Chapter 3

Multiaxial representation (MAR) and classification of spin-$j$ systems

3.1 Introduction

Generalization of MR has been a long standing open problem due to the difficulties faced in the construction of a Majorana like geometric representation for symmetric mixed state because the number of parameters required to characterize $N$-qubit mixed state namely $N(N + 2)$ is much larger than the $2N$ parameters required to characterize $N$-qubit pure state. This problem was solved by Ramachandran& Ravishankar (1986) by constructing a MAR of the $2j$ Fano statistical tensor parameters [Fano (1951, 1953)] which characterize the spin-$j$ assembly. We focus on the language of the density matrix for the symmetric states as it can be applied with equal ease to pure as well as mixed spin systems.

One way of studying unitary equivalence of multipartite mixed states is, using the singular value decomposition method [Wang et al. (2008)] and another way is by evaluating the LUI. We propose a scheme for classifying the most general symmetric $N$-qubit mixed states under LU transformation by evaluating the LUI based on the MAR [Ramachandran& Ravishankar (1986)]. In addition to the two parameters defined for the entanglement classification of the symmetric pure states based on MR [Bastin et al. (2009)], namely, diversity degree and degeneracy configuration, we show that another parameter called rank needs to be introduced for symmetric mixed state classification. Therefore every symmetric $N$-qubit state is in general characterized by $N$ configurations. Further, we consider classification of uniaxial, Biaxial and triaxial symmetric two qubit mixed states which can be produced in the laboratory.


3.2 Multiaxial representation of pure and mixed states

In the case of most general spin-\( j \) state, both pure as well as mixed, \( \rho(\vec{J}) \) is given by (Eq. 1.6). Thus \( \rho \) can be parametrized in terms of \( 2j + 1 \) spherical tensors \( t^k_q ; k = 0, 1, 2, \ldots 2j \), \( q = -k \) to \( +k \). Consider a rotation \( R(\phi, \theta, 0) \) of the frame of reference such that \( t^k_k \) in the rotated frame vanishes. i.e from (Eq. 1.13)

\[
(t^k_k)^R = 0 = \sum_{q=-k}^{+k} D^k_{qk}(\phi, \theta, 0) t^k_q. \tag{3.1}
\]

Again using the Wigner expression for \( D^j \) matrices, (Eq. 2.6) in (Eq. 3.1), we obtain

\[
\sum_{q=-k}^{+k} e^{-iq\phi} (-1)^{k-q} \sqrt{2k} C^k_{k+q} t^k_q \left( \cos \frac{\theta}{2} \right)^{k+q} (-1)^{k-q} \left( \sin \frac{\theta}{2} \right)^{k-q} = 0 \tag{3.2}
\]

or

\[
\mathcal{A} \sum_{q=-k}^{+k} (-1)^{2(k-q)} \sqrt{2k} C^k_{k+q} t^k_q Z^{k-q} = 0. \tag{3.3}
\]

where

\[
Z = \tan \left( \frac{\theta}{2} \right) e^{i\phi}
\]

and the overall coefficient

\[
\mathcal{A} = \cos^{2k} \left( \frac{\theta}{2} \right) e^{-ik\phi}.
\]

Thus the polynomial equation \( P(Z) \) is given by

\[
P(Z) = \sum_{q=-k}^{+k} (-1)^{2(k-q)} \sqrt{2k} C^k_{k+q} t^k_q Z^{k-q} = 0, \tag{3.4}
\]

which for every \( k \) leads to \( 2k \) solutions namely

\[
\{(\theta_1, \phi_1), (\theta_2, \phi_2), \ldots, (\theta_k, \phi_k), (\pi - \theta_1, \pi + \phi_1), \ldots, (\pi - \theta_k, \pi + \phi_k)\}.
\]

Thus the \( 2k \) solutions constitute \( k \) axes or \( k \) double headed arrows. Therefore, every \( t^k_q \) can be constructed as follows:

\[
t^k_q = r_k (\ldots (\hat{Q}(\theta_1, \phi_1) \otimes \hat{Q}(\theta_2, \phi_2))^2 \otimes \hat{Q}(\theta_3, \phi_3))^3 \otimes \ldots)^{k-1} \otimes \hat{Q}(\theta_k, \phi_k))_{q}^k \tag{3.5}
\]
where

\[(\hat{Q}(\theta_1, \phi_1) \otimes \hat{Q}(\theta_2, \phi_2))^2 = \sum_{q_1} C(11k; q_1q_2) (\hat{Q}(\theta_1, \phi_1))_{q_1}^1 (\hat{Q}(\theta_2, \phi_2))_{q_2}^1 \quad (3.6)\]

and the spherical components of \(\hat{Q}\) are given by,

\[(\hat{Q}(\theta, \phi))_{q}^1 = \sqrt{\frac{4\pi}{3}} Y_q^1(\theta, \phi). \quad (3.7)\]

Here \(Y_q^1(\theta, \phi)\) are the well known spherical harmonics.

Observe that from (Eq. 3.2) we can also have

\[A' + k \sum_{q=-k}^{+k} (-1)^{2(k-q)} \sqrt{2k} C_{k+q}^q t^k_q Z'^k+q = 0 \quad (3.8)\]

where

\[A' = \sin^{2k}\left(\frac{\theta}{2}\right) e^{ik\phi}\]

and

\[Z' = \frac{1}{Z} = \cot\left(\frac{\theta}{2}\right) e^{-i\phi}.\]

Therefore,

\[P(Z') = \sum_{q=-k}^{+k} (-1)^{2(k-q)} \sqrt{2k} C_{k+q}^q t^k_q Z'^k+q = 0 \quad (3.9)\]

for every \(k\), leading to the same set of \(2k\) solutions as obtained from (Eq. 3.4).

Thus in MAR, the symmetric state of \(N\)-qubit assembly can be represented geometrically by a set of \(N = 2j\) spheres of different radii \(r_1, r_2, \ldots, r_k\) corresponding to each value of \(k\).

The \(k^{th}\) sphere in general consists of a constellation of \(2k\) points on its surface specified by \(\hat{Q}(\theta_i, \phi_i)\) and \(\hat{Q}(\pi - \theta_i, \pi + \phi_i); i = 1, 2, \ldots, k\). In other words, every \(t^k\) is specified by \(k\) axes in a sphere of radius \(r_k\).

On the other hand, consider a spin-\(j\) density matrix which is characterized by non-zero \(t^k_0\) \((k = 1, 2 \ldots 2j)\) only. In a rotated frame we have from (Eq. 3.1)

\[(t^k_q)^R = D^k_{q0}(\phi, \theta, 0) t^k_0. \quad (3.10)\]
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Since $D_{0q}^{k}(\phi, \theta, 0) = (-1)^q \sqrt{\frac{4\pi}{2k+1}} Y_q^k(\theta, \phi)$ [Varshalovich (1988)],

$$(t_q^k)^R = (-1)^q \sqrt{\frac{4\pi}{2k+1}} t_0^k Y_q^k(\theta, \phi)$$  \hspace{1cm} (3.11)$$

where $t_0^k$ is a real number. It is very well-known [Varshalovich (1988)] that

$$Y_q^k(\theta, \phi) = \frac{1}{r^k} \sqrt{\frac{(2k+1)!!}{4\pi k!}} \left(...\left(\hat{Q}(\theta, \phi) \otimes \hat{Q}(\theta, \phi)\right)^2 \otimes \hat{Q}(\theta, \phi)\right)^3 \otimes \ldots \hat{Q}(\theta, \phi)\right)_q^k$$  \hspace{1cm} (3.12)$$

where $Y_q^k(\theta, \phi)$ are the spherical harmonics. Thus every $t_q^k$ in the rotated frame is characterized by $k$ axes ($k = 1, 2\ldots 2j$) which are collinear and every axis is given by $(\theta, \phi)$ and $(\pi - \theta, \pi + \phi)$. In the unrotated coordinate frame, it is obvious that $t_0^k$'s are characterized by $k$ axes collinear to the $z$-axis. In this case, the MAR consists of $r_k$ spheres and each sphere has $k$ collinear axes.

3.2.1 Local Unitary Invariants (LUI)

It has been shown [Adiga (2012); Sirsi & Adiga (2011)] that since $(\hat{Q}(\theta_i, \phi_i) \otimes \hat{Q}(\theta_j, \phi_j))_0^0$ is an invariant under rotation, one can construct in general $j^{(2j+1)}C_2$ invariants out of $j(2j + 1)$ axes together with $2j$ real positive scalars specifying a spin-$j$ density matrix. Here $j^{(2j+1)}C_2$ denotes binomial coefficient.

For example, spin-1 or symmetric two qubit state is in general parametrized in terms of 3 axes and 2 real scalars and possess $3C_2+2=5$ invariants. spin-3/2 or symmetric three qubit state is represented by 6 axes and 3 real scalars and has $6C_2+3 = 18$ invariants and spin-2 or symmetric four qubit state is characterized by 10 axes and 4 real scalars and has $10C_2+4=49$ invariants.

The importance of LUI in the context of LU classification is brought out in the next section.
3.3 Classification of Pure and Mixed States based on Multiaxial Representation

Since the most general symmetric state $\rho(\vec{J})$ is parametrized in terms of spherical tensors $t^k$ ($k = 0, 1, \ldots, 2j$) and $t^k$'s are characterized by $k$ axes, it is but natural that the two parameters employed in the entanglement classification of symmetric $N$-qubit pure states based on MR viz, the degeneracy configuration and the diversity degree, are defined for $t^k$'s. Thus the degeneracy number here represents the number of identical axes characterizing the given spherical tensor parameter $t^k$. Further, we define the degeneracy configuration $\mathcal{D}_{\{n_i\}}$ of $t^k$ as the set of degeneracy numbers $\{n_i\}$ ordered by convention in the decreasing order. The number of $n_i$'s define the diversity degree of the given $t^k$ and we have $\sum_{i=1}^{k} n_i = k$ and $k = 1, 2, \ldots, 2j$. Therefore, the degeneracy configuration here is also the partition of $k$ as introduced in Bastin et al. (2009) and the number of different configurations is given by the partition function $p(k)$.

In addition to this, in the case of symmetric mixed system we need to define another number called the rank $k$ which refers to the rank of the spherical tensor parameter $t^k$. Thus the notation for the degeneracy configuration of $t^k$ becomes $\mathcal{D}_{\{n_i\}}^k$. Therefore every symmetric $N$-qubit state is in general characterized by $N$ configurations.

For example, in the case of a symmetric two qubit system, the density matrix is characterized by $t^1$ and $t^2$. In the case of $t^1$, there is only one axis. Thus $t^1 \in \mathcal{D}_1$. In the case of $t^2$, there are two axes in general. If the two axes are identical then $t^2 \in \mathcal{D}_2$ and if the axes are not collinear then $t^2 \in \mathcal{D}_{1,1}^2$. Thus, in general, a symmetric two-qubit state belongs to either of the two following classes:

$$\{\mathcal{D}_1^1, \mathcal{D}_2^2\} \text{ or } \{\mathcal{D}_1^1, \mathcal{D}_{1,1}^2\}.$$

Similarly, a symmetric three qubit system is characterized by $t^1$, $t^2$ and $t^3$. Thus the spin-3/2 or symmetric three qubit density matrix in general belong to one of the following classes:

$$\{\mathcal{D}_1^1, \mathcal{D}_2^2, \mathcal{D}_{1,1}^3\}.$$
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configurations:

\begin{align*}
\{D_1^1, D_2^2, D_3^3\}, \\
\{D_1^1, D_2^2, D_3^3\}, \{D_1^1, D_2^2, D_{1,1,1}^1\}, \\
\{D_1^1, D_2^2, D_3^3\}, \{D_1^1, D_{1,1,1}^1, D_{2,1,1}^1\}, \{D_1^1, D_{1,1,1}^1, D_{1,1,1}^1\}.
\end{align*}

Two density matrices are LU equivalent provided they have the same set of invariants. It is obvious from our classification scheme, that density matrices having different sets of degeneracy configurations can never be LU equivalent as they have different set of invariants. Therefore LU equivalent density matrices need to have the same set of degeneracy configurations.

Let us now consider some well known examples of two qubit and three qubit entangled pure states to demonstrate our method.

### 3.3.1 Pure Entangled States

**Bell State:** Consider

\[
|\psi_{\text{Bell}_1}\rangle = |10\rangle \equiv \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}
\]

which is a symmetric state. The corresponding density matrix in $|1m\rangle$ basis; $m = 1, 0, -1$ is,

\[
\rho_{\text{Bell}_1} = \begin{pmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0
\end{pmatrix}.
\] (3.13)

Since

\[
t_q^k = \sum_{m=-j}^{+j} \rho_{mm'} [k] C(jk; m q m'), \quad \text{with} \quad m' = m + q.
\]

The only non-zero $t_q^k$ is

\[
t_0^2 = \sqrt{2}.
\] (3.14)
Solving the polynomial equation for \( t^2 \), we get

\[
\sqrt{4C_2^1 t^2} Z^2 = 0,
\]

Or

\[
Z^2 = 0. \tag{3.15}
\]

which shows that the two axes are collinear to \( z \)-axis. Thus \( t^2 \) belongs to \( D_2^2 \).

Therefore according to MAR, \( \rho \in \{D_2^2\} \) in contrast to the degeneracy configuration of the Bell state based on MR namely \( \{D_{1,1}^2\} \).
Figure 3.1: MAR of the Bell state $|\psi\rangle = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}}$. The two axes representing the Bell state are along the z-axis and shown by the double headed arrows.
Bell states: Consider
\[ |\psi_{\text{Bell}}\rangle = \frac{|11⟩ + |1 \downarrow⟩}{{\sqrt{2}}} = \frac{|\uparrow\uparrow⟩ + |\downarrow\downarrow⟩}{{\sqrt{2}}}. \]

Corresponding density matrix is
\[ \rho_{\text{Bell}_2} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \] (3.16)

The non-zero \( t^k_q \)s are
\[ t^2_0 = \frac{1}{\sqrt{2}}, \quad t^2_2 = \frac{\sqrt{3}}{2}, \quad \text{and} \quad t^2_{-2} = \frac{\sqrt{3}}{2}. \]

Solving the polynomial equation for \( t^2 \), we get
\[ \sqrt{C^4_0 t^2_{-2}} + \sqrt{C^4_1 t^2_0} Z^2 + \sqrt{C^4_4 t^2_2} Z^4 = 0, \] (3.17)
\[ Z^4 + 2Z^2 + 1 = 0, \]
or
\[ (Z^2 + 1)^2 = 0, \]
\[ Z_{1,2,3,4} = \pm i. \]

Since, \( Z = \tan \frac{\theta}{2} e^{i\phi} = \pm i \), the corresponding two axes are collinear and given by
\[ \{(\frac{\pi}{2}, \frac{\pi}{2}), (\frac{\pi}{2}, 3\frac{\pi}{2})\}. \]

Thus the two axes are collinear to \( Y \)-axis.

Therefore, \( t^2 \) belongs to \( D^2_2 \).
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Figure 3.2: MAR of the Bell state \( |\psi\rangle = \frac{|↑↑\rangle + |↓↓\rangle}{\sqrt{2}} \). The two axes representing the Bell state are along the \( Y \)-axis and shown by the double headed arrows.
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**Bell State:** Consider

\[
|\psi_{\text{Bell}}\rangle_3 = \frac{|11\rangle - |11\rangle}{\sqrt{2}} = \frac{|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle}{\sqrt{2}}.
\]

Corresponding density matrix is

\[
\rho_{\text{Bell}_3} = \frac{1}{2} \begin{pmatrix}
1 & 0 & -1 \\
0 & 0 & 0 \\
-1 & 0 & 1
\end{pmatrix}.
\] (3.18)

The Non-zero \( t^k \)'s are

\[
t^0_2 = \frac{1}{\sqrt{2}}, \quad t^2_2 = -\frac{\sqrt{3}}{2}, \quad \text{and} \quad t^2_{-2} = -\frac{\sqrt{3}}{2}.
\]

Solving the polynomial equation for \( t^2 \)

\[
\sqrt{C_0^4 t_{-2}^2} + \sqrt{C_1^4 t_0^2} Z^2 + \sqrt{C_4^4 t_2^2} Z^4 = 0,
\] (3.19)

\[
Z^4 - 2Z^2 + 1 = 0,
\]

or

\[
(Z^2 - 1)^2 = 0,
\]

we get

\[
Z^2 = 1
\]

or

\[
Z_{1,2,3,4} = \pm 1.
\] (3.20)

The corresponding axes are

\[
\{(\frac{\pi}{2}, 0) (\frac{\pi}{2}, \pi)\}
\]

which shows that the two axes are collinear to \( X \)-axis.

Thus \( t^2 \) belongs to \( D^2_2 \).
Figure 3.3: MAR of the Bell state $|\psi\rangle = \frac{|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle}{\sqrt{2}}$. The two axes representing the Bell state are along the $X$-axis and shown by the double headed arrows.
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**W state:**

Consider the symmetric three qubit state,

\[
|\psi_W\rangle \equiv \frac{|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle}{\sqrt{3}} = |3/2 - 1/2\rangle.
\]

The corresponding density matrix in \(|^{\frac{3}{2}}m\rangle\) basis; \(m = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}\) is,

\[
\rho_{W_1} = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\]

(3.21)

Since

\[t^k_q = \rho_{\pm\frac{1}{2} \pm\frac{1}{2}} [k] C(\frac{3}{2}k, \frac{3}{2}; -\frac{1}{2}q, -\frac{1}{2}),\]

the non-zero \(t^k_q\)’s are

\[t^1_0 = -\frac{1}{\sqrt{5}}, \quad t^2_0 = -1, \quad t^3_0 = \frac{3}{\sqrt{5}}\]

(3.22)

Here \(t^1_{\pm 1} = 0\) and \(t^1_0 = \frac{2}{\sqrt{5}}\), hence there is one axis along \(z\)-axis.

Again, \(t^2_{\pm 2} = 0\) and \(t^2_0 = -1\), therefore there are two axes collinear to \(z\)-axis.

Also, \(t^3_{\pm 3} = 0\) and \(t^3_0 = \frac{3}{\sqrt{5}}\), thus three axes are along \(z\)-axis.

Since all the 6 axes are collinear and parallel to \(z\)-axis, \(t^1 \in D^1_1, t^2 \in D^2_2\) and \(t^3 \in D^3_3\) and hence

\[\rho \in \{D^1_1, D^2_2, D^3_3\}.\]

Similarity consider

\[
|\psi_{W_2}\rangle \equiv \frac{|\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle}{\sqrt{3}} = |3/2 1/2\rangle.
\]

The corresponding density matrix in angular momentum basis is,
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\[
\rho_{W_2} = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\]  

(3.23)

the non-zero \(t^k_q\)s are

\[
t_0^1 = \frac{1}{\sqrt{5}}, \quad t_0^2 = -1, \quad t_0^3 = \frac{-3}{\sqrt{5}}.
\]  

(3.24)

Therefore, \(|\psi_{W_2}\rangle\) also represented by the same set of axes and belongs to the same class as that of \(|\psi_{W_1}\rangle\).
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Figure 3.4: Multiaxial representation of \(t^1\), \(t^2\) and \(t^3\) characterizing the W state.
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**GHZ state:**

Consider the GHZ state which is a symmetric three qubit state, given by

$$\ket{\psi_{\text{GHZ}}_1} = \frac{\ket{\frac{3}{2}, \frac{3}{2}} + \ket{\frac{3}{2}, -\frac{3}{2}}}{\sqrt{2}} = \frac{\ket{\uparrow\uparrow\uparrow} + \ket{\downarrow\downarrow\downarrow}}{\sqrt{2}}.$$  

Corresponding density matrix in the angular momentum $j = \frac{3}{2}$ basis is,

$$\rho_{\text{GHZ}_1} = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$  \hspace{1cm} (3.25)

$$t_q^k = \sum_{m=-j}^{+j} \rho_{mm'} [k] C(jkj;mqm'), \quad \text{with} \quad m' = m + q. \quad (3.26)$$

The non-zero $t_q^k$'s are

$$t_0^2 = 1, \quad t_3^2 = -1, \quad t_{-3}^2 = 1. \quad (3.27)$$

Since, $t_2^2 = t_{-2}^2 = 0$, the two axes characterizing $t^2$ are parallel to the $Z$ axis. Thus $t^2 \in D_2^2$.

Solving the polynomial equation for $t_3^3$,

$$\sqrt{6}C_0 t_3^{3} - \sqrt{6}C_6 t_3^{3} Z^6 = 0 \quad (3.28)$$

we get

$$Z^6 = 1,$$

and hence

$$Z = e^{\frac{2\pi i}{6}}, \quad r = 0, 1...5.$$

Thus, the three distinct axes are

$$\{\left(\frac{\pi}{2}, 0\right), \left(\frac{\pi}{2}, \pi\right)\}, \quad \{\left(\frac{\pi}{2}, \frac{\pi}{3}\right), \left(\frac{\pi}{2}, \frac{4\pi}{3}\right)\}, \quad \{\left(\frac{\pi}{2}, \frac{2\pi}{3}\right), \left(\frac{\pi}{2}, \frac{5\pi}{3}\right)\}.$$  

Therefore $t^2 \in D_2^2$, $t^3 \in D_{111}^3$ and $\rho \in \{D_2^2, D_{111}^3\}$.

Similarity, consider

$$\ket{\psi_{\text{GHZ}}_2} = \frac{\ket{\frac{3}{2}, \frac{3}{2}} - \ket{\frac{3}{2}, -\frac{3}{2}}}{\sqrt{2}} = \frac{\ket{\uparrow\uparrow\uparrow} - \ket{\downarrow\downarrow\downarrow}}{\sqrt{2}}.$$  

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Corresponding density matrix in the angular momentum $j = \frac{3}{2}$ basis is,

$$
\rho_{GHZ_2} = \frac{1}{2} \begin{pmatrix}
1 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 1
\end{pmatrix}.
$$

(3.29)

The non-zero $t^k_q$'s are

$$
t^2_0 = 1, \quad t^3_3 = 1, \quad t^3_{-3} = -1.
$$

(3.30)

Solving the polynomial equation for $t^3_q$, we get

$$
Z^6 = 1,
$$

and hence

$$
Z = e^{\frac{2\pi i r}{6}}, \quad r = 0, 1, \ldots, 5.
$$

Both GHZ states have the same set of axes and classification.
Figure 3.5: Multiaxial representation of $t^2$ and $t^3$ characterizing the GHZ state.
Triaxial Pure State:

This state can be generated by the time evolution operator $U(t, t_0)$ commonly found in quantum optics processes involving two intense laser beams with the same arbitrary amplitude modulation. The three level systems interacting with these laser fields have in general unequal Rabi frequencies [Pegg (1983)]. Consider,

$$|\psi\rangle = U(t, t_0)|11\rangle$$

with

$$U(t, t_0) = 1 - \frac{1}{\nu} H_0 \sin\left(\nu \int_{t_0}^{t} f(\tau)d\tau\right) + \frac{1}{\nu^2} H_0^2 \cos\left(\nu \int_{t_0}^{t} f(\tau)d\tau - 1\right).$$ (3.31)

Here $f(\tau)$ is the common amplitude modulation factor, $\nu = \sqrt{a^2 + b^2}$, $a$ and $b$ are the steady resonant Rabi frequencies and $H_0$ in spin-1 representation is given by

$$H_0 = aJ_x + b(J_zJ_x + J_xJ_z).$$

Choosing the pulse area to be

$$\nu \int_{t_0}^{t} f(\tau)d\tau = \pi,$$

$$U(t, t_0) = 1 - \frac{2}{\nu^2} H_0^2$$

and

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} \frac{4a^2b^2}{\nu^4} & 0 & \frac{2ab}{\nu^2}(a^2 - b^2) \\ 0 & 0 & 0 \\ \frac{2ab}{\nu^2}(a^2 - b^2) & 0 & \frac{1}{\nu^4}(a^2 - b^2)^2 \end{pmatrix}.$$ (3.32)

The non-zero $t_0^{k\ell}$’s are

$$t_0^{11} = -\sqrt{\frac{3}{2}} + \frac{4\sqrt{6}a^2b^2}{\nu^4},$$
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\[
t_0^2 = \frac{1}{\sqrt{2}},
\]
\[
t_{\pm 2}^2 = \frac{2\sqrt{3}ab}{\nu^4} (a^2 - b^2).
\]

\(t_0^1\) is characterized by an axis collinear to \(z\)-axis. Two axes characterizing \(t^2\) are not collinear and depend on the values of \(a\) and \(b\).

For \(a = b\), \(t_{\pm 2}^2 = 0\) and \(t_0^2 \neq 0\), therefore \(t^2 \in \mathcal{D}_2^2\) and hence \(\rho \in \{\mathcal{D}_1^1, \mathcal{D}_2^2\}\).

For \(a \neq b, t^2 \in \mathcal{D}_{1,1}^2\) and hence \(\rho \in \{\mathcal{D}_1^1, \mathcal{D}_{1,1}^2\}\).

### 3.3.2 Classification of some Mixed states

Let us now consider density matrices representing some well-known spin-1 systems belonging to different LU classes and study their classification in terms of LUI's \(r_1, r_2\) and the axes. These density matrices also represent symmetric two qubit mixed states whose entanglement can be studied in terms of the \(r_k'\)'s \((k = 1, 2)\) and the axes. Here we make use of the Positive Partial Transpose (PPT) criterion\(^1\) [Peres (1996)] to characterize entanglement.

#### Uniaxial Systems

The density matrix representing a uniaxial system is characterized by \(t_0^1 \neq 0, t_{\pm 1}^1 \neq 0, t_q^2 = 0\) \((q = 0, \pm 1, \pm 2)\). In the context of nuclear physics, such a system is said to be purely vector polarized with single axis of cylindrical symmetry. It can be produced in the laboratory by the interaction of a spin-1 assembly with an external dipole magnetic field [Sirsi (1995)]. Here the most general density matrix corresponding to this class is

\[
\rho = \frac{1}{3} \left[ t_{0,0}^0 + t_{0,-1}^1 + t_{1,1}^1 + t_{-1,-1}^1 \right] \\
= \frac{1}{3} \left[ 1 + r_1 Q_0^1(\theta_1, \phi_1) + r_1 Q_1^1(\theta_1, \phi_1) + r_1 Q_{-1}^1(\theta_1, \phi_1) \right]. \tag{3.33}
\]

\(^1\)see appendix B
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Since

\[ t_q^1 = r_1 \hat{Q}_q^1(\theta, \phi) = r_1 \sqrt{\frac{4\pi}{3}} Y_q^1(\theta, \phi), \]

thus

\[
\rho = \frac{1}{3} \left[ 1 + r_1 \cos \theta_1 \tau_0^1 \right. \\
+ r_1 \frac{-1}{\sqrt{2}} \sin \theta_1 e^{i\phi_1} \tau_1^1 + r_1 \frac{1}{\sqrt{2}} \sin \theta_1 e^{-i\phi_1} \tau_{-1}^1 \left. \right]. \tag{3.34}
\]

The density matrix corresponding to this class in the \(|1m\rangle\) basis is given by\(^2\)

\[
\rho = \frac{1}{3} \begin{pmatrix}
1 + \sqrt{\frac{2}{3}} r_1 \cos \theta_1 & \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{-i\phi_1} & 0 \\
\frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & 1 & \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{-i\phi_1} \\
0 & \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & 1 - \sqrt{\frac{3}{2}} r_1 \cos \theta_1
\end{pmatrix}. \tag{3.35}
\]

\(\rho\) is found to be positive semi-definite\(^3\) iff

\[ 0 < r_1 \leq \sqrt{\frac{2}{3}}. \]

The non-zero \(t_q^k\)'s are

\[ t_0^1 = r_1 \cos \theta_1 , \ t_{\pm 1}^1 = \frac{r_1}{\sqrt{2}} \sin \theta_1 e^{\mp i\phi_1}. \]

and the only LU invariant is \(r_1\).

To characterize entanglement properties of uniaxial system, we need to use partial transpose of the density matrix. Therefore, the density matrix in computational basis, \(\rho'\) is given by

\[ \rho' = \mathcal{U}^\dagger \rho \mathcal{U}, \]

\(^2\)Matrix representation of \(\tau_q^1\) are given in appendix A.

\(^3\)see appendix C
where unitary transformation from angular momentum basis $|11\rangle$, $|10\rangle$, $|1 - 1\rangle$, $|00\rangle$ to computational basis $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ is

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}.$$ 

i.e.,

$$\rho' = \frac{1}{3} \begin{pmatrix} 1 + \sqrt{2} r_1 \cos \theta_1 & \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{-i\phi_1} & \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{-i\phi_1} & 0 \\ \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & \frac{1}{2} & \frac{1}{2} & \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{-i\phi_1} \\ \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & \frac{1}{2} & \frac{1}{2} & \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{-i\phi_1} \\ 0 & \frac{1}{2} \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & \frac{1}{2} \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & 1 - \sqrt{2} r_1 \cos \theta_1 \end{pmatrix}. \quad (3.36)$$

A necessary and sufficient condition for separability in this case is that a matrix $\rho'^{PT}$, obtained by partial transposition of $\rho'$, has only non-negative eigenvalues. In the other words, if any one of the eigen values of $\rho'^{PT}$ is negative, the state is entangled. Corresponding to the density matrix in computational basis (Eq. 3.36), eigen values of partially transposed density matrix

$$\rho'^{PT} = \frac{1}{3} \begin{pmatrix} 1 + \sqrt{2} r_1 \cos \theta_1 & \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{-i\phi_1} & \frac{1}{3} \\ \frac{1}{2} \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & \frac{1}{2} & 0 & \frac{1}{2} \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{-i\phi_1} \\ \frac{1}{2} \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & 0 & \frac{1}{2} & \frac{1}{2} \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{-i\phi_1} \\ \frac{1}{2} & \frac{1}{2} \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & \frac{1}{2} \frac{\sqrt{3}}{2} r_1 \sin \theta_1 e^{i\phi_1} & 1 - \sqrt{2} r_1 \cos \theta_1 \end{pmatrix}. \quad (3.37)$$

are

$$\lambda_{1,2} = \frac{1}{6},$$

$$\lambda_3 = \frac{1}{6} \left( 2 + \sqrt{1 + 6r_1^2} \right),$$

and

$$\lambda_4 = \frac{1}{6} \left( 2 - \sqrt{1 + 6r_1^2} \right).$$
Therefore, $\lambda_4$ is negative for $rac{1}{\sqrt{2}} < r_1 \leq \sqrt{\frac{2}{3}}$ for all values of $\theta$ ($0 \leq \theta \leq \pi$). Here,

$$Tr(\rho^2) = \frac{1}{3} [1 + r_1^2] < 1,$$

and hence this class consist of mixed states only.

Since

$$t^1 \in D^1_1, \quad \rho \in \{D^1_1\},$$
Figure 3.6: Eigenvalue of $\lambda_4$ as a function of $r_1$. $\lambda_4 < 1$ indicates entanglement.
Figure 3.7: $Tr(\rho^2)$ as a function of $r_1$. $Tr(\rho^2) < 1$ indicate mixed states.
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**Biaxial Systems**

Here \( t_q^1 = 0 \) (\( q = 0, \pm 1 \)), \( t_0^2 \neq 0, t_{\pm 2}^2 \neq 0, t_{\pm 1}^2 = 0 \) and the two axes which characterize \( \rho \) in the Principal Axes of Alignment frame (PAAF) \cite{Ramachandran} are \{\( (\theta, 0), (\pi - \theta, \pi) \)\} and \{\( (\theta, \pi), (\pi - \theta, 0) \)\}. Thus \( \rho \) is said to be Biaxial. Since \( \rho \) in this case is parametrized in terms of second rank tensor parameters only, namely \( t_0^2 \) and \( t_{\pm 2}^2 \), it is said to be purely tensor polarized. Such a system can be produced by the interaction of a spin-1 nuclei with an external electric quadrupole field \cite{Ramachandran}. The density matrix in PAAF is given by

\[
\rho = \frac{1}{3} \left[ t_0^{\tau_0^0} + t_0^{\tau_0^{2^1}} + t_1^{\tau_1^{2^1}} + t_{-1}^{\tau_{-1}^{2^1}} + t_2^{\tau_2^{2^1}} + t_{-2}^{\tau_{-2}^{2^1}} \right]
\]

\[= \frac{1}{3} \left[ 1 + r_2 \left( Q(\theta, 0) \otimes Q(\theta, \pi) \right)^2 \tau_0^{2^1} + r_2 \left( Q(\theta, 0) \otimes Q(\theta, \pi) \right)^2 \tau_1^{2^1}
+ r_2 \left( Q(\theta, 0) \otimes Q(\theta, \pi) \right)^2 \tau_{-1}^{2^1} + r_2 \left( Q(\theta, 0) \otimes Q(\theta, \pi) \right)^2 \tau_2^{2^1}
+ r_3 \left( Q(\theta, 0) \otimes Q(\theta, \pi) \right)^2 \tau_{-2}^{2^1} \right] \tag{3.38}
\]

Thus,

\[
\rho = \frac{1}{3} \left[ 1 + r_2 \left( C(112; 000) \hat{Q}_0^1(\theta, 0) \hat{Q}_0^1(\theta, \pi)
+ C(112; 1 - 10) \hat{Q}_1^1(\theta, 0) \hat{Q}_{-1}^1(\theta, \pi) + C(112; -110) \hat{Q}_{-1}^1(\theta, 0) \hat{Q}_1^1(\theta, \pi) \right) \tau_0^{2^1}
+ r_2 \left( C(112; 011) \hat{Q}_0^1(\theta, 0) \hat{Q}_1^1(\theta, \pi) + C(112; 000) \hat{Q}_0^1(\theta, 0) \hat{Q}_0^1(\theta, \pi) \right) \tau_1^{2^1}
+ r_2 \left( C(112; -10 - 1) \hat{Q}_{-1}^1(\theta, 0) \hat{Q}_0^1(\theta, \pi) + C(112; -112) \hat{Q}_0^1(\theta, 0) \hat{Q}_1^1(\theta, \pi) \right) \tau_{-1}^{2^1}
+ r_2 \left( C(112; 112) \hat{Q}_0^1(\theta, 0) \hat{Q}_{-1}^1(\theta, \pi) \right) \tau_{-2}^{2^1}
\right]. \tag{3.39}
\]
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i.e;

\[
\rho = \frac{1}{3} \left[ 1 + r_2 \left( \sqrt{\frac{2}{3}} \cos^2 \theta + \frac{1}{\sqrt{6}} \sin^2 \theta \right) \tau_{0}^{2\dagger} \right. \\
+ r_2 \left( -\frac{1}{2} \sin \theta \cos \theta + \frac{1}{2} \sin \theta \cos \theta \right) \tau_{1}^{2\dagger} \\
+ r_2 \left( -\frac{1}{2} \sin \theta \cos \theta + \frac{1}{2} \sin \theta \cos \theta \right) \tau_{-1}^{2\dagger} \\
+ r_2 \left( \frac{1}{2} \sin^2 \theta \right) \tau_{2}^{2\dagger} + r_2 \left( \frac{1}{2} \sin^2 \theta \right) \tau_{-2}^{2\dagger} \left. \right] .
\] (3.40)

Or

\[
\rho = \frac{1}{3} \left[ 1 + r_2 \left( \sqrt{\frac{2}{3}} \cos^2 \theta + \frac{1}{\sqrt{6}} \sin^2 \theta \right) \tau_{0}^{2\dagger} \right. \\
+ r_2 \left( \frac{1}{2} \sin^2 \theta \right) \tau_{2}^{2\dagger} + r_2 \left( \frac{1}{2} \sin^2 \theta \right) \tau_{-2}^{2\dagger} \left. \right] .
\] (3.41)

Therefore, the density matrix in \(|1m\) basis is\(^4\),

\[
\rho = \frac{1}{3} \begin{pmatrix}
1 + \frac{1}{2\sqrt{3}} r_2 (1 + \cos^2 \theta) & 0 & -\frac{\sqrt{3}}{2} r_2 \sin^2 \theta \\
0 & 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) & 0 \\
-\frac{\sqrt{3}}{2} r_2 \sin^2 \theta & 0 & 1 + \frac{1}{2\sqrt{3}} r_2 
\end{pmatrix} .
\] (3.42)

\(\rho\) is positive semi-definite\(^5\) iff

\[0 < r_2 \leq \sqrt{3}\]

and the range of \(\theta\) then depends on \(r_2\).

The non-zero \(t_{kq}^{\dagger}\)’s are

\[t_{0}^{2} = \frac{r_2}{\sqrt{6}} (1 + \cos^2 \theta) , \ t_{\pm2}^{2} = -\frac{r_2}{2} \sin^2 \theta .\]

For \(0 < \theta < \frac{\pi}{2}\) and \(\frac{\pi}{2} < \theta < \pi\),

\[t^{2} \in \mathcal{D}_{1,1}^{2}\]

\(\text{Matrix representation of } \tau_{q}^{2}\) are given in appendix A.

\(\text{see appendix C}\)
and hence

\[ \rho \in \{ D_{1,1}^2 \}. \]

For \( \theta = 0, \frac{\pi}{2}, \pi, \)

\[ t^2 \in D_2^2 \]

and hence

\[ \rho \in \{ D_2^2 \}. \]

The density matrix in computational basis and its partial transpose is given in (Eq. 3.43) and (Eq. 3.44), respectively

\[
\rho' = \frac{1}{3} \begin{pmatrix}
1 + \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) & 0 & 0 & \frac{\sqrt{3}}{2} r_2 \sin^2 \theta \\
0 & \frac{1}{2} \left[ 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \right] & \frac{1}{2} \left[ 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \right] & 0 \\
0 & \frac{1}{2} \left[ 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \right] & \frac{1}{2} \left[ 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \right] & 0 \\
\frac{-\sqrt{3}}{2} r_2 \sin^2 \theta & 0 & 0 & 1 + \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \\
\end{pmatrix}
\]

(Eq. 3.43)

and

\[
\rho'^{P,T} = \frac{1}{3} \begin{pmatrix}
1 + \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) & 0 & 0 & \frac{1}{2} \left[ 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \right] \\
0 & \frac{1}{2} \left[ 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \right] & \frac{\sqrt{3}}{2} r_2 \sin^2 \theta & 0 \\
0 & \frac{-\sqrt{3}}{2} r_2 \sin^2 \theta & \frac{1}{2} \left[ 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \right] & 0 \\
\frac{1}{2} \left[ 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \right] & 0 & 0 & 1 + \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \\
\end{pmatrix}
\]

(Eq. 3.44)

The eigen values of partially transposed density matrix (Eq. 3.44) are

\[ \lambda_1 = \frac{1}{2}, \]

\[ \lambda_2 = \frac{1}{18} \left( 3 + 3\sqrt{3} r_2 + \sqrt{3} r_2 \cos 2\theta \right). \]
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\[
\lambda_3 = \frac{1}{36} \left( 6 - 3\sqrt{3} r_2 - \sqrt{3} r_2 \cos 2\theta 
- \sqrt{39 r_2^2 - 54 r_2^2 \cos 2\theta + 3 r_2^2 \cos^2 2\theta + 12 r_2^2 \cos 4\theta} \right)
\]

\[
\lambda_4 = \frac{1}{36} \left( 6 - 3\sqrt{3} r_2 - \sqrt{3} r_2 \cos 2\theta 
+ \sqrt{39 r_2^2 - 54 r_2^2 \cos 2\theta + 3 r_2^2 \cos^2 2\theta + 12 r_2^2 \cos 4\theta} \right).
\]

Numerical solutions indicate that in the case of Biaxial systems, \(\rho\) is positive semi-definite and separable iff \(0 < r_2 \leq \sqrt{\frac{3}{4}}\) and \(0 \leq \theta \leq \pi\). For \(r_2 = \sqrt{3}\) and \(\theta = \frac{\pi}{2}\), \(\rho\) is pure as well as entangled.

Some values of \(r_2\) and \(\theta\) for which \(\rho\) is positive semi-definite and corresponding entanglement region are shown in table (3.1).

**Table 3.1:** Positive semidefinite and entanglement region for biaxial system

<table>
<thead>
<tr>
<th>Positive semidefinite region</th>
<th>Entanglement region</th>
</tr>
</thead>
<tbody>
<tr>
<td>(r_2 = \frac{1}{\sqrt{3}}) 0 (\leq \theta \leq \pi)</td>
<td>(\frac{\pi}{4} \leq \theta &lt; \frac{3\pi}{4})</td>
</tr>
<tr>
<td>(r_2 = \sqrt{\frac{3}{2}}) 0 (\leq \theta \leq \pi)</td>
<td>0 (\leq \theta &lt; \pi)</td>
</tr>
<tr>
<td>(r_2 = \sqrt{3}) (\theta = \frac{\pi}{2})</td>
<td>(\theta = \frac{\pi}{2})</td>
</tr>
</tbody>
</table>
Figure 3.8: Eigenvalues $\lambda_1, \lambda_2, \lambda_3$ and $\lambda_4$ as function of $\theta$ for $r_2 = \frac{\sqrt{3}}{4}$ in the case of Biaxial system. $\lambda > 0$ indicates non entanglement.
Figure 3.9: Eigenvalue $\lambda_3$ as a function of $\theta$ for $r_2 = \frac{1}{\sqrt{3}}$ in the case of Biaxial system. $\lambda_3 < 0$ indicates entanglement.
Figure 3.10: Eigenvalue $\lambda_3$ as a function of $\theta$ for $r_2 = \frac{\sqrt{3}}{2}$ in the case of Biaxial system. $\lambda_3 < 0$ indicates entanglement.
Triaxial Systems

Here $t_0^1 \neq 0$, $t_{\pm 1}^1 = 0$, $t_0^2 \neq 0$, $t_{\pm 2}^2 = 0$, $t_{\pm 1}^2 = 0$. Such a system is realized when a spin-$1$ nucleus with non-zero quadrupole moment is exposed to a combined external dipole and electric quadrupole field found in suitable crystal lattice [Usha et al. (1997)].

Consider a special case of the density matrix belonging to this class such that the axes are $\{(\theta_1 = 0), (\theta_1 = \pi)\}$, $\{(\theta, 0), (\pi - \theta, \pi)\}$ and $\{(\theta, \pi), (\pi - \theta - 0)\}$. Such a $\rho$ is called triaxial.

The density matrix corresponding to this class is explicitly given by

$$
\rho = \frac{1}{3} \left[ t_0^0 \tau_0^0 + t_0^1 \tau_1^1 + t_1^1 \tau_{-1}^1 + t_0^2 \tau_0^2 + t_1^2 \tau_1^2 + t_{-1}^2 \tau_{-1}^2 + t_2^2 \tau_{-2}^2 + t_{-2}^2 \tau_{-2}^2 \right]
$$

Using (Eq. 3.34) and (Eq. 3.41), we have

$$
\rho = \frac{1}{3} \left[ 1 + r_1 Q_0^1(\theta = 0) \tau_0^1 + r_1 Q_1^1(\theta = 0) \tau_1^1 + r_1 Q_{-1}^1(\theta = 0) \tau_{-1}^1 + r_2 \left( Q(\theta, 0) \otimes Q(\theta, \pi) \right)^2 \tau_0^2 + r_2 \left( Q(\theta, 0) \otimes Q(\theta, \pi) \right)^2 \tau_1^2 + r_2 \left( Q(\theta, 0) \otimes Q(\theta, \pi) \right)^2 \tau_{-1}^2 + r_2 \left( Q(\theta, 0) \otimes Q(\theta, \pi) \right)^2 \tau_{-2}^2 \right]. 
$$

Thus, the density matrix in $|1m\rangle$ basis is

$$
\rho = \frac{1}{3} \begin{pmatrix}
1 + \sqrt{\frac{2}{3}} r_1 + \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) & 0 & \frac{-\sqrt{2} r_2 \sin^2 \theta}{\sqrt{3}} \\
0 & 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) & 0 \\
\frac{\sqrt{2} r_2 \sin^2 \theta}{\sqrt{3}} & 0 & 1 - \sqrt{\frac{2}{3}} r_1 + \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta)
\end{pmatrix}
$$
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\(\rho\) is positive semi-definite\(^6\) iff

\[
0 < r_1 \leq \sqrt{\frac{3}{2}},
\]

and

\[
0 < r_2 < \sqrt{3},
\]

and the range of \(\theta\) then depends on \(r_1\) and \(r_2\).

The non-zero \(t^k_q\)’s corresponding to this \(\rho\) are

\[
t^1_0 = r_1, \quad t^2_0 = \frac{r^2}{\sqrt{6}} (1 + \cos^2 \theta),
\]

and

\[
t^2_{\pm 2} = -\frac{r^2}{2} \sin^2 \theta.
\]

Since \(t^1 \in D^1_1\) and \(t^2 \in D^2_1\) for \(0 < \theta < \frac{\pi}{2}\) and \(\frac{\pi}{2} < \theta < \pi\), \(\rho \in \{D^1_1, D^2_{1.1}\}\).

Since \(t^1 \in D^1_1\) and \(t^2 \in D^2_2\) for \(\theta = 0, \frac{\pi}{2}, \pi\), \(\rho \in \{D^1_1, D^2_2\}\).

A necessary and sufficient condition to entanglement is that the partial transpose of \(\rho\) has negative eigenvalues. Therefore, we will study eigenvalues of \(\rho^{\text{P.T}}\) to indicate entanglement. (Eq. 3.48) and (Eq. 3.49) represent the density matrix of triaxial system in computational basis and its partial transpose, respectively.

\(^6\)appendix B
\[ \rho' = \frac{1}{3} \begin{pmatrix}
1 + \sqrt{\frac{3}{2}} r_1 + \frac{1}{2\sqrt{3}} r_2(1 + \cos^2 \theta) & 0 & 0 & -\frac{\sqrt{3}}{2} r_2 \sin^2 \theta \\
0 & \frac{1}{2} \left[1 - \frac{1}{\sqrt{3}} r_2(1 + \cos^2 \theta)\right] & \frac{1}{2} \left[1 - \frac{1}{\sqrt{3}} r_2(1 + \cos^2 \theta)\right] & 0 \\
0 & \frac{1}{2} \left[1 - \frac{1}{\sqrt{3}} r_2(1 + \cos^2 \theta)\right] & \frac{1}{2} \left[1 - \frac{1}{\sqrt{3}} r_2(1 + \cos^2 \theta)\right] & 0 \\
-\frac{\sqrt{3}}{2} r_2 \sin^2 \theta & 0 & 0 & 1 - \sqrt{\frac{3}{2}} r_1 + \frac{1}{2\sqrt{3}} r_2(1 + \cos^2 \theta) \end{pmatrix} \]
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\[
\begin{pmatrix}
\frac{1}{2} \left[ 1 - \frac{1}{\sqrt{3}} r_1 (1 + \cos^2 \theta) \right] & 0 & 0 \\
0 & \frac{1}{2} \left[ 1 - \frac{1}{\sqrt{3}} r_2 (1 + \cos^2 \theta) \right] & 0 \\
0 & 0 & 1 - \sqrt{\frac{2}{3}} r_1 + \frac{1}{2} \sqrt{\frac{2}{3}} r_2 (1 + \cos^2 \theta)
\end{pmatrix}
\]

(3.49)
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The eigenvalues corresponding to \(\rho_{P,T}^{\prime}\), are

\[
\lambda_1 = \frac{1}{36} \left( 6 - 3\sqrt{3} r_2 - \sqrt{3} r_2 \cos 2\theta \\
\quad - \sqrt{36 + 216 r_1^2 - 36 \sqrt{3} r_2 - 12 \sqrt{3} r_2 \cos 2\theta + 27 r_2^2 + 18 r_2^2 \cos 2\theta + 3 r_2^2 \cos^2 2\theta} \right),
\]

\[
\lambda_2 = \frac{1}{36} \left( 6 - 3\sqrt{3} r_2 - \sqrt{3} r_2 \cos 2\theta \\
\quad + \sqrt{36 + 216 r_1^2 - 36 \sqrt{3} r_2 - 12 \sqrt{3} r_2 \cos 2\theta + 27 r_2^2 + 18 r_2^2 \cos 2\theta + 3 r_2^2 \cos^2 2\theta} \right),
\]

\[
\lambda_3 = \frac{1}{36} \left( 6 - 3\sqrt{3} r_2 - \sqrt{3} r_2 \cos 2\theta \\
\quad - \sqrt{39 r_2^2 - 54 r_2^2 \cos 2\theta + 3 r_2^2 \cos^2 2\theta + 12 r_2^2 \cos 4\theta} \right),
\]

\[
\lambda_4 = \frac{1}{36} \left( 6 - 3\sqrt{3} r_2 - \sqrt{3} r_2 \cos 2\theta \\
\quad + \sqrt{39 r_2^2 - 54 r_2^2 \cos 2\theta + 3 r_2^2 \cos^2 2\theta + 12 r_2^2 \cos 4\theta} \right).
\]

On the other hand,

\[
\text{Tr}(\rho^2) = \frac{1}{9} \left[ 3 + 3 r_1^2 + \frac{r_2^2}{4} (7 + \cos 4\theta) \right]. \tag{3.50}
\]

Thus, For \(r_1 = \sqrt{\frac{3}{2}}\) and \(r_2 = \frac{\sqrt{3}}{2}\), the density matrix of triaxial system is found to be pure and separable for two values of \(\theta\) only, namely \(\theta = 0\) and \(\theta = \pi\).

For all other values of \(\theta\), ie; \(0 < \theta < \pi\), \(\rho\) is found to be mixed and entangled.

Some values of \(r_1\), \(r_2\) and \(\theta\) for which \(\rho\) is positive semi-definite and corresponding entanglement region are shown in table 3.2.
Table 3.2: Positive semidefinite and entanglement region for triaxial system

<table>
<thead>
<tr>
<th>Positive semidefinite region</th>
<th>Entanglement region</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r_1 = \frac{1}{4} \sqrt{\frac{3}{2}} ), ( r_2 = \frac{\sqrt{3}}{4} )</td>
<td>( 0 \leq \theta \leq \pi )</td>
</tr>
<tr>
<td>( r_1 = \frac{1}{4} \sqrt{\frac{3}{2}} ), ( r_2 = \frac{\sqrt{3}}{3} )</td>
<td>( 0 \leq \theta \leq \pi )</td>
</tr>
<tr>
<td>( r_1 = \frac{1}{4} \sqrt{\frac{3}{2}} ), ( r_2 = \frac{\sqrt{3}}{2} )</td>
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</tr>
<tr>
<td>( r_1 = \frac{1}{2} \sqrt{\frac{3}{2}} ), ( r_2 = \frac{\sqrt{3}}{4} )</td>
<td>( 0 \leq \theta \leq \pi )</td>
</tr>
<tr>
<td>( r_1 = \frac{1}{4} \sqrt{\frac{3}{2}} ), ( r_2 = \frac{\sqrt{3}}{3} )</td>
<td>( 0 \leq \theta \leq \pi )</td>
</tr>
<tr>
<td>( r_1 = \frac{1}{2} \sqrt{\frac{3}{2}} ), ( r_2 = \frac{\sqrt{3}}{2} )</td>
<td>( 0 \leq \theta \leq \pi )</td>
</tr>
<tr>
<td>( r_1 = \sqrt{\frac{3}{2}} ), ( r_2 = \frac{\sqrt{3}}{2} )</td>
<td>( \theta = 0, \ \theta = \pi )</td>
</tr>
</tbody>
</table>
Figure 3.11: $\lambda_3$ as a function of $r_2$ and $\theta$ for a fixed $r_1 = \frac{1}{4}\sqrt{\frac{3}{2}}$. Since $\lambda_3 > 0$ for $0 < r_2 < \frac{\sqrt{3}}{4}$, the triaxial system is separable.
Chapter 3. Multiaxial representation (MAR) and classification of spin-$j$ systems

Figure 3.12: Entanglement region for triaxial system. \( r_1 = \frac{1}{4} \sqrt{\frac{3}{2}} \) and \( \frac{\sqrt{3}}{4} \leq r_2 < \frac{\sqrt{3}}{2} \).

\( \lambda_3 < 0 \) indicates entanglement.