Lemma

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Lemma: *Let $\mathbb{A}_N$ be the vector space of $N \times N$ Hermitean matrices with no diagonal entries.*

$$\mathbb{A}_N \equiv \Big\{ A \in C_H^{N\times N} \;\Big|\; A_{ii} = 0 \Big\}$$

Also, let $\mathcal{A}_N$ be the following convex set

$$\mathcal{A}_N \equiv \Big\{ A \in \mathbb{A}_N \;\Big|\; \mathbb{I} + A \geq 0 \Big\}$$

Then for any $A \in \operatorname{ext}\big(\mathcal{A}\big)$, we have $\operatorname{rank}(\mathbb{I} + A) \leq \sqrt{N}$.

Corollary: *For $N < 4$, since $\mathbb{I} + A^{ext.}$ is of unit rank and has unit diagonal, we may write*

$$A_{ij}^{ext.} = e^{i(\phi_i - \phi_j)} - \delta_{ij}$$

Proof: A is an extreme point for $\mathcal{A}$ iff for any $A' \in \mathbb{A}$, the line $A + tA'$ falls outside $\mathcal{A}$ either for $t > 0$ or $t < 0$. Now for any $A \in \operatorname{ext}(\mathcal{A})$, let $k \equiv \operatorname{rank} \mathbb{I} + A > 0$, then

$$\mathbb{I} + A = \sum_{\alpha=1}^{k} \lambda_\alpha \left| u_\alpha \right\rangle \left\langle u_\alpha \right|; \quad \lambda_\alpha > 0; \;\; \left\langle u_\alpha \middle| u_\beta \right\rangle = \delta_{\alpha\beta}$$

then in the eigen-basis for A we may write

$$\mathbb{I} + A + tA' = \begin{pmatrix} \Lambda + tV & tB \\ tB^\dagger & tC \end{pmatrix}$$

where $\Lambda = \operatorname{diag}[\lambda_\alpha]$, and B and C are Hermitean matrices of sizes $k \times k$ and $(N-k) \times (N-k)$ respectively. For $C \neq 0$, the matrix is always non positive semi definite for either $t > 0$ or $t < 0$. Therefore, the extremity of A is determined only by A' that make $C = 0$. Next, we see that we also need $B = 0$. In that regard consider

$$(t\vec{a}^\dagger, \mu\vec{b}^\dagger) \begin{pmatrix} \Lambda + tV & tB \\ tB^\dagger & 0 \end{pmatrix} \begin{pmatrix} t\vec{a} \\ \mu\vec{b} \end{pmatrix} = t^2 \Big[\vec{a}^\dagger \Lambda \vec{a} + \mu\big(\vec{a}^\dagger B \vec{b} + \vec{b}^\dagger B^\dagger \vec{a} \big) \Big] + \mathcal{O}(t^3)$$

For nonzero B, there is always a choice of μ and $\vec{b}$ that make this negative for small t. Therefore, if any A' work as a witness for $non-extremeity$ of A they must have $B = 0$. Finally we may write such an A' with only V components as

$$A' = \sum_{\alpha\beta} V_{\alpha\beta} \left| u_\alpha \right\rangle \left\langle u_\beta \right|$$

$A' \in \mathbb{A}$ also insists that

$$\sum_{\alpha\beta} u_{\alpha,i}^* u_{\beta,i} V_{\alpha\beta} = 0; \quad \forall 1 \leq i \leq N \tag{1}$$

Finally, we have proved that extremity of A is equivalent to (1) having no non-trivial (i.e. other than $V_{\alpha\beta} = 0$) solutions. Since this is a linear system with k^2 unknowns and N equations, we must at least have $k^2 \leq N$ or there WILL be nontrivial solutions. QED.

We just showed that A *could* be extreme only if $\text{rank}(\mathbb{I}+A) \leq \sqrt{N}$. Note that A *would* be extreme if the following $k \times k$ matrices are linearly independent. (w.r.t the field $\mathbb{C}$)

$$M^{(i)}_{\alpha\beta} \equiv u^*_{\alpha,i} u_{\beta,i} \qquad 1 \leq i \leq N$$

Let us finish with an extreme point in $\mathcal{A}_4$ that has $\text{rank}(\mathbb{I}+A) = 2$. Here it is

$$A = \begin{pmatrix} 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} & -i/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 & \frac{1-i}{2} \\ 1/\sqrt{2} & i/\sqrt{2} & \frac{1+i}{2} & 0 \end{pmatrix}$$

$$\mathbb{I}+A = 2\sum_{\alpha=1}^{2} \vec{u}_\alpha \vec{u}^\dagger_\alpha$$

with

$$\vec{u}_1 = \begin{pmatrix} 1/\sqrt{2} \\ 0 \\ 1/2 \\ 1/2 \end{pmatrix}; \quad \vec{u}_2 = \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ 1/2 \\ i/2 \end{pmatrix}$$

this *is* extreme because the following are linearly independent

$$M^{(1)} = 1/2 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}; \quad M^{(2)} = 1/2 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$M^{(3)} = 1/4 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}; \quad M^{(4)} = 1/4 \begin{pmatrix} 1 & i \\ -i & -1 \end{pmatrix}$$

Conjecture:

$$\forall\, 1 \leq k \leq \sqrt{N}\ \exists\, A \in \text{ext}(\mathcal{A}_N)\ \ s.t.\ \ \text{rank}(\mathbb{I}+A) = k$$

Remark: Note that the last counter example shows that not any $K > 0$ with $K_{ii} = 1$ may be written as

$$K_{ij} = \left\langle e^{i(\theta_i - \theta_j)} \right\rangle = \int d\mu(\vec{\theta}) e^{i(\theta_i - \theta_j)}$$

For some probability measure μ. In other words there are universal constraints on $K_{ij} = e^{i(\theta_i - \theta_j)}$ other than positivity and unit diagonal entries. Yet in other words

$$\begin{pmatrix} 1 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 1 & 1/\sqrt{2} & -i/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} & 1 & \frac{1-i}{2} \\ 1/\sqrt{2} & i/\sqrt{2} & \frac{1+i}{2} & 1 \end{pmatrix}$$

is not in the form $\left\langle e^{i(\theta_i - \theta_j)} \right\rangle$ for any distribution.