Separability bounds on multiqubit moments due to positivity under partial transpose

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Abstract

Positivity of the density operator reflects itself in terms of sequences of inequalities on observable moments. Uncertainty relations for non-commuting observables form a subset of these inequalities. In addition, criterion of positivity under partial transposition (PPT) imposes distinct bounds on moments, violations of which signal entanglement. We present bounds on some novel sets of composite moments, consequent to positive partial transposition of the density operator and report their violation by entangled multiqubit states. In particular, we derive separability bounds on a multiqubit moment matrix (based on PPT constraints on bipartite divisions of the density matrix) and show that three qubit pure states with non-zero tangle violate these PPT moment constraints. Further, we recover necessary and sufficient condition of separability in a multiqubit Werner state through PPT bounds on moments.

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Quantum description of nature departs from classical one at various levels. Uncertainty relations (UR) exhibit quantum feature in a fundamental manner. Entanglement is another peculiar quantum signature, which has evoked much interest from the point of view of its applicability in quantum information science [1] - in addition to promoting a deeper conceptual understanding. While UR bring out explicit constraints placed on first and second moments of two non-commuting observables, it is a complex issue to specify how inseparability manifests itself through observable moments. Exploring such practical entanglement tests forms an active field of research [2, 3, 4, 5, 6].

A hierarchy of inequalities for the observable moments could be formulated based on the non-negativity of the density operator characterizing the quantum system [7, 8, 9] - uncertainty principle occurring as a particular attribute of this property. In the case of composite quantum systems, appropriately chosen matrix of moments associated with the set of all states, which are positive under partial transpose (PPT) [10], get additional restrictions - thus paving way for distinguishing them from the class of quantum entangled states that are non-positive under partial transpose (PT). It may be emphasized that the PPT constraints on composite moments are equivalent to the positivity of the associated partially transposed density matrix (when PT on bipartite divisions of the system are considered). The reformulation of the problem of testing entanglement in terms of observable moments has been successful in the case of two-mode gaussian states, where necessary and sufficient conditions of entanglement get encrypted as inequalities [11, 12] on second order moments of canonical observables ($\hat{q}$, $\hat{p}$; $\hat{q}'$, $\hat{p}'$). It is a complex issue to find a general prescription to identify appropriate basic operators associated with composite systems, which reveal entanglement in terms of optimal bounds on observable moments. However, operators exhibiting simple transformation properties under PT serve as useful tools in exploring how inseparability gets encoded in observable moments [6, 11, 12, 13].

The purpose of the present paper is to investigate separability bounds on composite moments associated with multiqubit systems, by exploiting simple transformation properties of the basic qubit operators under PT. With suitable choices of operators, we recover necessary and sufficient conditions for separability in multiqubit systems of interest - formulated here as PPT inequalities on moments. More specifically, we recover inseparability conditions of
Horodecki et. al. [14] on the state parameters of entangled two qubit systems as violation of PPT bounds on a given moment matrix. We construct a generalized multiqubit moment matrix involving basic observables of the system, and show that PPT moment inequalities are violated by GHZ-like pure states. Inseparable multiqubit Werner states are also shown to necessarily violate the PPT moment constraints.

The organization of this paper is as follows: In Sec. II a general description to find PPT bounds on the matrix of moments is outlined. In Sec. III suitable matrices of two qubit moments are investigated and PT restrictions on moments are derived. Entangled two qubit states are shown to violate these PPT bounds on moments. In Sec. IV a special $4 \times 4$ multiqubit moment matrix is proposed and restriction on it due to partial transpose on bipartite divisions of the system is identified. Entangled three qubit pure states with non-zero tangle are shown to necessarily violate the PPT bounds on the moments. Further, we recover necessary and sufficient condition for separability in multiqubit Werner state through PPT moment restrictions. Sec. V has a summary of results.

II. GENERAL DESCRIPTION OF PPT INEQUALITIES ON MOMENTS

Consider a set of linearly independent, hermitian observables $\{ \hat{A}_i, \ i = 0, 1, 2, \ldots \}$, with $\hat{A}_0 = \hat{I}$ being the identity operator, arranged in the form of an operator column (row) $\hat{\xi} (\hat{\xi}^T)$ as,

$$\hat{\xi}^T = \left( \hat{A}_0 \ \hat{A}_1 \ \ldots \ \hat{A}_n \right).$$

(1)

The moment matrix [9], $M(\hat{\rho}) = \text{Tr}[\hat{\rho} \hat{\xi} \hat{\xi}^\dagger]$, formed by taking quantum averages of operator entries of $\hat{\xi} \hat{\xi}^\dagger$ in a density operator $\hat{\rho}$ is given by,

$$M(\hat{\rho}) = \begin{pmatrix}
1 & \langle \hat{A}_1 \rangle & \langle \hat{A}_2 \rangle & \ldots & \ldots \\
\langle \hat{A}_1 \rangle & \langle \hat{A}_1^2 \rangle & \langle \hat{A}_1 \hat{A}_2 \rangle & \ldots & \ldots \\
\langle \hat{A}_2 \rangle & \langle \hat{A}_2 \hat{A}_1 \rangle & \langle \hat{A}_2^2 \rangle & \ldots & \ldots \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\vdots & \vdots & \vdots & \ddots & \vdots 
\end{pmatrix}.$$  

(2)

By virtue of its construction, $M(\hat{\rho}) \geq 0$, a condition imposed due to the non-negativity of $\hat{\rho}$. In other words, positive semi-definiteness of the density matrix $\hat{\rho}$ is reformulated in terms of observable moments of all orders. The well-known Schrodinger-Robertson (SR) uncertainty
relation for the observables $A_1$, $A_2$ i.e.,

$$\langle (\Delta \hat{A}_1)^2 \rangle \langle (\Delta \hat{A}_2)^2 \rangle \geq \frac{1}{4} \left( \langle [\hat{A}_1, \hat{A}_2] \rangle^2 + \langle \{\Delta \hat{A}_1, \Delta \hat{A}_2\} \rangle^2 \right),$$

(3)

(where $\Delta \hat{A}_i = \hat{A}_i - \langle \hat{A}_i \rangle$, and $\{\Delta \hat{A}_1, \Delta \hat{A}_2\} = \Delta \hat{A}_1 \Delta \hat{A}_2 + \Delta \hat{A}_2 \Delta \hat{A}_1$) emerges \[9\] as a consequence of the positive semi-definiteness of the $3 \times 3$ principle diagonal block of (2):

$$\begin{pmatrix}
1 & \langle \hat{A}_1 \rangle & \langle \hat{A}_2 \rangle \\
\langle \hat{A}_1 \rangle & \langle \hat{A}_1^2 \rangle & \langle \hat{A}_1 \hat{A}_2 \rangle \\
\langle \hat{A}_2 \rangle & \langle \hat{A}_2 \hat{A}_1 \rangle & \langle \hat{A}_2^2 \rangle
\end{pmatrix} \geq 0.$$

For the canonical observables $\hat{A}_1 = \hat{q}$, $\hat{A}_2 = \hat{p}$, satisfying the commutation relation $[\hat{q}, \hat{p}] = i \hbar$, this leads to an unsurpassable quantum limit

$$\langle (\Delta \hat{q})^2 \rangle \langle (\Delta \hat{p})^2 \rangle - \frac{1}{4} \langle \{\Delta \hat{q}, \Delta \hat{p}\} \rangle^2 \geq \frac{\hbar^2}{4},$$

which serves as both necessary and sufficient condition for a single mode Gaussian to be a legitimate quantum state. When more general states are considered it becomes a nontrivial task to identify a finite set of inequalities on moments, capturing the positivity of the quantum states \emph{completely}.

If a given multipartite quantum state is separable, i.e., when the state can be expressed as a convex sum of product states,

$$\hat{\rho}^{\text{sep}} = \sum_i p_i \hat{\rho}_{1i} \otimes \hat{\rho}_{2i} \otimes \ldots \otimes \hat{\rho}_{ni}, \quad \sum_i p_i = 1, \quad 0 \leq p_i \leq 1,$$

PT operation \[10\] on any bipartite division of the state preserves its hermiticity, positive semi-definiteness and unit trace, leading to another physically valid separable state. The moment matrix $M(\hat{\rho}^{\text{sep}})$ as well as the corresponding matrix $M((\hat{\rho}^{\text{sep}})^{\text{PT}})$, constructed using partially transposed separable density operator are bound to be non-negative. Therefore, separability implies additional restriction viz., $M(\hat{\rho}^{\text{PT}}) \geq 0$ on the moments, which is stronger, in general, than the usual moment matrix positivity condition $M(\hat{\rho}) \geq 0$.

If the PT map is transferred to operators i.e.,

$$\text{Tr}[\hat{\rho}^{\text{PT}} \mathcal{O}] = \text{Tr}[\hat{\rho} \mathcal{O}^{\text{PT}}] \quad \text{with} \quad \mathcal{O} \longrightarrow \mathcal{O}^{\text{PT}},$$

(4)

positivity of the moment matrix in a separable state may be expressed as,

$$M((\hat{\rho}^{\text{sep}})) \geq 0, \quad M^{\text{PT}}((\hat{\rho}^{\text{sep}})) \geq 0,$$

(5)
where \( M^{\text{PT}}(\hat{\rho}^{\text{sep}}) = M((\hat{\rho}^{\text{sep}})^{\text{PT}}) \).

An equivalent of SR inequality (3) in a partially transposed separable state is readily obtained by demanding positivity of the 3 \( \times \) 3 principle diagonal block of \( M^{\text{PT}}(\hat{\rho}^{\text{sep}}) \):

\[
\langle((\triangle \hat{A}_1)^2)^{\text{PT}}\rangle \langle((\triangle \hat{A}_2)^2)^{\text{PT}}\rangle \geq \frac{1}{4} |\langle[\triangle \hat{A}_1, \triangle \hat{A}_2]^{\text{PT}}\rangle|^2 \]

Gillet et. al. [6] considered special observables \( \hat{A}_1 \) and \( \hat{A}_2 \) satisfying the property

\[
(\hat{A}_1^2)^{\text{PT}} = (\hat{A}_1^{\text{PT}})^2, \quad (\hat{A}_2^2)^{\text{PT}} = (\hat{A}_2^{\text{PT}})^2,
\]

in which case the LHS of the inequality (6) involves a product of variances \( \langle((\triangle \hat{A}_1)^2)^{\text{PT}}\rangle \langle((\triangle \hat{A}_2)^2)^{\text{PT}}\rangle \) and the resulting Schrodinger-Robertson partial transpose (SRPT) inequality is, in general, stronger compared to the traditional SR uncertainty for the operators \( A_1^{\text{PT}}, A_2^{\text{PT}} \). SRPT inequality [6] is necessarily obeyed by the set of all separable states and its violation would therefore be sufficient to detect entanglement. Using special observables satisfying (7), a wide class of entangled pure bipartite, tripartite states of qubits, angular momentum states of harmonic oscillators, cat states, etc. are shown [6] to violate the SRPT inequality. In general, violation of PPT bounds \( M^{\text{PT}}((\hat{\rho}^{\text{sep}})) \geq 0 \) provide a series of constraints on observable moments, which leads to operational tests of entanglement.

It is worth noting that the implications of PT on observables is established as "local time-reversal" in the case of canonical pair of observables \( \{\hat{q}_\alpha, \hat{p}_\alpha\} \) of continuous variable (CV) states and also for basic qubit observables \( \vec{\sigma}_\alpha \):

\[
\text{PT on CV observables (w.r.t \( \alpha^{\text{th}} \) subsystem)}:\]

\[
\hat{q}_\alpha, \hat{p}_\alpha \rightarrow \hat{q}_\alpha, -\hat{p}_\alpha
\]

\[
\hat{q}_\beta, \hat{p}_\beta \rightarrow \hat{q}_\beta, \hat{p}_\beta, \quad \beta \neq \alpha
\]

\[
\text{PT on qubit observables}:
\]

\[
\vec{\sigma}_\alpha \rightarrow -\vec{\sigma}_\alpha
\]

\[
\vec{\sigma}_\beta \rightarrow \vec{\sigma}_\beta, \quad \beta \neq \alpha.
\]

For bipartite CV states, non-negativity of the moment matrix \( M(\hat{\rho}) = \langle \hat{\xi} \hat{\xi}^T \rangle \) constructed using the operator column \( \hat{\xi}^T = (\hat{I}, \hat{\zeta}^T) \) of basic canonical pair of observables \( \hat{\zeta}^T = (\hat{q}_1, \hat{p}_1; \hat{q}_2, \hat{p}_2) \), leads to uncertainty condition on the variance matrix of the two mode CV state:

\[
V + \frac{i}{2} \beta \geq 0,
\]

(10)
where $V$ denotes the $4 \times 4$ real symmetric variance matrix with elements, $V_{ab} = \frac{1}{2}<\{\Delta \hat{\varsigma}_a, \Delta \hat{\varsigma}_b\}>$ and the matrix $\beta$ is defined through $i (\beta)_{ab} = <[\hat{\varsigma}_a, \hat{\varsigma}_b]>$. The PT map on the canonical observables, leads to a structurally similar uncertainty-like restriction on the variance matrix expressed compactly as [11]

\[ V^{PT} + \frac{i}{2} \beta \geq 0, \quad V^{PT} = \Omega V \Omega, \tag{11} \]

where $\Omega = \text{diag}(1, -1, 1, 1)$, for partial transpose taken on the first system. Separable bipartite CV states never violate the inequality (11) and its violation signals entanglement of a bipartite CV state. Moreover, violation of (11) serves as both necessary and sufficient inseparability condition for an arbitrary two mode Gaussian state [11]. Inequalities on higher order moments of bipartite CV states, involving canonical pairs of observables have been formulated by Shchukin and Vogel (SV) [3], based on the positivity of corresponding moment matrix $M^{PT}(\hat{\rho})$. SV result provided a common basis for many other CV inseparability criteria [11, 12, 13] derived previously, including those, which appeared to be independent of the PPT condition.

In the following, we investigate the PPT bounds on some specially constructed moment matrices associated with multiqubit operators, which exhibit well defined PT maps and explore violation of PPT bounds imposed on them.

### III. TWO QUBIT PPT MOMENT INEQUALITIES

An arbitrary two-qubit density operator belonging to the Hilbert-Schmidt space $\mathcal{H} = \mathcal{C}^2 \otimes \mathcal{C}^2$ has the form,

\[ \rho = \frac{1}{4} \left[ I \otimes I + \vec{\sigma} \cdot \vec{s}^{(1)} \otimes I + I \otimes \vec{\sigma} \cdot \vec{s}^{(2)} + \sum_{i,j=1,2,3} \sigma_i \otimes \sigma_j t_{ij} \right], \tag{12} \]

where $\sigma_i$ are the standard Pauli spin matrices; $I$ denotes the $2 \times 2$ unit matrix. Here, qubit averages are given by,

\[ \vec{s}^{(1)} = \text{Tr} (\rho \vec{\sigma} \otimes I), \quad \vec{s}^{(2)} = \text{Tr} (\rho I \otimes \vec{\sigma}) \tag{13} \]

and

\[ t_{ij} = \text{Tr} (\rho \sigma_i \otimes \sigma_j), \tag{14} \]
are elements of the real $3 \times 3$ two qubit correlation matrix

$$T = \begin{pmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix}. \quad (15)$$

A direct examination of positivity bounds on the moment matrix may be done by considering a basic column of qubit operators $\hat{\xi}_1^T = (I \otimes I, \sigma_i \otimes I, I \otimes \sigma_j)$. We construct a real symmetric moment matrix $M_1(\hat{\rho}) = \langle \hat{\xi}_1^T \hat{\xi}_1 \rangle$, expressed in a suitable block form as,

$$M_1(\hat{\rho}) = \begin{pmatrix} 1 & s^{(1)T} & s^{(2)T} \\ s^{(1)} & I & T \\ s^{(2)} & T^T & I \end{pmatrix} = \begin{pmatrix} 1 & C^T \\ C & B \end{pmatrix}, \quad (16)$$

where $B = \begin{pmatrix} I & T \\ T^T & I \end{pmatrix}$, $C^T = \begin{pmatrix} s^{(1)T}, s^{(2)T} \end{pmatrix}$

where $s^{(1)}$, $s^{(2)}$ denote three componental columns of qubit averages: $s^{(1)T} = (s_1^{(1)}, s_2^{(1)}, s_3^{(1)})$, $s^{(2)T} = (s_1^{(2)}, s_2^{(2)}, s_3^{(2)})$, and $I$ denotes $3 \times 3$ identity matrix.

A congruence transformation

$$M_1(\hat{\rho}) \longrightarrow L M_1(\hat{\rho}) L^T = \begin{pmatrix} 1 & 0 \\ 0 & B - C C^T \end{pmatrix} \quad (17)$$

with $L = \begin{pmatrix} 1 & 0 \\ -C & I \oplus I \end{pmatrix}$ leads to the identification that

$$M_1(\hat{\rho}) \geq 0 \iff B - C C^T \geq 0$$

i.e.,

$$\begin{pmatrix} I - s^{(1)T} & T - s^{(1)T} \\ T^T - s^{(2)T} & I - s^{(2)T} \end{pmatrix} \geq 0. \quad (18)$$

The corresponding PT moment matrix $M_1^{PT}(\hat{\rho}) \equiv M_1(\hat{\rho}^{PT})$ is obtained by using $[9]$ (with PT operation on the first qubit) and after some simple algebra we obtain,

$$M_1^{PT}(\hat{\rho}) = \begin{pmatrix} 1 & -s^{(1)T} & s^{(2)T} \\ -s^T & I & -T \\ s^2 & -T^T & I \end{pmatrix}. \quad (19)$$
Following similar arguments illustrated above, we identify that

\[ M_1^{PT}(\hat{\rho}) \geq 0 \iff \]

\[
\begin{pmatrix}
    \mathcal{I} - s^{(1)}s^{(1)T} & - (T - s^{(1)}s^{(2)T}) \\
    -(T^T - s^{(2)s^{(1)T}}) & \mathcal{I} - s^{(2)}s^{(2)T}
\end{pmatrix} \geq 0. \quad (20)
\]

An examination of (18) and (20) reveals that for two qubit states with random subsystems i.e., \( s^{(1)} = 0 = s^{(2)} \), we have \( M_1(\hat{\rho}) \geq 0 \Rightarrow M_1^{PT}(\rho) \geq 0 \). In other words, the PPT bound (20) does not impose stronger restriction on moments other than the usual positivity constraints (18) and thus, it fails to capture the inseparability of the two qubit state with disordered subsystems.

A suitable moment matrix, PPT constraints on which allow a clear distinction between separable and entangled two qubit states, could indeed be realized and is discussed in the following: We construct a \( 4 \times 4 \) moment matrix \( M_2(\hat{\rho}) = \text{Tr}[\hat{\rho} \hat{\xi}_2 \hat{\xi}_2^\dagger] \), where the operator column \( \hat{\xi}_2 \) is chosen to be,

\[
\hat{\xi}_2 = \begin{pmatrix}
    I \otimes I \\
    \vec{\sigma} \cdot \vec{k}_1 \otimes \vec{\sigma} \cdot \vec{k}_2 \\
    \vec{\sigma} \cdot \vec{l}_1 \otimes \vec{\sigma} \cdot \vec{l}_2 \\
    \vec{\sigma} \cdot \vec{m}_1 \otimes \vec{\sigma} \cdot \vec{m}_2
\end{pmatrix}
\]

with \( \{\vec{k}_1, \vec{l}_1, \vec{m}_1\} \) and \( \{\vec{k}_2, \vec{l}_2, \vec{m}_2\} \) denoting two sets of mutually orthogonal real three dimensional unit vectors. The moment matrix associated with the operator column (21) takes the following explicit form:

\[
M_2(\hat{\rho}) = \begin{pmatrix}
    1 & t_{k_1k_2} & t_{l_1l_2} & t_{m_1m_2} \\
    t_{k_1k_2} & 1 & -t_{m_1m_2} & -t_{l_1l_2} \\
    t_{l_1l_2} & -t_{m_1m_2} & 1 & -t_{k_1k_2} \\
    t_{m_1m_2} & -t_{l_1l_2} & -t_{k_1k_2} & 1
\end{pmatrix}, \quad (22)
\]

where we have denoted \( t_{k_1k_2} = k_1^T T k_2 \), \( t_{l_1l_2} = l_1^T T l_2 \), \( t_{m_1m_2} = m_1^T T m_2 \) with \( T \) corresponding to the two qubit correlation matrix given by (15); \( k_\alpha, l_\alpha, m_\alpha, \alpha = 1, 2 \) being 3 componental columns involving components of unit vectors \( \vec{k}_\alpha, \vec{l}_\alpha, \vec{m}_\alpha \).

Partial transpose operation with respect to first qubit leads to the partial time reversal transformation (9) on the qubit operators and the corresponding moment matrix is given
explicitly by,

\[
M_2^{PT}(\rho) = \begin{pmatrix}
1 & -t_{k_1} - t_{l_1} - t_{m_1} \\
-t_{k_1} & 1 & t_{m_1} \\
-t_{l_1} & t_{m_1} & 1 \\
-t_{m_1} & t_{l_1} & t_{k_1} \\
\end{pmatrix}.
\] (23)

The PPT bound \( M_2^{PT}(\rho) \geq 0 \) is violated if any of the eigenvalues

\[
\begin{align*}
\mu_1^{PT} &= 1 + t_{k_1} - t_{l_1} - t_{m_1} \\
\mu_2^{PT} &= 1 - t_{k_1} + t_{l_1} - t_{m_1} \\
\mu_3^{PT} &= 1 - t_{k_1} - t_{l_1} + t_{m_1} \\
\mu_4^{PT} &= 1 + t_{k_1} + t_{l_1} + t_{m_1}.
\end{align*}
\] (24)

of (23) assume negative values. We illustrate the power of this choice by way of examples.

Consider a two-qubit Werner state

\[
\hat{\rho}_W = \frac{(1 - x)}{4} I \otimes I + x |\Psi(-)\rangle \langle \Psi(-)|, \ 0 \leq x \leq 1
\] (25)

where \(|\Psi(-)\rangle = \frac{1}{\sqrt{2}} |0, 1\rangle - |1, 0\rangle\) is a two qubit Bell state. The two qubit correlation matrix is readily found to be \(T = \text{diag}(-x, -x, -x)\) and with a choice \(k_1^T = (1, 0, 0) = k_2^T, l_1^T = (0, 1, 0) = l_2^T, m_1^T = (0, 0, 1) = m_2^T,\)

it is easy to find the eigenvalues of \(M_2^{PT}(\rho_W)\):

\[
\begin{align*}
\mu_1^{PT} &= 1 - 3x, \ \mu_2^{PT} = \mu_3^{PT} = \mu_4^{PT} = 1 + x.
\end{align*}
\] (26)

Clearly, \(M_2^{PT}(\rho_W)\) respects the PPT bound, when \(0 \leq x \leq \frac{1}{3}\), which is the well-known separability domain [10] for the two qubit Werner state.

We also recover the inseparability conditions of Horodecki et. al., [14] through non-positivity of the eigenvalues (24). In order to see this, we recall that the two qubit state parameters \(\{s_i^{(1)}, s_i^{(2)}, t_{ij}\}\) (defined in (13), (14)) transform under local unitary operations \(U_1 \otimes U_2\) on the qubits as follows [14]:

\[
\begin{align*}
s_i^{(1)'} &= \sum_{j=x,y,z} O_{ij}^{(1)} s_{1j}, \quad s_i^{(2)'} = \sum_{j=x,y,z} O_{ij}^{(2)} s_{2j}, \\
t_{ij}' &= \sum_{k,l=x,y,z} O_{ik}^{(1)} O_{jl}^{(2)} t_{kl} \quad \text{or} \quad T' = O^{(1)} T O^{(2)} T,
\end{align*}
\] (27)

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where $O^{(a)} \in SO(3)$ denote the $3 \times 3$ real orthogonal rotation matrices, corresponding uniquely to the $2 \times 2$ unitary matrices $U_\alpha \in SU(2)$. As the entanglement properties of the two qubit state remain unaltered under local unitary operations one may choose to specify the state parameters $\vec{s}^{(a)}$, ($\alpha = 1, 2$) and $T$ in a basis in which $T$ is diagonal. This is possible because the real $3 \times 3$ correlation matrix $T$ can always be transformed to a diagonal form with the help of an appropriate local transformation $U_1 \otimes U_2$:

$$T^d = O^{(1)} T O^{(2)T} = \text{diag} (t_1, t_2, t_3).$$

(28)

Let us arrange the mutually orthogonal unit column vectors $k_\alpha, l_\alpha, m_\alpha$, $\alpha = 1, 2$ (involved in the definition (21) of the operator column $\hat{\xi}_2$) to form $3 \times 3$ real orthogonal matrices

$$O^{(1)} = \begin{pmatrix} k_1^T \\ l_1^T \\ m_1^T \end{pmatrix}, \quad O^{(2)} = \begin{pmatrix} k_2^T \\ l_2^T \\ m_2^T \end{pmatrix}.$$  (29)

With an appropriate choice of unit vectors $k_\alpha, l_\alpha, m_\alpha$ we may thus transform the two qubit correlation matrix $T$ to its diagonal form

$$T^d = O^{(1)} T O^{(2)T}$$

$$= \text{diag} \left( t_{k_1k_2} = t_1, \quad t_{l_1l_2} = t_2, \quad t_{m_1m_2} = t_3 \right).$$

It is readily found that the non-positivity of the eigenvalues (24) of the PT matrix of moments $M_2^{PT}(\hat{\rho})$ reduce to the inseparability conditions of Horodecki et. al. [14] i.e.,

$$1 + t_1 - t_2 - t_3 < 0, \quad 1 - t_1 + t_2 - t_3 < 0,$$

$$1 - t_1 - t_2 + t_3 < 0, \quad 1 + t_1 + t_2 + t_3 < 0.$$  (30)

IV. PPT BOUNDS ON A MULTIQUBIT MOMENT MATRIX

Now we discuss a special multiqubit moment matrix, which has a distinct and stronger PPT bound than the conventional one. Important class of entangled pure and mixed multiqubit states are shown to violate this PPT bound.

Consider the following four componental column (row) of $N$-qubit operators:

$$\hat{\xi}^T = \left( \bigotimes_{\alpha=1}^N I, \Sigma_1, \Sigma_2, \Sigma_3 \right)$$  (31)
where
\[
\Sigma_1 = \bigotimes_{\alpha=1}^{N} \sigma_{+}^{k_{\alpha}l_{\alpha}} + \bigotimes_{\alpha=1}^{N} \sigma_{-}^{k_{\alpha}l_{\alpha}}
\]
\[
\Sigma_2 = -i \left( \bigotimes_{\alpha=1}^{N} \sigma_{+}^{k_{\alpha}l_{\alpha}} - \bigotimes_{\alpha=1}^{N} \sigma_{-}^{k_{\alpha}l_{\alpha}} \right)
\]
\[
\Sigma_3 = \frac{1}{2^N} \left( \bigotimes_{\alpha=1}^{N} (I + \vec{\sigma} \cdot \vec{m}_\alpha) - \bigotimes_{\alpha=1}^{N} (I - \vec{\sigma} \cdot \vec{m}_\alpha) \right).
\]

(32)

Here, we have denoted
\[
\sigma_{\pm}^{k_{\alpha}l_{\alpha}} = \frac{1}{2} \vec{\sigma} \cdot [\vec{k}_\alpha \pm i \vec{l}_\alpha]
\]
and \{\vec{k}_\alpha, \vec{l}_\alpha, \vec{m}_\alpha\}, \alpha = 1, 2, \ldots, N correspond to sets of mutually orthogonal three dimensional (real) unit vectors.

We give below a more explicit structure of the operators (32) in the case of two and three qubits:

Two qubits:
\[
\Sigma_1 = \frac{1}{2} \left( (\vec{\sigma} \cdot \vec{k}_1) \otimes (\vec{\sigma} \cdot \vec{k}_2) - (\vec{\sigma} \cdot \vec{l}_1) \otimes (\vec{\sigma} \cdot \vec{l}_2) \right)
\]
\[
\Sigma_2 = \frac{1}{2} \left( (\vec{\sigma} \cdot \vec{k}_1) \otimes (\vec{\sigma} \cdot \vec{l}_2) + (\vec{\sigma} \cdot \vec{l}_1) \otimes (\vec{\sigma} \cdot \vec{k}_2) \right)
\]
\[
\Sigma_3 = \frac{1}{2} (\vec{\sigma} \cdot \vec{m}_1 \otimes I + I \otimes \vec{\sigma} \cdot \vec{m}_2)
\]

Three qubits:
\[
\Sigma_1 = \frac{1}{4} \left( (\vec{\sigma} \cdot \vec{k}_1) \otimes (\vec{\sigma} \cdot \vec{k}_2) \otimes (\vec{\sigma} \cdot \vec{k}_3) - (\vec{\sigma} \cdot \vec{l}_1) \otimes (\vec{\sigma} \cdot \vec{l}_2) \otimes (\vec{\sigma} \cdot \vec{k}_3) - (\vec{\sigma} \cdot \vec{k}_1) \otimes (\vec{\sigma} \cdot \vec{l}_2) \otimes (\vec{\sigma} \cdot \vec{l}_3) - (\vec{\sigma} \cdot \vec{l}_1) \otimes (\vec{\sigma} \cdot \vec{k}_2) \otimes (\vec{\sigma} \cdot \vec{l}_3) + i (\vec{\sigma} \cdot \vec{l}_1) \otimes (\vec{\sigma} \cdot \vec{l}_2) \otimes (\vec{\sigma} \cdot \vec{l}_3) \right)
\]
\[
\Sigma_2 = \frac{1}{4} \left( (\vec{\sigma} \cdot \vec{k}_1) \otimes (\vec{\sigma} \cdot \vec{l}_2) \otimes (\vec{\sigma} \cdot \vec{k}_3) - (\vec{\sigma} \cdot \vec{l}_1) \otimes (\vec{\sigma} \cdot \vec{k}_2) \otimes (\vec{\sigma} \cdot \vec{l}_3) - (\vec{\sigma} \cdot \vec{k}_1) \otimes (\vec{\sigma} \cdot \vec{k}_2) \otimes (\vec{\sigma} \cdot \vec{l}_3) \right)
\]
\[
\Sigma_3 = \frac{1}{4} \left( (\vec{\sigma} \cdot \vec{m}_1) \otimes I \otimes I + I \otimes (\vec{\sigma} \cdot \vec{m}_2) \otimes I + I \otimes I \otimes (\vec{\sigma} \cdot \vec{m}_3) + (\vec{\sigma} \cdot \vec{m}_1) \otimes (\vec{\sigma} \cdot \vec{m}_2) \otimes (\vec{\sigma} \cdot \vec{m}_3) \right).
\]
The operators (32) satisfy the following properties
\[
\Sigma_i \Sigma_j = i \epsilon_{ijk} \Sigma_k, \quad i \neq j = 1, 2, 3
\]
\[
\Sigma_i^2 = \frac{1}{2^N} \left( \bigotimes_{\alpha=1}^{N} (I + \vec{\sigma}_\alpha \cdot \vec{m}_\alpha) + \bigotimes_{\alpha=1}^{N} (I - \vec{\sigma}_\alpha \cdot \vec{m}_\alpha) \right)
\]
\[
i = 1, 2, 3.
\] (34)

As will be shown in the foregoing, this novel construction encodes the separability properties of pure three qubit states with non-zero tangle and also in mixed \(N\)-qubit Werner state.

Partial transpose on, say first \(r\) qubits, corresponds to the following PT map on the operators (32) (see Eq. (9)):
\[
\Sigma_{1}^{\text{PT}} = (-1)^r \Sigma_1, \quad \Sigma_{2}^{\text{PT}} = (-1)^r \Sigma_2,
\]
\[
\Sigma_{3}^{\text{PT}} = \frac{1}{2^N} \left( \bigotimes_{\alpha=1}^{r} (I - \vec{\sigma}_\alpha \cdot \vec{m}_\alpha) \bigotimes_{\nu=r}^{N} (I + \vec{\sigma}_\nu \cdot \vec{m}_\nu) \right.
\]
\[
- \bigotimes_{\alpha=1}^{r} (I + \vec{\sigma}_\alpha \cdot \vec{m}_\alpha) \bigotimes_{\nu=r}^{N} (I - \vec{\sigma}_\nu \cdot \vec{m}_\nu) \right),
\]
\[
(\Sigma_i \Sigma_j)^{\text{PT}} = i \epsilon_{ijk} \Sigma_k^{\text{PT}}, \quad i \neq j = 1, 2, 3
\]
\[
(\Sigma_i^2)^{\text{PT}} = \frac{1}{2^N} \left( \bigotimes_{\alpha=1}^{r} (I - \vec{\sigma}_\alpha \cdot \vec{m}_\alpha) \bigotimes_{\nu=r}^{N} (I + \vec{\sigma}_\nu \cdot \vec{m}_\nu) \right.
\]
\[
+ \bigotimes_{\alpha=1}^{r} (I + \vec{\sigma}_\alpha \cdot \vec{m}_\alpha) \bigotimes_{\nu=r}^{N} (I - \vec{\sigma}_\nu \cdot \vec{m}_\nu) \right),
\]
\[
i = 1, 2, 3.
\] (35)

The moment matrix \(M(\hat{\rho})\) constructed with the set of operators (32) and its PT analogue \(M^{\text{PT}}(\hat{\rho})\) have identical structures:
\[
M(\hat{\rho}) = \begin{pmatrix}
1 & \langle \Sigma_1 \rangle & \langle \Sigma_2 \rangle & \langle \Sigma_3 \rangle \\
\langle \Sigma_1 \rangle & \langle \Sigma_0 \rangle & i \langle \Sigma_3 \rangle & -i \langle \Sigma_2 \rangle \\
\langle \Sigma_2 \rangle & -i \langle \Sigma_3 \rangle & \langle \Sigma_0 \rangle & i \langle \Sigma_1 \rangle \\
\langle \Sigma_3 \rangle & i \langle \Sigma_2 \rangle & -i \langle \Sigma_1 \rangle & \langle \Sigma_0 \rangle 
\end{pmatrix},
\] (36)
\[
M^{\text{PT}}(\hat{\rho}) = \begin{pmatrix}
1 & \langle \Sigma_{1}^{\text{PT}} \rangle & \langle \Sigma_{2}^{\text{PT}} \rangle & \langle \Sigma_{3}^{\text{PT}} \rangle \\
\langle \Sigma_{1}^{\text{PT}} \rangle & \langle \Sigma_{0}^{\text{PT}} \rangle & i \langle \Sigma_{3}^{\text{PT}} \rangle & -i \langle \Sigma_{2}^{\text{PT}} \rangle \\
\langle \Sigma_{2}^{\text{PT}} \rangle & -i \langle \Sigma_{3}^{\text{PT}} \rangle & \langle \Sigma_{0}^{\text{PT}} \rangle & i \langle \Sigma_{1}^{\text{PT}} \rangle \\
\langle \Sigma_{3}^{\text{PT}} \rangle & i \langle \Sigma_{2}^{\text{PT}} \rangle & -i \langle \Sigma_{1}^{\text{PT}} \rangle & \langle \Sigma_{0}^{\text{PT}} \rangle 
\end{pmatrix},
\] (37)
where we have denoted $\Sigma_1^2 = \Sigma_2^2 = \Sigma_3^2 = \Sigma_0$.

The eigenvalues of $M^{\text{PT}}(\hat{\rho})$ are given by,

$$
\mu_{1 \pm}^{\text{PT}} = \langle \Sigma_0^{\text{PT}} \rangle \pm \sqrt{\langle \Sigma_1^2 \rangle + \langle \Sigma_2^2 \rangle + \langle \Sigma_3^2 \rangle},
$$

$$
\mu_{2 \pm}^{\text{PT}} = \frac{1}{2} (1 + \langle \Sigma_0^{\text{PT}} \rangle) \pm \frac{1}{2} \left[ (1 + \langle \Sigma_0^{\text{PT}} \rangle)^2 + 4(\langle \Sigma_1^2 \rangle + \langle \Sigma_2^2 \rangle + \langle \Sigma_3^2 \rangle^2 - \langle \Sigma_0^{\text{PT}} \rangle) \right]^{\frac{1}{2}}.
$$

It may be readily seen (from (38)) that the PPT bound $M^{\text{PT}}(\hat{\rho}) \geq 0$ imposes the following restriction on separable states:

$$
\langle \Sigma_0^{\text{PT}} \rangle \geq \sqrt{\langle \Sigma_1^2 \rangle + \langle \Sigma_2^2 \rangle + \langle \Sigma_3^2 \rangle}.
$$

(39)

Entangled multiqubit states will be shown to violate the PPT constraint (39) on the moments. Specializing (32) for a random pair of qubits drawn from a symmetric multiqubit system, it is found [16] that spin squeezing [17] occurs as a consequence of violation of the PPT bound (39). This will be addressed in a separate communication [16].

We consider here the example of an arbitrary pure state of three qubits expressed in the Schmidt decomposed form as [18]

$$
|\Psi\rangle = \lambda_0 |0,0,0\rangle + \lambda_1 e^{i\phi} |1,0,0\rangle + \lambda_2 |1,0,1\rangle + \lambda_3 |1,1,0\rangle + \lambda_4 |1,1,1\rangle
$$

(40)

where $\lambda_i \geq 0$, $0 \leq \phi \leq \pi$, $\sum_i \lambda_i^2 = 1$.

Choosing the unit vectors

$$
\vec{k}_\alpha = (1, 0, 0), \quad \vec{l}_\alpha = (0, 1, 0), \quad \vec{m}_\alpha = (0, 0, 1)
$$

(41)

in Eqs. (32), (33), we obtain (with a PT operation on the first qubit),

$$
\langle \Sigma_1 \rangle = \lambda_0 \lambda_4, \quad \langle \Sigma_2 \rangle = 0,
$$

$$
\langle \Sigma_3^{\text{PT}} \rangle = \lambda_1^2, \quad \langle (\Sigma_0^{\text{PT}}) \rangle = \lambda_1^2.
$$

(42)

The PPT inequality (39) is violated if and only if

$$
\lambda_0 \lambda_4 > 0.
$$

(43)

Recalling that the 3-tangle [19], a measure of genuine three qubit entanglement, is given by

$$
\tau_3 = 4\lambda_0^2 \lambda_4^2
$$

(44)
We find an interesting result: the PPT bound (39) is violated iff an arbitrary three qubit state has non-vanishing tangle.

We also find that \( N \)-qubit GHZ-like states

\[
|\Psi_N\rangle = \sqrt{p}|0,0,\ldots,0\rangle + e^{i\phi}\sqrt{1-p}|1,1,\ldots,1\rangle,
\]

(45)

(where \( 0 \leq p \leq 1, \; 0 \leq \phi \leq 2\pi \)) violate the separability bound (39) on moments for all values of \( p \neq 0,1 \), as

\[
\langle \Sigma_1 \rangle = 2\sqrt{p(1-p)} \cos \phi,
\]

\[
\langle \Sigma_2 \rangle = 2\sqrt{p(1-p)} \sin \phi,
\]

\[
\langle \Sigma^\text{PT}_3 \rangle = 0, \quad \langle \Sigma^\text{PT}_0 \rangle = 0.
\]

(46)

in the state (45) - with unit vectors \((k_\alpha,l_\alpha,m_\alpha)\) chosen as in (41).

We now show that the PPT bound (39) can be used to detect entanglement in mixed states too. For this purpose we consider a \( N \)-qubit Werner state,

\[
\hat{\rho}_N(x) = x|\text{GHZ}\rangle_N\langle \text{GHZ}| + \frac{(1-x)}{2^N} \bigotimes_{\alpha=1}^N I,
\]

(47)

where \(|\text{GHZ}\rangle_N = \frac{1}{\sqrt{2}}[|0,0,\ldots,0\rangle + |1,1,\ldots,1\rangle]\) and \( 0 \leq x \leq 1 \). Fixing the unit vectors as in (41) and performing PT operation on the first qubit, we obtain,

\[
\langle \Sigma^\text{PT}_1 \rangle = -x, \quad \langle \Sigma^\text{PT}_2 \rangle = 0,
\]

\[
\langle \Sigma^\text{PT}_3 \rangle = 0, \quad \langle \Sigma^\text{PT}_0 \rangle = \frac{(1-x)}{2^{N-1}}.
\]

(48)

The PPT bound (39) is satisfied by the multiqubit Werner state if and only if

\[
0 \leq x \leq \frac{1}{2^{N-1}+1},
\]

(49)

which is the necessary and sufficient condition [20] for separability of the state (47). It is worth pointing out here that entanglement witness employed in Ref. [21] leads to weaker regimes of inseparability for this state. Thus, it is significant that a novel set of composite multiqubit moments given by Eqs. (32),(35) capture the inseparability behavior of the state (47) completely.
V. SUMMARY

We have analyzed bounds imposed on matrix of multiqubit moments due to positivity under partial transpose of density operator. These PPT bounds, in general, place additional stronger restrictions on the moments, than the conventional ones imposed due to positivity of the quantum state. While the set of all separable states obey PPT bounds on moments, violation of these constraints are sufficient to detect entanglement in bipartite divisions of the density operator. By constructing an appropriate PT matrix of moments we have recovered inseparability conditions of Horodecki et. al., [14] for entangled two qubit states. We have also investigated a generalized matrix of moments for multiqubit states and derived its PPT bounds. It is shown that an arbitrary pure three qubit state violates PPT restrictions on this generalized moment matrix if and only if its three tangle [19] is non-zero. As yet another consequence of violation of these PPT bounds, we recover the necessary and sufficient condition for entanglement in \( N \) qubit Werner state. It is for the first time that inequalities involving composite multiqubit moments are shown to capture the complete inseparability status of this important class of mixed states.

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