taking values from 0 to $r - 1$. For each coordinate we define the usual addition and multiplication mod $r$ thus obtaining the structure of a finite mathematical field $F_r$ with $r$ elements (0, 1, ..., $r-1$). If the dimension is $N = r^n$, with $r$ prime and $n$ an integer greater than 1, the discrete phase space can be built in two ways, both giving a discrete phase space formed by a $N \times N$ grid: the first involves the extension $F_N$ of the primitive field $F_r$ \[\{7, 21\}\], while the second is based on performing the $n$-fold cartesian product of $r \times r$ phase spaces \[\{1\}\]. In the present article we will use this last definition of discrete phase-space (entailing the definition of WF given in \[\{1\}\]). The choice of phase-space structure is justified by the direct connection with the tensor-product structure of the Hilbert space ensuing from the decomposition of the system in two or more subsystems, which is a useful feature for studying the entanglement. According to this definition, the phase-space points $\alpha$ are labelled as $n$-tuple $(\alpha_1, \alpha_2, ..., \alpha_n)$ of coordinates, each $\alpha_i$ pertaining to the $i$-th subsystem. In each subsystem with prime dimension $r$ we can build standard lines as set of points satisfying equation $(uq + vp)_{modr} = c$. However, we cannot define uniquely lines over the entire phase space (with modular arithmetic): in reference \[\{7\}\] there is an example of two sets of points which form two parallel ”lines” but intersect in two distinct points. Nevertheless, we can define the alternative concept of slice \[\{1\}\]: given a set of $n$ lines \{$\lambda_i$\} (one for each subsystem), the slice is the set of all points $\alpha = (\alpha_1, \alpha_2, ..., \alpha_n)$, where $\alpha_i \in \lambda_i$. A weaker notion of parallelism can be defined: two slices are parallel if each of the $n$ lines forming the first slice are parallel to the corresponding $n$ lines of the second slice.

2.1. Definition of the discrete WF

The discrete WF relevant to a $N = r^n$-dimensional system can be defined \[\{1\}\] by means of the set of discrete phase-point operators $\hat{A}(\alpha)$ (or $\Delta(\alpha)$ \[\{9\}\]). Consistently with the definition of phase space in terms (of cartesian product) of constituent subspaces \[\{1\}\], phase-point operators $\hat{A}(\alpha)$ are defined as tensor product of phase-point operators relevant to the corresponding subsystems: $\hat{A}(\alpha) \equiv \hat{A}(\alpha_1) \otimes \hat{A}(\alpha_2) \otimes ... \otimes \hat{A}(\alpha_n)$. Since they form a complete orthogonal basis for the Hermitian $N \times N$ matrices, any density matrix can be written as $\hat{\rho} = \sum_\alpha W(\alpha)\hat{A}(\alpha)$, where the real-valued coefficients

$$W(\alpha) = \frac{1}{N} tr[\hat{\rho}\hat{A}(\alpha)]$$ (1)
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represent the discrete Wigner function (also called the discrete Weyl symbol). Phase-
point operators exhibit two basic properties: i) for any couple of points \((\alpha_1, \alpha_2)\)

\[
tr[\hat{A}(\alpha_1)\hat{A}(\alpha_2)] = N\delta(\alpha_1, \alpha_2),
\]

(2)

ii) given any slice \(\lambda\) in the phase space, the projector relevant to \(\lambda\) can be written as

\[
\hat{P}_\lambda = \frac{1}{N} \sum_{\alpha \in \lambda} \hat{A}(\alpha).
\]

(3)

The latter definition implies that the set of all \(\hat{P}_\lambda\), for which \(\lambda\) is parallel to \(\lambda\) forms a set of mutually orthogonal projection operators. Moreover, given the slice \(\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_n)\), then \(\hat{P}_\lambda\) is the tensor product \(\hat{P}_{\lambda_1} \otimes \hat{P}_{\lambda_2} \otimes \cdots \otimes \hat{P}_{\lambda_n}\) of projectors relevant to the subsystems. Such properties, analogous to those characterizing continuous phase-point operators \[1\], can be used to derive the discrete-WF properties. Owing to formulas \[2\] and \[3\] discrete WF’s feature two crucial properties. First, if \(W(\alpha)\), \(W'(\alpha)\) correspond to density matrices \(\rho\), \(\rho'\), respectively, then formula \[2\] entails that

\[
N \sum_{\alpha} W(\alpha)W'(\alpha) = tr(\rho\rho').
\]

(4)

Second, due to equation \[3\] given a complete set of \(N\) parallel slices, for each slice \(\lambda\), the \(N\) real numbers \(p_\lambda = \sum_{\alpha \in \lambda} W_\alpha\) are the probabilities of the outcomes of a specific measurement associated with \(\lambda\). Hence \(\sum_\alpha W_\alpha = 1\) (normalization property).

Let us consider first the simple case \(N = 2\) (single qubit). The phase-point operators can be written in terms of Pauli matrices as \[1\]

\[
\hat{A}(\alpha) = \frac{1}{2} \left[I + (-1)^q \sigma_z + (-1)^p \sigma_x + (-1)^{q+p} \sigma_y\right], \quad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}
\]

and \(\sigma_z = [\sigma_x, \sigma_y]/2i\). The single-qubit phase space is the set of points \(\alpha = (q, p)\), where \(q, p = 0, 1\), exhibiting properties of \(F_2\). Since the density matrix for a general one-qubit state can be written (within the standard computational basis) in terms of three independent real elements \(\rho_{00}, Re(\rho_{01}), Im(\rho_{01})\), we have

\[
W(q, p) = \frac{1}{4} \left\{[1 + (-1)^q] \rho_{00} + [1 - (-1)^q] \rho_{11} + (-1)^p 2 Re(\rho_{01}) + (-1)^{q+p} 2 Im(\rho_{01})\right\}.
\]

In the case of two qubits, the WF has a more complex expression. Upon noting that the phase space operators are defined as \(\hat{A}(\alpha_1, \alpha_2) = \hat{A}(\alpha_1) \otimes \hat{A}(\alpha_2)\), the WF becomes

\[
W(q_1, q_2, p_1, p_2) = \frac{1}{4} tr[\hat{\rho} \hat{A}(q_1, p_1) \otimes \hat{A}(q_2, p_2)].
\]

(5)

When necessary, we shall write \(W_\rho\), where the subscript means that the WF is associated to density matrix \(\rho\).

2.2. The discrete characteristic function

The set \(\{I, \sigma_x, \sigma_y, \sigma_z\}\) forms an orthogonal basis for the set of hermitian operators acting on a single qubit. Thus any density matrix \(\rho\) for a single qubit can be written as

\[
\rho = \frac{1}{2} \sum_{uv} \chi(u, v) \hat{S}(u, v)
\]

while the characteristic function for a single qubit is

\[
\chi(u, v) = tr[\rho \hat{S}(u, v)]
\]

(6)
where $\hat{S}(0,0) = I$, $\hat{S}(1,0) = \sigma_x$, $\hat{S}(0,1) = \sigma_z$, and $\hat{S}(1,1) = \sigma_y$. When necessary, we write the argument $\beta$ instead of $(u,v)$, or the single index $i$, where $i = u + 2v$ assuming integer values from 0 to 3. In the case of two qubits, any density matrix can be written as $\rho = \frac{1}{4} \sum_{\beta_1,\beta_2} \chi(\beta_1,\beta_2) S(\beta_1) \otimes S(\beta_2)$. The two-qubit characteristic function is thus defined as $\chi(\beta_1,\beta_2) = tr[\rho \hat{S}(\beta_1) \otimes \hat{S}(\beta_2)]$. Function $\chi(\beta)$ is connected with the discrete WF by a discrete Fourier transform. For example, in the single-qubit case ($r = 2$), $W(q,p) = \frac{1}{4} \sum_{\beta} (-1)^{(qu+pv)} \chi(u,v)$, and in the two-qubit case

$$W(q_1,q_2,p_1,p_2) = \frac{1}{16} \sum_{u_1,u_2,v_1,v_2} (-1)^{(q_1u_1+p_1v_1)+(q_2u_2+p_2v_2)} \chi(u_1,u_2,v_1,v_2).$$

It is worth noting that the determination of $\chi(\beta)$ is connected to a specific tomographic technique $[6]$. For example, in the case of spin $\frac{1}{2}$ particles, it consists of repeated measures of spin “up vs down” along three directions relevant to each particle. The WF can be determined via the previous equations from the characteristic function. The Inner Product Rule for $\chi(\beta)$ corresponding to formula $[4]$ is

$$\frac{1}{N} \sum_{\beta} \chi(\beta) \chi'(\beta) = tr(\rho \rho').$$

Operators $\hat{S}$ can be thought as translation operators. The single-qubit WF relevant to $\hat{\rho}' = \hat{S}(a,b) \hat{\rho} \hat{S}(a,b)\dagger$ is $W_{\rho'}(q,p) = W_{\rho}(q+a,p+b)$, where the sum in the argument is mod2. In the two-qubit case, operators $\hat{S}$ act as translation operators on each single-qubit phase space. This formalism supplies a useful tool for recognizing the translational covariance of the WF $[9, 10]$. 

2.3. Graphical representation, pure and mixed states.

The phase space of the single qubit is represented in table $[11]$ left panel. A simple example of WF is given by the spin $j = 1/2$ coherent state $|\xi\rangle = (|0\rangle + |1\rangle)/\sqrt{1 + |\xi|^2}$ (where $|0\rangle$ and $|1\rangle$ are the spin-up and the spin-down state, respectively), which is known to be the most general pure state for a single qubit. Given $|\xi\rangle$, the corresponding WF is depicted in table $[11]$ right panel. The WF can have only one negative element (otherwise, at least one probability associated to a direction would be negative) determined by $|\text{Re}(\xi) + \text{Im}(\xi)| > 1$ or $|\text{Re}(\xi) - \text{Im}(\xi)| > |\xi|^2$. An important observation is that, while most positive value of the single-qubit WF is 1/2, the most negative value $(1 - \sqrt{3})/4$ is assumed in correspondence to state $|\xi\rangle$ with $\xi = (1+i)/(1-\sqrt{3})$ $[6]$. These extremal values are useful to write a simple separability criterion.

In table $[2]$ we illustrate $W_\alpha = W(q_1,q_2,p_1,p_2)$ on the discrete phase-space points for the two qubit case, where the phase-space label is $\alpha = (\alpha_1,\alpha_2) = (q_1,q_2,p_1,p_2)$. This table is useful to clarify the notation we adopt for the WF (which differs from that of reference $[7]$). The purity character of a state can be evinced both from the WF and from the characteristic functions. From the general equations $[4]$ and $[7]$ we find

$$\frac{1}{N} \leq N \sum_\alpha W(\alpha)^2 = \frac{1}{N} \sum_\beta \chi(\beta)^2 = tr(\rho^2) \leq 1,$$

$\text{(8)}$
Table 1. Left panel: graphical representation of the discrete WF for one qubit. Right panel: an example of WF for SU(2) coherent state with $j = 1/2$ (up to a factor $1/2(1 + |\xi|^2)$)

| $p$ | $q$ | $W(0,0)$ | $W(1,0)$ | $W(0,1)$ | $W(1,1)$ | $1 - \text{Re}(\xi) - \text{Im}(\xi)$ | $|\xi|^2 - \text{Re}(\xi) + \text{Im}(\xi)$ | $1 + \text{Re}(\xi) + \text{Im}(\xi)$ | $|\xi|^2 + \text{Re}(\xi) - \text{Im}(\xi)$ |
|-----|-----|-----------|-----------|-----------|-----------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| 1   | 0   | W(0,1)    | W(1,1)    |           |           |                                 |                                 |                                 |                                 |
| 0   | 1   | W(0,0)    | W(1,0)    |           |           |                                 |                                 |                                 |                                 |

Table 2. Graphical representation of the discrete WF for two qubits $(p_1, p_2)$

| $(p_1, p_2)$ | W(00,00) | W(01,00) | W(10,00) | W(11,00) | W(00,01) | W(01,01) | W(10,01) | W(11,01) | W(00,10) | W(01,10) | W(10,10) | W(11,11) |
|-------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| (00, 01)    | W(00,00) | W(01,00) | W(10,00) | W(11,00) | W(00,01) | W(01,01) | W(10,01) | W(11,01) | W(00,10) | W(01,10) | W(10,10) | W(11,11) |

where the equality holds for pure states whereas the inequality is involved by mixed states. In order to define a ”mixed state” we recall that, upon introducing the basis $\{|e\rangle : \rho|e\rangle = p_e|e\rangle\}$ relevant to a given density matrix $\rho$, a state is ”mixed” when more than one eigenvalue $p_e$ is nonzero. In this case the system state is represented by $\rho = \sum_e p_e|e\rangle\langle e|$ where probabilities $p_e$ evidence the characteristic lack of information about the relative phases of the state superposition. An interesting feature of formula 8 is that the pseudo-probability WF can not be concentrated in a too small region of phase space. We will see that this is equivalent to the Uncertainty Principle.

2.4. Axis operators

In the single-qubit case the axis operators are defined as $\hat{\xi}_i = \frac{1}{2} \sum_{q,p} \xi_i(q,p) \hat{A}(q,p)$, where $\hat{A}(q,p) = (q + p)_{mod2}$, and $\xi_i(q,p) := q$ while $\hat{\xi}_1 = \hat{p}$, $\hat{\xi}_2 = \hat{d}$, and $\hat{\xi}_3 = \hat{q}$, (relevant to vertical, diagonal and horizontal lines) are the vertical, diagonal and horizontal axis operators, respectively. The explicit form of operators $\hat{\xi}_i$ reads

$$\hat{\xi}_i = \frac{1}{2} [I - \hat{S}(i)].$$

where $\hat{S}(i)$ is defined after formula 8. In this case operators $\hat{q}$ and $\hat{p}$ play the role of (discrete) position and momentum operators, respectively. The spectrum of such axis operators is completely determined by the (two-eigenvalue) spectrum of $\sigma_z$ and $\sigma_x$, respectively. In the sequel operator $\hat{d}$ will be named diagonal-direction (or simply diagonal) operator, since it is connected to the diagonal lines. Notice that $\hat{\xi}_i$ obey commutators $[\hat{\xi}_i, \hat{\xi}_j] = 2i\epsilon_{ijk}\hat{\xi}_k$ showing the SU(2) algebraic structure. Thus they have essentially the same physical meaning of the three Pauli matrices which is to describe two-level systems. The only difference is that the relevant eigenvalues are 0 and 1 (rather than $\pm1/2$) that are more useful for treating quantum information applications.
Analogously to the continuous case, we can define the anticommutator
\[
\{\hat{\xi}_i, \hat{\xi}_j\}_S = \frac{1}{2} (\hat{\xi}_i \hat{\xi}_j + \hat{\xi}_j \hat{\xi}_i)
\]
(where the label $S$ stands for standard). Differently from the continuous case, the mean value $\text{tr}(\rho \{\hat{\xi}_i, \hat{\xi}_j\}_S)$ cannot be written as sum over the phase-space points of $qpW(q,p)$. We thus introduce an alternative definition of anticommutator
\[
\{\hat{\xi}_i, \hat{\xi}_j\}_D = \frac{1}{2} (\hat{\xi}_i + \hat{\xi}_j - |\epsilon_{ijk}|k),
\]
where $D$ stands for discrete. This definition allows one to express the symmetrized product $\{\hat{q}_i, \hat{p}_j\}_D$ as a sum over the phase space of $W(q,p)$ multiplied by $qp$. In general,
\[
\langle \hat{\xi}_i \rangle = \sum_{q,p} \xi_i W(q,p), \quad \langle \{\hat{\xi}_i, \hat{\xi}_j\}_D \rangle = \sum_{q,p} \xi_i \xi_j W(q,p).
\]
The introduction of the symmetrized product (11) is motivated by the identity $\xi_i \xi_j = \frac{1}{2} [\xi_i + \xi_j - (\xi_i + \xi_j)_{mod2}]$ (with $\xi_i = q,p,d \in 0,1$).

In the two-qubit case ($N = 4$) we can perform nine possible measurements (nine combinations of Pauli matrices), corresponding to the nine striations of phase space. This tomographic scheme is not the most efficient since five orthogonal measurements suffice to determine the state. Nevertheless, we will consider such scheme (involving nine striation operators $\hat{\xi}_i \otimes \hat{\xi}_j$) in that it leads to a definition of the WF exhibiting more interesting entanglement properties.

3. Entanglement properties in two qubit systems

Given a two-qubit density matrix $\rho$, such a state is said to be separable if there exists a decomposition $\rho = \sum_k p_k |\psi_k\rangle \langle \psi_k| \otimes |\phi_k\rangle \langle \phi_k|$ (with the probabilities $\sum_k p_k = 1$). A nonseparable state is said to be entangled. If a state can be written as a density-matrix product $\rho = \rho' \otimes \rho''$ ($\rho', \rho''$ relevant to the two constituent subsystems) then the corresponding WF is written as $W(q_1, q_2, p_1, p_2) = W_{\rho'}(q_1, p_1)W_{\rho''}(q_2, p_2)$. Thus the WF associated to a separable state is
\[
W(q_1, q_2, p_1, p_2) = \sum_k p_k W'_k(q_1, p_1)W''_k(q_2, p_2).
\]
In this perspective —so far scarcely considered in the literature— an entangled state exhibits a WF that cannot be written in the form (13). If a classical probability distribution can be written non-trivially as $p(q_1, q_2, p_1, p_2) = \sum_i p_i t'_i(q_1, p_1)p''_i(q_2, p_2)$, the presence of more than one $p_k \geq 0$ indicates a (classical) correlation. The WF representation (13) clearly evidences that separable states display a classical-like correlation since the related WF’s have the same form of a classical distribution, whereas entangled states embody a different type of correlation named quantum correlation. We investigate the entanglement properties of two-qubit WF within 1) the negativity approach 2) a direct reformulation of PT criterion in terms of WF, 3) the study of non-negativity of WF relevant both to the density matrix and to its partial trasposed (deriving from the PT criterion) 3) the Local Uncertainty Relation (LUR) approach and 4) the Generalized Uncertainty Principle (GUP) of the continuous case.
Table 3. Left panel: graphical representation of the discrete WF for a two-qubits separable state with the most negative values. Right panel: graphical representation of the discrete WF for the singlet state

|       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|
| W(α_1) | W(α_2) | W(α_1)W(α_2) | singlet WF |
| + 0    | 0.394 | 0.394 |       |       |       |
| + 0    | -0.183 | 0.394 |       |       |       |
| -0.0915 | 0.197 | 0.197 | 0 0 0 0 |
| 0.197 | 0.197 | 0 0 0 0 |
| -0.0915 | 0.197 | 0 0 0 0 |

3.1. Negativity of WF and entanglement

We show that the negativity of $W_ρ$ can be connected to the non-separability. We give a sufficient condition for non-separability, based on the observations of subsection 2.3, where it is shown that any single-qubit WF assumes $(1 - \sqrt{3})/8$ as most negative value and 1/2 as most positive value. We can get a two-qubit WF with negative elements considering the product of WF’s of single qubit $W(α_1)W(α_2)$, where $W(α_1)$ has negative elements, while $W(α_2)$ is positive. The most negative value of such a two-qubit WF is given by considering the most negative value for $W(α_1)$ and the most positive value for $W(α_2)$, as exemplified in table 3 left panel. The minimum value we get is $(1 - \sqrt{3})/8 \approx -0.0915$, which is the lower limit not only for WF relevant to product states. It is easy to show that any convex combination of i.e. separable states have, as most negative value, $(1 - \sqrt{3})/8$. However, the value we have found is not in general the most negative value of a WF, as we can see in table 3 right panel. The state represented is the singlet state (a particular the Bell state), which results to be maximally entangled. Thus if the WF has a negative value $W(α) < (1 - \sqrt{3})/8$, the state is entangled. Of course, it a WF has all the values $W(α) \geq (1 - \sqrt{3})/8$, then the state can be entangled or separable. The Partial Transposition criterion, analyzed in next two sections, will be useful in such cases.

3.2. Partial transposition criterion

For all bipartite states (both discrete and continuous), the well-known partial-transposition (PT) criterion [29, 30] turns out to be a necessary condition for separability. In the 2 × 2 and 2 × 3 dimensional cases, it is also a sufficient condition.

In the discrete case, the transposition action on a single-qubit WF and on its characteristic function gives respectively $W_ρ^{T}(q,p) = W_ρ(q,p) - (-1)^{q+p} tr(\hat{ρ}\hat{σ}_y)$ and $χ_ρ^{T}(1,1) = -χ_ρ(1,1)$ (where $χ$ is unchanged for $(u,v) \neq (1,1)$). In the two-qubit case, the PT with respect to the second subsystem of $ρ$ provides the new operator $ρ^{T_2}$ whose matrix elements are $ρ^{T_2}_{mn} = ρ_{mn}$, where latin (greek) indices refer to the first (second) subsystem. The WF $W_ρ^{T_2}(α_1, α_2)$ corresponding to $ρ^{T_2}$ reads

$$\frac{1}{4} \sum_{mnμν} ρ_{mnμν} A^*_μν(α_1) A^*_μν(α_2) = \frac{1}{4} tr [ρA(α_1) \otimes A^*(α_2)]$$
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Table 4. Application of the PT criterion to a Werner state.

| \( W_\rho(\alpha) \) | \( W_{\rhoT}(\alpha) \) | \( W_{\Phi^+}(\alpha) \) |
|---------------------|---------------------|---------------------|
| \( 1-x/16 \) | \( 1-x/16 \) | \( 1-x/16 \) |
| \( 1-x/16 \) | \( 1-x/16 \) | \( 1-x/16 \) |
| \( 1-x/16 \) | \( 1-x/16 \) | \( 1-x/16 \) |
| \( 1-x/16 \) | \( 1-x/16 \) | \( 1-x/16 \) |

where partial transposition is shown to be equivalent to the substitution \( \hat{A}_{\alpha_1} \otimes \hat{A}_{\alpha_2} \rightarrow \hat{A}_{\alpha_1} \otimes \hat{A}_{\alpha_2}^* \). Interestingly, the latter is connected to the alternative definition \([6,7]\) of WF involving tomographic properties that differ from those discussed in section 2.4. As to the action of PT on a WF and its characteristic function we find

\[
W_{\rhoT}(\alpha) = W_\rho(\alpha) - \tau_\rho(\alpha), \quad \chi_{\rhoT}(\alpha_1, 11) = -\chi_\rho(\alpha_1, 11),
\]

(14)

where the trace-like term \( \tau_\rho(\alpha_1, \alpha_2) = (-1)^{\alpha_1+\alpha_2} tr(\hat{A}_{\alpha_1} \otimes \hat{\sigma}_y)/2 \) in equations 13 embodies the effect of the PT. It is known that the operator \( \rho^T \) relevant to a separable-state density operator possesses non-negative eigenvalues. In view of the properties just discussed, the PT criterion can be reformulated within the WF approach. If \( \rho^T \) has all nonnegative eigenvalues, then \( tr(\rho^T \rho') \geq 0 \), for all density matrices \( \rho' \), thus giving

\[
\sum_\alpha W_{\rhoT}(\alpha)W_{\rho'}(\alpha) = \sum_\alpha \chi_{\rhoT}(\alpha)\chi_{\rho'}(\alpha) \geq 0, \forall W_{\rho'}(\alpha), \chi_{\rho'}(\alpha),
\]

(15)

which is a necessary and sufficient condition for separability. To illustrate this result, we consider the Werner (mixed) state \( \rho = x|\Psi^-\rangle\langle\Psi^-| + (1-x)I/4 \), where \( |\Psi^-\rangle = (|0,1\rangle - |1,0\rangle)/\sqrt{2} \) and assume \( \rho' \) to be the pure state \( |\Phi^+\rangle = (|0,0\rangle + |1,1\rangle)/\sqrt{2} \). It is easy to show that (see table 4) \( \sum_\alpha W_{\rhoT}(\alpha)W_{\Phi^+}(\alpha) = (1-3x)/16 \), consistent with the well known separability of the Werner state for \( x \leq 1/3 \). This method states that the separability of \( \rho \) is ensured when inequality (15) holds for any \( W_\alpha' \) thus having a limited operational value. Nevertheless, it is important in that 1) its violation for some \( W_\alpha' \) entails that \( \rho \) is entangled, and 2) it is useful to link in a direct way the non-negativity of the WF to the entanglement properties, as we show in the next section.

3.3. Non-negativity of WF and separability

We now return to the difficult problem of establishing a connection between the non-negativity (negativity) of WF and the separability (non-separability) of the corresponding state. The starting point consists in observing that any Bell state has a WF with negative elements, whereas a Werner state has non-negative WF for any \( x \leq 1/3 \) (separable cases) (this is illustrated in table 4). In this respect, however, we know that exist separable states with negative WF such as the state in table 3.1 left panel. On the other hand, one might conjecture that the non-negativity of WF is a sufficient condition for separability. Unfortunately, one can show that non-negative WF’s exist which correspond to entangled states. As a possible strategy for solving
we note that the last inequality can be rewritten as
\[ \sum \alpha W^\rho(\alpha) < 0 \]  
(this entails, using \[ 15 \] that the state is entangled). We show that these assumptions lead to a contradiction. First we note that the last inequality can be rewritten as
\[ \sum \alpha W^\rho(\alpha) < \sum \alpha \tau^\rho(\alpha) W^{\rho'}(\alpha) \]  
On the other hand, the non-negativity of both \[ W^\rho \] and \[ W^{\rho'} \], and equation \[ 14 \] [which gives \[ W^\rho(\alpha) \geq \tau^\rho(\alpha) \] for all \( \alpha \)] imply that \[ \sum \alpha W^\rho(\alpha) W^{\rho'}(\alpha) \geq \sum \alpha \tau^\rho(\alpha) W^{\rho'}(\alpha) \] which clearly involves a contradiction.

It follows that, given a state \( \rho \), if both \( W^\rho \) and \( W_{\rho^{T_2}} \) have non-negative elements, than \( \rho \) is separable. Viceversa, if a state \( \rho \) is entangled, then \( W^\rho \) or \( W_{\rho^{T_2}} \) has negative values. Such a result –which is a necessary condition to ensure entanglement (sufficient condition for separability)– relates the nonclassic character of entangled states to the presence of negative elements in \( W^\rho \) and \( W_{\rho^{T_2}} \). This criterion has been confirmed by testing it on thousands of randomly-generated density matrices and on the Werner state (for \( x \leq 1/3 \) both \( W^\rho \) and \( W_{\rho^{T_2}} \) are positive, which implies separability).

### 3.4. Local Uncertainty Relation

It is known that the violation of local uncertainty relations (LUR’s) is a signature of entanglement \[ 27, 28 \]. Given two qubits 1 and 2, the inequalities
\[ \sum_i U[\xi_i^{(1)}] \geq \frac{1}{2} \quad \text{and} \quad \sum_i U[\xi_i^{(2)}] \geq \frac{1}{2} , \tag{16} \]
are known to be uncertainty relations relevant to the single qubit systems \( k = 1, 2 \), where \( U[\xi_i^{(k)}] = \langle \xi_i^{(k)} \rangle^2 - \langle \xi_i^{(k)} \rangle^2 \) are the uncertainties relevant to the set of axis operators \( \xi_i^{(k)} \) defined in formula \[ 9 \]. We note that simple calculations prove the equivalence between formula \[ 16 \] and \[ 8 \] entailing that the pseudo-probability can not be concentrated in a too small region of the phase space. As shown in \[ 27 \], in the two-qubit case, separable states are constrained by the single-qubits uncertainty relations
\[ \sum_i U[\xi_i^{(1)} \otimes I + I \otimes \xi_i^{(2)}] \geq 1 . \tag{17} \]
As a consequence, a state appears to be entangled if inequality \[ 17 \] is violated.
LUR inequalities can be formulated in terms of WF, by defining the first-order covariance matrix of single-qubit WF

\[
V_{ij}^{(X)} = \left\langle \{ \Delta \hat{\xi}_i, \Delta \hat{\xi}_j \} \right\rangle_X = \left\langle \{ \hat{\xi}_i \hat{\xi}_j \} \right\rangle_X - \left\langle \hat{\xi}_i \right\rangle \left\langle \hat{\xi}_j \right\rangle,
\]

where we use the axis operators \( \hat{\xi}_i = \hat{p}_i, \hat{d}_i, \hat{q}_i \) and \( \Delta \hat{\xi}_i = \hat{\xi}_i - \left\langle \hat{\xi}_i \right\rangle \). Moreover, the label \( X = S, D \), linking to the two types of anticommutator defined in formulas 10 and 11, leads to two different covariance matrices. Nevertheless, the following results are independent from definition of anticommutator, and we will write the parameter \( X \) only when necessary. Recalling that matrix \( V_{ij} \) is a \( 3 \times 3 \) semi-definite positive symmetric matrix and that diagonal elements \( V_{ii} \), named variances, coincide with the uncertainties \( U[\hat{\xi}_i] \), then the sum of diagonal elements \( V_{ii} \) is positive, consistent with 16.

Following the scheme of reference [32] for the continuous case, the covariance matrix of two qubits is built by writing formula 18 with the enlarged set \( \hat{\xi} = (\hat{p}_1, \hat{d}_1, \hat{q}_1, \hat{p}_2, \hat{d}_2, \hat{q}_2) \) giving a \( 6 \times 6 \) matrix. A compact version of covariance matrix is given by

\[
V = \begin{bmatrix}
A & C \\
C^T & B
\end{bmatrix},
\]

where \( A, B, C \) are \( 3 \times 3 \) matrices. Notice that matrix elements of \( A \) and \( B \) represent the covariance matrix \( V_{ij} \) relevant to qubit 1 and to qubit 2, respectively, while matrix \( C \) represents the inter-qubit correlations between axis operators \( \hat{\xi}_i^{(1)} \) and \( \hat{\xi}_i^{(2)} \). Two-qubit covariance matrix can be easily computed by means of equations 12 once the WF is known. It is easy to show that the inter-qubit correlations \( C_{ii} \) measure the degree of correlation between spin observables \( \hat{\sigma}_i^{(1)} \) and \( \hat{\sigma}_i^{(2)} \). Hence their operational meaning is the establish the interdependence of the two constituent subsystems. At this point, the WF formulation of LUR’s is easily achieved. Upon observing that

\[
U[\hat{\xi}_i^{(1)} \otimes I + I \otimes \hat{\xi}_i^{(2)}] = U[\hat{\xi}_i^{(1)}] + U[\hat{\xi}_i^{(2)}] + 2\left\langle \hat{\xi}_i^{(1)} \otimes \hat{\xi}_i^{(2)} \right\rangle - \left\langle \hat{\xi}_i^{(1)} \right\rangle \left\langle \hat{\xi}_i^{(2)} \right\rangle,
\]

the LUR relevant to the axis operators becomes

\[
trA + trB + 2trC \geq 1,
\]

where only diagonal elements of submatrices are involved, thus making the formula independent from the definition of anticommutator. This equation has the following interpretation: if the correlations \( C_{ii} \) are negative and their absolute values are sufficiently large, than the inequality is violated and the state is entangled. This evidences that non-separability strongly depends on the inter-qubit correlations described by \( tr \ C \). An important problem that deserves to be clarified is raised by those entangled states where correlations \( C_{ii} \) are positive. To answer to this question, in table we consider covariance matrices relevant to both the WF of Werner’s state (including as well the singlet state with weight \( x \)) and the WF of the Bell state \( |\Phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2} \). In the first case, formula 20 is violated for \( x \leq 1/3 \), which is a correct result. Instead, in the second case, formula 20 is not violated, thought the Bell state is known to be maximally entangled. We can show that, except for the singlet state, no Bell state violates formula 20 and the criterion does not supply information about separability.
The singlet case (corresponding in the table to the $x = 1$ case) differs from the other Bell states in that all the diagonal elements of matrix $C$ are negative. The other Bell states have elements $C_{ii}$ with alternating sign, which makes the violation of formula (20) impossible. Nevertheless, it is clear that such correlations, thought not negative, contain a large amount of information on non-separability. We thus propose the following modified inequality as a necessary condition for separability

$$\sum_i |C_{ii}| \leq \frac{trA + trB - 1}{2},$$

(21)

whose main feature is to replace the diagonal elements of $C$ with their absolute values. The effectiveness of formula (21) is confirmed by the fact that it is violated by any Bell states. The quantum-mechanical meaning is also clear in that, if a state is separable, then the absolute value of the correlations must be bounded from above. We easily prove that this inequality follows from equation (17) by resorting to the more general operator $\hat{\xi}_i^{(1)} \otimes I + \epsilon_i I \otimes \hat{\xi}_i^{(2)}$ where $\epsilon_i = \pm 1$. With such a choice, the LUR condition written in terms of covariance matrix reads $trA + trB + 2 \sum_i \epsilon_i C_{ii} \geq 1$. To obtain inequality (21) it is sufficient to consider $\epsilon_i = -1$ when $C_{ii}$ is positive. As a final comment, we notice that the sum of correlations (21) thus exhibits an upper limit for separable states: entangled states may overcome it, and the exceeding part is an indicator of quantum correlation.

3.5. Generalized Uncertainty Principle (GUP) and PT criterion

In the continuous case, a well-known separability criterion \cite{31, 32} is obtained by combining the Generalized Uncertainty Principle (GUP) with the application of the PT criterion to the variance matrix relevant to position and momentum operators. For a system of two (one-dimensional) particles in a continuous space, the GUP-based criterion states that, if a state $\rho$ is separable, one can construct a matrix $M = tr(\rho \xi_i \xi_j)$ which is semi-deﬁnite positive under PT, namely \cite{32}

$$M = V + i \frac{\Omega}{2} \geq 0,$$

(22)

where $V_{\alpha\beta} = \langle \{\Delta \hat{\xi}_\alpha, \Delta \hat{\xi}_\beta\} \rangle$ is the covariance matrix, $\Delta \hat{\xi}_\alpha = \hat{\xi}_\alpha - \langle \hat{\xi}_\alpha \rangle$, $\hat{\xi}_\alpha = \{\hat{q}_1, \hat{p}_1\}$ and $[\hat{\xi}_\alpha, \hat{\xi}_\beta] = i \Omega_{\alpha\beta}$ with

$$\Omega = \begin{bmatrix} J & 0 \\ 0 & J \end{bmatrix}, \quad J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$ 

Following the PT criterion, given a separable state $\hat{\rho}$ and its WF $W_\rho$, the PT generates a nonnegative operator $\hat{\rho}^{T2}$ and a genuine WF $W_{\rho^{T2}}$ still satisfying the equation (22).

The extension of the previous GUP-based criterion to the discrete case requires that each separable state can be associated to a matrix $M$ semi-deﬁnite positive under PT. Considering first the single-qubit case, we define the matrix $M_{ij} = [tr(\hat{\rho} \hat{\xi}_i \hat{\xi}_j)]$ written in terms of the list of operators $\hat{\xi}_i = \hat{I}, \hat{p}, \hat{d}, \hat{q}$. It can be easily shown that $\rho \geq 0$ entails $M \geq 0$. The latter is equivalent to the condition

$$V^{S}_{jk} + \frac{i}{2} \epsilon_{jkl} \chi_l \geq 0,$$

(23)
of the $3 \times 3$ condition under partial transposition. This result will be discussed in a separate paper.

where covariance matrix $V^{(S)}$ in equation $18$ in the present case, is a $3 \times 3$ matrix and is related to the standard definition of anticommutator $10$. Condition $23$ implies $\text{tr}(V) \geq 1/2$, which is equivalent to the LUR equation for single qubit $27$. It is worth observing how any other choice for the set $\{\xi_i\}$ implies that $M \geq 0$ iff $\rho \geq 0$ provided $\{\xi_i\}$ forms a complete basis of the space of hermitian matrices for a single-qubit.

In the case of two qubits, once more in analogy with the continuous case, it seems quite natural to derive $M$ from the set $\xi = (I, \hat{p}_1, \hat{d}_1, \hat{q}_1, \hat{p}_2, \hat{d}_2, \hat{q}_2)$. Following the standard prescriptions $32$ for calculating the GUP inequality, we have that $M \geq 0$ and, equivalently,

$$
\begin{bmatrix}
A_{jk} + \frac{i}{2} \epsilon_{jkl} \xi_l^{(1)} & C_{jn} \\
C_{km} & B_{mn} + \frac{i}{2} \epsilon_{mns} \xi_s^{(2)}
\end{bmatrix} \geq 0 .
$$

The matrix on the left-hand side is a $6 \times 6$ matrix that can be written in terms of the $3 \times 3$ matrices $A$, $B$, $C$ appearing in equation $19$. Similar calculations show how $\tilde{M} = \text{tr}(\rho T^2 \xi_i \xi_j)$ is such that $\tilde{M} \geq 0$ if $\rho T^2 \geq 0$. Then we conclude that the separability condition for a state $\rho$ (achieved within the PT criterion when both $\rho \geq 0$ and $\rho T^2 \geq 0$ are satisfied) is now ensured by $M \geq 0$ and $\tilde{M} \geq 0$. Notice that condition $\tilde{M} \geq 0$ can be reduced as well to the equivalent form

$$
\begin{bmatrix}
A_{jk} + \frac{i}{2} \epsilon_{jkl} \chi_l^{(1)} & \tilde{C}_{jn} \\
\tilde{C}_{km} & \tilde{B}_{mn} + \frac{i}{2} \epsilon_{mns} \chi_s^{(2)}
\end{bmatrix} \geq 0 ,
$$

where $\tilde{B}, \tilde{C}$ are determined using once more the PT operation. Formula $25$ containing the axis-operator covariance matrix is the core of the two-qubit PT criterion. In table $6$ we illustrate the application of the present criterion to the Werner state. In this case $V = M$ and the eigenvalues of matrix $\tilde{M}$ (relevant to $\rho T^2$) are positive for $x \geq 1$ (rather than for $x \geq 1/3$). Unfortunately, this means that the GUP is not violated so that the criterion does not give information about separability. This can be explained with the fact that, when using the set of operators $(\hat{p}_1, \hat{d}_1, \hat{q}_1, \hat{p}_2, \hat{d}_2, \hat{q}_2)$, the nonnegativity of $\tilde{M}$ is only a necessary condition for separability. In order to cure this problem we have generalized the GUP-based criterion by using the enlarged set of operators $\xi_i \otimes \xi_j$, which leads to a $9 \times 9$ matrix $M$. In this case, we could have a violation of the positivity condition under partial transposition. This result will be discussed in a separate paper.

| Table 6. An example of GUP in the two-qubit case. |

\[
\begin{pmatrix}
\frac{1}{4} & 0 & 0 & -\frac{x}{4} & 0 & 0 \\
0 & \frac{1}{4} & 0 & 0 & -\frac{x}{4} & 0 \\
0 & 0 & \frac{1}{4} & 0 & 0 & -\frac{x}{4} \\
-\frac{x}{4} & 0 & 0 & \frac{1}{4} & 0 & 0 \\
0 & -\frac{x}{4} & 0 & 0 & \frac{1}{4} & 0 \\
0 & 0 & -\frac{x}{4} & 0 & 0 & \frac{1}{4}
\end{pmatrix} \quad \begin{pmatrix}
\frac{1}{4} & 0 & 0 & -\frac{x}{4} & 0 & 0 \\
0 & \frac{1}{4} & 0 & 0 & -\frac{x}{4} & 0 \\
0 & 0 & \frac{1}{4} & 0 & 0 & -\frac{x}{4} \\
-\frac{x}{4} & 0 & 0 & \frac{1}{4} & 0 & 0 \\
0 & -\frac{x}{4} & 0 & 0 & \frac{1}{4} & 0 \\
0 & 0 & -\frac{x}{4} & 0 & 0 & \frac{1}{4}
\end{pmatrix}
\]
4. Conclusions

In the present work, we have considered the WF defined in [1] focusing our attention on two properties of the two-qubit WF, the negativity and the covariance matrix, which are useful in the characterization of entanglement. After reformulating/generalizing the PT, LUR, and GUP-based separability criteria in the WF formalism, we have tried to evidence what features of the WF and of its covariance matrix are able to reveal the presence of entanglement.

In section 3.1 we have found that a two-qubit WF relevant to a separable state can not assume values lower than \((1 - \sqrt{8})/4\). In section 3.2 we have recast the PT criterion in terms of WF by means of inner-product rule 4. Based on this result, in section 3.3 we have shown that the non-separability of \(\rho\) entails the presence of negative elements in \(W_\rho\) or in \(W_{\rho^{T_2}}\). Interestingly, these facts relate the main non-classical feature of the WF (the presence of negative values) to the presence of entanglement in the two-qubit system. Considering the separability problem within the LUR criterion, in section 3.4 we have reformulated it in terms of covariance-matrix elements of WF. In particular, we have found a stronger version of the LUR criterion (illustrated by formula 21) once more involving the covariance matrix. This generalized criterion, which has been tested both on Bell states and on Werner states, evidences that the presence of strong correlations can be used to detect non-separability. Finally, in section 3.5 we have studied the analogue of the GUP-based separability criterion (continuous case) from the viewpoint of discrete WF’s. We have shown that adopting the same procedure of the continuous case leads to criterion 25. The latter does not succeed in detecting entanglement as a consequence of the fact that the set of operators used to build the discrete GUP is too small. In order to cure this problem, we have enlarged such an operator set thus obtaining that \(\tilde{M} \geq 0 \iff \rho^{T_2} \geq 0\). Such an equivalence provides the basis to extend in an effective way the GUP-based separability criterion from the continuous to the discrete case.

Future work about entanglement properties of the two-qubit WF will be developed in two directions. Our first objective is to derive, relying on equation 25, the explicit form of a generalized GUP-based separability criterion from a suitably enlarged operator set. A second important problem which deserves to be deepen is to establish how the presence of negative elements in WF’s \(W_\rho\) (and \(W_{\rho^{T_2}}\)) relevant to entangled states is related to the violation of inequality 21 issued from the LUR condition. Such aspects will be investigated in a separate paper.

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