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Entanglement reflected in Wigner functions

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Abstract

We construct an Abelian algebra built by maximally entangled pure states. The partial transposition maps this algebra for odd dimensions into a full matrix algebra. ppt-states are in one-to-one correspondence to states with a positive definite Wigner function. Special extremal ppt-states correspond to projections of various dimensions. In particular, we recover the projections corresponding to a complete set of mutually unbiased bases in prime dimensions.

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1. Introduction

In quantum information theory we usually work in finite-dimensional Hilbert spaces and with the algebra acting on it. We are especially interested in the structure of the state space over this algebra with respect to various view points. The study of these Hilbert spaces has a long history [1, 2]. An important problem is the task to consider the noncommutative algebra as a replacement of the classical algebra over the phase space that is now reduced to a lattice. The probability distributions over the classical lattice are replaced by suitable Wigner functions. One can demand various properties that these Wigner functions should satisfy [3–5]. We can concentrate on the geometric interpretation. Replacing the algebra over $L^2(R, dx)$ as considered by Wigner by a finite-dimensional matrix algebra M_d the task is to express location and momentum by a two-dimensional lattice of length d such that a state over $\mathcal{M}_d$ corresponds to a real functional over the lattice. Positivity can in general not be preserved. This approach is followed in [5] and especially for odd dimensions a concrete construction for the Wigner function is offered. In addition, [3] asks for a function that remains closer to a probability in the sense that for a sufficiently large class of states it remains positive. Based on a different construction than those of [5], namely based on a complete set of mutually unbiased bases, they offer a solution. However, only for dimensions $d = p^r$, p prime, such a set is shown to exist. In other dimensions it is conjectured that such a set cannot exist.

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Another task in the framework of noncommutative information theory is the characterization of entangled states. Especially here our understanding in higher dimensions is rather limited. A well analysed example is the Werner states [6], characterized by a high symmetry and depending on just one parameter. The high symmetry allows to calculate the entanglement quantitatively and especially to fix the point where separable states turn into entangled states [7, 8]. Other examples are offered in two, three and four dimensions [9–12]. The symmetry group was slightly reduced. In two dimensions we have total control on the set of states inside this class: it is possible to describe the set of states as lying in a tetrahedron in which the entangled states are imbedded in the form of an octahedron [9, 10].

In this paper we will show that the two problems, characterization of separable states in a suitable class of states and construction and positivity of Wigner functions, are related. We will consider the analogous set of states chosen in [10] in higher dimensions. The geometric description where entanglement sets in is less obvious. We will extrapolate it from the Werner states on the boundary of the separable states. Their tangent functionals also form part of the boundary of the ppt-states and we will find the extremal separable states on these tangent planes. In addition, we will show that in this restricted class of states the edges of the ppt-states, i.e. the states that remain positive under partial transposition [14] are separable so that here the boundary of the ppt-states and separable states coincide.

But even more we will see that the partial transposition serves to relate the two concepts, Wigner functions and entanglement. It gives a natural map from an Abelian algebra of dimension d^2 to a non-Abelian algebra of the same geometric dimension. This non-Abelian algebra is the full matrix algebra if the dimension is odd; otherwise it is the matrix algebra of dimension $\left(\frac{d}{2}\right)^2$ tensorized with an Abelian algebra of dimension 4. This is in correspondence with the results in [5], where the possibility of constructing Wigner functions also differs for odd and even dimensions.

From this map we can gain additional insight into the structure of the states: our map from the Abelian to the non Abelian algebra also serves as a map from a probability distribution over the Abelian algebra into a Wigner function belonging to the non-Abelian algebra. This Wigner function defines a real linear functional over the non-Abelian algebra which can uniquely be decomposed into a difference of two positive functionals, orthogonal to one another. The correspondence between the original state over the tensor product of the two matrix algebras and the state over the new matrix algebra is such that ppt-states on the original algebra are mapped into states on the non-Abelian algebra, whereas distillably entangled states are mapped into real functionals that are not strictly positive. Decomposing these functionals into their positive and negative part corresponds to the optimal decomposition of the original state into the difference of weighted separable states, a decomposition that can also be used as characterization of the amount of entanglement [15].

In addition, we can make more concrete statements about the properties of the operators in the commuting algebra and their counterpart in the noncommuting algebra: a state on the boundary of ppt-states determines a tangent space that corresponds to a ppt-witness. This ppt-witness belongs to the Abelian algebra and therefore has a counterpart in the matrix algebra. It turns out that this counterpart defines a projector. In this way we obtain from Werner states in a fairly natural way a class of projection operators of dimension $(d-1)/2$ that is related to the choice of the Weyl algebra in the full matrix algebra. Further decomposition of extremal separable Werner states allows for dimension d prime to construct all projections that correspond to a complete set of mutually unbiased bases in the matrix algebra. As a further consequence this implies that for d prime the definitions for the Wigner functional given in [5] and in [3] coincide.

2. The passage from the Abelian to the non-Abelian algebra

2.1. The set of states

In [10] we considered the subset of states over two qubits that correspond to density matrices $\frac{1}{4} + \sum_i^3 \lambda_i \sigma_i \otimes \tau_i$. These states reduced to the subsystems give the tracial state, i.e. the state that is maximally mixed. Furthermore we note that these density matrices form a maximal Abelian subalgebra of the two-qubit algebra. In [11] $\mathcal{M}_2$ was replaced by $\mathcal{M}_3$ and the Pauli matrices were replaced by Gell–Mann matrices. In this paper we want to replace the qubit algebra by $\mathcal{M}_d \otimes \mathcal{M}_d$ where $\mathcal{M}_d$ is the full matrix algebra of dimension d, and as analogue of the above states we look for a set of d^2 vector states, where each vector corresponds to a maximally entangled state and different vectors are orthogonal to one another.

Such a set of states can in fact be constructed. One possibility for such a construction is based on the choice of a set of vectors that form an orthogonal basis $|s\rangle$, $s = 0, \ldots, d-1$, in one factor M_d. A maximally entangled state $|\Omega\rangle$ (that in the following we will keep fixed) implements a corresponding basis in the other factor such that $|\Omega\rangle = \frac{1}{\sqrt{d}} \big|\sum_0^{d-1} s \otimes s\big\rangle$. Every other maximally entangled state can be obtained as $U \otimes 1|\Omega\rangle$ with U unitary in M_d. The new vector is orthogonal to the original one if $tr U = 0$. In order to obtain an orthogonal basis of maximally entangled states we can use the results of [2]. We take the vectors $|\Omega_{r_1,r_2}\rangle = U_{r_1,r_2} \otimes 1|\Omega\rangle$, $r_i = 0, 1, \ldots, d-1$, where we take the Weyl operators U_{r_1,r_2} in M_d that are determined by the choice of the orthonormal basis in $\mathcal{H}_d$ and are defined by

$$\langle s|U_{r_1,r_2}|s'\rangle = \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} r_1 s} \delta_{s-s'+r_2,0}. \tag{1}$$

They satisfy the algebraic relations

$$U_{r_1,r_2} U_{t_1,t_2} = \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} t_1 r_2} U_{r_1+t_1,r_2+t_2} \tag{2}$$

$$U^*_{r_1,r_2} = \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} r_1 r_2} U_{-r_1,-r_2}. \tag{3}$$

On the other hand, these algebraic relations (2, 3) determine the Weyl operators up to unitary equivalence. They satisfy $\mathrm{tr}\, U_{r_1,r_2} = d\delta_{r_1,,0}\delta_{r_2,0}$ and therefore serve for the construction of the other maximally entangled states.

The projection on $|\Omega\rangle$ is an operator in $\mathcal{M}_d \otimes \mathcal{M}_d = \mathcal{M}_{d^2}$. It can be expressed in terms of the Weyl operators in $\mathcal{M}_d \otimes 1$ together with those in $1 \otimes \mathcal{M}_d$ as

$$|\Omega\rangle\langle\Omega| = \frac{1}{d^2} \sum_{0,0}^{d-1,d-1} U_{l_1,l_2} \otimes U_{-l_1,l_2}, \tag{4}$$

which can be seen by evaluating

$$\langle\Omega|s\rangle\langle s'| \otimes |t\rangle\langle t'|\Omega\rangle = \frac{1}{d}\delta_{st}\delta_{s't'} = \frac{1}{d^2}\,\mathrm{tr} \sum_{0,0}^{d-1,d-1} U_{l_1,l_2} \otimes U_{-l_1,l_2}|s\rangle\langle s'| \otimes |t\rangle\langle t'|.$$

The other maximally entangled states correspond to the projection operators in $\mathcal{M}_d \otimes \mathcal{M}_d$,

$$\begin{aligned} P_{r_1,r_2} = \big|\Omega_{r_1,r_2}\big\rangle\big\langle\Omega_{r_1,r_2}\big| &= \frac{1}{d^2}\big(U_{r_1,r_2} \otimes 1\big)\left(\sum_{0,0}^{d-1,d-1} U_{l_1,l_2} \otimes U_{-l_1,l_2}\right)\big(U^*_{r_1,r_2} \otimes 1\big) \\ &= \frac{1}{d^2} \sum_{0,0}^{d-1,d-1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d}(l_1 r_2 - l_2 r_1)}\big(U_{l_1,l_2} \otimes U_{-l_1,l_2}\big). \end{aligned} \tag{5}$$

Commutativity of the projections is a consequence of the orthogonality, but also can be verified by direct calculation using (2), (3).

2.2. The Abelian algebra

We consider the Abelian algebra $\mathcal{M}^0_{d^2}$ as subalgebra of $\mathcal{M}_d \otimes \mathcal{M}_d$, constructed in this way either as $\{P_{r_1,r_2}\}''$, the algebra built by the projections, or as $\{U_{l_1,l_2} \otimes U_{-l_1,l_2}\}''$, the algebra built by the unitaries. Since it has dimension d^2 it is maximally Abelian. It is unique up to isomorphisms implemented by local unitaries $U \otimes \tilde{U}$ if we keep $|\Omega\rangle$ fixed (where the map $U \to \tilde{U}$ as defined in [6] depends on $|\Omega\rangle$).

If we also vary $|\Omega\rangle$, then all unitaries $U \otimes V$ implement possible isomorphisms between $\mathcal{M}^0_{d^2}$. However, this does not exhaust all possibilities of constructing a maximally Abelian algebra whose one-dimensional projections define states that are tracial on the subalgebras. If e.g. the dimension d is not prime we can consider another possibility of constructing $\mathcal{M}^0_{d^2}$: with $d = p_1, \ldots, p_l$ we can decompose the algebra into its factors $\mathcal{M}_d = \mathcal{M}_{p_1} \otimes \cdots \otimes \mathcal{M}_{p_l}$ and construct in each factor the Weyl operators. Then we can take as the unitaries used for the construction of the projectors in $\mathcal{M}_{d^2}$ the tensor products of the Weyl operators. Relations between these two constructions of unitaries representing a phase-space are discussed in [16].

We return to our algebra built by the projections (5). Convex combinations of these projections define density matrices belonging to $\mathcal{M}^0_{d^2}$. They can be written as

$$\sum_{0,0}^{d-1,d-1} c_{l_1,l_2} P_{l_1,l_2} = \sum_{0,0}^{d-1,d-1} \tilde{c}_{-r_2,r_1} U_{r_1,r_2} \otimes U_{-r_1,r_2}, \tag{6}$$

with $\tilde{c}$ the Fourier transform of c given as

$$\tilde{c}_{r_1,r_2} = \frac{1}{d^2} \sum_{0,0}^{d-1,d-1} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d}(l_1 r_1 + l_2 r_2)} c_{l_1,l_2}. \tag{7}$$

On the two subfactors $\mathcal{M}_d \otimes 1$ and $1 \otimes \mathcal{M}_d$ they implement the tracial state $\omega(U_{r_1,r_2}) = \operatorname{tr} \sum_{0,0}^{d-1,d-1} c_{l_1,l_2} P_{l_1,l_2}(U_{r_1,r_2} \otimes 1) = \delta_{r_1 0}\delta_{r_2 0}$. As density matrices they define a positive cone in the set of real linear functionals over $\mathcal{M}_d \otimes \mathcal{M}_d$, but we can also think of these functionals restricted to the subalgebra $\mathcal{M}^0_{d^2}$. This cone has dimension d^2 just as the states over the matrix algebra $\mathcal{M}_d$.

2.3. The map to the non-Abelian algebra

A density matrix is distillably entangled if it does not stay positive under the partial transposition $T \otimes 1$ over $\mathcal{M}_d \otimes \mathcal{M}_d$. Since our density matrix is expressed in terms of Weyl operators we can easily calculate the effect of the partial transposition. In one factor the transposition acts on the Weyl operators as

$$\langle s|U^T_{r_1,r_2}|s'\rangle = \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} r_1 s'} \delta_{s'-s+r_2,0} = \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} r_1 (s-r_2)} \delta_{s-s'+r_2,0} = \mathrm{e}^{-\frac{2\pi \mathrm{i}}{d} r_1 r_2} \langle s|U_{r_1,-r_2}|s'\rangle. \tag{8}$$

Therefore

$$T \otimes 1(U_{r_1,r_2} \otimes U_{-r_1,r_2}) = \mathrm{e}^{-\frac{2\pi \mathrm{i}}{d} r_1 r_2} U_{r_1,-r_2} \otimes U_{-r_1,r_2}. \tag{9}$$

The Abelian algebra $\mathcal{M}^0_{d^2}$ is mapped into $(T \otimes 1)\mathcal{M}^0_{d^2} = \mathcal{A}$. $\mathcal{A}$ is to be taken as a linear vectorspace which is a subspace of $\mathcal{M}_d \otimes \mathcal{M}_d$. But as a subset of $\mathcal{M}_d \otimes \mathcal{M}_d$ also multiplication is defined and maps $\mathcal{A}$ into itself, so that $\mathcal{A}$ is also an algebra. The typical multiplication rule is

$$U_{r_1,-r_2} \otimes U_{-r_1,r_2} U_{t_1,-t_2} \otimes U_{-t_1,t_2} = \mathrm{e}^{-\frac{2\pi \mathrm{i}}{d} 2 t_1 r_2} U_{r_1+t_1,-r_2-t_2} \otimes U_{-r_1-t_1,r_2+t_2}. \tag{10}$$

Apart from the factor 2 in the exponent we recover the commutation relations between the Weyl operators (2). Due to this factor we have to distinguish between even and odd dimensions.

Let d be odd. Then we introduce as the Weyl operator $W_{r_1,r_2} \in \mathcal{A}$

$$W_{r_1,-2r_2} = U_{r_1,-r_2} \otimes U_{-r_1,r_2}. \tag{11}$$

Since $s_2 = 2r_2 \bmod(d)$ has a unique solution r_2 for given s_2 we get the complete set of Weyl operators in $\mathcal{M}_d$. Therefore, the algebra $\mathcal{A}$ built by $\mathrm{e}^{-\frac{2\pi \mathrm{i}}{d} r_1 r_2} U_{r_1,-r_2} \otimes U_{-r_1,r_2}$ is isomorphic to $\mathcal{M}_d$.

Let $d = 2^m$. Then we can use the other method mentioned to construct $\mathcal{M}^0_{d^2}$. Let $\sigma_{r_i}, r_i = 0, 1, 2, 3$, be the spin matrices including the identity. Then we can choose the unitaries in $\mathcal{M}_d$ as $U_{r_1,\ldots,r_m} = \sigma_{r_1} \otimes \cdots \otimes \sigma_{r_m}$. Similar to (2) they satisfy

$$U_{r_1,\ldots,r_m} U_{s_1,\ldots,s_m} = \exp\left(\frac{\mathrm{i}\pi}{2} \sum_{i=j}^{m} f(r_j, s_j, t_j)\right) \sigma_{t_1} \otimes \cdots \otimes \sigma_{t_m}, \qquad |f| = 1, \tag{12}$$

where $t = t(r, s)$ is determined by $(r.s)$, i.e. $t(r, r) = 0, t(0, s) = s, t(r, 0) = r, t(r \neq 0, s \neq 0, r) \neq 0, r, s$. We do not specify f; it is sufficient to note that it is an integer and that a product is again of the same form with an additional factor being either $\pm 1, \pm \mathrm{i}$. Further $\operatorname{tr} U_{r_1,\ldots,r_m} = \delta_{r_1,0} \cdots \delta_{r_m,0}$. Again with an appropriate integer $f(r_1, \ldots, r_m)$

$$|\Omega\rangle\langle\Omega| = \frac{1}{4^m} \sum (-1)^{f(r_1,\ldots,r_m)} U_{r_1,\ldots,r_m} \otimes U_{r_1,\ldots,r_m}. \tag{13}$$

Therefore all maximally entangled states $U_{r_1,\ldots,r_m} \otimes 1|\Omega\rangle\langle\Omega|U^*_{r_1,\ldots,r_m} \otimes 1$ are of the form (13) with varying sign function f. According to the multiplication rule (12) all $U_{r_1,\ldots,r_m} \otimes U_{r_1,\ldots,r_m}$ commute with one another and the projections form our Abelian $\mathcal{M}^0_{2^m}$. But now the transposition acts as $T(U_{r_1,\ldots,r_m}) = \pm U_{r_1,\ldots,r_m}$. Therefore the partial transposition maps the Abelian $\mathcal{M}^0_{2^m}$ into itself. Especially for $m = 2$ this algebra was studied in [12]. Ppt-states could be characterized, and in addition it was shown that bound entanglement is possible.

Let d be even and $\frac{d}{2^m}$ odd. Then we can introduce $\mathcal{M}_d \simeq \mathcal{M}_{\frac{d}{2^m}} \otimes \mathcal{M}_{2^m}$. We construct the Weyl operators on $\mathcal{M}_{\frac{d}{2^m}}$ and the corresponding Abelian algebra, whereas for $\mathcal{M}_{2^m}$ we choose the above construction. As projections we take the tensor product of projections belonging to the two Abelian algebras $\mathcal{M}^0_{\frac{d^2}{2^{2m}}} \subset \mathcal{M}_{\frac{d}{2^m}} \otimes \mathcal{M}_{\frac{d}{2^m}}$ respectively to $\mathcal{M}^0_{2^{2m}} \subset \mathcal{M}_{2^m} \otimes \mathcal{M}_{2^m}$. They define again an orthonormal set of maximally entangled states. The transposition $T_d = T_{\frac{d}{2^m}} \otimes T_{2^m}$ respects the tensor product and we get $T \otimes 1\big(\mathcal{M}^0_{\frac{d^2}{2^{2m}}} \otimes \mathcal{M}^0_{2^{2m}}\big) \simeq \mathcal{M}_{\frac{d}{2^m}} \otimes \mathcal{M}^0_{2^m}$.

An alternative is to keep the algebra built by (9). Then $\forall r_1, r_2$

$$\begin{aligned}\big[U_{r_1,-r_2} \otimes U_{-r_1,r_2}, U_{\frac{d}{2},-\frac{d}{2}} \otimes U_{-\frac{d}{2},\frac{d}{2}}\big] &= \big[U_{r_1,-r_2} \otimes U_{-r_1,r_2}, U_{0,-\frac{d}{2}} \otimes U_{0,\frac{d}{2}}\big] \\ &= \big[U_{r_1,-r_2} \otimes U_{-r_1,r_2}, U_{\frac{d}{2},0} \otimes U_{-\frac{d}{2},0}\big] = 0\end{aligned} \tag{14}$$

Therefore, the algebra has a centre of dimension 4, built by the operators $\big(U_{0,-\frac{d}{2}}, U_{\frac{d}{2},0}, U_{\frac{d}{2},-\frac{d}{2}}, 1\big)$. The total algebra $(T \otimes 1)M^0_{d^2} \simeq \mathcal{M}_{\frac{d}{2}} \otimes \mathcal{M}^0_4$ where we can construct the Weyl operators W_{l_1,l_2} creating $M_{\frac{d}{2}}$ by

$$W_{l_1,l_2} = \sum_{\alpha_1,\alpha_2} U_{r_1,-r_2} \otimes U_{-r_1,r_2}, \qquad l_1, l_2 = 0, \ldots, \frac{d}{2}, \qquad \alpha_1, \alpha_2 = 0, 1; \quad r_k = l_k + \alpha_k \frac{d}{2}. \tag{15}$$

They satisfy the multiplication rules (2), (3) for $\frac{d}{2}$ and act in the subspace determined by the projection $W_{0,0}$ that belongs to the centre like the matrix algebra $\mathcal{M}_{\frac{d}{2}}$.

In the following we will concentrate on d being odd, not only because then the mapping into the matrix algebra is more transparent, but also because the construction of the Wigner functional offered in [5] becomes unique only for odd dimensions.

2.4. The Wigner function

The algebra is linearly spanned by the Weyl operators and it suffices therefore to know the expectation values of the Weyl operators. However, the passage to the Wigner function is favoured because they remain real and in comparison to a classical distribution over the phase space only the positivity is lost. In this sense they remain closer to the classical description.

There exists an immense literature on the Wigner functions. See e.g. the review [13]. We collect some basic facts. Given a state respectively a density matrix ρ for the infinite system the Wigner distribution $\mathcal{P}(x, p)$ corresponding to this state is defined as

$$\mathcal{P}(x, p) = \frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{d}y \langle x - y|\rho|x + y\rangle\, \mathrm{e}^{2\mathrm{i}py}. \tag{16}$$

We prefer to express the distribution as expectation value over the Weyl operators

$$\mathcal{P}(x, p) = 2\mathrm{i} \int \mathrm{d}y\, \mathrm{d}\alpha\, \mathrm{tr}\, \rho\, \mathrm{e}^{-2\mathrm{i}(\hat{P}-p)y}\, \mathrm{e}^{\mathrm{i}\alpha(\hat{X}-x)}\, \mathrm{e}^{-\mathrm{i}\alpha y}, \tag{17}$$

where $\hat{X}$, $\hat{P}$ are the location and momentum operators. Therefore, the natural replacement as it is obtained in [5] reads

$$\mathcal{P}_{\mathcal{A},\rho}(l_1, l_2) = \sum_{0,0}^{d-1,d-1} \mathrm{tr}\, \rho W(r_1, 2r_2)\, \mathrm{e}^{\frac{2\pi \mathrm{i}}{d}(r_1 l_1 - 2r_2 l_2 + r_1 r_2)}, \tag{18}$$

with ρ the density matrix in $\mathcal{M}_d$ defining the state over $\mathcal{M}_d$. It is easy to check using (3) that this expression is real. We can read it as a real function over the lattice, depending linearly on the state over the matrix algebra. Again we can recover the expectation value of the Weyl operators from $\mathcal{P}(l_1, l_2)$ via the Fourier transform provided d is odd. It should be noted that [3, 4] concentrate on other properties of the Wigner function: the Wigner function should be a real linear function over a lattice, linearly given by the density matrix, that mimics a kind of set in the classical phase space such that the Wigner functions corresponding to these projections should be positive definite. If it is possible to find a set of mutually unbiased basis it is not necessary to refer to the Weyl operators.

Let us return to our map from an Abelian algebra to a non-Abelian algebra. We restrict ourselves to odd dimensions, so that the non-Abelian algebra is a full matrix algebra for which the Wigner function in the sense of [5] exists. The partial transposition maps a density matrix ρ in $\mathcal{M}_d \otimes \mathcal{M}_d$ into a self-adjoint operator that is not necessarily positive. The corresponding state ω over $\mathcal{M}_d \otimes \mathcal{M}_d, \omega(B) = \mathrm{tr}\, \rho B, B \in \mathcal{M}_d \otimes \mathcal{M}_d$ is therefore mapped into a real linear functional ω^T over $\mathcal{M}_d \otimes \mathcal{M}_d, \omega^T(A) = \mathrm{tr}(T \otimes 1)\rho A = \mathrm{tr}\, \rho(T \otimes 1)A$. Reduced to $\mathcal{M}^0_{d^2} = \{P_{l_1,l_2}\}''$ it remains a real linear function. Similarly, we can consider a state restricted to the linear subset $\mathcal{A}$. $\omega(A), A \in \mathcal{A} = (T \otimes 1)\mathcal{M}^0_{d^2}$, in general be a real linear functional but not a state over the algebra $\mathcal{A}$. Combined with the partial transposition we obtain $\omega^T(A)$, which is again a state over $\mathcal{A}$. This state respectively a real linear functional defines the Wigner function according to (18) over $\mathcal{A}$ with the Weyl operators given by (11). If however we examine the details of the map and combine (5), (7), (9) and (12), then we note that the Wigner functions that correspond to the new real linear functional over $\mathcal{A}$ coincide with the original state over $\mathcal{M}^0_{d^2}$ in the sense that

$$\omega(P_{-2l_2,l_1}) = \mathrm{tr}\, \rho P_{-2l_2,l_1} = \mathrm{tr}(T \otimes 1)\rho(T \otimes 1)(P_{-2l_2,l_1}) = \mathcal{P}_{\mathcal{A},(T\otimes 1)\rho}(l_1, l_2), \tag{19}$$

where only now $(T \otimes 1)\rho$ has to be inserted in (18) and is not a positive density matrix but corresponds to the possibly not positive definite $\omega \circ (T \otimes 1)$. Also the trace has to be taken in the larger $\mathcal{M}_d \otimes \mathcal{M}_d$.

As a consequence we can conclude that

Theorem 2. *A density matrix of* $\mathcal{M}_{d^2}$ *implements a functional* ω *over* $\mathcal{A} = (T \otimes 1)M^0_{d^2} \subset M_{d^2}$ *via* $\omega(A) = \mathrm{tr}(T \otimes 1)\rho A$, $A \in \mathcal{A}$. *The corresponding Hermitian linear functional* $\omega \circ (T \otimes 1)$ *(which is not necessarily positive) leads to a positive definite Wigner function.*

Proof. $\omega(T \otimes 1) \circ (T \otimes 1)(P_{-2l_1,l_2}) = \mathcal{P}_{\mathcal{A}}(l_2, l_1)$ is positive definite, since it coincides with the expectation of a projector in a state. Interpreted as the Wigner function related to $\mathcal{A}$ it is positive and corresponds to a Hermitian functional. $\omega(T \otimes 1)\big(U_{l_1,l_2} \otimes U_{-l_1,l_2}\big) = \omega\big(W_{l_1,-2l_2}\big)$ defines a state over the algebra $\mathcal{A}$. □

The positive Wigner function corresponds to a Hermitian linear functional that can be decomposed into the difference of two positive linear functionals. This difference is unique provided we demand that the two corresponding density matrices are orthogonal to one another. There are some positive Wigner functions for which this decomposition is trivial, i.e. the negative part is 0. These Wigner functions form a convex set, and the corresponding states, i.e. those that have positive Wigner functions, form the corresponding convex set in state space. Let us call these states pW-states in analogy with the ppt-states. We can copy the considerations of [14] and conclude that the set is determined by its tangent functionals. It remains to search for the relation between the ppt-states and pW-states.

3. Entanglement witnesses versus projectors

A ppt-state ω is a state ω for which $\omega \circ T \otimes 1$ remains positive as a state over $\mathcal{M}_{d^2}$. Since we are interested in it as a state over $\mathcal{M}^0_{d^2}$ we have to make sure that violation of positivity is already felt on $\mathcal{M}^0_{d^2}$. This is in fact the case. We argue with the tangent functionals:

Theorem 3. *Consider the intersection of states given by density matrices from* $\mathcal{M}^0_{d^2}$ *and ppt-states. They form a convex set* $\mathcal{C}_0$ *in the convex set* $\mathcal{C}$ *of ppt-states. We characterize the boundary of* $\mathcal{C}$ *by its tangent planes. The tangent planes at a boundary point* ω_e *of* $\mathcal{C}$ *(we include the possibility that there are several tangent planes) are defined by entanglement witnesses* $A_{\omega_e} \in \mathcal{M}_{d^2}$ *such that* $\omega_e\big(A_{\omega_e}\big) = 0$ *and* $\omega\big(A_{\omega_e}\big) > 0$ *for all* ω *in the interior of* $\mathcal{C}$. *For* $\omega_e \subset \mathcal{C}_0$ *it follows that among the possible tangent functionals (that can be unique) there is one with* $A_{\omega_e} \in M^0_{d^2}$.

Proof. Let A correspond to a tangent functional for the set of ppt-states corresponding to the extremal ppt-state ω_e. Then for all unitaries $U, V \in \mathcal{M}_d$ the state $\bar{\omega}_e(B) = \omega_e(U^* \otimes V^* B U \otimes V)$ is also a ppt-state on the boundary of $\mathcal{C}.U \otimes VAU^* \otimes V^*$ defines its corresponding tangent functional. If $\bar{\omega}_e = \omega_e$, i.e. if the corresponding density matrix ρ commutes with $U \otimes V$, then every convex superposition of the two possible entanglement witnesses $\lambda A + (1 - \lambda)U \otimes VAU^* \otimes V^*$, $0 \leqslant \lambda \leqslant 1$, also gives a tangent functional. Let us take an ω_e whose density matrix belongs to $M^0_{d^2}$. All unitaries of $M^0_{d^2}$ are of the desired tensor product form and in addition commute with the chosen density matrix. Therefore, we can take the invariant mean η with respect to all unitaries in $M^0_{d^2} : \eta(A) = \sum_{l_1,l_2} \big(U_{l_1,l_2} \otimes U_{-l_1,l_2} A U^*_{l_1,l_2} \otimes U^*_{-l_1,l_2}\big)$ and still obtain a tangent functional for ω_e that in addition commutes with $M^0_{d^2}$. But this algebra is maximally Abelian: all operators that commute with $\mathcal{M}^0_{d^2}$ belong to $\mathcal{M}^0_{d^2}$. Therefore the so constructed tangent functional corresponds to a witness belonging to $M^0_{d^2}$. It follows that $\mathcal{C}_0$ is the set of states determined by a density matrix $\rho \in \mathcal{M}^0_{d^2}$ for which also $(T \otimes 1)\rho$ remains a density matrix, though not belonging to $\mathcal{M}^0_{d^2}$. □

If we combine theorem 2 and theorem 3, we obtain

Theorem 4. *The set of real linear functionals over* $\mathcal{M}^0_{d^2}$ *and the set of real linear functionals over* $\mathcal{M}_d$ *are in one-to-one correspondence by the map* $\omega \to \omega \circ T \otimes 1$. *Under this map ppt-states correspond to pW-states.*

Proof. For a ppt-state both ω and $\omega \circ T \otimes 1$ is a state. According to (19) it follows that $\mathcal{P}_{\mathcal{A},\rho}(l_1, l_2)), \mathcal{P}_{\mathcal{A},(T\otimes 1)\rho}(l_1, l_2)$ is positive $\forall (l_1, l_2)$ which by definition is the case for a pW-state. Note that in (18) it was not necessary to assume $\rho \in \mathcal{M}^0_{d^2}$. □

We want to learn more about the geometry of the ppt-states or equivalently the pW-states and their tangent functionals, where both viewpoints might give additional insight. Assume that we have found an extremal ppt-state $\omega_{0,0}$ with entanglement witness $A^t_{0,0}$. Then $\omega_{r_1,r_2}(B) = \omega_{00}\big((U_{r_1,r_2} \otimes 1)B(U^*_{r_1,r_2} \otimes 1)\big)$ is also an extremal ppt-state and $(U^*_{r_1,r_2} \otimes 1)A^t_{0,0}(U_{r_1,r_2} \otimes 1)$ is its entanglement witness. There remains the possibility that the two states belong to the same tangent space or equivalently that $A^t_{0,0}$ commutes with $U_{r_1,r_2} \otimes 1$. On the other hand not all entanglement witnesses have to be connected by these unitary transformations. From a geometric viewpoint there remains as the extreme case that to every tangent space there exists only one extremal ppt-state. For geometric reasons we only know that the number of tangent spaces must be $\geqslant d^2$ (compare the octahedron for $d = 2$ where in addition to the obvious symmetry relation we have a reflection).

We turn to the image of the entanglement witnesses in M_d. We know that with $\omega_{0,0}$ a ppt-state on the boundary $\omega_{0,0} \circ T \otimes 1$ defines a state over M_d, but for an arbitrary small perturbation becomes only a real functional. This functional corresponds to a Hermitian operator that can uniquely be decomposed into its positive and negative parts and therefore also gives a unique decomposition of the real functional into the difference of two positive functionals $\omega_+ - \omega_-$. Then $\frac{\omega_-}{\|\omega_-\|}$ has accumulation points, and similarly ω_+ has a limit point that is orthogonal to the accumulation points of the negative part. Therefore a state on the boundary defines a projection operator on its nontrivial orthogonal complement. Let us call it $Q_{0,0}$. In the limit we keep

$$\omega_{0,0}(T \otimes 1 Q_{0,0}) = 0. \tag{20}$$

Note however that we do not conclude so far that $Q_{0,0}$ defines a tangent functional.

On the other hand, as for the ppt-states the set of linear functionals that remain positive is a convex set characterized by its tangent planes that in this context correspond to the images by $T \otimes 1$ of the optimal entanglement witnesses. Do the images of the ppt-witnesses that coincide with the pW-witnesses reflect the projection operators that are the characteristic of the extremal pW-states?

3.1. Werner states and their images

We study the above question on special states where we know the explicit form of the extremal ppt-states and can also construct the corresponding ppt-witness.

The set of states that we consider contains especially the Werner states with density matrices

$$\rho = \left(\frac{1-c}{d^2}\right) 1 + c P_{r_1,r_2}. \tag{21}$$

For simplicity we concentrate on $P_{0,0}$. The other Werner states and according to theorem 3 also their ppt-witnesses can be obtained according to (5) by applying $U_{r_1,r_2} \otimes 1$. The entangled states are those for which $\frac{1}{d+1} \leqslant c \leqslant 1$ where the upper bound guarantees positivity whereas the lower bound can be found in [8, 9]. A Werner state is characterized by the fact that it is invariant under $U \otimes \tilde{U}$ $\forall U \in M_d$ where the details on how $\tilde{U}$ is determined by U depend on the set (r_1, r_2). As a consequence every optimal entanglement witness is mapped by $U \otimes \tilde{U}$ into an optimal entanglement witness. Especially averaging over all permitted rotations $U \otimes \tilde{U}$ generates again an optimal entanglement witness that commutes with $U \otimes \tilde{U}$. Since we know that for the Werner state there exists only one tangent space, the entanglement witness is unique and of the form $1 + g P_{0,0}$. With

$$\mathrm{tr}\left(\frac{1}{d(d+1)} + \frac{1}{d+1} P_{0,0}\right)(1 + g P_{0,0}) = \left(\frac{d^2}{d(d+1)}\right) + \frac{1}{d+1} + g\left(\frac{1}{d+1} + \frac{1}{d(d+1)}\right) = 0 \tag{22}$$

we obtain $g = -d$. Therefore the tangent plane for the pW-states over M_d is determined by

$$T \otimes 1(1 - d P_{0,0}) = 1 - \frac{1}{d} \sum_{r_1,r_2} \mathrm{e}^{2\pi \frac{\mathrm{i}}{d} r_1 r_2} U_{r_1,-r_2} \otimes U_{-r_1,r_2}. \tag{23}$$

Calculating

$$\begin{aligned}
&\sum_{r_1,r_2} \mathrm{e}^{2\pi \frac{\mathrm{i}}{d} r_1 r_2} U_{r_1,-r_2} \otimes U_{-r_1,r_2} \sum_{t_1,t_2} \mathrm{e}^{2\pi \frac{\mathrm{i}}{d} t_1 t_2} U_{t_1,-t_2} \otimes U_{-t_1,t_2} \\
&\qquad = \sum_{r_1,r_2,t_1,t_2} \mathrm{e}^{2\pi \frac{\mathrm{i}}{d}(r_1 r_2 + t_1 t_2 + 2 t_1 r_2)} U_{r_1+t_1,-r_2-t_2} \otimes U_{-r_1-t_1,r_2+t_2} \\
&\qquad = \sum_{r_1,r_2,t_1,t_2} \delta_{r_1+t_1,0} \delta_{r_2+t_2,0} = d^2
\end{aligned} \tag{24}$$

we observe that $\left(1 - \frac{1}{d} \sum_{r_1,r_2} \mathrm{e}^{2\pi \frac{\mathrm{i}}{d} r_1 r_2} U_{r_1,-r_2} \otimes U_{-r_1,r_2}\right)^2 = 2\left(1 - \frac{1}{d} \sum_{r_1,r_2} \mathrm{e}^{2\pi \frac{\mathrm{i}}{d} r_1 r_2} U_{r_1,-r_2} \otimes U_{-r_1,r_2}\right)$ and therefore proportional to a projector $\beta Q \otimes 1$. Evaluating $\mathrm{tr}\, \beta Q \otimes 1 = d(d-1)$ we conclude that the dimension of Q equals $\frac{d-1}{2}$.

If however we examine the matrices over M_d that belong to the Werner states, then we get

$$T \otimes 1\left(\frac{1}{d(d+1)} + \frac{1}{d+1} P\right) = \frac{1}{d(d+1)} + \frac{1}{d^2(d+1)} \sum_{r_1,r_2} \mathrm{e}^{2\pi \frac{\mathrm{i}}{d} r_1 r_2} U_{r_1,-r_2} \otimes U_{-r_1,r_2}. \tag{25}$$

Using (20) the density operator is again proportional to a projector $\alpha \bar{Q}$ with $\alpha^2 = 2\frac{1}{d(d+1)}$. Evaluating its dimension we use $\mathrm{tr}_{M_{d^2}} \alpha \bar{Q} \otimes 1 = 1$ and obtain $\frac{1}{\alpha d} = \frac{d+1}{2}$. Evidently $\bar{Q} Q = 0$ in correspondence with the fact that Q defines a tangent space, and $Q = 1 - \bar{Q}$.

The other tangent space corresponding to $c = 1$ describes the border line where the functional over M_{d^2} stops to be positive, without referring to the partial transposition. Therefore, we cannot expect and it is also not true that the corresponding functional over M_d violates positivity and defines a projection.

Note that $A_g = T \otimes 1\left(1 + g P_{r_1,r_2}\right) = \beta Q$ with Q being a projection according to (24) has as only solutions $g = \pm d$. Therefore also on this basis we find the borderline between entangled states and ppt-states respectively the border of pW-states. In fact, in this special setting the projection operator that corresponds to the border already coincides with the operator defining the tangent functional.

It remains to study the relation between the operators

$$Q_{r_1,r_2} = \frac{1}{2}\left(1 - \frac{1}{d} \sum_{l_1,l_2} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d}(l_1 r_2 - l_2 r_1 + l_1 l_2)} U_{l_1,-l_2} \otimes U_{-l_1,l_2}\right). \tag{26}$$

We evaluate

$$\operatorname{tr} Q_{r_1,r_2} Q_{t_1,t_2} = \frac{1}{4}\left(d^2 - 2d + \frac{1}{d^2}\sum_{l_1,l_2} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d}(l_1 r_2 - l_2 r_1 - l_1 t_2 + l_2 t_1)}\right)$$
$$= \frac{d^2 - 2d}{4} = \frac{d(d-2)}{4}, \qquad (r_1, r_2) \neq (t_1, t_2). \tag{27}$$

Therefore the projections are homogeneously distributed. Especially for $d = 3$ they are one dimensional, but they do not serve to assign lines in phase space as it is desired in [3].

4. The geometry of extremal ppt-states

Let us first consider $d = 2^m$. We choose the Abelian algebra built by (13). In detail this algebra is studied in [12] for $m = 2$. The picture is more transparent if we remove the normalization of states and consider instead linear functionals. Since all operators commute we can use the classical picture. Therefore the set of positive functionals is a cone in the set of functionals, built by d^2 hyperplanes, corresponding to positive operators orthogonal to one of the Werner states. The partial transposition maps the Abelian algebra into itself and acts as a partial reflection. Therefore it transforms the set of positive functionals into another cone with the same origin built by other d^2-dimensional hyperplanes. These hyperplanes are tangent functionals to the set of ppt-states and are determined by the d^2 points, where the linear combination of a Werner state and the tracial state turns from a ppt-state to a non-ppt-state. This transition point is known. In addition, we know that for this class of states we do not have to distinguish between ppt-states and separable states. The total set of ppt-states is therefore the intersection of the two cones with common origin and thus again a cone, now built by $2d^2$ hyperplanes, and there are no other restrictions. In particular, the additional hyperplanes correspond to entanglement witnesses A_r, and the extremal ppt states can be characterized by satisfying

$$\exists r \in \{1, \ldots, d^2\}, \qquad \omega_e(A_r) = 0. \tag{28}$$

However, as is shown in [12] even in this transparent situation the set of separable states is smaller than the set of ppt-states. A complete description of separable states is missing.

This consideration remains only partly true in other dimensions: the boundary of the ppt-states splits into two parts, one where the linear functional f stops being positive, the other, where $f \circ T \otimes 1$ stops being positive. One corresponds to a cone with d^2 hyperplanes as boundary; the other is given by the geometry of pure states over a d-dimensional matrix algebra, which can also be characterized by tangent planes. The set of ppt-states is again the intersection of these two sets.

4.1. The structure of the tangent planes for odd dimension

We now turn to d odd and analyse the boundary in more detail. Then we can conclude that

Lemma. *All states satisfying*

$$\omega\big(T \otimes 1\big(1 - dP_{r_1,r_2}\big)\big) = 0 \tag{29}$$

for some (r_1, r_2) do not belong to the interior of the set of ppt-states.

More precisely, looking for candidates on the boundary of the set of ppt-states we have to look for states corresponding to a density matrix $\rho = \sum_{l_1,l_2} c_{l_1,l_2} P_{l_1,l_2}$ satisfying

$$\sum_{l_1,l_2} c_{l_1,l_2} \operatorname{tr} P_{l_1,l_2}\big(1 - dP_{s_1,s_2}\big) \leqslant 0, \qquad \exists\{r_1, r_2\}, \sum_{l_1,l_2} c_{l_1,l_2} \operatorname{tr} P_{l_1,l_2}\big(1 - dP_{r_1,r_2}\big) = 0.$$

It follows that $0 \leqslant c_{l_1,l_2} \leqslant c_{r_1,r_2} = \frac{1}{d}$. This is a sufficient condition for belonging to the boundary of ppt-states. We concentrate on the extremal states that under this condition cannot further be decomposed. These are the states characterized by a set Λ such that the corresponding density matrix $\rho_\Lambda = \sum_{l_1,l_2} c_{l_1,l_2} P_{l_1,l_2}$ with $c_{l_1,l_2} = \frac{1}{d}$, $\{l_1, l_2\} \subset \Lambda$. It follows that the size of Λ is $|\Lambda| = d$ and $\sum_{(l_1,l_2)\subset\Lambda} \frac{1}{d} P_{l_1,l_2}$ therefore corresponds to d-dimensional projection operators in $M^0_{d^2}$. We will search for those Λ for which the corresponding state is separable. According to (29) it is also on the boundary of ppt-states. The convex combinations of all these states form a subset of the separable states. We expect that it is really smaller than the set of separable states, and that in addition also ppt-states exist, which are not separable. We leave this problem for further investigation. However, already the considered states determined by the permitted Λ will give insight into the Wigner functions. Therefore we hope that the interplay of the description will give further understanding on one hand of the Wigner functions, and on the other hand of a refined description of separable and ppt-states.

We start with a pure separable state

$$|\Psi\rangle\langle\Psi| = \sum_{r,r's,s'} a_r \bar{a}_s b_{r'} \bar{b}_{s'} |r, r'\rangle\langle s, s'| = |a\rangle\langle a| \otimes |b\rangle\langle b|.$$

This state will not belong to the class of states in $M^0_{d^2}$. But we can create a separable density matrix in $M^0_{d^2}$ that corresponds to this state by taking the invariant mean with respect to the group $M^0_{d^2}$:

$$\begin{aligned}\sum_{l_1,l_2} U_{l_1,l_2} \otimes U_{-l_1,l_2} |\Psi\rangle\langle\Psi| U^*_{l_1,l_2} \otimes U^*_{-l_1,l_2} \\ &= \sum_{r,s,r',s',l_1,l_2} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} l_1(r-s-r'+s')} a_r \bar{a}_s b_{r'} \bar{b}_{s'} |r + l_2, r' + l_2\rangle\langle s + l_2, s' + l_2| \\ &= d \sum_{u,u',v,l_2} a_{u-l_2} \bar{a}_{v-l_2} b_{u'-l_2} \bar{b}_{u'-u+v-l_2} |u, u'\rangle\langle v, u' - u + v|. \end{aligned} \tag{30}$$

The so obtained state is separable but not necessarily extremal separable. However, all extremal separable states in $M^0_{d^2}$ are of this type: assume that such an extremal separable state can be written as $\sum_i |\Psi_i\rangle\langle\Psi_i|$. Taking the invariant mean does not change the state but produces a nontrivial decomposition into separable states belonging to $\mathcal{M}^0_{d^2}$ if the averages over the different $|\Psi_i\rangle\langle\Psi_i|$ do not coincide. Therefore, we can start with a state of the type (30) and compare it with

$$\begin{aligned}\sum_{r_1,r_2} c_{r_1,r_2} P_{r_1,r_2} &= \frac{1}{d} \sum_{r_1,r_2} c_{r_1,r_2} U_{r_1,r_2} \otimes 1 \left| \sum_j j, j \right\rangle \left\langle \sum_k k, k \right| \\ &= \sum_{r_1,u,u',v} \frac{1}{d} c_{r_1,u-u'} \, \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} r_1(u-v)} |u, u'\rangle\langle v, u' - u + v|. \end{aligned} \tag{31}$$

(30) and (31) gives

$$\sum_{r_1} c_{r_1,u-u'} \, \mathrm{e}^{\frac{2\pi \mathrm{i}}{d} r_1(u-v)} = \sum_{l_2} a_{u-l_2} \bar{a}_{v-l_2} b_{u'-l_2} \bar{b}_{u'-u+v-l_2}$$

or

$$c_{r_1,r_2} = \frac{1}{d} \sum_{t,z} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{d} z r_1} a_t \bar{a}_{t-z} b_{t+r_2} \bar{b}_{t+r_2-z} = \frac{1}{d} \left| \langle a| U_{\frac{r_1}{2},r_2} |b\rangle \right|^2 \tag{32}$$

where $r_1/2$ is the solution of $2s_1 = r_1 \,\mathrm{mod}(d)$. Especially for normalized $\|\Psi\| = 1$ we can control

$$0 \leqslant \frac{1}{d}\sum_{t,z} a_t \bar{a}_{t-z} b_t \bar{b}_{t-z} = c_{00} \leqslant \frac{1}{d}$$
$$\frac{1}{d}\sum_{r_1,r_2,t,z} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{d} z r_1} a_t \bar{a}_{t-z} b_{t+r_2} \bar{b}_{t+r_2-z} = 1$$

as it should be. Let us concentrate on our condition that the separable state lies on the tangent plane corresponding to the Werner state with $c_{00} = \frac{1}{d}$.

$$c_{00} = \frac{1}{d} = \frac{1}{d}\sum_{t,z} a_t \bar{a}_{t-z} b_t \bar{b}_{t-z} = \frac{1}{d}\langle \bar{b}|a\rangle\langle a|\bar{b}\rangle.$$

This is only satisfied for

$$|\bar{b}\rangle = \mathrm{e}^{\mathrm{i}\alpha_{0,0}}|a\rangle \tag{33}$$

where without loss of generality we may assume that $\alpha_{0,0} = 0$. Similarly

$$c_{r_1,r_2} = \frac{1}{d} = \frac{1}{d}\sum_{t,z} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{d} z r_1} a_t \bar{a}_{t-z} b_{t+r_2} \bar{b}_{t+r_2-z}$$

demands

$$|\bar{b}\rangle = \mathrm{e}^{\mathrm{i}\alpha_{r_1,r_2}} U_{r_1/2,r_2}|a\rangle. \tag{34}$$

If both $c_{0,0} = c_{r_1,r_2} = \frac{1}{d}$, then we can use (33), (34) and continue to

$$|a\rangle = \mathrm{e}^{\mathrm{i}\alpha_{nr_1,nr_2}} U_{nr_1/2,nr_2}|a\rangle. \tag{35}$$

Inserting this into (32) we conclude that also $c_{nr_1,nr_2} = \frac{1}{d}$. It follows that the sets Λ that correspond to separable states on the chosen hyperplane have to contain $\{nr_1, nr_2, n = 0, \ldots, d-1\}$. Especially for d prime they have to be equal to $\{nr_1, nr_2, n = 0, \ldots, d-1\}$ for given (r_1, r_2), since $|\Lambda| = d$. It remains to find $|a\rangle$, which satisfies (35). The explicit form of the vector depends on (r_1, r_2). Solutions to (35) are given by

$$\begin{aligned} &\Lambda = \{n = 0, \ldots, d-1; 0\}: \quad a_t = \delta_{t,0} \\ &\Lambda = \{n, nl_2; n = 0, \ldots, d-1\}: \quad a_t = \frac{1}{\sqrt{d}}\mathrm{e}^{\frac{2\pi \mathrm{i}}{d} l_2 t^2} \end{aligned} \tag{36}$$

and these are all permitted sets Λ.

We have therefore found states that are both extremal ppt-states and extremal separable states. They belong to the tangent plane. As a consequence the boundary of the ppt-states and that of separable states contain d^2 planes of dimensions $d+1$ and the two boundaries coincide on these planes.

Next we study the counterpart in $\mathcal{M}_d$ of the extremal separable states we have found. The structure will turn out to be more familiar. We restrict our analysis to d prime. In this situation (36) describes all sets Λ that belong to the tangent plane with witness $(1 - dP_{0,0})$. We look which states on $\mathcal{M}_d$ correspond to the extremal ppt-states that we have constructed. The density matrices of the extremal pW-states

$$\begin{aligned} Q_{r_1,r_2} = \sum_n (T\otimes 1)P_{nr_1,nr_2} &= \frac{1}{d^2}\sum_{n,l_1,l_2} \mathrm{e}^{\frac{2\pi \mathrm{i}}{d}(nl_1r_2 - nl_2r_1 - l_1l_2)} U_{l_1,-l_2}\otimes U_{-l_1,l_2} \\ &= \frac{1}{d}\sum_{l_1r_2 - l_2r_1 = 0} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{d} l_1 l_2} U_{l_1,-l_2}\otimes U_{-l_1,l_2} \end{aligned} \tag{37}$$

turn out to be one-dimensional projection operators and we can distinguish $(d+1)$ of them (every set contains d points, among them (0, 0), all others different). They satisfy

$$\frac{1}{d}\mathrm{tr}_{d^2} Q_{1,r} Q_{1,s} = \frac{1}{d} = \mathrm{tr}_d Q_{1,r} Q_{1,s}, \qquad r \neq s$$

$$\mathrm{tr}_d Q_{0,1} Q_{1,r} = \frac{1}{d}.$$

Here we can take the trace either as considering Q to be an operator in $\mathcal{M}_{d^2}$ or as an operator lying in $\mathcal{M}_d$. Therefore, we can interpret them as projections belonging to different mutually unbiased bases. So far we have found the extremal ppt-states corresponding to the entanglement witness $(1 - dP_{0,0})$. The extremal ppt-states corresponding to $\left(1 - dP_{s_1,s_2}\right)$ can be obtained by the unitary transformation with $U_{s_1,s_2} \otimes 1$. The corresponding extremal states with the positive Wigner function are given by the projections

$$Q^{s_1,s_2}_{r_1,r_2} = \frac{1}{d} \sum_{l_1 r_2 - l_2 r_1 = 0} \mathrm{e}^{-\frac{2\pi \mathrm{i}}{d}(l_1 l_2 + s_1 l_2 + s_2 l_1)} U_{l_1,-l_2} \otimes U_{-l_1,l_2} \qquad (38)$$

Again they satisfy, e.g.,

$$\mathrm{tr}\, Q^{t_1,t_2}_{0,1} Q^{s_1,s_2}_{1,n} = \frac{1}{d}, \qquad \{s_1, s_2\} \neq \{t_1, t_2\},$$

but now

$$Q_{1,n} Q^{s_1,s_2}_{1,n} = 0, \qquad \{s_1, s_2\} \neq \{0, 0\}$$

Further

$$Q^{s_1,s_2}_{r_1,r_2} = Q^{t_1,t_2}_{r_1,r_2}, \qquad \forall\, r_1 s_1 + r_2 s_2 = r_1 t_1 + r_2 t_2.$$

These equalities are consequences of (38). (r_1, r_2) determine, which (l_1, l_2) contribute, the appropriate relations between (s_1, s_2) and (t_1, t_2) guarantee that they contribute with the same phase factor. Altogether we have found $d(d+1)$ separable states on the boundary of ppt-states that cannot be further decomposed into states on the boundary, and these states correspond in M_d to $d(d+1)$ projections that define the desired $d+1$ mutually unbiased bases in the sense of [3, 4]. But even more, in [17] it is shown that these are the vertices such that every state for which the Wigner function compatible with the mutually unbiased bases in the sense of [3] is positive, is a convex combination of these pure states. Since more Wigner functions are taken into account, this set is an intersection of sets in our context. This supports the conjecture that the corresponding polyhedron in the set of separable states does not cover all separable states. On the other hand it raises the question whether separable states give some characteristic features to the corresponding Wigner functions. Further we keep the additional boundary corresponding to states over $M^0_{d^2}$ of the form $1 - \frac{1}{d^2} P_{r_1,r_2}$, but also those determining the boundary of the ppt-states. Again our special convex set of separable states covers a subset of ppt-states.

5. Conclusion

Starting with a maximally Abelian algebra that represents maximally entangled states we moved via the partial transposition to a non-Abelian algebra that for odd dimensions is the full matrix algebra. The states on the Abelian algebra define functionals on the non-Abelian algebra. With the appropriate and natural choice of Weyl operators this partial transposition maps the initial state considered as a restricted state over a classical lattice into the Wigner functions offered in [5]. Ppt-states and states with positive Wigner function are in one-to-one correspondence. The decomposition into extremal separable states that is fairly well under control can be used to define operators in the matrix algebra. At least for d prime these operators turn out to be the projections on the set of unbiased bases which is the starting point for the definition of the Wigner functions as proposed in [3]. As a consequence the definition of the Wigner functions in the sense of [5] can be considered as a generalization of the definition of [3] to dimensions that are not prime. The decomposition into extremal separable states can be used to find a replacement in these dimensions for the mutually unbiased bases. This is under investigation.

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