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Unitary Transformations in 3-D Vector Representation of Qutrit States

by Vinod K Mishra

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14. ABSTRACT The qutrit comes next in complexity after qubit as a resource for quantum information processing. The qubit density matrix can be easily visualized using Bloch sphere representation of its states. This simplicity is unavailable for the 8-D state space of a qutrit. Recently a 3-D vector was used to visualize the qutrit states. In current work we derive the transformation of these vectors under unitary transformations.					
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1. Introduction

A qutrit density matrix is of order 3 and depends on 8 parameters. There are many attempts at visualizing the state space of a qutrit¹⁻⁴:

- 1) Using all 8 Gell–Mann matrices, which form a complete set for expressing 3×3 SU(3) matrices;
- 2) Using 6 Gell–Mann matrices supplemented by different matrices in place of 2 diagonal ones; and
- 3) Bloch matrices and their principal minors.

The Bloch matrix approach leads to many complicated constraints on the qutrit parameters. Previous work in this area focused on understanding the structure of 8-D parameter spaces through 2- and 3-sections. On the other hand, the 3-D Bloch ball state space of qubits are easily visualized. Developing geometrical tools to visualize the state space of qutrits in a similar way will be very useful. In this report, we present a scheme for representing qutrit state space (QtSS) in 3-D.

2. Unitary Transformations

2.1 General Qutrit States

The most general qutrit density matrix can be represented using the special unitary group SU(3) invariant form as

$$\rho = \frac{1}{3}I_3 + \vec{n} \cdot \vec{\lambda}. \quad (1)$$

Here I_3 is 3×3 unit matrix, $\vec{n} = (n_1, n_2, \dots, n_8)$ are 8 real parameters, and $\vec{\lambda} = (\lambda_1, \lambda_2, \dots, \lambda_8)$ are 3×3 Gell–Mann matrices. Using them one obtains

$$\rho = \begin{bmatrix} \frac{1}{3} + n_3 + \frac{n_8}{\sqrt{3}} & n_1 - in_2 & n_4 - in_5 \\ n_1 + in_2 & \frac{1}{3} - n_3 + \frac{n_8}{\sqrt{3}} & n_6 - in_7 \\ n_4 + in_5 & n_6 + in_7 & \frac{1}{3} - \frac{2n_8}{\sqrt{3}} \end{bmatrix}. \quad (2)$$

2.2 Matrix Exponential for Density Matrix

Given a Hamiltonian H and an angle-like parameter θ , the corresponding unitary transformation is given as $U = e^{i\theta\rho}$. In general ρ is a Hermitian matrix. For traceless and Hermitian H matrices the exponentials are widely known. The

calculation becomes more involved for a general 3×3 matrix, which is the case with the density matrix under consideration.

The characteristic equation (CE) of ρ derived from Eq. 2 is given as follows:

$$\mu^3 - \mu^2 + c_2\mu - c_3 = 0. \quad (3)$$

Using the definition $r_i^2 = \frac{1}{4} (a_i^2 + q_i^2)$, the coefficients of the CE are given by

$$c_2 = \frac{1}{2}\{1 - Tr(\rho^2)\}. \quad (4)$$

$$c_3 = \frac{1}{6}\{1 - 3Tr(\rho^2) + 2Tr(\rho^3)\}. \quad (5)$$

Expressing the CE in terms of its eigenvalues,

$$(\mu - \mu_0)(\mu - \mu_1)(\mu - \mu_2) = 0. \quad (6)$$

It leads to alternate expressions for the CE coefficients:

$$c_2 = \mu_0\mu_1 + \mu_1\mu_2 + \mu_2\mu_0, c_3 = \mu_0\mu_1\mu_2. \quad (7)$$

So the eigenvalues are expressible in terms of the density matrix elements. These coefficients are further constrained by the following inequalities:

$$0 \leq c_2 \leq \frac{1}{3}, 0 \leq c_3 \leq \frac{1}{27}. \quad (8)$$

One can derive the constraints on the traces also by

$$0 \leq Tr(\rho^2) \leq \frac{1}{3}, 0 \leq Tr(\rho^3) \leq \frac{1}{9}. \quad (9)$$

It is possible to express any function of the density matrix (including the exponential for the unitary transformation) using the method of projectors as given in de Zela.¹ Let μ_k and $|\mu_k\rangle$ denote the eigenvalues and eigenvectors of the density matrix. Denoting the 3-D identity matrix by I_3 , we can write,

$$I_3 = \sum_{k=0}^2 |\mu_k\rangle\langle\mu_k|, \rho = \sum_{k=0}^2 \mu_k |\mu_k\rangle\langle\mu_k|. \quad (10)$$

The matrices $|\mu_k\rangle\langle\mu_k|$ ($k = 0, 1, 2$) can be expressed as a combination of eigenvalues (μ_k) and powers of density matrix (ρ). Also any function of density matrix can then be written as

$$f(\rho) = \sum_{k=0}^2 f(\mu_k) |\mu_k\rangle\langle\mu_k|, \quad (11)$$

The unitary operator takes the following form:

$$U = e^{i\theta\rho} = \sum_{k=0}^2 e^{i\theta\mu_k} |\mu_k\rangle \langle \mu_k|. \quad (12)$$

2.3 Unitarily Transformed Density Matrix

The density matrix transformed by the unitary operator is given as

$$U\rho U^+ = e^{i\theta\rho} \rho e^{-i\theta\rho} = \left(\sum_{k=0}^2 e^{i\theta\mu_k} |\mu_k\rangle \langle \mu_k| \right) \rho \left(\sum_{k=0}^2 e^{-i\theta\mu_k} |\mu_k\rangle \langle \mu_k| \right). \quad (13)$$

One needs to use a relation for density matrix due to the Cayley-Hamilton Theorem.

$$\rho^3 = \rho^2 - c_2\rho + c_3. \quad (14)$$

Its use reduces the higher powers of density matrix to, at most, the quadratic.

2.4 Unitary Transformation for Special Cases

Details about the calculation are given in the Appendix. Here we enumerate the results under a common scheme.

Case I: Roots: 0, 0, 1

CE:	$\mu^2(\mu - 1) = 0$
Constraints on CE coefficients:	$c_2 = 0, c_3 = 0$
Unitary operator:	$U = e^{i\theta\rho} = I_3 + (e^{i\theta} - 1)\rho$
Transformed density matrix:	$U\rho U^+ = e^{i\theta\rho} \rho e^{-i\theta\rho} = \rho$

Case II: Roots: 0, μ_1 , μ_2 ($\mu_2 > \mu_1$)

CE:	$\mu(\mu - \mu_1)(\mu - \mu_2) = 0$
	$\mu_1 = \frac{1}{2} - \alpha, \mu_2 = \frac{1}{2} + \alpha$ (with $\alpha = \sqrt{\frac{1}{4} - c_2}$)
Constraints on CE coefficients:	$c_2 < \frac{1}{4}, c_3 = 0$
Unitary operator:	$U = e^{i\theta\rho} = e^{i\theta/2} \left[\cos\theta\alpha + i \left(\frac{\sin\theta\alpha}{\alpha} \right) \left(\rho - \frac{1}{2} \right) \right]$
Transformed density matrix:	$U\rho U^+ = e^{i\theta\rho} \rho e^{-i\theta\rho} = \rho$

Case III: Roots: 0, $\mu_1 = \mu_2 = \frac{1}{2}$

CE:	$\mu(\mu - \mu_1)^2 = 0$
Constraints on CE coefficients:	$c_2 = \frac{1}{4}, c_3 = 0$

$$\begin{aligned} \text{Unitary operator:} \quad & U = e^{i\theta\rho} = e^{i\theta/2} \\ \text{Transformed density matrix:} \quad & U\rho U^+ = e^{i\theta\rho}\rho e^{-i\theta\rho} = e^{i\theta/2}\rho e^{-i\theta/2} = \rho \end{aligned}$$

Case IV: Roots: $\mu_0 = \mu_1 = \mu_2$

$$\begin{aligned} \text{CE:} \quad & (\mu - \mu_0)^3 = 0 \\ \text{Constraints on CE coefficients:} \quad & c_2^3 = 27c_3^2 \\ \text{Examples:} \quad & (c_2, c_3) = \left(\frac{1}{4}, \frac{1}{24\sqrt{3}}\right), \left(\frac{1}{3}, \frac{1}{27}\right), \left(\frac{1}{2}, \frac{1}{6\sqrt{6}}\right), \text{ etc.} \\ \text{Unitary operator:} \quad & U = e^{i\theta\rho} = e^{i\theta\mu_0} \\ \text{Transformed density matrix:} \quad & U\rho U^+ = e^{i\theta\mu_0}\rho e^{-i\theta\mu_0} = \rho \end{aligned}$$

Case V: Roots: $\mu_0, \mu_1 = \mu_2$

$$\begin{aligned} \text{CE} \quad & (\mu - \mu_0)(\mu - \mu_1)^2 = 0, \\ \text{Constraints on CE coefficients:} \quad & c_3 = \frac{1}{27}[9c_2 - 2 + 2(1 - 3c_2)^{3/2}] \\ \text{Examples:} \quad & (c_2, c_3) = \left(\frac{1}{4}, \frac{1}{54}\right), \left(\frac{8}{27}, \frac{20}{729}\right), \left(\frac{8}{25}, \frac{112}{3375}\right), \text{ etc.} \end{aligned}$$

$$\begin{aligned} \text{Also,} \quad & \mu_1 = \mu_2 = \frac{1}{3}(1 + \beta), \beta = \sqrt{1 - 3c_2} \\ & \mu_0 = \frac{1-4c_2+9c_3}{1-3c_2}, \mu_1 = \mu_2 = \frac{c_2-9c_3}{2(1-3c_2)} \mu_0 = \frac{1}{3}(1 - 2\beta), \end{aligned}$$

$$\begin{aligned} \text{Unitary operator:} \quad & U = e^{i\theta\rho} = \frac{1}{\beta} [e^{i\theta\mu_1}(\rho - \mu_0) + e^{i\theta\mu_0}(\mu_1 - \rho)] \\ \text{Transformed density matrix:} \quad & U\rho U^+ = e^{i\theta\rho}\rho e^{-i\theta\rho} \end{aligned}$$

$$= \rho + \left(\frac{\sin\beta\theta/2}{\beta/2}\right)^2 \left[c_3 - \frac{1}{9}(2 + \beta - \beta^2)\rho + \frac{1}{3}(1 + \beta)\rho^2 \right]$$

2.5 Unitary Transformation for General Case

The general case with all 3 real roots ($\mu_0 < \mu_1 < \mu_2$) leads to both coefficients of the CE being nonzero. So we get a complicated expression for the roots of the resulting cubic equation. One has to solve the following equations to calculate the density matrix and related functions.

$$I_3 = |\mu_0 \rangle \langle \mu_0| + |\mu_1 \rangle \langle \mu_1| + |\mu_2 \rangle \langle \mu_2|, \quad (15)$$

$$\rho = \mu_0|\mu_0\rangle\langle\mu_0| + \mu_1|\mu_1\rangle\langle\mu_1| + \mu_2|\mu_2\rangle\langle\mu_2|, \quad (16)$$

and
$$\rho^2 = \mu_0^2|\mu_0\rangle\langle\mu_0| + \mu_1^2|\mu_1\rangle\langle\mu_1| + \mu_2^2|\mu_2\rangle\langle\mu_2|. \quad (17)$$

Their solution allows one to write the unitary transformation operator as

$$\begin{aligned} U &= e^{i\theta\rho} = e^{i\theta\mu_0}|\mu_0\rangle\langle\mu_0| + e^{i\theta\mu_1}|\mu_1\rangle\langle\mu_1| + e^{i\theta\mu_2}|\mu_2\rangle\langle\mu_2| \\ &= e^{i\theta\mu_0} \frac{(\mu_1-\rho)(\mu_2-\rho)}{(\mu_1-\mu_0)(\mu_2-\mu_0)} - e^{i\theta\mu_1} \frac{(\mu_0-\rho)(\mu_2-\rho)}{(\mu_1-\mu_0)(\mu_2-\mu_1)} + e^{i\theta\mu_2} \frac{(\mu_0-\rho)(\mu_1-\rho)}{(\mu_2-\mu_0)(\mu_2-\mu_1)}. \end{aligned} \quad (18)$$

Rewriting Eq. 14,

$$(\mu_1 - \mu_0)(\mu_2 - \mu_0)(\mu_2 - \mu_1)U = e^{i\theta\mu_0}a - e^{i\theta\mu_1}b + e^{i\theta\mu_2}c, \quad (19)$$

with

$$a = (\mu_2 - \mu_1)(\mu_2 - \rho)(\mu_1 - \rho), \quad (20)$$

$$b = (\mu_2 - \mu_0)(\mu_2 - \rho)(\mu_0 - \rho), \quad (21)$$

and
$$c = (\mu_1 - \mu_0)(\mu_1 - \rho)(\mu_0 - \rho). \quad (22)$$

Then the transformed density matrix can be expressed as

$$\begin{aligned} &(\mu_1 - \mu_0)^2(\mu_2 - \mu_0)^2(\mu_2 - \mu_1)^2 U \rho U^\dagger \\ &= [e^{i\theta\mu_0}a - e^{i\theta\mu_1}b + e^{i\theta\mu_2}c][e^{-i\theta\mu_0}a - e^{-i\theta\mu_1}b + e^{-i\theta\mu_2}c]\rho \\ &= a^2 + b^2 + c^2 - 2abc\cos(\mu_1 - \mu_0)\theta - 2bcc\cos(\mu_2 - \mu_1)\theta + 2cac\cos(\mu_2 - \mu_0)\theta \\ &= (a - b + c)^2 + 4absin^2\frac{(\mu_1 - \mu_0)\theta}{2} + 4bcsin^2\frac{(\mu_2 - \mu_1)\theta}{2} - 4casin^2\frac{(\mu_2 - \mu_0)\theta}{2}. \end{aligned} \quad (23)$$

We use the following relations,

$$\mu_0 + \mu_1 + \mu_2 = 1, c_2 = \mu_0\mu_1 + \mu_1\mu_2 + \mu_2\mu_0, c_3 = \mu_0\mu_1\mu_2, \quad (24)$$

to find that each of the combinations ab , bc , and ca vanishes. One also gets $(\mu_1 - \mu_0)^2(\mu_2 - \mu_0)^2(\mu_2 - \mu_1)^2 = (a - b + c)^2$. Finally, the transformed density matrix reduces to the following:

$$U\rho U^\dagger = e^{i\theta\rho}\rho e^{-i\theta\rho} = \rho. \quad (25)$$

This rather surprising result says that the density matrix ρ with 3 real and distinct eigenvalues describes a pure state.

3. Effect of Unitary Transformations on 3-D Vectors for Qutrit States

For a density matrix to represent a physical qutrit, it must satisfy some constraints:

- 1) Positivity of diagonal elements

$$0 \leq \frac{1}{3} \pm n_3 + \frac{n_8}{\sqrt{3}} \leq 1, 0 \leq \frac{1}{3} - \frac{2n_8}{\sqrt{3}} \leq 1. \quad (26)$$

- 2) Normalization

$$\text{Tr}(\rho) = 1. \quad (27)$$

- 3) Constraint on the length of the state vector

$$\vec{n} \cdot \vec{n} \leq \frac{1}{3}. \quad (28)$$

- 4) Nonnegativity of the determinant

$$\det \rho \geq 0. \quad (29)$$

Earlier attempts at visualizing these general constraints focused on 8-D Cartesian space as shown by Sarbicki and Bengtsson,² Mendas,³ Goyal et al.,⁴ and Bengtsson et al.⁵ The 2- and 3-sections of these 8-D objects (only 2 and 3 nonzero elements) have been found, classified, and characterized by these authors. Beyond 3 dimensions it is impossible to visualize the state space, so attempts have been made to find alternative schemes. In this work, such a scheme is presented.

3.1 Qutrit Constraints for Spin-1 Representation as 3-D Vectors

Following the formalism of Kurzynski et al.⁶ and Kurzynski⁷, an alternative representation of the qutrit density matrix based on the symmetric part of the 2 qubit is our starting point. Define:

$$d_i = (q_i + ia_i)/2, \bar{d}_i = (q_i - ia_i)/2. \quad (30)$$

Then the Bloch matrix representing a spin-1 state is given by

$$\rho = \begin{bmatrix} \omega_1 & -d_3 & -\bar{d}_2 \\ -\bar{d}_3 & \omega_2 & -d_1 \\ -d_2 & -\bar{d}_1 & \omega_3 \end{bmatrix}. \quad (31)$$

The parameters in this representation are connected to spin-1 observables.

$$\omega_i = \langle S_i^2 \rangle = \text{Tr}(\rho S_i^2), \quad (32)$$

$$a_i = \langle S_i \rangle = \text{Tr}(\rho S_i), \quad (33)$$

$$\text{and } q_k = \langle S_i S_j + S_j S_i \rangle = \text{Tr}\{\rho(S_i S_j + S_j S_i)\}, k \neq i, j. \quad (34)$$

Comparison of this parametrization of this qutrit density matrix with the earlier one based on the Gell–Mann matrices gives the following identities:

$$n_1 = \frac{1}{2}q_3, n_2 = \frac{1}{2}a_3, n_4 = \frac{1}{2}q_2, n_5 = \frac{1}{2}a_2, n_6 = -\frac{1}{2}q_1, n_7 = \frac{1}{2}a_1, \quad (35)$$

$$\text{and } n_3 = \frac{1}{2}(\omega_1 - \omega_2), n_8 = \sqrt{3} \left[-\frac{1}{3} + \frac{1}{2}(\omega_1 + \omega_2) \right]. \quad (36)$$

Then the constraints in Eq. 20 take the following forms:

1) Positivity of diagonal elements implies

$$\omega_1 \geq 0, \omega_2 \geq 0, \omega_3 \geq 0. \quad (37)$$

2) $\text{Tr}(\rho) = 1$ implies

$$\omega_1 + \omega_2 + \omega_3 = 1. \quad (38)$$

3) $\text{Tr}(\rho^2) \leq 1$ implies

$$\sum_{i=1}^3 (\omega_i^2 + 2r_i^2) \leq 1. \quad (39)$$

Here $r_i^2 = \frac{1}{4}(a_i^2 + q_i^2)$ and equality sign hold for the pure states.

4) $\det \rho \geq 0$ implies

$$[\sum_{i=1}^3 (3\omega_i^2 - 2\omega_i^3 + 6\omega_i r_i^2) - \Delta] \leq 1. \quad (40)$$

Here $\Delta = \frac{1}{4}(a_2 a_3 q_1 + a_3 a_1 q_2 + a_1 a_2 q_3 - q_1 q_2 q_3)$, and equality sign hold for

the pure states. The relation to CE coefficients is given as

$$c_2 = \frac{1}{2}\{1 - \text{Tr}(\rho^2)\} = (\omega_2 \omega_3 + \omega_3 \omega_1 + \omega_1 \omega_2) - \sum_{i=1}^3 r_i^2, \quad (41)$$

$$\text{and } c_3 = \frac{1}{6}\{1 - 3\text{Tr}(\rho^2) + 2\text{Tr}(\rho^3)\} = \omega_1 \omega_2 \omega_3 - \sum_{i=1}^3 \omega_i r_i^2 + \Delta. \quad (42)$$

It is apparent that the 3 constraints can be rewritten in terms of the following 3-D vectors:

1) $\vec{u} = \{u_1, u_2, u_3\}$ such that

$$u^2 = \frac{1}{2}\{3\text{Tr}(\rho^2) - 1\} = \frac{3}{2}\sum_{i=1}^3 (\omega_i^2 + 2r_i^2) - \frac{1}{2}, \quad (43)$$

$$u_1 = \sqrt{\frac{3}{2}(\omega_1^2 + 2r_1^2) - \frac{1}{6}}, \quad (44)$$

$$u_2 = \sqrt{\frac{3}{2}(\omega_2^2 + 2r_2^2) - \frac{1}{6}}, \quad (45)$$

and

$$u_3 = \sqrt{\frac{3}{2}(\omega_3^2 + 2r_3^2) - \frac{1}{6}}. \quad (46)$$

2) $\vec{v} = \{v_1, v_2, v_3\}$ such that

$$v^2 = \frac{1}{8}\{9Tr(\rho^3) - 1\} = \frac{9}{8}\sum_{i=1}^3\{\omega_i^3 + 3r_i^2 - 3\omega_i r_i^2 + 3\Delta\} - \frac{1}{8}, \quad (47)$$

$$v_1 = \sqrt{\frac{9}{8}\{\omega_1^3 + 3(1 - \omega_1)r_1^2 + \Delta\} - \frac{1}{24}}, \quad (48)$$

$$v_2 = \sqrt{\frac{9}{8}\{\omega_2^3 + 3(1 - \omega_2)r_2^2 + \Delta\} - \frac{1}{24}}, \quad (49)$$

and

$$v_3 = \sqrt{\frac{9}{8}\{\omega_3^3 + 3(1 - \omega_3)r_3^2 + \Delta\} - \frac{1}{24}}. \quad (50)$$

3) $\vec{w} = \{w_1, w_2, w_3\}$ such that

$$w^2 = \omega_1 + \omega_2 + \omega_3 = 1, \quad (51)$$

and

$$\vec{w} = \{\sqrt{\omega_1}, \sqrt{\omega_2}, \sqrt{\omega_3}\}. \quad (52)$$

These vectors have the desired properties such that for pure states $u^2 = 1 = v^2$, and for maximum mixed states $u^2 = 0 = v^2$, and they also obey the constraints $0 \leq u^2 \leq 1$ and $0 \leq v^2 \leq 1$. The 3rd vector \vec{w} is always of unit length. The original 8 degrees of freedom of a general qutrit state is distributed as 3+3+2 among the 3 vectors. They are always in the positive octant of a 3-D sphere of unit radius. The mixed states reside inside the volume interior to the “pure qutrit state surface”. This is similar to the Bloch ball of a qubit.

3.2 Effect of Unitary Transformation on the QtSS Vectors

It was found earlier that almost all the cases lead to no change in the density matrix. The special case with one double root with CE: $(\mu - \mu_0)(\mu - \mu_1)^2 = 0$ is the only case when this does not hold true. The transformed density matrix is given as the following:

$$U\rho U^\dagger = e^{i\theta\rho} \rho e^{-i\theta\rho} = \rho + \left(\frac{\sin\beta\theta/2}{\frac{\beta}{2}}\right)^2 \left[c_3 - \frac{1}{9}(2 + \beta - \beta^2)\rho + \frac{1}{3}(1 + \beta)\rho^2\right]. \quad (53)$$

It is clear from the definitions that $\beta = u$ and $c_3 = \frac{1}{27} - \frac{1}{3}u^2 + \frac{8}{27}v^2$, and so the connection with 3-D vectors can be easily established.

4. Conclusion

In this work we have shown that the 8-D qutrit state space can be alternatively visualized in 3 dimensions using 3-D vectors, and unitary transformations affect their lengths and directions. In the future it will be interesting to see if the QtSS 3-D vectors offer advantages over traditional methods for visualizing the properties and quantifying measures of the entangled qutrits.

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Appendix. Unitary Transformation for Special Cases

Results for some special cases are as follows:

(I) Both coefficients are zero.

$$\mathbf{c}_2 = \mathbf{0}, \quad \mathbf{c}_3 = \mathbf{0}. \quad (\text{A-1})$$

These are all pure states with eigenvalues $\mu = 0,0,1$.

(II) Second coefficient is zero.

$$\mathbf{c}_2 \neq \mathbf{0}, \quad \mathbf{c}_3 = \mathbf{0}. \quad (\text{A-2})$$

Which gives $Tr(\rho^3) = 1 - 3c_2$. The characteristic equation (CE) for this case is given by

$$\mu^3 - \mu^2 + c_2\mu = \mu(\mu^2 - \mu + c_2) = 0. \quad (\text{A-3})$$

It has 3 roots out of which one is always zero. The other 2 roots can be either 2 reals or 1 complex conjugate pair. This leads to the following special cases:

(IIa) Two real nonzero roots ($c_2 < 1/4$ or $Tr(\rho^2) > 1/2$)

Define $\alpha = \sqrt{1 - 4c_2}$, then the roots are 0, $(1 + \alpha)/2$, and $(1 - \alpha)/2$,

and
$$\rho = \text{diag}(0, (1 + \alpha)/2, (1 - \alpha)/2). \quad (\text{A-4})$$

The Cayley-Hamilton Theorem can be used according to which the density matrix itself satisfies the CE. Then we find that

$$U = e^{i\theta\rho} = e^{i\theta/2}[\cos(\theta\alpha/2) - (i/\alpha)\sin(\theta\alpha/2) + (2/\alpha)\sin(\theta\alpha/2)\rho]. \quad (\text{A-5})$$

(IIb) One double root ($c_2 = 1/4$ or $Tr(\rho^2) = 1/2$)

The roots are $\alpha = 0$ and $\rho = \text{diag}(0, 1, 1)$. There is a single root of 0 and a double root of $1/2$. The unitary transformation matrix is

$$U = e^{i\theta\rho} = I - 2(1 - e^{i\theta/2})\rho. \quad (\text{A-6})$$

(IIc) Pair of complex conjugate roots ($c_2 > 1/4$ or $Tr(\rho^2) < 1/2$)

Define $\alpha' = \sqrt{4c_2 - 1}$ then the roots are 0, $(1 + i\alpha')/2$, and $(1 - i\alpha')/2$,

and,
$$\rho = \text{diag}(0, (1 + i\alpha')/2, (1 - i\alpha')/2). \quad (\text{A-7})$$

We also get

$$U = e^{i\theta\rho} = e^{i\theta/2}[\cosh(\theta\alpha'/2) + (i/\alpha')\sinh(\theta\alpha'/2) - (2/\alpha')\sinh(\theta\alpha'/2)\rho]. \quad (\text{A-8})$$

(III) Unitary Transformation for case with 2 nonzero roots ($c_2 < 1/4$)

The general unitary transformation is given by

$$U\rho U^+ = e^{i\theta\hat{\rho}}\rho e^{-i\theta\hat{\rho}}. \quad (\text{A-9})$$

Here ρ' is the original 3×3 matrix and $e^{i\theta\rho}$ is the diagonal matrix exponential for the case with real roots (the complex root situation is similar). It can be recalled that for a qubit this results in the rotation of the 3-dimensional Bloch vector. Rewriting

$$\alpha U = (A_1 + B_1\hat{\rho}) + i(A_2 + B_2\hat{\rho}). \quad (\text{A-10})$$

Where

$$A_1 = \alpha \cos(\theta\alpha/2) \cos(\theta/2) + \sin(\theta\alpha/2) \sin(\theta/2), \quad (\text{A-11})$$

$$A_2 = \alpha \cos(\theta\alpha/2) \sin(\theta/2) - \sin(\theta\alpha/2) \cos(\theta/2), \quad (\text{A-12})$$

and $B_1 = -2\sin(\theta\alpha/2)\sin(\theta/2), B_2 = -2\sin(\theta\alpha/2)\cos(\theta/2).$ (\text{A-13})

We get

$$\begin{aligned} \alpha^2 U\rho U^+ &= (A_1^2 + A_2^2)\rho + (A_1B_1 + A_2B_2)(\hat{\rho}\rho + \rho\hat{\rho}) + \\ &(B_1^2 + B_2^2)\hat{\rho}\rho\hat{\rho} + i(A_1B_2 - A_2B_1)(\hat{\rho}\rho - \rho\hat{\rho}). \end{aligned} \quad (\text{A-14})$$

with

$$A_1^2 + A_2^2 = \alpha^2 \cos^2(\theta\alpha/2) + \sin^2(\theta\alpha/2), \quad (\text{A-15})$$

$$B_1^2 + B_2^2 = 4\sin^2(\theta\alpha/2), \quad (\text{A-16})$$

$$A_1B_1 + A_2B_2 = -4\sin^2(\theta\alpha/2), \quad (\text{A-17})$$

and $A_1B_2 - A_2B_1 = 2\alpha \sin\left(\frac{\theta\alpha}{2}\right) \cos\left(\frac{\theta\alpha}{2}\right).$ (\text{A-18})

Also let $D = \{\cos(\theta\alpha/2) + (i/\alpha)\sin(\theta\alpha/2)\}$. Then the unitarily transformed density matrix is given as

$$U\rho U^+ = \begin{bmatrix} D\bar{D}\omega_1 & \bar{D}e^{-i\theta\alpha/2}(-d_3) & \bar{D}e^{i\theta\alpha/2}(-\bar{d}_2) \\ De^{i\theta\alpha/2}(-\bar{d}_3) & \omega_2 & e^{i\theta\alpha/2}(-d_1) \\ De^{-i\theta\alpha/2}(-d_2) & e^{-i\theta\alpha/2}(-\bar{d}_1) & \omega_3 \end{bmatrix}. \quad (\text{A-19})$$

Comparing this with Eq. 31, it is seen that under a unitary transformation the density matrix elements get multiplied by various trigonometric functions. This induces changes in the lengths and angles of the vectors $(\mathbf{u}, \mathbf{v}, \mathbf{w})$.

List of Symbols, Abbreviations, and Acronyms

3-D	3-dimensional
8-D	8-dimensional
CE	characteristic equation
QtSS	qutrit state space
SU	special unitary group

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