Geometry of the space of density matrices #NYAJ

1 General Matrices

Let $\mathcal{D} \equiv M_d(\mathbb{C}) = \{d \times d$ matrices with complex entries$\}$. $(d > 1)$.

Let $x \in \mathcal{D}$ be an arbitrary $d \times d$ matrix with complex entries, and let

$$\rho(x) = \tfrac{1}{d}\, \mathbb{I} + \sqrt{\tfrac{d-1}{d}}\; x\ .$$

Proposition 1.1. The map $\rho : \mathcal{D} \to \mathcal{D}$ by $x \mapsto \rho(x)$ is a bijection with inverse

$$x(\rho) = \sqrt{\tfrac{d}{d-1}}\; (\rho - \tfrac{1}{d}\, \mathbb{I})\ .$$

Thus each ρ is specified by exactly one x.

Proof. It is trivial to show that $\rho = \rho'$ implies $x = x'$, and that for any $\rho' \in \mathcal{D}$ the matrix $x(\rho')$ is also in $\mathcal{D}$ such that $\rho(x(\rho')) = \rho'$, which proves the assertion. ∎

Proposition 1.2. Some properties.

1. $\rho^\dagger = \rho \iff x^\dagger = x$.
2. $\mathrm{Tr}\ \rho = 1 \iff \mathrm{Tr}\ x = 0$.

Proof. Trivial. ∎

Proposition 1.3. (FALSE) Let $\rho^\dagger = \rho$ and $\mathrm{Tr}\ \rho = 1$. Then the following are equivalent: (FALSE)

1. $z^\dagger\, \rho\, z \geq 0$ for all d-dimensional complex vectors z (ρ is positive definite),
2. $\mathrm{Tr}\ (\rho^2) \leq 1$,
3. $\mathrm{Tr}\ (x^2) \leq 1$.

Proof. $(1 \to 2)$ and $(2 \leftrightarrow 3)$ are true. But $(2 \to 1)$ is false for $d > 2$, as shown by the counterexample $\rho = \mathrm{diag}(-.2, .6, .6)$, which obeys $\mathrm{Tr}\ (\rho) = 1$ and $\mathrm{Tr}\ (\rho^2) = .76 < 1$ and $\mathrm{Tr}\ (x) = 0$ and $\mathrm{Tr}\ (x^2) \approx .427 < 1$ but is not positive semi-definite because it has a negative eigenvalue. ∎

2 Bipartite System

An arbitrary hermitian matrix Q_{AB} of size $d_A d_B$ can be written in the form

$$Q_{AB} = c_{00}\, \frac{\mathbb{I}_{AB}}{d_A d_B} + \left(\frac{A}{d_B} \oplus \frac{B}{d_A} \right) + \sum_{mn} c_{mn}\ (A_m \otimes B_n) \tag{1}$$

where A and B are arbitrary traceless hermitian matrices of sizes d_A and d_B, and A_m and B_n are bases for the spaces of traceless hermitian matrices of sizes d_A and d_B, and c_{mn} are real numbers, and $m = 1, 2 \ldots d_A^2 - 1$ and $n = 1, 2 \ldots d_B^2 - 1$. To show this fact, first show that $L(V \otimes W) \cong L(V) \otimes L(W)$ and that the same goes for the hermitian spaces. Then choose a basis for hermitian matrices such that the zeroth basis element is the identity matrix, and the rest are traceless.

It follows that

$$\mathrm{Tr}\ Q_{AB} = c_{00} \qquad Q_A = \mathrm{Tr}_B Q_{AB} = c_{00}\,\frac{\mathbb{I}_A}{d_A} + A \qquad Q_B = \mathrm{Tr}_A Q_{AB} = c_{00}\,\frac{\mathbb{I}_B}{d_B} + B \tag{2}$$

Therefore we may write an arbitrary density matrix as

$$\begin{aligned}
\rho_{AB} &= \frac{\mathbb{I}_{AB}}{d_A d_B} + \sqrt{\tfrac{d_A d_B - 1}{d_A d_B}}\left[\left(\sqrt{\tfrac{d_B(d_A-1)}{d_A d_B - 1}}\,\frac{x_A}{d_B} \oplus \sqrt{\tfrac{d_A(d_B-1)}{d_A d_B - 1}}\,\frac{x_B}{d_A}\right) + y_{AB}\right] &(3)\\
&= \tfrac{\mathbb{I}}{d} + \sqrt{\tfrac{d-1}{d}}\ \left[(\alpha\, x_A \oplus \beta\, x_B) + y_{AB}\right] &(4)\\
&= \tfrac{\mathbb{I}}{d} + \sqrt{\tfrac{d-1}{d}}\ x_{AB} &(5)
\end{aligned}$$

along with the condition that $\rho_{AB} \geq 0$. The matrix y_{AB} is defined as above, and

$$\mathrm{Tr}\ \rho_{AB} = 1 \qquad \rho_A = \frac{\mathbb{I}_A}{d_A} + \sqrt{\tfrac{d_A-1}{d_A}}\ x_A \qquad \rho_B = \frac{\mathbb{I}_B}{d_B} + \sqrt{\tfrac{d_B-1}{d_B}}\ x_B \tag{6}$$

We find that

$$x_{AB}^2 = \left(\alpha^2\, x_A^2 \oplus \beta^2\, x_B^2\right) + 2\alpha\beta\,(x_A \otimes x_b) + y_{AB}^2 + z_{AB} \tag{7}$$

where

$$\begin{aligned}
z_{AB} &= (\alpha x_A \oplus \beta x_B) y_{AB} + y_{AB}(\alpha x_A \oplus \beta x_B) &(8)\\
&= \sum_{mn} c_{mn}\left[\alpha\,(x_A A_m + A_m x_A) \otimes B_n + \beta\, A_m \oplus (x_B B_n + B_n x_B)\right] &(9)
\end{aligned}$$

and then since $\mathrm{Tr}\ z_{AB} = 0$ we find

$$\mathrm{Tr}\ x_{AB}^2 = \alpha^2\, d_B\, \mathrm{Tr}\ x_A^2 + \beta^2\, d_A\, \mathrm{Tr}\ x_B^2 + \mathrm{Tr}\ y_{AB}^2\ . \tag{10}$$

The conditions $\rho_{AB}, \rho_A, \rho_B \geq 0$ imply $(\mathrm{Tr}\ x_A^2, \mathrm{Tr}\ x_A^2, \mathrm{Tr}\ y_{AB}^2) \leq 1$ along with

$$\alpha^2\, d_B\, \mathrm{Tr}\ x_A^2 + \beta^2\, d_A\, \mathrm{Tr}\ x_B^2 + \mathrm{Tr}\ y_{AB}^2 \leq 1 \tag{11}$$

Assigning the inner product $(A, B) = \mathrm{Tr}\ A^\dagger B$ and choosing orthonormal bases for the spaces of traceless hermitian matrices, the system can be described by three bloch vectors: one for A, one for B, and a mutual vector. Each lies within a ball of radius one.