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ON THE TIGHTNESS OF THE PARTHASARATHY AND SCHMIDT RANK BOUNDS FOR EXTREMAL TRACIAL COUPLINGS

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ABSTRACT. Let $2 \leq a \leq b$ be positive integers, and let ρ_A, ρ_B be density operators on $\mathbb{C}^a, \mathbb{C}^b$, respectively. Let $\mathcal{C}(\rho_A, \rho_B)$ denote the set of bipartite couplings on $\mathbb{C}^a \otimes \mathbb{C}^b$ with marginals ρ_A and ρ_B. A result of Parthasarathy asserts that the rank of every extreme coupling is bounded above by $\mathrm{KRP}(a,b) := \lfloor \sqrt{a^2+b^2-1} \rfloor$, and it is not known for which dimension pairs (a,b) this bound is tight.

In this article, we restrict our attention to the tracial case, $\rho_A = I_a/a$, $\rho_B = I_b/b$. In the context of the Parthasarathy bound, we construct extreme couplings of rank r from pairs of finite unit-norm tight frames (FUNTFs) of length r in $\mathbb{C}^a$ and $\mathbb{C}^b$ which satisfy a transversality condition. As a consequence, we obtain an extreme coupling of rank b for every $2 \leq a < b$, whence the Parthasarathy bound is tight whenever $a < b$ and $b \geq (a^2-1)/2$; in particular, it is tight along the entire qubit-qudit line $(2,b)$, $b \geq 3$. This subsumes the two previously known tracial cases with $a < b$, namely, $(2,3)$ and $(3,4)$.

Using the Schmidt decomposition and the subadditivity of rank, we note that the rank of every tracial coupling (extreme or not) is bounded below by $\mathrm{ES}(a,b) := \lceil b/a \rceil$, which we refer to as the Schmidt bound. In the context of the Schmidt bound, we make use of sparse Kraus operators built from weighted partial permutation matrices. With $r := \mathrm{ES}(a,b)$, we construct an extreme coupling of rank r whenever $b-(r-1)a$ divides a. For $a < b \leq 2a$, where this condition reads $b - a = \gcd(a,b)$, we show that it is also necessary; in fact, when it fails, there is no tracial coupling of rank 2 at all, extreme or not. Furthermore, for $b > a(a-1)$, we show that the divisibility condition is superfluous and the Schmidt bound is attained for every such b. Thus, for each fixed a, the attainability of both bounds remains open for only finitely many $b \geq a$.

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1. Introduction

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be the finite-dimensional Hilbert spaces of two quantum systems, A and B, of dimensions a and b, respectively, with $2 \leq a \leq b$. A *density operator* on a finite-dimensional Hilbert space $\mathcal{H}$ is a positive semidefinite operator with unit trace, and is used to represent quantum states. We denote the set of all density operators on $\mathcal{H}$ by $\mathcal{D}(\mathcal{H})$. We identify $\mathcal{H}_A$ with $\mathbb{C}^a$ and $\mathcal{H}_B$ with $\mathbb{C}^b$, each equipped with the standard inner product.

Let $\rho_A \in \mathcal{D}(\mathbb{C}^a)$ and $\rho_B \in \mathcal{D}(\mathbb{C}^b)$ be density operators. The corresponding *coupling set* with the prescribed marginal states ρ_A and ρ_B is defined as

$$\mathcal{C}(\rho_A, \rho_B) = \left\{\rho \in \mathcal{D}(\mathbb{C}^a \otimes \mathbb{C}^b) : \mathrm{Tr}_B(\rho) = \rho_A,\ \mathrm{Tr}_A(\rho) = \rho_B\right\},$$

where Tr_A and Tr_B denote the partial traces over subsystems A, B, respectively.

The extremality criterion for couplings (for example, see Theorem 2.10) is rooted in Choi's characterization of extreme completely positive maps [Cho75], and was later adapted to this setting by Rudolph [Rud04] and Price–Sakai [PS07]. In [Par05, Corollary, p. 261], Parthasarathy proved that the rank of every extremal coupling, ρ, is bounded above by

$$\mathrm{rank}\,\rho \ \leq\ \mathrm{KRP}(a, b) := \left\lfloor \sqrt{a^2 + b^2 - 1} \right\rfloor, \tag{1}$$

and also established a slackness in the bound for the tracial two-qubit case, showing that every extremal tracial coupling in $\mathcal{C}(I_2/2, I_2/2)$ has rank $1 < \mathrm{KRP}(2, 2) = 2$ (see [Par05, Theorem 3.1]). Subsequently, in [Rud04], Rudolph raised the question of when this upper bound is attained.

In this article, we focus exclusively on the case of *tracial couplings*,

$$\mathcal{C}(I_a/a, I_b/b),$$

where both marginal states are the maximally mixed quantum states (tracial states) in $\mathcal{D}(\mathbb{C}^a)$ and $\mathcal{D}(\mathbb{C}^b)$, respectively. We denote the maximum rank attained by an extreme point of $\mathcal{C}(I_a/a, I_b/b)$, by $R_{\max}(a, b)$. We say that the pair (a, b) is *KRP-tight* if

$$R_{\max}(a, b) = \mathrm{KRP}(a, b),$$

meaning that the Parthasarathy upper bound is achieved by an extremal tracial coupling. We emphasize that the term KRP-tight is reserved for tracial marginals; when the bound is achieved by an extreme point of $\mathcal{C}(\rho_A, \rho_B)$ for some other pair of marginals, we simply say that the Parthasarathy bound is *attained* at (a, b).

Prior work on the attainment of the Parthasarathy bound may be divided into two kinds, namely, constructions of extremal tracial couplings, and constructions that achieve the bound only with non-tracial marginals. We briefly survey these results below.

In [Ohn10], Ohno computed $R_{\max}(3,3) = 4$ and $R_{\max}(4,4) = 5$ (see [Ohn10, Theorems 2.6 and 2.7]), and established the diagonal lower bound, $R_{\max}(a,a) \geq a$, for $a \geq 3$ (see [Ohn10, Theorem 2.8]). In [KS21], Kanmani and Satyanarayana settled the qubit-qutrit pair in the tracial setting by showing that $R_{\max}(2,3) = \mathrm{KRP}(2,3) = 3$. In [DDD26], Devendra, Dey, and Dey consider tensor products of known extreme points and check whether the result remains extreme in the appropriate dimension, which allows them to build new examples from Ohno's extreme points. In this manner, they have shown that the pairs $(5,5)$, $(9,9)$, and $(12,12)$, the amplified families $(5k,5k)$ with $3 \leq k \leq 14$, and the rectangular pair $(3,4)$ are KRP-tight. For the qubit-qudit family $(2,b)$ with $b \geq 4$, however, the Parthasarathy bound is attained in [DDD26] only after deforming the first marginal away from $I_2/2$, so that the construction is non-tracial except at $b = 3$, where it coincides with the tracial case. In [BR26], Bala and Rana have shown that the Parthasarathy bound is attained for the infinite rectangular family $(a, a+m)$ with $a \geq 3$ and $m > (a^2 - 2a - 2)/2$, for the qubit case $(2, 2+m)$ with $m \geq 1$, and for the single pair $(6,6)$. It is worth pointing out that in their rectangular families, these constructions have a non-tracial marginal when $m > 1$, and are tracial when $m = 1$.

A central role in our discussion is played by a marginal-normalized version, J_m, of the Choi–Jamiołkowski isomorphism (see Theorem 2.7). When ρ_A is invertible, J_m identifies a coupling $\rho \in \mathcal{C}(\rho_A, \rho_B)$ with a completely positive (CP) map $\Phi : M_a(\mathbb{C}) \to M_b(\mathbb{C})$ satisfying the marginal constraints, $\Phi^*(I_b) = I_a$, $\Phi(\rho_A^T) = \rho_B$. Under this identification, the extreme points of $\mathcal{C}(\rho_A, \rho_B)$ correspond to the extreme points of this set of CP maps, and the rank of ρ is equal to the Choi rank of Φ. In the tracial case, we have $J_m(\Phi) = \frac{1}{a} J(\Phi)$, where $J(\Phi)$ denotes the usual Choi matrix of Φ. If $K_1, \ldots, K_r$ are the Kraus operators in a minimal Kraus representation of Φ, then the marginal constraints take the form,

$$\sum_{i=1}^{r} K_i^* K_i = I_a, \qquad \sum_{i=1}^{r} K_i K_i^* = \frac{a}{b} I_b. \tag{2}$$

For most of this article, we find it convenient to work directly with Kraus operators rather than with couplings or Choi matrices. The simplest case to consider is that of an equal-weight, rank-one collection,

$$K_i = \sqrt{\frac{a}{r}}\, |v_i\rangle\langle u_i|,$$

with unit vectors $\{u_i\}_{i=1}^r \subset \mathbb{C}^a$ and $\{v_i\}_{i=1}^r \subset \mathbb{C}^b$; in this case, the constraints in (2) reduce to the defining identities for tight frames in $\mathbb{C}^a$ and $\mathbb{C}^b$.

Recall that a *finite unit-norm tight frame (FUNTF)* of length r in $\mathbb{C}^a$ is a collection of r unit vectors $\{u_i\}_{i=1}^r$ whose synthesis matrix U satisfies $UU^* = \frac{r}{a} I_a$. Such frames were introduced by Benedetto and Fickus [BF03]; their geometry has since been studied extensively (see [DS06, CMS17]) and they play an important role in signal processing.

Given a pair of FUNTFs, $\{u_i\}_{i=1}^r \subset \mathbb{C}^a$ and $\{v_i\}_{i=1}^r \subset \mathbb{C}^b$, of the same length r, we consider the bipartite state,

$$\rho := \frac{1}{r} \sum_{i=1}^{r} |\bar{u}_i\rangle\langle\bar{u}_i| \otimes |v_i\rangle\langle v_i|. \tag{3}$$

From the tight-frame identities, it immediately follows that $\mathrm{Tr}_B(\rho) = I_a/a$ and $\mathrm{Tr}_A(\rho) = I_b/b$, so that ρ is a tracial coupling.

In Theorem 3.2, we show that the question of whether ρ is an extremal tracial coupling of rank r is governed by the Gram matrices, G_U and G_V, of its constituent frames. More precisely, ρ is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ with $\operatorname{rank}\rho = r$ if and only if the linear map, $\Theta_{U,V} : M_r(\mathbb{C}) \to M_a(\mathbb{C}) \oplus M_b(\mathbb{C})$, given by

$$\Theta_{U,V}(X) := \Big(U(X^T \circ G_V)U^*,\ V(X \circ G_U)V^*\Big),$$

is injective; in fact, the injectivity of $\Theta_{U,V}$ already forces $\operatorname{rank}\rho = r$ (see Theorem 3.2-(i)).

We say that a pair of FUNTFs (U, V) is *transversal* if $\ker\Theta_{U,V} = \{0\}$. Thus our strategy for attaining the Parthasarathy bound at a given dimension pair (a, b) is to construct a transversal pair of FUNTFs of length $r = \mathrm{KRP}(a, b)$. The underlying linear-independence criterion (see Theorem 2.10) goes back to Choi, and has been applied via explicit vector constructions in [Ohn10, Rud04]. To the best of our knowledge, the reduction to a single transversality map between two tight frames is new.

In Theorem 4.1, for every $2 \le a < b$, we construct a transversal pair of FUNTFs of length b in $\mathbb{C}^a, \mathbb{C}^b$, which yields an extremal tracial coupling of rank b. Thus we have the lower bound, $R_{\max}(a, b) \ge b$ (see Corollary 4.2), which supplements Ohno's result (see [Ohn10, Theorem 2.8]). It immediately follows that the Parthasarathy bound is tight, that is, $R_{\max}(a, b) = \mathrm{KRP}(a, b) = b$, along the qubit-qudit line $(2, b)$, $b \ge 3$, and throughout the region, $a \ge 3$, $b \ge \frac{a^2-1}{2}$ (see Corollary 4.3). Note that this region subsumes the isolated known cases, such as the tracial $(3, 4)$ pair. Over the integers, our boundary condition, $b \ge \frac{a^2-1}{2}$, is equivalent to the bound $m > (a^2 - 2a - 2)/2$ of Bala and Rana [BR26]. For $m > 1$, their displayed construction has a non-tracial marginal, whereas for $m = 1$ it is already tracial; in contrast, our construction achieves extremality directly within the tracial setting throughout the stated region.

Unfortunately, for square dimension pairs in low dimensions, our rank-one construction runs into obstructions. From Proposition 4.4 and Corollary 4.9, it follows that there are no transversal pairs of FUNTFs of length $\mathrm{KRP}(a, a)$ for the pairs $(2, 2)$, $(3, 3)$, and $(4, 4)$. Nevertheless, from Ohno's results, we know that $(3, 3)$ and $(4, 4)$ are KRP-tight, which leaves $(2, 2)$ as the only dimension pair known to be **not** KRP-tight (see Theorem 2.12).

In Figure 1, we summarize the KRP-tight region established in this article. The pairs $(2, 2)$, $(3, 3)$, and $(4, 4)$, for which no transversal pair of FUNTFs of length $\mathrm{KRP}(a, a)$ exists, are also marked; recall that $(2, 2)$ is not KRP-tight, whereas $(3, 3)$ and $(4, 4)$ are KRP-tight by Ohno's constructions. For the sake of comparison, we also show the earlier results of Kanmani–Satyanarayana and Devendra–Dey–Dey that our work recovers or complements.

In view of the above discussion, we conjecture that a transversal pair of FUNTFs of length $\mathrm{KRP}(a, b)$ exists for every dimension pair (a, b) outside the set $\{(2, 2), (3, 3), (4, 4)\}$ (see Conjecture 6.1). In particular, echoing a similar question posed by Devendra, Dey, and Dey in [DDD26], we conjecture that $(2, 2)$ is the only dimension pair which is not KRP-tight (see Conjecture 6.2).

On another note, while the Parthasarathy bound limits the rank of an extremal coupling from above, in this article we also study a companion lower bound (see Theorem 2.3-(iii)). A straightforward application of the Schmidt decomposition and the subadditivity of rank shows that every tracial coupling ρ, extremal or not, satisfies $\operatorname{rank}\rho \ge \mathrm{ES}(a, b) := \lceil b/a \rceil$; we refer to this as the *Schmidt bound*. This naturally leads us to the following counterpart of Rudolph's question: For which dimension pairs is the Schmidt bound attained by an extremal tracial coupling?

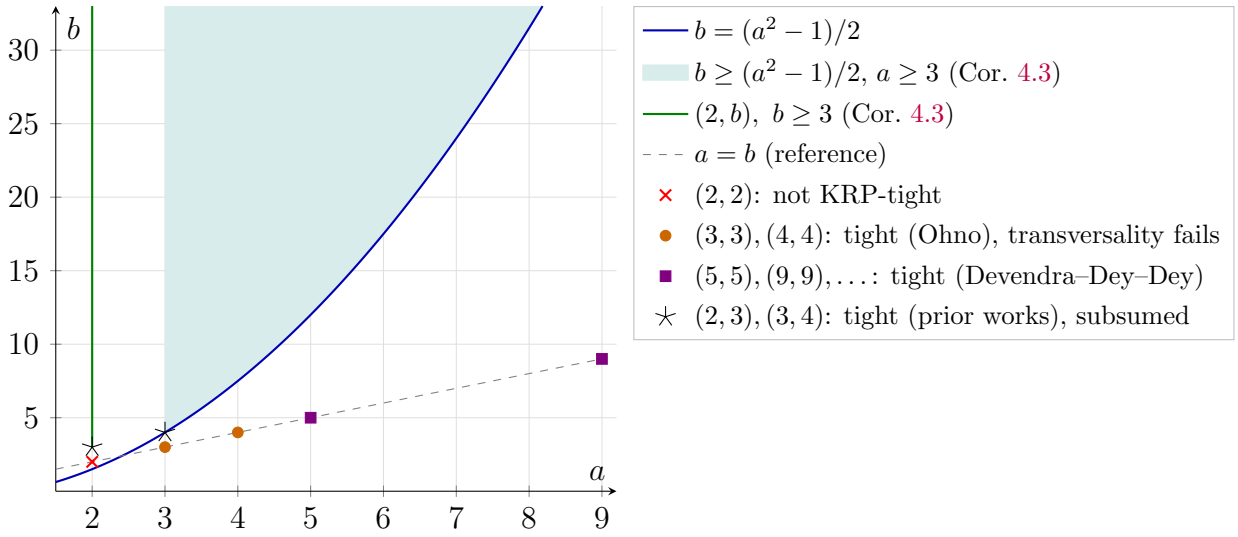


FIGURE 1. The dimension pairs (a, b) for which KRP-tightness is settled. In Corollary 4.3, we show that (a, b) is KRP-tight whenever $a < b$ and $b \geq (a^2-1)/2$. For $a \geq 3$, these are the pairs in the shaded region, which lies on or above the curve $b = (a^2-1)/2$. For $a = 2$, these are the qubit-qudit pairs $(2, b)$ with $b \geq 3$, shown by the vertical line at $a = 2$. In both cases the extreme points come from Theorem 4.1. The point $(2, 2)$ is not KRP-tight, while $(3, 3)$ and $(4, 4)$ are KRP-tight but cannot be realized by the equal-weight rank-one construction considered here. Square pairs resolved by Devendra–Dey–Dey are shown for context. The pairs $(2, 3)$ and $(3, 4)$, previously settled by Kanmani–Satyanarayana and Devendra–Dey–Dey respectively, lie on the boundaries of the regions resolved here.

We denote the minimum rank attained by an extreme point of $\mathcal{C}(I_a/a, I_b/b)$, by $R_{\min}(a, b)$. We say that the dimension pair (a, b) is *ES-tight* if

$$R_{\min}(a, b) = \mathrm{ES}(a, b),$$

meaning that the Schmidt lower bound is achieved by an extremal tracial coupling.

When a divides b, in Proposition 5.2 we obtain an extremal tracial coupling of rank $\mathrm{ES}(a, b) = \frac{b}{a}$, by taking as Kraus operators a family of $\frac{b}{a}$ partial isometries from $\mathbb{C}^a$ into $\mathbb{C}^b$ with mutually orthogonal ranges. For $a < b \leq 2a$, where $\mathrm{ES}(a, b) = 2$, we give a complete characterization in Theorem 5.13, by showing that the Schmidt bound is attained by an extreme point if and only if $b - a = \gcd(a, b)$. Thus, every consecutive pair $(a, a+1)$ attains the Schmidt bound, whereas a pair such as $(3, 5)$ does not. Interestingly, the obstruction has little to do with extremality; in Proposition 5.12, we show that when $b - a \neq \gcd(a, b)$, the set $\mathcal{C}(I_a/a, I_b/b)$ contains no coupling of rank 2 whatsoever, so that the Schmidt bound is not attained even by a non-extreme tracial coupling. More generally, with $r := \mathrm{ES}(a, b)$, in Theorem 5.10 we construct a collection of weighted partial permutation Kraus operators that attains the Schmidt bound whenever $b-(r-1)a$ divides a. This recovers the sufficiency part of the $r = 2$ characterization as a special case, and guarantees that for every $k \geq 2$, the window $(k-1)a < b < ka$ contains an integer b such that (a, b) is an ES-tight pair.

For $b > a(a-1)$, the divisibility hypothesis becomes superfluous. In fact, in Theorem 5.15, we show that the Schmidt bound is attained for every such b, via an explicit tight-frame construction. Thus, from Theorems 5.10 and 5.15, for each a there are only finitely many values of $b \geq a$ for which we do not know whether the Schmidt bound is attained. We describe these values in §6.

Our techniques for attaining the Schmidt bound in §5 are different from those used for the Parthasarathy bound in §3. In place of rank-one Kraus operators and tight frames, we use weighted partial permutation matrices and similar sparse operators. In each case, we prove extremality using the same lemma, which we call the isolation lemma (see Lemma 5.6).

Organisation. This article is organized as follows. In §2, we describe the coupling set as a compact convex set, and prove the Parthasarathy and Schmidt rank bounds, and the extremality criterion for tracial couplings. In §3, we introduce the tight-frame construction, and show that extremality is characterized by the injectivity of the linear map $\Theta_{U,V}$. With this criterion as the main tool, in §4 we construct a transversal pair of FUNTFs for every $a < b$; en route, we also note some obstructions to transversality for square dimension pairs. Finally, in §5, we turn our attention to the companion lower bound, namely, the Schmidt bound, where we obtain a complete characterization when $\mathrm{ES}(a, b) = 2$, and a general construction for higher values of $\mathrm{ES}(a, b)$.

1.1. **Notation.** Below we document the conventions and notation needed to follow the discussion in this article. For the reader's convenience, the notation that is used repeatedly is collected in Table 1.

Symbol	Definition
$M_a(\mathbb{C}), M_{a,b}(\mathbb{C})$	The space of $a \times a$, $a \times b$ complex matrices, respectively.
$\mathcal{C}(\rho_A, \rho_B)$	The coupling set; the space of all bipartite quantum states with marginals ρ_A and ρ_B.
$\mathrm{KRP}(a, b)$	Parthasarathy's KRP bound $\lfloor\sqrt{a^2+b^2-1}\rfloor$, an upper bound on the rank of an extreme coupling.
$R_{\max}(a, b)$	The maximal rank of an extreme point of $\mathcal{C}(I_a/a, I_b/b)$.
$CP(M_a(\mathbb{C}), M_b(\mathbb{C}))$	Completely positive maps from $M_a(\mathbb{C})$ to $M_b(\mathbb{C})$.
U, V	Synthesis matrices of Finite Unit-Norm Tight Frames (FUNTFs) in $\mathbb{C}^a$ and $\mathbb{C}^b$, respectively.
G_U, G_V	The Gram matrices of the frames U and V, given by U^*U and V^*V.
P_U, P_V	The scaled Gram projections, $P_U = \frac{a}{r}G_U$ and $P_V = \frac{b}{r}G_V$.
$\Theta_{U,V}$	The linear map $\Theta_{U,V} : M_r \to M_a \oplus M_b$ whose injectivity characterizes extremality at rank r (see Theorem 3.2).

TABLE 1. Notation used throughout this article.

A note on conventions. All of our inner products are conjugate-linear in the first argument and linear in the second (the Dirac convention), which is the standard convention in the quantum information literature. A vector is denoted interchangeably in ket form, such as $|e_k\rangle$, or in bare form, such as e_k. We use the ket form inside Dirac expressions (for example,

$|e_k\rangle\langle e_k|$), and the bare form when the vector appears as the argument of an operator in ordinary notation (for example, $K_i e_k$); it helps to keep in mind that both forms denote the same vector.

Our primary reference for background material on completely positive maps, the Choi–Jamiołkowski isomorphism, and vectorization is Watrous's *The Theory of Quantum Information* [Wat18], and we freely use the results therein. For notational convenience, our conventions differ from those of [Wat18] in one respect. In [Wat18], the vectorization of an operator $K \in L(X, Y)$ lies in $Y \otimes X$, and the Choi representation is defined using $\Phi \otimes \mathcal{I}$, so that $J(\Phi) \in L(Y \otimes X)$. In this article, the vectorization of a $b \times a$ matrix $K : \mathbb{C}^a \to \mathbb{C}^b$ lies in $\mathbb{C}^a \otimes \mathbb{C}^b$ (domain first, codomain second), and the Choi matrix is defined using $\mathcal{I} \otimes \Phi$, so that $J(\Phi) \in M_a(\mathbb{C}) \otimes M_b(\mathbb{C})$ for $\Phi : M_a(\mathbb{C}) \to M_b(\mathbb{C})$. This agrees with the order in which we write the coupling set $\mathcal{C}(\rho_A, \rho_B)$ and the subsystems $\mathbb{C}^a, \mathbb{C}^b$. Thus, whenever we cite a result from [Wat18], the two tensor factors must be interchanged; this does not affect the mathematical content.

2. The coupling set and its convex geometry

In this section, we document some basic results about the coupling set, viewed as a compact convex set, which are needed to follow the discussion in this article. In Lemma 2.2, we give a criterion for a coupling to be an extreme point, and use it to prove the Parthasarathy bound in Theorem 2.3, where we also prove the Schmidt bound. In Theorem 2.10, we give a second criterion for extremality, for tracial couplings, in terms of Kraus operators. Finally, in Theorem 2.12, we show that the qubit-qubit pair is not KRP-tight.

2.1. The Parthasarathy and Schmidt rank bounds.

Below we give a linear-algebraic formulation for the extreme points of $\mathcal{C}(\rho_A, \rho_B)$, which leads to the Parthasarathy bound. Let Herm_n denote the real vector space of Hermitian $n \times n$ matrices, so that $\dim_{\mathbb{R}} \mathrm{Herm}_n = n^2$. Let $2 \le a \le b$ be the dimensions of the two subsystems. We denote the combined marginal map by

$$\Lambda : \mathrm{Herm}_{ab} \longrightarrow \mathrm{Herm}_a \times \mathrm{Herm}_b, \qquad \Lambda(X) := (\mathrm{Tr}_B X,\ \mathrm{Tr}_A X).$$

In this language, note that $\mathcal{C}(\rho_A, \rho_B) = \{X \in \mathrm{Herm}_{ab} : X \succeq 0,\ \Lambda(X) = (\rho_A, \rho_B)\}$ is the intersection of the closed convex cone of positive semidefinite matrices with an affine subspace, and hence is closed and convex. Since every $X \succeq 0$ with $\mathrm{Tr}\, X = 1$ has operator norm at most 1, it is also bounded. Thus $\mathcal{C}(\rho_A, \rho_B)$ is a compact convex set.

Proposition 2.1. *The image of Λ is equal to the hyperplane*

$$\big\{(P, Q) \in \mathrm{Herm}_a \times \mathrm{Herm}_b : \mathrm{Tr}\, P = \mathrm{Tr}\, Q\big\} \ \subset\ \mathrm{Herm}_a \times \mathrm{Herm}_b,$$

which has real dimension $a^2 + b^2 - 1$.

Proof. For any $H \in \mathrm{Herm}_{ab}$, we have $\mathrm{Tr}(\mathrm{Tr}_B H) = \mathrm{Tr}\, H = \mathrm{Tr}(\mathrm{Tr}_A H)$, so that $\Lambda(H) = (\mathrm{Tr}_B H, \mathrm{Tr}_A H)$ lies in the hyperplane. Hence $\mathrm{range}\,\Lambda$ is contained in the hyperplane.

Recall the partial-trace identities $\mathrm{Tr}_B(H_A \otimes H_B) = \mathrm{Tr}(H_B)\, H_A$ and $\mathrm{Tr}_A(H_A \otimes H_B) = \mathrm{Tr}(H_A)\, H_B$. Let $(P, Q) \in \mathrm{Herm}_a \times \mathrm{Herm}_b$ with $\mathrm{Tr}\, P = \mathrm{Tr}\, Q$, and set

$$H_{AB} := P \otimes \frac{I_b}{b} + \frac{I_a}{a} \otimes Q - \mathrm{Tr}(P)\, \frac{I_a}{a} \otimes \frac{I_b}{b}.$$

Using $\mathrm{Tr}(Q) = \mathrm{Tr}(P)$, we see that,

$$\mathrm{Tr}_B(H_{AB}) = P + \mathrm{Tr}(Q)\,\frac{I_a}{a} - \mathrm{Tr}(P)\,\frac{I_a}{a} = P.$$

Similarly, $\mathrm{Tr}_A(H_{AB}) = Q$. Thus $\Lambda(H_{AB}) = (P, Q)$, and we conclude that range Λ is equal to the hyperplane. Note that this hyperplane is the kernel of the non-zero linear functional, $(P, Q) \mapsto \mathrm{Tr}(P) - \mathrm{Tr}(Q)$, on $\mathrm{Herm}_a \times \mathrm{Herm}_b$, and hence has real dimension $a^2 + b^2 - 1$. □

For a complex subspace $W \subseteq \mathbb{C}^{ab}$, we define,

$$\mathrm{Herm}(W) := \{H \in \mathrm{Herm}_{ab} : \mathrm{range}\, H \subseteq W\}.$$

Note that this is a real vector space of dimension $(\dim_{\mathbb{C}} W)^2$, since it is the space of self-adjoint maps from W to itself. With this notation, we have the following characterization of extremality.

Lemma 2.2. *A coupling $X \in \mathcal{C}(\rho_A, \rho_B)$ is extreme if and only if*

$$\ker \Lambda \cap \mathrm{Herm}(\mathrm{range}\, X) = \{0\}.$$

Proof. Suppose that $\ker \Lambda \cap \mathrm{Herm}(\mathrm{range}\, X) = \{0\}$ and $X = \frac{1}{2}(Y_1 + Y_2)$ with $Y_1, Y_2 \in \mathcal{C}(\rho_A, \rho_B)$. Let $\xi \in \ker(X)$, so that $\langle X\xi, \xi\rangle = 0$. The positivity of Y_1, Y_2 forces $\langle Y_i\xi, \xi\rangle = 0$ as well, so $\ker(X) \subseteq \ker(Y_i)$ which implies $\mathrm{range}\, Y_i \subseteq \mathrm{range}\, X$, for $i = 1, 2$. Thus $Y_1, Y_2 \in \mathrm{Herm}(\mathrm{range}\, X)$. Hence $Y_1 - X \in \ker \Lambda \cap \mathrm{Herm}(\mathrm{range}\, X)$ which implies that $Y_1 = X = Y_2$. We conclude that X is an extreme point of $\mathcal{C}(\rho_A, \rho_B)$.

Conversely, let $H \neq 0$ be an element of $\ker \Lambda \cap \mathrm{Herm}(\mathrm{range}\, X)$. Since $\mathrm{range}\, H \subseteq \mathrm{range}\, X$, for all sufficiently small $\varepsilon > 0$ both $X + \varepsilon H$ and $X - \varepsilon H$ are positive semidefinite and satisfy $\Lambda(X \pm \varepsilon H) = \Lambda(X) = (\rho_A, \rho_B)$. In other words, $X \pm \varepsilon H \in \mathcal{C}(\rho_A, \rho_B)$. Thus, X being the midpoint of $X - \varepsilon H, X + \varepsilon H$, is not an extreme point of $\mathcal{C}(\rho_A, \rho_B)$. □

We are now in a position to give a conceptual proof of the Parthasarathy upper bound for the ranks of extremal couplings, which is different from the original proof due to Parthasarathy.

Theorem 2.3. *Let $a \leq b$ be positive integers, and $\rho_A \in \mathcal{D}(\mathbb{C}^a), \rho_B \in \mathcal{D}(\mathbb{C}^b)$ be states. Then the following assertions hold:*

(i) For any $\rho \in \mathcal{C}(\rho_A, \rho_B)$, $\mathrm{rank}\, \rho \leq (\mathrm{rank}\, \rho_A)(\mathrm{rank}\, \rho_B)$.

(ii) (cf. [Par05, Corollary, p. 261]) If ρ is an extreme point of $\mathcal{C}(\rho_A, \rho_B)$, then

$$\mathrm{rank}\, \rho \;\leq \left\lfloor \sqrt{a^2 + b^2 - 1} \right\rfloor.$$

(iii) For every $\rho \in \mathcal{C}(\rho_A, \rho_B)$,

$$\mathrm{rank}\, \rho \;\geq\; \left\lceil \frac{\mathrm{rank}\, \rho_B}{a} \right\rceil.$$

In particular, if ρ is a tracial coupling, then

$$\mathrm{rank}\, \rho \geq \left\lceil \frac{b}{a} \right\rceil.$$

Proof. (i) Let P_A, P_B be the orthogonal projections onto $\mathrm{range}(\rho_A), \mathrm{range}(\rho_B)$, respectively, and let $P := P_A \otimes P_B$. Let $\xi \in \mathbb{C}^a$ be any vector orthogonal to $\mathrm{range}(\rho_A)$. Since $\mathrm{Tr}_B(\rho) = \rho_A$ and $\langle \xi | \rho_A | \xi \rangle = 0$, we have $\langle \xi \otimes \eta | \rho | \xi \otimes \eta \rangle = 0$ for every $\eta \in \mathbb{C}^b$; as $\rho \succeq 0$, this forces $\rho(|\xi\rangle \otimes |\eta\rangle) = 0$ for every $\eta \in \mathbb{C}^b$. Using $\mathrm{Tr}_A(\rho) = \rho_B$, by the same argument we have $\rho(|\xi\rangle \otimes |\eta\rangle) = 0$ for every $\xi \in \mathbb{C}^a$ and every $\eta \in \mathbb{C}^b$ orthogonal to $\mathrm{range}(\rho_B)$. (When

ρ_A or ρ_B is invertible, as is the case for tracial couplings, the corresponding assertion is vacuous.) Since the vectors of the above two kinds span the orthogonal complement of $\operatorname{range}(P) = \operatorname{range}(\rho_A) \otimes \operatorname{range}(\rho_B)$, we get $\rho = \rho P$, and taking adjoints, $\rho = P\rho P$, whence

$$\operatorname{rank}\rho \leq \dim \operatorname{range}(P) = \dim\big(\operatorname{range}(\rho_A) \otimes \operatorname{range}(\rho_B)\big) = (\operatorname{rank}\rho_A)(\operatorname{rank}\rho_B).$$

(ii) Let $W := \operatorname{range}\rho$. From Lemma 2.2, we observe that $\Lambda|_{\mathrm{Herm}(W)}$ is injective. Since its domain, $\mathrm{Herm}(W)$, has real dimension $\dim_{\mathbb{C}}(W)^2 = (\operatorname{rank}\rho)^2 = r^2$ and its codomain has real dimension $a^2 + b^2 - 1$, we obtain the bound,

$$r^2 \leq a^2 + b^2 - 1.$$

(iii) Let $\rho = \sum_{i=1}^{r} p_i |\psi_i\rangle\langle\psi_i|$ be the spectral decomposition of ρ with $r = \operatorname{rank}\rho$ and $p_i > 0$ for $1 \leq i \leq r$. Taking the partial trace over A, we get

$$\rho_B = \sum_{i=1}^{r} p_i \operatorname{Tr}_A\big(|\psi_i\rangle\langle\psi_i|\big).$$

For every $1 \leq i \leq r$, the reduced state $\operatorname{Tr}_A(|\psi_i\rangle\langle\psi_i|)$ is the marginal of a pure state, whence its rank is bounded above by a (see [Wat18, Theorem 2.10]). Using the subadditivity of rank, we have

$$\operatorname{rank}\rho_B \;\leq\; \sum_{i=1}^{r} \operatorname{rank}\big(\operatorname{Tr}_A(|\psi_i\rangle\langle\psi_i|)\big) \;\leq\; ra,$$

so that $r \geq (\operatorname{rank}\rho_B)/a$. Since r is an integer, we get the desired bound. Finally, when ρ is a tracial coupling, $\rho_B = I_b/b$ has rank b, and we get $\operatorname{rank}\rho \geq \lceil b/a \rceil$. □

In the rest of this article, we restrict our attention to the tracial case, that is, $\rho_A = \frac{1}{a} I_a, \rho_B = \frac{1}{b} I_b$.

Definition 2.4. Let $2 \leq a \leq b$ be positive integers. Motivated by the theorem above, we define

$$\mathrm{KRP}(a,b) := \lfloor \sqrt{a^2 + b^2 - 1} \rfloor, \qquad \mathrm{ES}(a,b) := \left\lceil \frac{b}{a} \right\rceil,$$

named after the initials of K. R. Parthasarathy and E. Schmidt, respectively.

Definition 2.5. Let $2 \leq a \leq b$ be positive integers. We denote the maximum (minimum, respectively) of the ranks of extremal tracial couplings in $\mathcal{C}(I_a/a, I_b/b)$ by $R_{\max}(a,b), R_{\min}(a,b)$, respectively. We call the dimension pair (a,b) *KRP-tight* (*ES-tight*, respectively) if $R_{\max}(a,b) = \mathrm{KRP}(a,b), (R_{\min}(a,b) = \mathrm{ES}(a,b))$, respectively.

2.2. **The Choi–Jamiołkowski correspondence and the extremality criterion.**

2.2.1. *Vectorization.* For a linear operator $K : \mathbb{C}^a \to \mathbb{C}^b$, we define its *vectorization* as,

$$\operatorname{vec}(K) := (I_a \otimes K)|\eta\rangle \;\in\; \mathbb{C}^a \otimes \mathbb{C}^b,$$

where $|\eta\rangle := \sum_{j=1}^{a} |e_j\rangle \otimes |e_j\rangle \in \mathbb{C}^a \otimes \mathbb{C}^a$. Specializing to the rank-one case, for $u \in \mathbb{C}^a, v \in \mathbb{C}^b$, we get,

$$\operatorname{vec}\big(|v\rangle\langle u|\big) = |\bar{u}\rangle \otimes |v\rangle. \tag{4}$$

2.2.2. *The Choi matrix and the Choi–Kraus correspondence.* For a linear map $\Phi : M_a(\mathbb{C}) \to M_b(\mathbb{C})$, we define its *Choi matrix* as,

$$J(\Phi) := (\mathcal{I} \otimes \Phi)(|\eta\rangle\langle\eta|) \in M_a(\mathbb{C}) \otimes M_b(\mathbb{C}),$$

where as above $|\eta\rangle = \sum_{j=1}^{a} |e_j\rangle \otimes |e_j\rangle$.

The following result of Choi [Cho75] (see [Wat18, Theorem 2.22]) relates complete positivity, positivity of the Choi matrix, and the Kraus representation, and helps us define the notion of Choi rank.

Theorem 2.6 (Choi–Kraus correspondence)**.** *Let $\Phi : M_a(\mathbb{C}) \to M_b(\mathbb{C})$ be a linear map. Then the following are equivalent:*

(a) Φ is completely positive.
(b) $J(\Phi) \succeq 0$.
(c) (Kraus representation) $\Phi(X) = \sum_{i=1}^{r} K_i X K_i^*$ for some $r \geq 1$ and $K_i : \mathbb{C}^a \to \mathbb{C}^b$.

Moreover, $J : B\left(M_a(\mathbb{C}), M_b(\mathbb{C})\right) \to M_a(\mathbb{C}) \otimes M_b(\mathbb{C})$ is a linear bijection, restricting to a bijection between the completely positive maps $M_a(\mathbb{C}) \to M_b(\mathbb{C})$ and $\{Z \in M_a(\mathbb{C}) \otimes M_b(\mathbb{C}) : Z \succeq 0\}$. For a CP map Φ, the minimal number of terms r in a Kraus decomposition as in (c) equals rank $J(\Phi)$*; this common value is called the* Choi rank *of Φ, denoted $CR(\Phi)$, and any minimal Kraus decomposition $\{K_i\}_{i=1}^{CR(\Phi)}$ has $\{|\mathrm{vec}(K_i)\rangle\}$ a basis for* range $J(\Phi)$ *(and, a fortiori, linearly independent).*

If Φ has the Kraus form, $\Phi(X) = \sum_{i=1}^{r} K_i X K_i^*$ with $K_i : \mathbb{C}^a \to \mathbb{C}^b$, then

$$J(\Phi) = \sum_{i=1}^{r} |\mathrm{vec}(K_i)\rangle\langle\mathrm{vec}(K_i)|. \tag{5}$$

Thus a Kraus decomposition of Φ corresponds to a decomposition of $J(\Phi)$ into rank-one positive semidefinite pieces, $|\mathrm{vec}(K_i)\rangle\langle\mathrm{vec}(K_i)|$, with each non-zero Kraus operator recovered (up to a global phase) as $K_i = \sqrt{\lambda_i}\ \mathrm{unvec}(v_i)$, where λ_i is the non-zero eigenvalue of the i-th piece and v_i is a corresponding unit eigenvector.

Theorem 2.7 ([DDD26, Proposition 2.7])**.** *Let $\rho_A \in \mathcal{D}(\mathbb{C}^a)$ be invertible and let $\rho_B \in \mathcal{D}(\mathbb{C}^b)$. Let $J : B\left(M_a(\mathbb{C}), M_b(\mathbb{C})\right) \to M_a(\mathbb{C}) \otimes M_b(\mathbb{C})$ denote the Choi–Jamiołkowski map, and define*

$$J_m(\Phi) := (\rho_A^{1/2} \otimes I_b)\, J(\Phi)\, (\rho_A^{1/2} \otimes I_b).$$

Then we have the following:

(i) $J_m^{-1}\big(\mathcal{C}(\rho_A, \rho_B)\big) = \big\{\Phi \in CP\left(M_a(\mathbb{C}), M_b(\mathbb{C})\right) :\ \Phi^*(I_b) = I_a,\ \Phi(\rho_A^T) = \rho_B\big\}$, and this is a compact convex set.
(ii) For $\rho \in \mathcal{C}(\rho_A, \rho_B)$, ρ is an extreme point of $\mathcal{C}(\rho_A, \rho_B)$ if and only if $J_m^{-1}(\rho)$ is an extreme point of $J_m^{-1}(\mathcal{C}(\rho_A, \rho_B))$.
(iii) For every $\Phi \in CP(M_a(\mathbb{C}), M_b(\mathbb{C}))$, $\mathrm{rank}(J_m(\Phi)) = \mathrm{rank}(J(\Phi)) = CR(\Phi)$, the Choi rank of Φ.

Proof. (i) Since ρ_A is invertible, $\rho_A^{1/2} \otimes I_b$ is invertible, whence J_m, being a composition of J with conjugation by an invertible operator, is also a linear bijection. For $\Phi \in B\left(M_a(\mathbb{C}), M_b(\mathbb{C})\right)$, note that,

$$J_m(\Phi) = \sum_{i,j=1}^{a} (\rho_A^{1/2}|e_i\rangle\langle e_j|\rho_A^{1/2}) \otimes \Phi(|e_i\rangle\langle e_j|)$$

Below we compute the marginals of $J_m(\Phi)$.

$$\begin{aligned}
\mathrm{Tr}_A(J_m(\Phi)) &= \sum_{i,j=1}^{a} \mathrm{Tr}(\rho_A^{1/2}|e_i\rangle\langle e_j|\rho_A^{1/2})\Phi(|e_i\rangle\langle e_j|) = \sum_{i,j=1}^{a} \langle e_j|\rho_A|e_i\rangle\Phi(|e_i\rangle\langle e_j|) \\
&= \sum_{i,j=1}^{a} (\rho_A^T)_{ij}\Phi(|e_i\rangle\langle e_j|) = \Phi(\rho_A^T), \\
\mathrm{Tr}_B(J_m(\Phi)) &= \sum_{i,j=1}^{a} \rho_A^{1/2}|e_i\rangle\langle e_j|\rho_A^{1/2}\ \mathrm{Tr}\left(\Phi(|e_i\rangle\langle e_j|)\right) \\
&= \rho_A^{1/2}\Big(\sum_{i,j=1}^{a} \mathrm{Tr}\left(\Phi^*(I_b)|e_i\rangle\langle e_j|\right)|e_i\rangle\langle e_j|\Big)\rho_A^{1/2} \\
&= \rho_A^{1/2}(\Phi^*(I_b))^T\rho_A^{1/2}.
\end{aligned}$$

Thus, $J_m\big(\{\Phi \in CP\,(M_a(\mathbb{C}), M_b(\mathbb{C})) :\ \Phi^*(I_b) = I_a,\ \Phi(\rho_A^T) = \rho_B\}\big) = \mathcal{C}(\rho_A, \rho_B)$.

Since $\mathcal{C}(\rho_A, \rho_B)$ is compact and convex (§2.1) and J_m^{-1} is a linear bijection, $J_m^{-1}(\mathcal{C}(\rho_A, \rho_B))$ is compact and convex.

(ii) This follows from the general fact that an affine bijection carries extreme points to extreme points.

(iii) Since $\rho_A^{1/2} \otimes I$ is invertible, we have $\mathrm{rank}(J_m(\Phi)) = \mathrm{rank}(J(\Phi)) = CR(\Phi)$. □

Remark 2.8. For tracial marginals, note that J_m identifies the coupling set with the set of trace-preserving CP maps Φ satisfying $\Phi(I_a/a) = I_b/b$, and expresses a coupling as $\rho = \frac{1}{a}\sum_i |\mathrm{vec}(K_i)\rangle\langle\mathrm{vec}(K_i)|$. One may equally well normalize by the other marginal, as is done with the standard Choi matrix of a unital map (see [Rud04, DDD26]). Writing $\rho = \frac{1}{b}\sum_i |\mathrm{vec}(L_i)\rangle\langle\mathrm{vec}(L_i)|$, the marginal constraints take the form,

$$\sum_i L_i L_i^* = I_b, \qquad \sum_i L_i^* L_i = \frac{b}{a} I_a.$$

Clearly, the two descriptions differ only by the rescaling, $L_i = \sqrt{b/a}\, K_i$. In particular, for the rank-one tuples $c\,|v_i\rangle\langle u_i|$ considered in §3, both descriptions lead to the same pair of FUNTF identities, $\sum_i |u_i\rangle\langle u_i| = \frac{r}{a} I_a$ and $\sum_i |v_i\rangle\langle v_i| = \frac{r}{b} I_b$, with $c = \sqrt{a/r}$ in the trace-preserving normalization and $c = \sqrt{b/r}$ in the unital one. Throughout this article, we work with J_m, so that the maps Φ are trace-preserving and the constant is $c = \sqrt{a/r}$.

Remark 2.9. Specializing Theorem 2.7 to the tracial case, we observe that the marginal constraints in terms of the Kraus representation, $\Phi(X) = \sum_{i=1}^{r} K_i X K_i^*$, are precisely the constraints in (2) noted in the introduction, namely,

$$\sum_{i=1}^{r} K_i^* K_i = I_a, \qquad \sum_{i=1}^{r} K_i K_i^* = \frac{a}{b} I_b.$$

Below we give a proof of the extremality criterion for tracial couplings. A more general form of the theorem is proved in [Rud04] using a somewhat different approach.

Theorem 2.10 (cf. [Rud04, Theorem 1])**.** *Consider the compact convex set*

$$\mathcal{A} := \{\Phi \in CP\,(M_a(\mathbb{C}), M_b(\mathbb{C})) : \Phi^*(I_b) = I_a,\ \Phi(I_a/a) = I_b/b\}\,,$$

where Φ^* denotes the adjoint of Φ with respect to the Hilbert–Schmidt inner product $\langle A, B\rangle_{HS} = \mathrm{Tr}(A^*B)$ (see [Wat18, Ch. 2]). Let $\Phi \in \mathcal{A}$ have minimal Kraus representation $\Phi(X) = \sum_{i=1}^r K_i X K_i^*$, where $K_i : \mathbb{C}^a \to \mathbb{C}^b$. Define the linear map $\Gamma\colon M_r(\mathbb{C}) \to M_a(\mathbb{C}) \oplus M_b(\mathbb{C})$ by

$$\Gamma(X) = \Big(\sum_{i,j=1}^r x_{ij} K_j^* K_i,\ \sum_{i,j=1}^r x_{ij} K_i K_j^* \Big). \tag{6}$$

Then Φ is an extreme point of $\mathcal{A}$ if and only if $\ker \Gamma = \{0\}$.

Proof. For a Hermitian matrix $Y = (y_{ij}) \in M_r(\mathbb{C})$, let $\Psi_Y(\cdot) := \sum_{i,j=1}^r y_{ij} K_i(\cdot) K_j^*$, so that $\Psi_{I_r} = \Phi$. A straightforward computation of the Hilbert–Schmidt adjoint tells us that $\Psi_Y^*(Z) = \sum_{i,j=1}^r y_{ij} K_j^* Z K_i$ (using $\bar{y}_{ij} = y_{ji}$), whence

$$\Gamma(Y) = \big(\Psi_Y^*(I_b),\ \Psi_Y(I_a)\big). \tag{7}$$

In particular, note that

$$\Gamma(I_r) = (\Phi^*(I_b), \Phi(I_a)) = \left(I_a, \frac{a}{b} I_b\right),$$

encodes precisely the two conditions defining $\mathcal{A}$.

($\ker \Gamma \neq \{0\} \implies$ Non-extreme). Let $0 \neq X \in \ker \Gamma$. Since $\Gamma(X^*) = \Gamma(X)^*$ by (6), $\ker \Gamma$ is closed under taking adjoints. Thus, without loss of generality, we may assume that X is Hermitian, by replacing X with $X + X^*$ or $i(X - X^*)$ if necessary. Let $\varepsilon > 0$ be small enough so that $X_\pm := I_r \pm \varepsilon X \succ 0$, and let $S_\pm := \sqrt{X_\pm}$. Writing $(X_\pm)_{ij} = \sum_{l=1}^r (S_\pm)_{il} \overline{(S_\pm)_{jl}}$ and substituting into $\Psi_{X_\pm}$, we get the Kraus form,

$$\Psi_{X_\pm}(Y) = \sum_{l=1}^r \tilde{K}_l^\pm Y (\tilde{K}_l^\pm)^*, \qquad \tilde{K}_l^\pm := \sum_{i=1}^r (S_\pm)_{il} K_i,$$

so that $\Psi_\pm := \Psi_{X_\pm}$ is a CP map. By linearity, $\Gamma(X_\pm) = \Gamma(I_r) \pm \varepsilon \Gamma(X) = \Gamma(I_r)$. Since $X_\pm$ is Hermitian, from (7) we have $\big(\Psi_\pm^*(I_b), \Psi_\pm(I_a)\big) = (\Phi^*(I_b), \Phi(I_a)) = \big(I_a, \frac{a}{b} I_b\big)$; thus $\Psi_\pm \in \mathcal{A}$.

Since $X_+ + X_- = 2I_r$, we have $\Psi_+ + \Psi_- = 2\Psi_{I_r} = 2\Phi$, so that $\Phi = \frac{1}{2}(\Psi_+ + \Psi_-)$. Note that the map $C \mapsto \sum_{i,j=1}^r c_{ij} |\mathrm{vec}(K_i)\rangle\langle \mathrm{vec}(K_j)|$ from $M_r(\mathbb{C})$ to $M_{ab}(\mathbb{C})$ is injective, as the r vectorizations $|\mathrm{vec}(K_i)\rangle$ are linearly independent by the minimality of the Kraus decomposition. Since $X_+ \neq I_r$, it follows that $J(\Psi_+) \neq J(\Phi)$, that is, $\Psi_+ \neq \Phi$. Hence $\Phi = \frac{1}{2}(\Psi_+ + \Psi_-)$ is a non-trivial convex combination in $\mathcal{A}$, and we conclude that Φ is not an extreme point of $\mathcal{A}$.

(Non-extreme $\implies \ker \Gamma \neq \{0\}$). Suppose $\Phi = \frac{1}{2}(\Psi_+ + \Psi_-)$, with $\Psi_\pm \in \mathcal{A}$ and $\Psi_+ \neq \Phi$.

At the level of Choi matrices, $J(\Psi_-) \succeq 0$ implies that $J(\Psi_+) = 2J(\Phi) - J(\Psi_-) \preceq 2J(\Phi)$, whence $\mathrm{range}\, J(\Psi_+) \subseteq \mathrm{range}\, J(\Phi)$. Since the minimal Kraus operators of Φ form a basis for $\mathrm{range}\, J(\Phi) = \mathrm{span}\{|\mathrm{vec}(K_i)\rangle : 1 \le i \le r\}$, $J(\Psi_+)$ is supported within this subspace and, being Hermitian, may be expanded in this basis with a Hermitian coefficient matrix $X \in M_r(\mathbb{C})$:

$$J(\Psi_+) = \sum_{i,j=1}^r x_{ij} |\mathrm{vec}(K_i)\rangle\langle \mathrm{vec}(K_j)| \qquad \implies \qquad \Psi_+ = \Psi_X.$$

Since X is Hermitian, (7) applies at $Y = X$ and at $Y = I_r$, giving

$$\Gamma(X) = \big(\Psi_+^*(I_b),\ \Psi_+(I_a)\big), \qquad \Gamma(I_r) = \big(\Phi^*(I_b),\ \Phi(I_a)\big).$$

Since $\Psi_+, \Phi \in \mathcal{A}$, we note that $\Gamma(X) = \Gamma(I_r) = \left(I_a, \frac{a}{b} I_b\right)$, that is, $\Gamma(X - I_r) = 0$. Since $\Psi_+ \neq \Phi$, we have $X \neq I_r$, and thus $X - I_r$ is a non-zero element of $\ker \Gamma$. □

In §5, we shall only need to verify that the second component of Γ is injective. In the corollary below, we note the relevant consequence of Theorem 2.10; it is worth pointing out that the minimality of the Kraus representation is not presupposed.

Corollary 2.11. *Let $K_1, \ldots, K_r : \mathbb{C}^a \to \mathbb{C}^b$ satisfy the tracial marginal constraints (2). If the operators $\{K_i K_j^*\}_{1 \leq i,j \leq r}$ are linearly independent, then $K_1, \ldots, K_r$ are linearly independent, and the state*

$$\rho = \frac{1}{a} \sum_{i=1}^{r} |\mathrm{vec}(K_i)\rangle\langle \mathrm{vec}(K_i)|$$

is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ of rank r.

Proof. Let $t_1, \ldots, t_r$ be scalars such that $\sum_{i=1}^r t_i K_i = 0$. Then $\sum_{i=1}^r t_i K_i K_1^* = 0$, and from the linear independence of $\{K_i K_j^*\}$, it follows that $t_1 = \cdots = t_r = 0$. Thus $K_1, \ldots, K_r$ are linearly independent. Let $\Phi(X) := \sum_{i=1}^r K_i X K_i^*$. From (5), we observe that $J(\Phi)$ has rank r, so that $\{K_i\}_{i=1}^r$ is a minimal Kraus representation of Φ (see Theorem 2.6); moreover, from (2), Φ lies in the set $\mathcal{A}$ of Theorem 2.10. Note that the linear independence of $\{K_i K_j^*\}$ is precisely the assertion that the second component of Γ in (6) is injective. Thus $\ker \Gamma = \{0\}$, and Φ is an extreme point of $\mathcal{A}$. By Theorem 2.7, we conclude that $\rho = J_m(\Phi) = \frac{1}{a} J(\Phi)$ is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ of rank r. □

2.3. **The qubit-qubit pair.** With the Choi–Jamiołkowski correspondence at our disposal, we note below the only dimension pair for which the Parthasarathy bound is known to be **not** attained by an extremal tracial coupling.

Theorem 2.12. *$R_{\max}(2,2) = 1 < 2 = \mathrm{KRP}(2,2)$, that is, every extremal tracial coupling in the qubit-qubit case has rank 1.*

Proof. From Theorem 2.7 with $\rho_A = \rho_B = I_2/2$, we observe that the extreme points of $\mathcal{C}(I_2/2, I_2/2)$ correspond to the extreme points of the set of unital trace-preserving CP maps on $M_2(\mathbb{C})$ (that is, unital qubit channels), with the rank of a coupling being equal to the Choi rank of the corresponding map. It is well-known that every unital qubit channel is a convex combination of unitary conjugations (see [BPS93, LS93] and Remark 2.13). Hence every extreme point of the set of unital qubit channels is a unitary conjugation, which has Choi rank 1; the corresponding coupling is a maximally entangled pure state. □

Remark 2.13 (The Birkhoff property for qubit channels). The fact used in the proof of Theorem 2.12, namely that every unital trace-preserving qubit channel is a convex combination of unitary conjugations, is a Birkhoff-type theorem for doubly stochastic maps on $M_2(\mathbb{C})$ with an interesting history. The result was proved by Bhat, Pati and Sunder in 1993 [BPS93], and independently by Landau and Streater [LS93] in the same year. It appears to have been anticipated earlier by Tregub [Tre86]. The corresponding statement fails in dimensions $d \geq 3$. Kümmerer and Maassen [KM87] had exhibited extreme points of the set of unital channels on M_d, $d \geq 3$, that are not unitary conjugations. Consequently, the argument used in the proof of Theorem 2.12 does not extend beyond qubits; in fact, its conclusion already fails at $(3,3)$, where $R_{\max}(3,3) = 4 = \mathrm{KRP}(3,3)$ by Ohno's result [Ohn10]. For completeness, we note that a more direct proof of Theorem 2.12 was given by Parthasarathy [Par05].

Remark 2.14. The pair $(2,2)$ is, to our knowledge, the only pair known to be non-KRP-tight.

3. Construction of extremal tracial couplings using tight frames

In §2, we noted that Theorem 2.10 reduces extremality of tracial couplings to a linear-algebraic condition on the associated Kraus operators K_i. In this section, we pursue the simplest possible strategy of building extremal tracial couplings using linearly independent rank-one Kraus operators of the form $K_i = \sqrt{a/r}\,|v_i\rangle\langle u_i|$, with $\{u_i\}$ in $\mathbb{C}^a$ and $\{v_i\}$ in $\mathbb{C}^b$ being tight frames of the same length r. The marginal constraints are automatically satisfied on account of tightness. Thus the condition $\ker\Gamma = \{0\}$ of Theorem 2.10 reduces to the injectivity of an explicit linear map, $\Theta_{U,V}$, which depends only on the two frames.

3.1. **Frames.** Below we recall some basic definitions and facts about frames in $\mathbb{C}^a$. A sequence of vectors, $\{u_i\}_{i=1}^r$, in $\mathbb{C}^a$ is said to be a *frame* if there are constants $0 < A \le B < \infty$ such that

$$A\|x\|^2 \le \sum_{i=1}^{r} |\langle u_i, x\rangle|^2 \le B\|x\|^2 \qquad (x \in \mathbb{C}^a).$$

A frame is said to be *tight* if the above inequalities hold with $A = B$, or equivalently, if $\sum_{i=1}^r |u_i\rangle\langle u_i| = A\, I_a$. A tight frame is said to be a *finite unit-norm tight frame* (FUNTF) if $\|u_i\| = 1$ for all $1 \le i \le r$. Let $\{u_i\}_{i=1}^r$ be a FUNTF in $\mathbb{C}^a$. Taking the trace on both sides of the above identity, we get $A = r/a$. Thus we have the reconstruction formula,

$$x = \frac{a}{r}\sum_{i=1}^{r} \langle u_i, x\rangle\, u_i \qquad \text{for all } x \in \mathbb{C}^a.$$

It is well-known that there is a FUNTF of length r in $\mathbb{C}^a$ for every $r \ge a$ (for instance, see Lemma 5.14). Because of the unit-norm and tightness conditions, the state that we construct below from a pair of FUNTFs has maximally mixed marginals (see Theorem 3.1-(i)).

It is convenient to work with matrices. For a frame $\{u_i\}_{i=1}^r \subset \mathbb{C}^a$, the matrix $U \in \mathbb{C}^{a\times r}$ whose columns are the frame vectors $u_1, \ldots, u_r$ is called its *synthesis matrix*; note that $Uc = \sum_{i=1}^r c_i u_i$ for $c \in \mathbb{C}^r$. Below we list four objects associated with U that we use in this article.

- **Analysis operator** $U^* : \mathbb{C}^a \to \mathbb{C}^r$, which is the adjoint of U, and maps x to its sequence of coefficients $(\langle u_i, x\rangle)_{i=1}^r$.
- **Frame operator** $UU^* \in \mathbb{C}^{a\times a}$: tightness reads $UU^* = \frac{r}{a} I_a$.
- **Gram matrix** $G_U = U^*U \in \mathbb{C}^{r\times r}$, recording the pairwise inner products $(G_U)_{ij} = \langle u_i, u_j\rangle$. For a FUNTF, its diagonal entries are all 1.
- **Spectrum of** G_U: since G_U shares its non-zero eigenvalues with UU^*, a tight FUNTF has $\mathrm{sp}(G_U) = \{r/a \text{ (multiplicity } a),\ 0 \text{ (multiplicity } r-a)\}$.

For a second FUNTF, $\{v_i\}_{i=1}^r \subset \mathbb{C}^b$, of the same length r, we use similar notation, with synthesis matrix $V \in \mathbb{C}^{b\times r}$ and Gram matrix $G_V = V^*V$.

3.2. **The rank-one tuple and its extremality criterion.** With a pair of FUNTFs U, V of length r, we associate the equal-weight, rank-one Kraus tuple,

$$K_i = \sqrt{\frac{a}{r}}\,|v_i\rangle\langle u_i|, \qquad i = 1, \ldots, r. \tag{8}$$

The specific coefficient, $\sqrt{a/r}$, is dictated by the trace-preserving constraint, $\sum K_i^* K_i = I_a$, under the J_m correspondence (see Remark 2.8).

Note that $|\mathrm{vec}(K_i)\rangle = \sqrt{a/r}\,|\bar{u}_i\rangle \otimes |v_i\rangle$, and

$$|\mathrm{vec}(K_i)\rangle\langle\mathrm{vec}(K_i)| = \frac{a}{r}(|\bar{u}_i\rangle \otimes |v_i\rangle)(\langle\bar{u}_i| \otimes \langle v_i|) = \frac{a}{r}\,|\bar{u}_i\rangle\langle\bar{u}_i| \otimes |v_i\rangle\langle v_i|.$$

Consider the quantum channel given by $\Phi(X) = \sum_{i=1}^r K_i X K_i^*$. It is straightforward to verify that Φ satisfies the tracial marginal constraints in (2). Indeed, by tightness, we have $\sum_{i=1}^r |u_i\rangle\langle u_i| = \frac{r}{a} I_a$ and $\sum_{i=1}^r |v_i\rangle\langle v_i| = \frac{r}{b} I_b$. Since $K_i^* = \sqrt{a/r}\,|u_i\rangle\langle v_i|$ and $\|v_i\| = \|u_i\| = 1$, we observe that

$$K_i^* K_i = \frac{a}{r}\,\|v_i\|^2 |u_i\rangle\langle u_i| = \frac{a}{r}|u_i\rangle\langle u_i|, \qquad \sum_{i=1}^r K_i^* K_i = \frac{a}{r}\cdot\frac{r}{a} I_a = I_a,$$

$$K_i K_i^* = \frac{a}{r}\,\|u_i\|^2 |v_i\rangle\langle v_i| = \frac{a}{r}|v_i\rangle\langle v_i|, \qquad \sum_{i=1}^r K_i K_i^* = \frac{a}{r}\cdot\frac{r}{b} I_b = \frac{a}{b} I_b.$$

Using (5), we observe that the (normalized) Choi state of the quantum channel is

$$\rho := J_m(\Phi) = \frac{1}{a} J(\Phi) = \frac{1}{a}\sum_{i=1}^r |\mathrm{vec}(K_i)\rangle\langle\mathrm{vec}(K_i)| = \frac{1}{r}\sum_{i=1}^r |\bar{u}_i\rangle\langle\bar{u}_i| \otimes |v_i\rangle\langle v_i|. \tag{9}$$

Theorem 3.1. *Let $\{u_i\}_{i=1}^r \subset \mathbb{C}^a$ and $\{v_i\}_{i=1}^r \subset \mathbb{C}^b$ be finite unit-norm tight frames (FUNTFs) of the same length r, and let ρ be the state defined in (9),*

$$\frac{1}{r}\sum_{i=1}^r |\bar{u}_i\rangle\langle\bar{u}_i| \otimes |v_i\rangle\langle v_i|.$$

Then we have the following:

(i) $\rho \in \mathcal{C}(I_a/a, I_b/b)$.
(ii) $\operatorname{rank}\rho = \operatorname{rank}(\overline{G_U} \circ G_V)$, *where G_U and G_V are the Gram matrices of the frames.*
(iii) $\operatorname{rank}\rho = r$ *if and only if the product vectors $\bar{u}_i \otimes v_i$ are linearly independent.*

Proof. (i) Tracing out the second subsystem, we get

$$\mathrm{Tr}_B\,\rho = \frac{1}{r}\sum_{i=1}^r |\bar{u}_i\rangle\langle\bar{u}_i|\,\|v_i\|^2 = \frac{1}{r}\sum_{i=1}^r |\bar{u}_i\rangle\langle\bar{u}_i| = \frac{I_a}{a},$$

where we have used $\|v_i\| = 1$ and the tightness of $\{u_i\}$, that is, $\sum_{i=1}^r |u_i\rangle\langle u_i| = \frac{r}{a} I_a$. Similarly, tracing out the first subsystem, we get

$$\mathrm{Tr}_A\,\rho = \frac{1}{r}\sum_{i=1}^r \|\bar{u}_i\|^2\,|v_i\rangle\langle v_i| = \frac{1}{r}\sum_{i=1}^r |v_i\rangle\langle v_i| = \frac{I_b}{b},$$

where we have used $\|\bar{u}_i\| = \|u_i\| = 1$ and the tightness of $\{v_i\}$, that is, $\sum_{i=1}^r |v_i\rangle\langle v_i| = \frac{r}{b} I_b$. Hence $\rho \in \mathcal{C}(I_a/a, I_b/b)$.

(ii) Let $|w_i\rangle = |\bar{u}_i\rangle \otimes |v_i\rangle$ and let W be the matrix with columns $|w_1\rangle, \ldots, |w_r\rangle$, so that $\rho = \frac{1}{r} W W^*$ and $\operatorname{rank}\rho = \operatorname{rank}(W^*W)$. The matrix W^*W has entries

$$(W^*W)_{ij} = \langle w_i, w_j\rangle = \langle\bar{u}_i, \bar{u}_j\rangle\langle v_i, v_j\rangle = \overline{(G_U)_{ij}}\,(G_V)_{ij},$$

that is, $W^*W = \overline{G_U} \circ G_V$. Thus $\operatorname{rank}\rho = \operatorname{rank}(\overline{G_U} \circ G_V)$.

(iii) From the proof of part (ii), we observe that $\operatorname{rank}\rho = \operatorname{rank} W$ is equal to the dimension of the span of the r vectors $|w_i\rangle$, which is r if and only if they are linearly independent. □

The extremality of ρ depends on the inner products within the two frames, and in the theorem below, we make this dependence precise. Throughout, $\circ$ denotes the Hadamard (entrywise) product on $M_r(\mathbb{C})$.

Theorem 3.2 (Transversality criterion)**.** *Let $\{u_i\}_{i=1}^r \subset \mathbb{C}^a$ and $\{v_i\}_{i=1}^r \subset \mathbb{C}^b$ be FUNTFs of the same length r, with synthesis matrices U, V, and let*

$$\rho := \frac{1}{r}\sum_{i=1}^{r} |\bar{u}_i\rangle\langle\bar{u}_i| \otimes |v_i\rangle\langle v_i|$$

be the corresponding state, as in Theorem 3.1. Let $\Theta_{U,V} : M_r(\mathbb{C}) \to M_a(\mathbb{C}) \oplus M_b(\mathbb{C})$ be the linear map given by

$$\Theta_{U,V}(X) := \Big(U\,(X^T \circ G_V)\,U^*,\ V\,(X \circ G_U)\,V^*\Big).$$

Then the following assertions hold:

(i) If $\Theta_{U,V}$ is injective, then the product vectors $\bar{u}_i \otimes v_i$ are linearly independent, and consequently $\operatorname{rank}\rho = r$.

(ii) $\Theta_{U,V}$ is injective, that is, $\ker\Theta_{U,V} = \{0\}$, if and only if ρ is an extreme point of the coupling set $\mathcal{C}(I_a/a, I_b/b)$ and $\operatorname{rank}\rho = r$.

Proof. Let Γ be the mapping defined as in (6) of Theorem 2.10, using the tuple $K_1, \ldots, K_r$ of (8). Note that the formula for Γ makes sense for any Kraus tuple, and minimality is needed only for the conclusion of Theorem 2.10. To begin with, we express $\Theta_{U,V}$ in terms of Γ. Since $\frac{r}{a}K_j^*K_i = \langle v_j, v_i\rangle |u_j\rangle\langle u_i| = (G_V)_{ji}\,|u_j\rangle\langle u_i|$, and $x_{ij}(G_V)_{ji}$ is the (j,i)-th entry of $X^T \circ G_V$, we have

$$\frac{r}{a}\sum_{i,j=1}^{r} x_{ij}K_j^*K_i = \sum_{i,j=1}^{r} x_{ij}(G_V)_{ji}\,|u_j\rangle\langle u_i| = U(X^T \circ G_V)U^*.$$

Similarly, since $\frac{r}{a}K_iK_j^* = (G_U)_{ij}\,|v_i\rangle\langle v_j|$, and $x_{ij}(G_U)_{ij}$ is the (i,j)-th entry of $X \circ G_U$, we have

$$\frac{r}{a}\sum_{i,j=1}^{r} x_{ij}K_iK_j^* = V(X \circ G_U)V^*.$$

Comparing with (6), we observe that

$$\Theta_{U,V} = \frac{r}{a}\,\Gamma. \tag{10}$$

In particular, $\ker\Theta_{U,V} = \ker\Gamma$.

Proof of (i). Let $\Theta_{U,V}$ be injective, and let $c_1, \ldots, c_r \in \mathbb{C}$ be scalars such that $\sum_{i=1}^r c_iK_i = 0$; we write $c := (c_1, \ldots, c_r) \in \mathbb{C}^r$. Let $\{e_k\}_{k=1}^r$ be the standard basis of $\mathbb{C}^r$. For $1 \le k \le r$, let $X := |c\rangle\langle e_k|$, that is, $x_{ij} = c_i\delta_{jk}$. Then,

$$\sum_{i,j=1}^{r} x_{ij}K_j^*K_i = K_k^*\Big(\sum_{i=1}^{r} c_iK_i\Big) = 0, \qquad \sum_{i,j=1}^{r} x_{ij}K_iK_j^* = \Big(\sum_{i=1}^{r} c_iK_i\Big)K_k^* = 0,$$

so that $\Gamma(X) = 0$ by (6), and hence $\Theta_{U,V}(X) = 0$ by (10). Since $\Theta_{U,V}$ is injective, we have $X = 0$, whence $c = 0$. Thus the Kraus operators $K_1, \ldots, K_r$ are linearly independent. Since vectorization is a linear isomorphism which maps K_i to $\sqrt{a/r}\,\bar{u}_i \otimes v_i$, the product vectors $\bar{u}_i \otimes v_i$ are linearly independent, and from Theorem 3.1-(iii), we conclude that $\operatorname{rank}\rho = r$.

Proof of (ii). Let $\Phi(X) = \sum_{i=1}^{r} K_i X K_i^*$, so that $\rho = J_m(\Phi)$ by (9). From the computation preceding (9), note that Φ lies in the set $\mathcal{A}$ of Theorem 2.10.

To begin with, let us assume that $\Theta_{U,V}$ is injective. By part (i), $\operatorname{rank}\rho = r$ and $K_1, \dots, K_r$ are linearly independent, so that they form a minimal Kraus representation of Φ (see Theorem 2.6). Thus Theorem 2.10 is applicable to this representation, and from (10), we have $\ker\Gamma = \{0\}$. Hence Φ is an extreme point of $\mathcal{A}$, and by Theorem 2.7-(ii), we conclude that ρ is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$.

Conversely, let us assume that ρ is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ with $\operatorname{rank}\rho = r$. By Theorem 3.1-(iii), the product vectors $\bar{u}_i \otimes v_i$, and hence the operators K_i, are linearly independent, so that $K_1, \dots, K_r$ is again a minimal Kraus representation of Φ. Since ρ is extreme, Φ is an extreme point of $\mathcal{A}$, and from Theorem 2.10 we have $\ker\Gamma = \{0\}$. By (10), we conclude that $\Theta_{U,V}$ is injective. □

Definition 3.3 (Transversal pair)**.** A pair of FUNTFs U, V of the same length is said to be *transversal* if $\ker\Theta_{U,V} = \{0\}$.

Remark 3.4. We emphasize that the rank condition in Theorem 3.2-(ii) cannot be dropped. Let (U, V) be a transversal pair of length r, and let ρ be the corresponding state. Consider the synthesis matrices $U' := [\,U \;\; U\,]$ and $V' := [\,V \;\; V\,]$, obtained by repeating every frame vector. Then U', V' are FUNTFs of length $2r$, and the state corresponding to the pair (U', V') is again ρ. Note that ρ is an extreme point of rank r. Since $r < 2r$, from Theorem 3.2-(i), it follows that $\Theta_{U',V'}$ is **not** injective. In the rest of this article, we only use the fact that a transversal pair of length r gives an extreme point of rank r.

From Theorem 3.2, if there is a transversal pair of length r, then there is an extreme point of rank r in $\mathcal{C}(I_a/a, I_b/b)$. Thus, in order to show that a dimension pair (a, b) is KRP-tight, it suffices to find a transversal pair of length $r = \mathrm{KRP}(a, b)$.

Remark 3.5. It is worth pointing out that the rank-one, equal-weight form of the K_i's is a restriction that we impose; it is not forced by extremality, and we do not expect it to yield every KRP-tight state. For instance, Ohno's extreme points at $(3, 3)$ and $(4, 4)$ are built from Kraus operators of rank greater than one, and in Corollary 4.9 below, we show that no equal-weight rank-one tuple attains the Parthasarathy bound at these two pairs. We do not know whether rank-one Kraus operators with unequal weights can achieve this (see §6). The advantage of the restricted form is that extremality translates to the injectivity of the explicit map $\Theta_{U,V}$.

3.3. **The projection formulation.** The kernel of $\Theta_{U,V}$ admits a description in terms of two orthogonal projections, namely, the scaled Gram matrices,

$$P_U := \frac{a}{r} G_U, \qquad P_V := \frac{b}{r} G_V. \tag{11}$$

We refer to P_U, P_V as the *scaled Gram projections*; note that they are the orthogonal projections onto $\operatorname{range}(U^*), \operatorname{range}(V^*)$, respectively.

Lemma 3.6. *The matrices P_U and P_V are orthogonal projections satisfying:*

$$\operatorname{rank} P_U = a, \qquad \operatorname{rank} P_V = b, \qquad (P_U)_{ii} = \frac{a}{r}, \qquad (P_V)_{ii} = \frac{b}{r} \quad \text{for all } i.$$

Proof. Since U is a tight frame, its frame operator is given by $UU^* = \frac{r}{a} I_a$, whence

$$P_U^2 = \left(\frac{a}{r}\right)^2 U^*(UU^*)U = \left(\frac{a}{r}\right)^2 \frac{r}{a} U^*U = P_U.$$

Since G_U is Hermitian, we have $P_U = P_U^*$, so that P_U is an orthogonal projection. Note that the rank of P_U is a as U has full row rank, and its diagonal entries are equal to $\frac{a}{r}$ as the columns of U have unit norm. A similar argument applies to P_V. □

Lemma 3.7. *For $X \in M_r(\mathbb{C})$, $\Theta_{U,V}(X) = 0$ if and only if*

$$P_U(X^T \circ P_V)P_U = 0 \qquad \text{and} \qquad P_V(X \circ P_U)P_V = 0. \tag{12}$$

Consequently, transversality depends on the two scaled Gram projections P_U and P_V relative to the standard coordinate basis used for the Hadamard product.

Proof. Since the global scalar factors $\frac{a}{r}$ and $\frac{b}{r}$ do not alter the kernel, it suffices to show that for any matrix $A \in M_r(\mathbb{C})$, $VAV^* = 0$ is equivalent to $P_V A P_V = 0$, and that $UAU^* = 0$ is equivalent to $P_U A P_U = 0$. The assertion in (12) then follows from the definition of $\Theta_{U,V}$, by applying the first equivalence with $A = X \circ G_U$ and the second with $A = X^T \circ G_V$.

Since

$$VV^* = \frac{r}{b} I_b \quad \text{and} \quad UU^* = \frac{r}{a} I_a,$$

we have

$$VAV^* = 0 \Longrightarrow V^*VAV^*V = 0 \Longrightarrow P_V A P_V = 0$$

and

$$P_V A P_V = 0 \Longrightarrow V^*VAV^*V = 0 \Longrightarrow V(V^*VAV^*V)V^* = 0 \Longrightarrow VAV^* = 0,$$

which proves the first equivalence. By an identical argument, with U, P_U in place of V, P_V, we have $UAU^* = 0 \iff P_U A P_U = 0$. □

4. Tightness of the Parthasarathy rank bound

Our main goal in this section is to construct an extremal tracial coupling of rank b for every $a < b$, thereby establishing KRP-tightness in the region $b \geq (a^2 - 1)/2$ and along the qubit-qudit line $(2, b)$, $b \geq 3$. On the other hand, for frames of length $a + 1$ in $\mathbb{C}^a$, we show that the transversality map $\Theta_{U,V}$ always has non-trivial kernel, which obstructs our construction at the pairs $(3, 3)$ and $(4, 4)$.

4.1. **Extremal tracial couplings of rank b for $a < b$.** When the common length of the pair of FUNTFs is equal to b, note that the second frame is square, and a square FUNTF is unitary; in particular, $G_V = I_b$. In this case, the second component of $\Theta_{U,V}$ is given by $X \mapsto V(X \circ G_U)V^*$. Since conjugation by the unitary V is a bijection, this component is injective if and only if the mapping $X \mapsto X \circ G_U$ is injective, that is, if and only if G_U has no zero entries. Clearly, the injectivity of one component suffices for the injectivity of $\Theta_{U,V}$, and without loss of generality, we may assume that $V = I_b$. Thus it suffices to find a FUNTF U of length b in $\mathbb{C}^a$ whose Gram matrix has no zero entries. For every $2 \leq a < b$, we construct such a U as follows: we start with one fixed vector, together with $b - 1$ vectors at an equal angle to it, which are obtained from one another by rotating within its orthogonal complement via the $(b - 1)$-th roots of unity.

Theorem 4.1. *For every dimension pair (a, b) satisfying $2 \le a < b$, there exists a transversal pair of FUNTFs of length b in $\mathbb{C}^a$ and $\mathbb{C}^b$. Consequently, there is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ of rank b.*

Proof. Let $V = I_b$, which is a square unitary FUNTF, so that $G_V = I_b$ and $\Theta_{U,V}(X) = (U \operatorname{diag}(X) U^*,\ X \circ G_U)$. Note that the second component, $X \mapsto X \circ G_U$ on $M_b(\mathbb{C})$, is injective if and only if $G_U = U^*U$ has no zero entries, and the injectivity of the second component implies the injectivity of Θ_{U,I_b}. In fact, the converse is also true, though we do not need it here. Indeed, since the diagonal entries of G_U are equal to 1, if $X \circ G_U = 0$, then the diagonal entries of X are zero, so that the first component, $U \operatorname{diag}(X) U^*$, is also zero. Hence (U, I_b) is transversal if and only if G_U has no zero entries. Thus it suffices to construct a FUNTF $U \in \mathbb{C}^{a\times b}$ such that every entry of its Gram matrix is non-zero.

Let $\{|e_k\rangle\}_{k=0}^{a-1}$ denote the standard basis of $\mathbb{C}^a$, and let

$$\alpha = \frac{b-a}{a(b-1)}, \qquad \beta = \frac{b(a-1)}{a(b-1)}.$$

Note that $\alpha, \beta \in (0,1)$ as $2 \le a < b$, and $\alpha + \beta = 1$. Let $\zeta := e^{2\pi i/(b-1)}$, which is a primitive $(b-1)$-th root of unity. For $0 \le j \le b-2$, we define the unit vector $|w_j\rangle$ in $\operatorname{span}\{|e_1\rangle, \dots, |e_{a-1}\rangle\}$ by

$$|w_j\rangle = \frac{1}{\sqrt{a-1}} \sum_{k=1}^{a-1} \zeta^{kj} |e_k\rangle.$$

We define the b columns of U as follows,

$$|u_0\rangle = |e_0\rangle, \qquad |u_j\rangle = \sqrt{\alpha}\,|e_0\rangle + \sqrt{\beta}\,|w_{j-1}\rangle, \quad j = 1, \dots, b-1.$$

Since $\langle w_{j-1}|w_{j-1}\rangle = 1$ and $\alpha + \beta = 1$, clearly $|u_j\rangle$ is a unit vector for every $0 \le j \le b-1$.

Below we compute the matrix entries of $UU^* = |u_0\rangle\langle u_0| + \sum_{j=1}^{b-1} |u_j\rangle\langle u_j|$ relative to the standard basis. For $k, k' \in \{1, \dots, a-1\}$, we have

$$\langle e_k|UU^*|e_{k'}\rangle = \beta \sum_{j=1}^{b-1} \langle e_k|w_{j-1}\rangle\langle w_{j-1}|e_{k'}\rangle = \frac{\beta}{a-1} \sum_{m=0}^{b-2} \zeta^{(k-k')m} = \frac{\beta(b-1)}{a-1}\,\delta_{k,k'} = \frac{b}{a}\,\delta_{k,k'},$$

where we have re-indexed with $m = j-1$, and used the fact that $\zeta^{k-k'} \ne 1$ for $0 < |k-k'| \le a-2 < b-1$. For the off-diagonal entries involving $|e_0\rangle$ and $|e_k\rangle$ with $k \ge 1$, we have

$$\langle e_0|UU^*|e_k\rangle = \sqrt{\alpha\beta} \sum_{j=1}^{b-1} \langle w_{j-1}|e_k\rangle = \frac{\sqrt{\alpha\beta}}{\sqrt{a-1}} \sum_{m=0}^{b-2} \zeta^{-km} = 0,$$

since $\zeta^{-k} \ne 1$ as $1 \le k \le a-1 < b-1$. Finally,

$$\langle e_0|UU^*|e_0\rangle = 1 + (b-1)\alpha = \frac{b}{a}.$$

Thus $UU^* = \frac{b}{a} I_a$, and we conclude that U is a FUNTF of b vectors in $\mathbb{C}^a$.

Note that

$$\langle u_0|u_j\rangle = \sqrt{\alpha} \ne 0 \qquad \text{for every } j \ge 1.$$

For $1 \le j < j' \le b-1$, let $d := j' - j$ so that $1 \le d \le b-2$, and let $S(d) = \sum_{k=1}^{a-1} \zeta^{kd}$. Then

$$\langle u_j|u_{j'}\rangle = \alpha + \beta\,\langle w_{j-1}|w_{j'-1}\rangle = \alpha + \beta\,\frac{S(d)}{a-1}.$$

Since $S(d)$ is a sum of roots of unity, it is an algebraic integer. If the inner product $\langle u_j|u_{j'}\rangle$ were zero, we would have $S(d) = -(a-1)\alpha/\beta = -(b-a)/b$, which is rational but not an integer (as $0 < b-a < b$). Since a rational algebraic integer is necessarily an integer (see [DF03, Section 15.3, Proposition 28]), this is not possible. Hence $\langle u_j|u_{j'}\rangle \neq 0$ for all $j \neq j'$. Thus G_U has no zero entries, whence $\ker \Theta_{U,I_b} = \{0\}$, and (U, I_b) is a transversal pair of length b. By Theorem 3.2, we conclude that the corresponding state is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ of rank b. □

Corollary 4.2. *For $2 \leq a < b$, we have $R_{\max}(a,b) \geq b$. This supplements Ohno's result that $R_{\max}(a,a) \geq a$ for $a \geq 3$.*

Corollary 4.3. *If $2 \leq a < b$ and $\frac{a^2-1}{2} \leq b$, then $R_{\max}(a,b) = \mathrm{KRP}(a,b) = b$.*

Proof. Since $b \geq \frac{1}{2}(a^2-1)$, we have $b^2 \leq a^2 + b^2 - 1 < (b+1)^2$. Hence $\mathrm{KRP}(a,b) = \lfloor \sqrt{a^2+b^2-1} \rfloor = b$. By Theorem 4.1, there is an extreme coupling of rank b, so that $R_{\max}(a,b) = b$. In particular, the Parthasarathy bound is tight for the following pairs,

$$(2,b),\ b \geq 3; \qquad (3,b),\ b \geq 4; \qquad (4,b),\ b \geq 8; \qquad (5,b),\ b \geq 12. \qquad \square$$

4.2. **Some obstructions to transversality.**

Proposition 4.4. *For every pair of FUNTFs U, V of length a in $\mathbb{C}^a$, $\ker \Theta_{U,V}$ consists of the matrices with zeroes on the diagonal. Thus,*

$$\dim_{\mathbb{C}}(\ker \Theta_{U,V}) = a^2 - a.$$

Proof. Since U and V are FUNTFs of length $r = a$, their square synthesis matrices satisfy $UU^* = I_a$ and $VV^* = I_a$. Thus U and V are unitary matrices, whence $G_U = G_V = I_a$.

For any $X \in M_a(\mathbb{C})$, note that $X \circ I_a = X^T \circ I_a = \mathrm{diag}(X)$, so that the transversality map reduces to,

$$\Theta_{U,V}(X) = \Big(U\,(X^T \circ G_V)\,U^*,\ V\,(X \circ G_U)\,V^*\Big) = \Big(U\,\mathrm{diag}(X)U^*,\ V\,\mathrm{diag}(X)V^*\Big).$$

Since U and V are invertible, $\Theta_{U,V}(X) = 0$ if and only if $\mathrm{diag}(X) = 0$. We conclude that the kernel of $\Theta_{U,V}$ is the subspace of matrices with zeroes on the main diagonal, which has complex dimension $a^2 - a$. □

The failure at $(2,2)$ may be explained by the fact that there are no extreme points of rank 2 in $\mathcal{C}(I_2/2, I_2/2)$ at all, let alone one obtained from a transversal pair of FUNTFs. The cases of $(3,3)$ and $(4,4)$ are of a different nature, and rely on the following elementary facts about rank-one projections.

Lemma 4.5. *Let Q be a rank-one orthogonal projection on $\mathbb{C}^r$ all of whose diagonal entries are equal. Then every diagonal entry of Q is equal to $1/r$, and there is a vector $g \in \mathbb{C}^r$ with $|g_i| = 1$ for every $1 \leq i \leq r$, such that $Q = \frac{1}{r}|g\rangle\langle g|$.*

Proof. Since Q is a rank-one orthogonal projection, there is a unit vector $w \in \mathbb{C}^r$ such that $Q = |w\rangle\langle w|$. Note that the diagonal entries of Q are $|w_1|^2, \ldots, |w_r|^2$, and their sum is $\langle w|w\rangle = 1$. Since they are all equal, we have $|w_i|^2 = 1/r$ for every $1 \leq i \leq r$. Let $g := \sqrt{r}\,w$. Then $Q = \frac{1}{r}|g\rangle\langle g|$, and $|g_i|^2 = r|w_i|^2 = 1$ for every $1 \leq i \leq r$. □

Let U, V be FUNTFs of length $r = a + 1$ in $\mathbb{C}^a$. Note that the scaled Gram projections P_U, P_V (see Lemma 3.6) have rank $a = r-1$ and constant diagonal a/r, so that $I_r - P_U, I_r - P_V$ are rank-one orthogonal projections with constant diagonal. By Lemma 4.5, we have

$$I_r - P_U = \tfrac{1}{r}|g\rangle\langle g|, \qquad I_r - P_V = \tfrac{1}{r}|h\rangle\langle h|,$$

for some $g, h \in \mathbb{C}^r$ with unit-modulus entries (the Naimark complements of U, V, respectively). In order to rule out a transversal pair, it suffices to exhibit a non-zero element of $\ker \Theta_{U,V}$, which is our next goal.

By Lemma 3.7, with $P_U = I_r - \frac{1}{r}|g\rangle\langle g|$ and $P_V = I_r - \frac{1}{r}|h\rangle\langle h|$ as above, we seek a non-zero matrix $X \in M_r(\mathbb{C})$ such that

$$P_U(X^T \circ P_V)P_U = 0 \qquad \text{and} \qquad P_V(X \circ P_U)P_V = 0.$$

In the lemma below, we describe the solutions for X in either condition.

Lemma 4.6. *Let $P = I - \frac{1}{r}|h\rangle\langle h|$ be the orthogonal projection onto $(\operatorname{span}\{|h\rangle\})^\perp$ for a vector $h \in \mathbb{C}^r$ with $\langle h|h\rangle = r$. For any matrix $A \in M_r(\mathbb{C})$,*

$$PAP = 0 \quad \iff \quad A = |h\rangle\langle x| + |y\rangle\langle h| \text{ for some } x, y \in \mathbb{C}^r.$$

Proof. If $A = |h\rangle\langle x| + |y\rangle\langle h|$, then $PAP = (P|h\rangle)\langle x|P + P|y\rangle(\langle h|P) = 0$ since $P|h\rangle = 0$ and $\langle h|P = 0$. Conversely, if $PAP = 0$, the range of AP lies entirely in $\ker P = \operatorname{span}\{|h\rangle\}$. Thus, $AP = |h\rangle\langle \tilde{x}|$ for some vector $\tilde{x} \in \mathbb{C}^r$. Decomposing A via the projection yields $A = A(P + I - P) = AP + \frac{1}{r}A|h\rangle\langle h|$. Substituting $AP = |h\rangle\langle \tilde{x}|$ gives $A = |h\rangle\langle \tilde{x}| + \left(\frac{A|h\rangle}{r}\right)\langle h|$. Setting $x = \tilde{x}$ and $y = \frac{A|h\rangle}{r}$ recovers the desired form. □

Proposition 4.7. *For every pair of FUNTFs U, V of length $a + 1$ in $\mathbb{C}^a$, the map $\Theta_{U,V}$ has non-trivial kernel.*

Proof. Let $r := a + 1$. With $P_U = I_r - \frac{1}{r}|g\rangle\langle g|, P_V = I_r - \frac{1}{r}|h\rangle\langle h|$ for $g, h \in \mathbb{C}^r$ whose entries have unit modulus, by Lemma 4.6,

$$P_V(X \circ P_U)P_V = 0 \quad \iff \quad X \circ P_U = |h\rangle\langle x| + |y\rangle\langle h|$$

for some $x, y \in \mathbb{C}^r$. Note that every entry of P_U is non-zero, with $(P_U)_{ii} = \frac{r-1}{r}$, $(P_U)_{ij} = -\frac{1}{r}g_i\bar{g}_j$ for $i \neq j$ since g has entries of unit modulus. Making the simplest non-trivial choice, $x = 0$, $y = h$, we get $X \circ P_U = |h\rangle\langle h|$. Dividing entrywise by $(P_U)_{ij} = \delta_{ij} - \frac{1}{r}g_i\bar{g}_j$, we get

$$X := \frac{r^2}{r-1}I_r - r|s\rangle\langle s|, \qquad \text{where } s := \bar{g} \circ h.$$

Since g and h have unit-modulus entries, s does as well. Note that $X^T = \frac{r^2}{r-1}I_r - r|\bar{s}\rangle\langle \bar{s}|$, so that

$$(X^T \circ P_V)_{ii} = 1 = g_i\bar{g}_i \quad \text{and} \quad (X^T \circ P_V)_{ij} = (-r\bar{s}_i s_j)\left(-\frac{1}{r}h_i\bar{h}_j\right) = g_i\bar{g}_j, \quad \text{for} \quad i \neq j.$$

Hence, $X^T \circ P_V = |g\rangle\langle g|$. Since $P_V|h\rangle = 0$ and $P_U|g\rangle = 0$, both conditions of Lemma 3.7 are satisfied, whence $X \in \ker \Theta_{U,V}$. Finally,

$$\operatorname{Tr} X = \operatorname{Tr}\left(\frac{r^2}{r-1}I_r - r|s\rangle\langle s|\right) = \frac{r^3}{r-1} - r^2 = \frac{r^2}{r-1} > 0,$$

so that $X \neq 0$. □

Remark 4.8. Let $a \geq 2$ be a positive integer. The frame length relevant to KRP-tightness at (a, a) is $r = \mathrm{KRP}(a, a)$, and Proposition 4.7 applies precisely when $r = a + 1$, that is,

$$a + 1 \;\leq\; \sqrt{2a^2 - 1} \;<\; a + 2.$$

Squaring the above inequalities, we get

$$a^2 + 2a + 1 \leq 2a^2 - 1 < a^2 + 4a + 4,$$

or equivalently, $a^2 - 2a - 2 \geq 0$ and $a^2 - 4a - 5 < 0$. The first inequality holds for integers $a \geq \lceil 1 + \sqrt{3} \rceil = 3$, and the second holds for integers $a < 5$, so that $a \in \{3, 4\}$. Thus, among square dimension pairs, $\mathrm{KRP}(a, a) = a + 1$ occurs only at $(3, 3)$ and $(4, 4)$.

Corollary 4.9. *Every pair of FUNTFs U, V of length 4 in $\mathbb{C}^3$, and every pair of FUNTFs U, V of length 5 in $\mathbb{C}^4$, has $\ker \Theta_{U,V} \neq \{0\}$. Thus, there are no transversal pairs to be found in the $(3, 3)$ or $(4, 4)$ case.*

Proof. Both cases correspond to FUNTFs of length $n + 1$ in $\mathbb{C}^n$, with $n = 3$ and $n = 4$, respectively. The assertion follows immediately from Proposition 4.7. □

Remark 4.10. Corollary 4.9 explains why the transversal-pair construction cannot handle the dimension pairs $(3, 3)$ and $(4, 4)$. Nevertheless, both pairs are KRP-tight; indeed, Ohno's constructions in [Ohn10] give extreme points of rank 4, 5, respectively, using Kraus operators of rank greater than one.

5. Tightness of the Schmidt rank bound

From Theorem 2.3, we know that the rank of an extremal tracial coupling lies between the Schmidt bound, $\mathrm{ES}(a, b) = \lceil b/a \rceil$, and the Parthasarathy bound, $\mathrm{KRP}(a, b) = \lfloor \sqrt{a^2 + b^2 - 1} \rfloor$. In §4, we studied dimension pairs for which the Parthasarathy upper bound is attained. In this section, we explore the analogous question for the Schmidt bound: *For which values of (a, b) is this lower bound tight?*

5.1. Extremal tracial couplings with rank $\mathrm{ES}(a, b)$.

Let $2 \leq a \leq b$ be positive integers. To begin with, we consider the case where a divides b.

Proposition 5.1. *Let $2 \leq a$ be a positive integer. Then the dimension pair (a, a) is* ES-tight, *that is, $R_{\min}(a, a) = \mathrm{ES}(a, a) = 1$.*

Proof. Let $\psi := \frac{1}{\sqrt{a}} \sum_{i=1}^{a} |e_i\rangle \otimes |e_i\rangle$, and set $\rho := |\psi\rangle\langle\psi|$. A straightforward computation tells us that $\mathrm{Tr}_A(\rho) = \mathrm{Tr}_B(\rho) = I_a/a$, so that $\rho \in \mathcal{C}(I_a/a, I_a/a)$. Since ρ is a pure state, it is an extremal tracial coupling of rank 1, whence $R_{\min}(a, a) = \mathrm{ES}(a, a) = 1$. □

Proposition 5.2. *Let $a \leq b$ be positive integers such that a divides b, and set $r = \frac{b}{a}$. Then there exists an extreme point of the tracial coupling set $\mathcal{C}(I_a/a, I_b/b)$ of rank r.*

Proof. Since $b = ra$, we have an orthogonal decomposition of the target space, $\mathbb{C}^b = \bigoplus_{i=1}^{r} B_i$, where $\dim B_i = a$ for $1 \leq i \leq r$. For each i, let $V_i : \mathbb{C}^a \to \mathbb{C}^b$ be an isometry with range B_i. Note that $V_i^* V_j = \delta_{ij} I_a$ and $\sum_{i=1}^{r} V_i V_i^* = I_b$. Defining the Kraus operators as $K_i := \frac{1}{\sqrt{r}} V_i$, we observe that the marginal constraints are satisfied,

$$\sum_{i=1}^{r} K_i^* K_i = \frac{1}{r} \sum_{i=1}^{r} I_a = I_a, \qquad \sum_{i=1}^{r} K_i K_i^* = \frac{1}{r} \sum_{i=1}^{r} V_i V_i^* = \frac{a}{b} I_b.$$

Thus the Choi state ρ associated with $\{K_i\}_{i=1}^r$ is a tracial coupling. Next we show that ρ is an extreme point of rank r. Let $X = (x_{ij}) \in M_r(\mathbb{C})$ be such that $\sum_{i,j=1}^r x_{ij} K_i K_j^* = 0$. Multiplying on the left by V_ℓ^* and on the right by V_n, we get

$$V_\ell^* \left(\sum_{i,j=1}^r x_{ij} \frac{1}{r} V_i V_j^* \right) V_n = \frac{1}{r} x_{\ell n} I_a = 0,$$

whence $x_{\ell n} = 0$ for all ℓ, n. Thus the operators $\{K_i K_j^*\}$ are linearly independent, and by Corollary 2.11, we conclude that ρ is an extreme point of rank r. □

The following lemma will be useful in §5.2.

Lemma 5.3. *Let $a \le b$ and $r := \lceil \frac{b}{a} \rceil$. Let $K_1, \dots, K_r : \mathbb{C}^a \to \mathbb{C}^b$ satisfy the constraints $\sum_{i=1}^r K_i^* K_i = I_a$ and $\sum_{i=1}^r K_i K_i^* = \frac{a}{b} I_b$. Then $\operatorname{rank} K_i = a$ for every $1 \le i \le r$.*

Proof. Let $c := a/b$. Since $K_i K_i^* \ge 0$ and $\sum_{l=1}^r K_l K_l^* = c I_b$, we have $K_i K_i^* \le c I_b$, so that $\operatorname{sp}(K_i K_i^*) \subseteq [0, c]$. Since $K_i K_i^*$ and $K_i^* K_i$ have the same non-zero eigenvalues, it follows that $\operatorname{sp}(K_i^* K_i) \subseteq [0, c]$ as well, that is, $K_i^* K_i \le c I_a$, for every $1 \le i \le r$.

Let $1 \le j \le r$. Summing the above bound over the remaining indices and using $\sum_{i=1}^r K_i^* K_i = I_a$, we get

$$K_j^* K_j = I_a - \sum_{i \ne j} K_i^* K_i \ge I_a - (r-1) c I_a = \big(1 - (r-1)c\big) I_a.$$

By the definition of r, we have $r - 1 < \frac{b}{a} \le r$, so that $1 - (r-1)c > 0$. Thus $K_j^* K_j$ is invertible, whence $\ker K_j = \{0\}$, and by the rank-nullity theorem, $\operatorname{rank} K_j = a$. □

Definition 5.4. Let $A \in M_{b,a}(\mathbb{C})$. We say that A is a *partial permutation matrix* if it has entries from $\{0, 1\}$ with at most one 1 in each row and each column. More generally, we say that A is a *weighted partial permutation matrix* if it has at most one non-zero entry in each row and each column.

Observation 5.5. Let $a \le b$ be positive integers, and let $\{e_k\}_{k=1}^a$ and $\{f_m\}_{m=1}^b$ denote the standard bases of $\mathbb{C}^a$ and $\mathbb{C}^b$. With an injective mapping $\pi : \{1, \dots, a\} \to \{1, \dots, b\}$ and a mapping $w : \{1, \dots, a\} \to (0, \infty)$, we associate the $b \times a$ weighted partial permutation matrix,

$$A := \sum_{k=1}^a w(k) \, |f_{\pi(k)}\rangle\langle e_k|,$$

so that $\pi(k)$ is the row of the unique non-zero entry in column k, and $w(k)$ is its value. Below we note the action of A and A^* on the standard basis vectors, which we invoke repeatedly in our discussion,

$$A e_k = w(k) \, f_{\pi(k)} \quad (1 \le k \le a), \qquad A^* f_m = \begin{cases} w(k) \, e_k, & \text{if } m = \pi(k), \\ 0, & \text{if } m \notin \operatorname{range}(\pi). \end{cases}$$

Note that the index k in the first case is unique, as π is injective.

All of the sparse Kraus operators $K_1, \dots, K_r$ that we consider in this section have the following property in common. For each index j, there is a vector ξ_j in $\mathbb{C}^b$ such that $K_j^* \xi_j \ne 0$, and $K_n^* \xi_j = 0$ for every $n \ne j$. Let $\sum_{i,n} x_{in} K_i K_n^* = 0$ be a linear relation among the operators $K_i K_n^*$. Applying both sides to ξ_j, we observe that only the terms with $n = j$ survive, and

these involve only the j-th column of the coefficient matrix (x_{in}). Since ξ_j isolates the j-th column in this manner, we refer to the lemma below as the *isolation lemma*. It tells us that the above property, together with a mild independence condition, implies extremality, and we use it in all the extremality arguments in the rest of this section.

Lemma 5.6 (Isolation)**.** *Let $K_1, \dots, K_r$ be linear maps from $\mathbb{C}^a$ to $\mathbb{C}^b$, and let $\{e_1, \dots, e_a\}$ denote the standard basis of $\mathbb{C}^a$. Assume that for every $1 \le j \le r$, there is a vector $\xi_j \in \mathbb{C}^b$, an index $1 \le k_j \le a$, and a non-zero scalar c_j, satisfying the following conditions:*

(a) $K_j^* \xi_j = c_j\, e_{k_j}$, and $K_n^* \xi_j = 0$ for every $n \neq j$;
(b) the vectors $K_1 e_{k_j}, \dots, K_r e_{k_j}$ are linearly independent.

Then the operators $\{K_i K_n^*\}_{1 \le i,n \le r}$ are linearly independent. Moreover, if $K_1, \dots, K_r$ satisfy the tracial marginal constraints, $\sum_{i=1}^r K_i^* K_i = I_a$ and $\sum_{i=1}^r K_i K_i^* = \frac{a}{b} I_b$, then the Choi state of $\{K_i\}$ is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ of rank r.

Proof. Let $X = (x_{in}) \in M_r(\mathbb{C})$ be such that $\sum_{i,n=1}^r x_{in} K_i K_n^* = 0$, and let $j \in \{1, \dots, r\}$. Applying both sides to the vector ξ_j and using condition (a), we observe that only the terms with $n = j$ survive, so that

$$0 = \sum_{i,n=1}^{r} x_{in}\, K_i K_n^* \xi_j = c_j \sum_{i=1}^{r} x_{ij}\, K_i e_{k_j}.$$

Since $c_j \neq 0$, from condition (b) we have $x_{ij} = 0$ for every $1 \le i \le r$. As j was arbitrary, we conclude that $X = 0$. The last assertion is a direct consequence of Corollary 2.11. □

For weighted partial permutation matrices, the two conditions in Lemma 5.6 may be stated in terms of the injections π_i, which we note in the corollary below.

Corollary 5.7. *For $1 \le i \le r$, let $\pi_i : \{1, \dots, a\} \to \{1, \dots, b\}$ be an injective mapping, let $w_i : \{1, \dots, a\} \to (0, \infty)$ be a mapping, and let $K_i : \mathbb{C}^a \to \mathbb{C}^b$ be the weighted partial permutation matrix associated with (π_i, w_i) as in Observation 5.5. Assume that $\{K_i\}_{i=1}^r$ satisfies the tracial marginal constraints $\sum_{i=1}^r K_i^* K_i = I_a$ and $\sum_{i=1}^r K_i K_i^* = \frac{a}{b} I_b$, and that for every $j \in \{1, \dots, r\}$ there is a column index $k_j \in \{1, \dots, a\}$ such that:*

(a) the row index $m_j := \pi_j(k_j)$ is not in the range of any other π_n $(n \neq j)$;
(b) the row indices $\pi_1(k_j), \dots, \pi_r(k_j)$ are pairwise distinct.

Then the operators $\{K_i K_n^*\}_{1 \le i,n \le r}$ are linearly independent, and the Choi state of $\{K_i\}$ is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ of rank r.

Proof. It suffices to verify the hypotheses of Lemma 5.6 with $\xi_j := f_{m_j}$. From Observation 5.5, we have $K_j^* f_{m_j} = w_j(k_j)\, e_{k_j}$ with $w_j(k_j) > 0$, and $K_n^* f_{m_j} = 0$ for $n \neq j$ since $m_j \notin \text{range}(\pi_n)$. Thus hypothesis (a) of the lemma is satisfied. Again from Observation 5.5, the vectors $K_i e_{k_j} = w_i(k_j)\, f_{\pi_i(k_j)}$, $1 \le i \le r$, are non-zero multiples of standard basis vectors of $\mathbb{C}^b$, which are pairwise distinct by condition (b). Hence they are linearly independent, and hypothesis (b) of the lemma is satisfied. □

Below we illustrate Corollary 5.7 in the smallest non-trivial case, $(a, b) = (2, 3)$, which is a particular case of the general construction in Proposition 5.9.

Example 5.8. Consider the dimension pair $(a, b) = (2, 3)$. We first define the injective mappings $\pi_1, \pi_2 : \{1, 2\} \to \{1, 2, 3\}$ and the weight functions $w_1, w_2 : \{1, 2\} \to (0, \infty)$ as

follows:

$$\begin{aligned} \pi_1(1) &= 1, & w_1(1) &= \sqrt{1/3}, \\ \pi_1(2) &= 2, & w_1(2) &= \sqrt{2/3}; \\ \pi_2(1) &= 3, & w_2(1) &= \sqrt{2/3}, \\ \pi_2(2) &= 1, & w_2(2) &= \sqrt{1/3}. \end{aligned}$$

As given in Observation 5.5, to these pairs (π_i, w_i), we associate the weighted partial permutation matrices $K_1, K_2 : \mathbb{C}^2 \to \mathbb{C}^3$:

$$K_1 = \begin{pmatrix} \sqrt{1/3} & 0 \\ 0 & \sqrt{2/3} \\ 0 & 0 \end{pmatrix}, \qquad K_2 = \begin{pmatrix} 0 & \sqrt{1/3} \\ 0 & 0 \\ \sqrt{2/3} & 0 \end{pmatrix}.$$

A straightforward computation verifies the tracial marginal constraints,

$$K_1^* K_1 + K_2^* K_2 = I_2, \quad K_1 K_1^* + K_2 K_2^* = \frac{2}{3} I_3.$$

Below we verify the two conditions in Corollary 5.7.

(a) The range of π_1 is $\{1, 2\}$ and the range of π_2 is $\{1, 3\}$. Row index $m_1 = 2 = \pi_1(2)$ is exclusive to the range of π_1, so we take $k_1 = 2$; row index $m_2 = 3 = \pi_2(1)$ is exclusive to the range of π_2, so we take $k_2 = 1$.

(b) In column $k_1 = 2$ we have $\pi_1(2) = 2 \neq 1 = \pi_2(2)$, and in column $k_2 = 1$ we have $\pi_1(1) = 1 \neq 3 = \pi_2(1)$.

The resulting extreme point is the Choi state $\rho = \frac{1}{2} \sum_{i=1}^{2} |\mathrm{vec}(K_i)\rangle\langle \mathrm{vec}(K_i)|$. Vectorizing the operators, with $\{|e_j\rangle\}_{j=1}^{2}, \{|f_m\rangle\}_{m=1}^{3}$ denoting the standard bases of $\mathbb{C}^2, \mathbb{C}^3$, respectively, we get

$$\begin{aligned} |\mathrm{vec}(K_1)\rangle &= \frac{1}{\sqrt{3}} |e_1\rangle \otimes |f_1\rangle + \sqrt{\frac{2}{3}} |e_2\rangle \otimes |f_2\rangle, \\ |\mathrm{vec}(K_2)\rangle &= \sqrt{\frac{2}{3}} |e_1\rangle \otimes |f_3\rangle + \frac{1}{\sqrt{3}} |e_2\rangle \otimes |f_1\rangle. \end{aligned}$$

Relative to the lexicographic basis, $|e_1\rangle\otimes|f_1\rangle, |e_1\rangle\otimes|f_2\rangle, |e_1\rangle\otimes|f_3\rangle, |e_2\rangle\otimes|f_1\rangle, |e_2\rangle\otimes|f_2\rangle, |e_2\rangle\otimes|f_3\rangle$, we get the 6×6 bipartite density matrix,

$$\rho = \frac{1}{6} \begin{pmatrix} 1 & 0 & 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & \sqrt{2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 1 & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

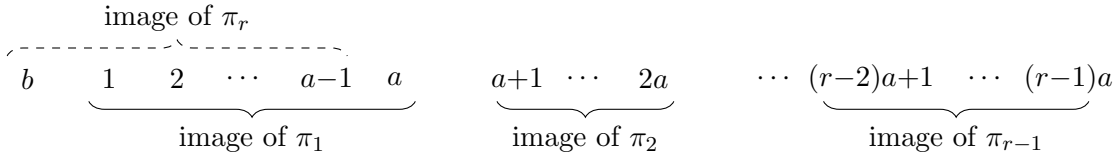
Proposition 5.9. *Let $2 \leq a \leq b$ be positive integers such that $b \equiv 1 \pmod{a}$, and let $r := \lceil \frac{b}{a} \rceil$. Then there exist weighted partial permutation matrices $K_1, \ldots, K_r : \mathbb{C}^a \to \mathbb{C}^b$ that satisfy the tracial marginal constraints (2) and for which the operators $\{K_i K_j^*\}_{1 \leq i,j \leq r}$ are linearly independent. In particular, $\mathcal{C}(I_a/a, I_b/b)$ contains an extreme point of rank $\lceil \frac{b}{a} \rceil$.*

Proof. Since $b \equiv 1 \pmod{a}$ and $b \geq a$, we have $b = (r-1)a+1$ with $r \geq 2$. For $1 \leq i \leq r-1$, we define $\pi_i : \{1, \ldots, a\} \to \{1, \ldots, b\}$ as translation by $(i-1)a$, that is,

$$\pi_i(k) = k + (i-1)a, \quad 1 \leq k \leq a.$$

We define π_r as the cyclic translation by $(r-1)a = b-1$, that is,

$$\pi_r(1) = b, \qquad \pi_r(k) = k-1 \quad (2 \leq k \leq a).$$



Note that each π_i is injective. We define the strictly positive weights,

$$w_i(k) := \begin{cases} \sqrt{k/b}, & i = 1, \\ \sqrt{a/b}, & 2 \leq i \leq r-1, \\ \sqrt{(a-k+1)/b}, & i = r; \end{cases}$$

on $\{1, \ldots, a\}$.

Let $\{|e_k\rangle\}_{k=1}^a$, $\{|f_m\rangle\}_{m=1}^b$ be the standard bases of $\mathbb{C}^a, \mathbb{C}^b$, respectively, and define

$$K_i := \sum_{k=1}^{a} w_i(k)\, |f_{\pi_i(k)}\rangle\langle e_k|.$$

Claim 1. For every $k \in \{1, \ldots, a\}$, the values $\pi_1(k), \ldots, \pi_r(k)$ are pairwise distinct.

Proof of Claim. For $i \leq r-1$, $\pi_i(k) = (i-1)a + k$ occupies the k-th position within the i-th of the $r-1$ disjoint length-a blocks pictured above. Since the blocks are disjoint, $\pi_1(k), \ldots, \pi_{r-1}(k)$ lie in different blocks, and hence are pairwise distinct. Thus it remains to show that $\pi_r(k)$ is different from $\pi_i(k)$ for every $1 \leq i \leq r-1$, and we consider two cases. If $k = 1$, then $\pi_r(1) = b$, whereas the last block ends at $(r-1)a = b-1$; thus $\pi_i(1) < \pi_r(1)$ for every $1 \leq i \leq r-1$. If $k \geq 2$, then $\pi_r(k) = k-1 < k = \pi_1(k)$, and since $\pi_1(k) \leq \pi_i(k)$ for every $1 \leq i \leq r-1$, we have $\pi_r(k) < \pi_i(k)$ for every $1 \leq i \leq r-1$. In either case, we conclude that $\pi_r(k)$ is different from $\pi_i(k)$ for every $1 \leq i \leq r-1$.

Claim 2. The operators $K_1, \ldots, K_r$ satisfy the tracial marginal constraints, that is, $\sum_{i=1}^r K_i^* K_i = I_a$ and $\sum_{i=1}^r K_i K_i^* = \frac{a}{b} I_b$. Moreover, for each i there is a column k_i such that the value $m_i := \pi_i(k_i)$ is attained by π_i but by no other π_j, that is, $m_i \in \mathrm{range}(\pi_i) \setminus \bigcup_{j \neq i} \mathrm{range}(\pi_j)$. (This is the hypothesis (a) of Corollary 5.7.) Explicitly,

$$m_1 = a \ \text{ at } k_1 = a, \qquad m_i = ia \ \text{ at } k_i = a \ (2 \leq i \leq r-1), \qquad m_r = b \ \text{ at } k_r = 1.$$

Proof of Claim. Since π_i is injective, we have $\langle f_{\pi_i(k)} | f_{\pi_i(k')} \rangle = \delta_{kk'}$, so that $K_i^* K_i = \sum_{k=1}^a w_i(k)^2 |e_k\rangle\langle e_k|$ is diagonal. For a fixed k, we have

$$\sum_{i=1}^{r} w_i(k)^2 = w_1(k)^2 + \sum_{i=2}^{r-1} w_i(k)^2 + w_r(k)^2 = \frac{k}{b} + (r-2)\frac{a}{b} + \frac{a-k+1}{b} = \frac{(r-1)a+1}{b} = 1,$$

whence $\sum_{i=1}^r K_i^* K_i = I_a$.

Next we turn our attention to the second identity. Since $K_i K_i^* = \sum_{k=1}^{a} w_i(k)^2 |f_{\pi_i(k)}\rangle\langle f_{\pi_i(k)}|$ for $1 \le i \le r$, collecting the ra terms (as i and k vary) according to the target row m, we have

$$\sum_{i=1}^{r} K_i K_i^* = \sum_{m=1}^{b} \Big(\sum_{(i,k):\pi_i(k)=m} w_i(k)^2 \Big) |f_m\rangle\langle f_m|.$$

Thus it suffices to show that the inner coefficient is equal to a/b for every $1 \le m \le b$, which we verify below by considering four cases.

- $1 \le m \le a-1$: exactly two pairs land on m, namely $(1, m)$ and $(r, m+1)$, contributing $w_1(m)^2 + w_r(m+1)^2 = \dfrac{m}{b} + \dfrac{a-m}{b} = \dfrac{a}{b}$;
- $m = a$: only $(1, a)$ lands, contributing $w_1(a)^2 = a/b$;
- $a+1 \le m \le (r-1)a$: writing $m = k + (i-1)a$ uniquely for $2 \le i \le r-1$, only (i, k) lands, contributing $w_i(k)^2 = a/b$;
- $m = b$: only $(r, 1)$ lands, contributing $w_r(1)^2 = a/b$.

Hence $\sum_{i=1}^{r} K_i K_i^* = \frac{a}{b} I_b$.

Note that the rows $m_1, \dots, m_r$ listed in the claim are precisely the singly-covered rows identified in the above case analysis ($m = a$, $m = ia$ for $2 \le i \le r-1$, and $m = b$), each of which is received precisely by the operator named.

From the above two claims, we observe that the hypotheses of Corollary 5.7 are satisfied with the columns $k_1, \dots, k_r$ of the second claim; indeed, hypothesis (a) is the exclusivity of the rows m_i, and hypothesis (b) holds in every column by the first claim. Hence the operators $\{K_i K_j^*\}$ are linearly independent, and the Choi state corresponding to $\{K_i\}$ is an extremal tracial coupling of rank r. □

Theorem 5.10. *Let $a \le b$ be positive integers, and $r := \lceil \frac{b}{a} \rceil$. If $b - (r-1)a$ divides a, then $\mathcal{C}(I_a/a, I_b/b)$ contains an extreme point of rank r.*

Proof. If $a = b$, then $r = 1$ and the assertion follows from Proposition 5.1. Thus we may assume that $b > a$. Let $p := b - (r-1)a > 0$. By our hypothesis, p divides a, and we write $a = pt$ with $t \ge 1$. Let $d := (r-1)t + 1$, so that $(a, b) = p(t, d)$ and $\lceil d/t \rceil = r$.

To begin with, we find Kraus operators $K'_1, \dots, K'_r : \mathbb{C}^t \to \mathbb{C}^d$ for the base pair (t, d) such that

$$\sum_{i=1}^{r} K_i'^* K_i' = I_t, \qquad \sum_{i=1}^{r} K_i' K_i'^* = \frac{t}{d} I_d, \qquad \{K_i' K_j'^*\}_{1 \le i,j \le r} \text{ is linearly independent.} \tag{13}$$

If $t \ge 2$, then $d \equiv 1 \pmod{t}$, and the existence of such operators follows from Proposition 5.9. If $t = 1$ (equivalently, $a \mid b$ and $d = r$), let $K'_i := \frac{1}{\sqrt{r}} |f_i\rangle\langle e_1|$, where $\{|f_i\rangle\}_{i=1}^{r}$ and $|e_1\rangle$ are the standard bases of $\mathbb{C}^r$ and $\mathbb{C}^1$, respectively. Then $K'_i K'^*_j = \frac{1}{r} |f_i\rangle\langle f_j|$, and it is straightforward to verify that $\sum_i K_i'^* K'_i = I_1$, $\sum_i K'_i K_i'^* = \frac{1}{r} I_r = \frac{t}{d} I_d$, and that the operators $K'_i K'^*_j$ are linearly independent.

Next we identify $\mathbb{C}^a$ with $\mathbb{C}^p \otimes \mathbb{C}^t$, and $\mathbb{C}^b$ with $\mathbb{C}^p \otimes \mathbb{C}^d$, and define

$$K_i := I_p \otimes K'_i, \qquad i = 1, \dots, r.$$

Since $K_i^* K_j = I_p \otimes K_i'^* K_j'$ and $K_i K_j^* = I_p \otimes K_i' K_j'^*$ for all i, j, taking $j = i$ and summing over i, we get

$$\sum_{i=1}^{r} K_i^* K_i = I_p \otimes I_t = I_a, \qquad \sum_{i=1}^{r} K_i K_i^* = I_p \otimes \frac{t}{d} I_d = \frac{a}{b} I_b.$$

Let $X = (x_{ij}) \in M_r(\mathbb{C})$ be such that $\sum_{i,j} x_{ij} K_i K_j^* = 0$. This may be rewritten as $I_p \otimes Y = 0$, where $Y = \sum_{i,j} x_{ij} K_i' K_j'^*$, whence $Y = 0$, and from the linear independence of $\{K_i' K_j'^*\}$, we get $X = 0$. Thus the operators $\{K_i K_j^*\}$ are linearly independent, and by Corollary 2.11, we conclude that the Choi state of $\{K_i\}$ is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ of rank r. □

5.2. **A complete characterization for $a < b \leq 2a$.** In this subsection, we consider the case $\mathrm{ES}(a, b) = 2$, which corresponds to $a < b \leq 2a$, and show that the divisibility condition in Theorem 5.10 is also necessary. In fact, the necessity has little to do with extremality; when the condition fails, we show that $\mathcal{C}(I_a/a, I_b/b)$ contains no coupling of rank 2 whatsoever (see Proposition 5.12). Our strategy is to compare the spectra of $K_1^* K_1$, $K_2^* K_2$ with those of $K_1 K_1^*$, $K_2 K_2^*$, respectively. This comparison yields a bijection between index sets with constant step $(b-a)/b$, and in Lemma 5.11, we show that such a bijection exists only if $b-a$ divides a.

Lemma 5.11. *Let p, q be positive integers, and let $n = p + q$. Let $S, T \subset \{1, \ldots, n\}$ with $|S| = |T| = q$ and $S \cup T = \{1, \ldots, n\}$. Let $\nu_1, \ldots, \nu_n, \alpha, \beta$ be real numbers such that $\nu_i = \alpha$ for $i \notin S$ and $\nu_j = \beta$ for $j \notin T$, with $\alpha \neq \beta$. If there exist a bijection $\phi : T \to S$ and a non-zero constant δ such that $\nu_i = \nu_{\phi(i)} + \delta$ for every $i \in T$, then $p \mid q$.*

Proof. Let us encode ϕ as a directed graph $G = (V, E)$ on the vertex set $V = \{1, \ldots, n\}$, with a directed edge $i \to \phi(i)$ for every $i \in T$. Since $\phi : T \to S$ is a bijection and $T \cup S = V$, we observe that:

- Every vertex in T has out-degree 1, while every vertex outside T ($i \notin T$) is a sink and has out-degree 0.
- Every vertex in S has in-degree 1, while every vertex outside S ($i \notin S$) is a source and has in-degree 0 in G.

At each step $i \to \phi(i)$ of a directed path in G, the relation $\nu_i = \nu_{\phi(i)} + \delta$ tells us that the value of ν changes by the non-zero constant $-\delta$. Thus G has no directed cycles.

Since $T \cup S = V$, there are no isolated vertices, and the graph G decomposes into a disjoint union of simple directed paths covering all of V. The number of sources in G is equal to $|V \setminus S| = n - |S| = (p + q) - q = p$ and similarly, the number of sinks in G is equal to p. It follows that there are p directed paths in the above decomposition of G.

Along each directed path in the decomposition, the value of ν drops by δ at each step. By definition, every source $i \notin S$ satisfies $\nu_i = \alpha$, and every sink $j \notin T$ satisfies $\nu_j = \beta$. Thus, every path in the decomposition has the same number of edges, $L = (\alpha - \beta)/\delta$.

Because each path in the decomposition consists of L edges and $L + 1$ vertices, and the p disjoint paths partition all n vertices, we have:

$$p + q = n = p(L + 1),$$

which implies that $q = pL$. Thus $p \mid q$. □

Proposition 5.12. *Let $a < b$ be positive integers. If $\mathcal{C}(I_a/a, I_b/b)$ contains a coupling of rank 2, extreme or not, then $b - a$ divides a (and in particular, $b \leq 2a$).*

Proof. Let $p := b - a$, and note that $p > 0$ as $a < b$ by our hypothesis. Since the given coupling has rank 2, from Theorem 2.3-(iii) we have $\lceil \frac{b}{a} \rceil \leq 2$, and as $a < b$, it follows that $\lceil \frac{b}{a} \rceil = 2$. In other words, the hypothesis can only be satisfied in the range $a < b \leq 2a$, where $0 < p \leq a$. If $p = a$, then $b - a$ divides a trivially; thus we may assume that $p < a$.

Via the correspondence in Theorem 2.7, the given coupling corresponds to a CP map of Choi rank 2. Let $K_1, K_2 : \mathbb{C}^a \to \mathbb{C}^b$ be the Kraus operators in a minimal Kraus representation of this map. From (2), we have

$$K_1K_1^* + K_2K_2^* = \frac{a}{b} I_b, \quad K_1^*K_1 + K_2^*K_2 = I_a.$$

Since they sum to a multiple of the identity, $K_1K_1^*$ and $K_2K_2^*$ commute with each other, and are simultaneously diagonalizable in $M_b(\mathbb{C})$; moreover, on every joint eigenspace, their eigenvalues add up to a/b.

Since $\lceil \frac{b}{a} \rceil = 2$, from Lemma 5.3 applied to K_1, K_2, we get $\operatorname{rank} K_1 = \operatorname{rank} K_2 = a$. Thus, 0 is an eigenvalue of $K_1K_1^*$ with multiplicity p. Let V_1 denote the p-dimensional 0-eigenspace for $K_1K_1^*$. Then V_1 is the same as the $\frac{a}{b}$-eigenspace of $K_2K_2^*$. Similarly, if V_2 denotes the 0-eigenspace for $K_2K_2^*$, the $\frac{a}{b}$-eigenspace of $K_1K_1^*$ is the same as V_2. Since $0 \neq a/b$, V_1 and V_2 are eigenspaces of the Hermitian operator $K_1K_1^*$ for two distinct eigenvalues, and are therefore mutually orthogonal. The space $\mathbb{C}^b \ominus (V_1 \oplus V_2)$ has dimension $q := b - 2p = a - p$ and the restrictions of both $K_1K_1^*$ and $K_2K_2^*$ to this space are invertible positive operators, thus possessing strictly positive eigenvalues.

Since the matrices $K_1^*K_1$ and $K_2^*K_2$ sum to I_a, they are simultaneously diagonalizable in $M_a(\mathbb{C})$. Let their joint eigenvalues be ν_i and $1 - \nu_i$, respectively, for $i = 1, \ldots, a$. The multiset of strictly positive eigenvalues of $K_\ell^*K_\ell$ is equal to that of $K_\ell K_\ell^*$ for both $\ell \in \{1, 2\}$. Thus, the multiset $\{\nu_i\}_{i=1}^a$ contains p copies of a/b alongside $a - p$ values strictly less than a/b, defining an index subset $S_1 \subset \{1, \ldots, a\}$ of size p where $\nu_i = a/b$. Symmetrically, the multiset $\{1 - \nu_i\}_{i=1}^a$ for $K_2^*K_2$ also contains p copies of a/b, defining an index subset $S_2 \subset \{1, \ldots, a\}$ of size p where $1 - \nu_i = a/b$, which gives us $\nu_i = 1 - a/b = p/b$.

Next we compare the eigenvalues of $K_2K_2^*$ and $K_2^*K_2$ which are different from a/b. Note that on the q-dimensional space $\mathbb{C}^b \ominus (V_1 \oplus V_2)$, the eigenvalues of $K_1K_1^*$ are given by $\{\nu_i \mid i \notin S_1\}$, whence the eigenvalues of $K_2K_2^* = \frac{a}{b} I_b - K_1K_1^*$ are given by $\{a/b - \nu_i \mid i \notin S_1\}$. Since the $\frac{a}{b}$-eigenspace of $K_2K_2^*$ is V_1, these are precisely the non-zero eigenvalues of $K_2K_2^*$ which are different from a/b. On the other hand, the eigenvalues of $K_2^*K_2$ which are different from a/b are precisely $\{1 - \nu_j \mid j \notin S_2\}$. Recall that the non-zero eigenvalues of $K_2^*K_2$ and $K_2K_2^*$ (counted with multiplicity) are identical, and each of these operators has a/b as an eigenvalue with multiplicity p (indexed by S_2, and with eigenspace V_1, respectively). Discarding these p copies of a/b on both sides, we observe that the remaining multisets, each of size q, are equal, that is,

$$\{1 - \nu_j \mid j \notin S_2\} = \{a/b - \nu_i \mid i \notin S_1\}.$$

Thus there is a bijection $\phi : \{1, \ldots, a\} \setminus S_2 \to \{1, \ldots, a\} \setminus S_1$ such that:

$$1 - \nu_j = \frac{a}{b} - \nu_{\phi(j)} \quad \text{for every } j \notin S_2.$$

Rearranging this equation yields:

$$\nu_j = \nu_{\phi(j)} + 1 - \frac{a}{b} = \nu_{\phi(j)} + \frac{p}{b}.$$

We are now ready to apply Lemma 5.11. Set $n = a$, and let

$$T = \{1, \dots, a\} \setminus S_2, \qquad S = \{1, \dots, a\} \setminus S_1.$$

Then $|S| = |T| = q = a - p$. The corresponding constant values are

$$\alpha = \frac{a}{b} \quad \text{for } i \notin S, \qquad \beta = \frac{p}{b} \quad \text{for } j \notin T.$$

Since $p < a$, we have $\alpha \neq \beta$ as well as $S_1 \cap S_2 = \varnothing$. Thus,

$$S \cup T = \{1, \dots, a\}.$$

Also, $p > 0$, so the step size $\delta = p/b$ is non-zero. Thus all the hypotheses of Lemma 5.11 are satisfied, and we see that

$$p \mid q = a - p$$

and hence $p \mid a$. Recalling that $p = b - a$, we obtain $b - a \mid a$, as required. □

Theorem 5.13. *Let a, b be positive integers such that $a < b \leq 2a$. Then the following are equivalent:*

(a) There is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ of rank 2.
(b) There is a coupling in $\mathcal{C}(I_a/a, I_b/b)$ of rank 2.
(c) $b - a = \gcd(a, b)$.

Proof. Since $a < b \leq 2a$, we have $r = \lceil \frac{b}{a} \rceil = 2$ and $b - (r-1)a = b - a$. Clearly, (a) implies (b). If (b) holds, then by Proposition 5.12, $b - a$ divides a; and if $b - a$ divides a, then by Theorem 5.10, (a) holds. Thus each of (a) and (b) is equivalent to the condition that $b - a$ divides a, and it remains to show that this condition is equivalent to (c).

If $b - a = \gcd(a, b)$, then $b - a$ divides a. Conversely, suppose $b - a$ divides a. Then it also divides $b = a + (b - a)$, so $b - a$ is a common divisor of a and b; hence $b - a \leq \gcd(a, b)$. But $\gcd(a, b)$ divides $b - a$ as well, giving $\gcd(a, b) \leq b - a$. We conclude that $b - a = \gcd(a, b)$. □

5.3. **An extremal tracial coupling of rank** $\mathrm{ES}(a, b)$ **for** $b > a(a-1)$**.** Our main goal in this subsection is to show that the divisibility hypothesis of Theorem 5.10 becomes superfluous once b is large enough (see Theorem 5.15). To this end, we need the following well-known lemma on the existence of harmonic frames.

Lemma 5.14 (Harmonic Frame)**.** *Let $a \geq 2$ be a positive integer, and let $1 \leq p \leq a$. Then there is a unit-norm tight frame, $\{v_1, \dots, v_a\}$, of length a in $\mathbb{C}^p$, that is, a collection of a unit vectors in $\mathbb{C}^p$ such that $\sum_{i=1}^{a} |v_i\rangle\langle v_i| = \frac{a}{p} I_p$.*

Proof. Let $\omega := e^{2\pi i/a}$, and let S be a subset of $\{0, \dots, a-1\}$ with $|S| = p$. We index the standard basis of $\mathbb{C}^p$ by S, and denote it by $\{|e_s\rangle\}_{s \in S}$. For $i = 1, \dots, a$, define

$$|v_i\rangle = \frac{1}{\sqrt{p}} \sum_{s \in S} \omega^{s(i-1)} |e_s\rangle.$$

Clearly, each $|v_i\rangle$ is a unit vector as $|\omega^{s(i-1)}| = 1$. The matrix entries of the frame operator are given by

$$\langle e_s| \left(\sum_{i=1}^{a} |v_i\rangle\langle v_i| \right) |e_{s'}\rangle = \frac{1}{p} \sum_{i=1}^{a} \omega^{(s-s')(i-1)} = \delta_{s,s'} \frac{a}{p},$$

since $0 < |s - s'| < a$ for distinct $s, s' \in S$. Hence $\sum_{i=1}^{a} |v_i\rangle\langle v_i| = \frac{a}{p} I_p$. □

Note that any linear map $K : \mathbb{C}^a \to \mathbb{C}^b$ may be written column by column as

$$K = \sum_{k=1}^{a} \lambda_k \, |z_k\rangle\langle e_k|,$$

with unit vectors $z_k \in \mathbb{C}^b$ and $\lambda_k \geq 0$. Writing each Kraus operator in this manner, $K_i = \sum_{k=1}^{a} \lambda_{i,k} |z_{i,k}\rangle\langle e_k|$, we get

$$K_i K_j^* = \sum_{k=1}^{a} \lambda_{i,k}\lambda_{j,k} \, |z_{i,k}\rangle\langle z_{j,k}|.$$

Thus, for strictly positive weights $\lambda_{i,k}$, the linear independence of $\{K_i K_j^*\}_{i,j=1}^{r}$ (which suffices for extremality, by Corollary 2.11) is governed by the ra column directions $z_{i,k} \in \mathbb{C}^b$. In the theorem below, we make a judicious choice of these directions.

Theorem 5.15. *Let $a \geq 2$ and let $b > a(a-1)$ be positive integers. Then there is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ of rank $\lceil \frac{b}{a} \rceil$.*

Proof. We first set up the notation used to construct the extreme point, working with its corresponding CP map and a minimal Kraus representation thereof, under the correspondence of Theorem 2.7.

Let $r := \lceil \frac{b}{a} \rceil$, $p := b - (r-1)a$ and $w_a := \frac{a}{b}$, $w_p := \frac{p}{b}$. Note that $0 < p \leq a$ and $(r-1)w_a + w_p = \frac{(r-1)a+p}{b} = 1$. It helps to keep in mind that the hypothesis $b > a(a-1)$ is equivalent to $r \geq a$, and it is only in this form that it enters the proof; it guarantees that every column index $k \in \{1, \ldots, a\}$ is also one of the operator indices $\{1, \ldots, r\}$, so that each column k has a 'diagonal' slot (k, k). Let $f_1, \ldots, f_b$ denote the standard basis vectors of $\mathbb{C}^b$, and define,

$$\Omega := \big\{(i,k) \in \{1, \ldots, r\} \times \{1, \ldots, a\} : k \neq i\big\}.$$

Since $r \geq a$, precisely a of the ra pairs (i, k) satisfy $k = i$, so that $|\Omega| = ra - a = a(r-1) < b$. Thus we may choose an injective map $\sigma : \Omega \to \{1, \ldots, b\}$. Let

$$V := \operatorname{span}\{f_{\sigma(i,k)} : (i,k) \in \Omega\}, \qquad W := V^{\perp},$$

so that $\dim V = a(r-1)$ and $\dim W = p$, and let E_V, E_W denote the orthogonal projections from $\mathbb{C}^b$ onto V, W, respectively. Using Lemma 5.14, we fix a tight frame $\{v_1, \ldots, v_a\} \subset W$ with $\sum_{i=1}^{a} |v_i\rangle\langle v_i| = \frac{a}{p} E_W$, $\|v_i\| = 1$.

Let $e_1, \ldots, e_a$ denote the standard basis vectors of $\mathbb{C}^a$. For $1 \leq i \leq r$, $1 \leq k \leq a$, set

$$z_{i,k} := \begin{cases} f_{\sigma(i,k)}, & k \neq i, \\ v_i, & k = i, \end{cases} \qquad \lambda_{i,k} := \begin{cases} \sqrt{w_a}, & k \neq i, \\ \sqrt{w_p}, & k = i, \end{cases}.$$

Note that $(i,k) \notin \Omega$ if and only if $k = i$. Since $r \geq a$, for every column $1 \leq k \leq a$ this happens for exactly one operator index, namely $i = k$, and thus

$$\sum_{i=1}^{r} \lambda_{i,k}^2 = w_p + (r-1)w_a = 1. \tag{14}$$

Define $K_1, \ldots, K_r : \mathbb{C}^a \to \mathbb{C}^b$ by

$$K_i := \sum_{k=1}^{a} \lambda_{i,k} \, |z_{i,k}\rangle\langle e_k|.$$

Claim 3. If $(i,k) \in \Omega$, then $z_{i,k} \perp z_{i',k'}$ for every $(i',k') \neq (i,k)$. In particular, $z_{i,k} \perp z_{i,k'}$ for $k \neq k'$ and $1 \leq i \leq r$, and $z_{i,k} \perp z_{i',k}$ for $i \neq i'$ and $1 \leq k \leq a$.

Proof of Claim. If also $(i',k') \in \Omega$, then $\sigma(i',k') \neq \sigma(i,k)$ since σ is injective and $(i',k') \neq (i,k)$, so $z_{i,k} = f_{\sigma(i,k)}$ and $z_{i',k'} = f_{\sigma(i',k')}$ are distinct standard basis vectors. If instead $(i',k') \notin \Omega$, then $z_{i',k'} = v_{i'} \in W$, while $z_{i,k} = f_{\sigma(i,k)} \in V$, and $V \perp W$.

For $(i,k), (i',k') \notin \Omega$ the vectors $z_{i,k} = v_i$ and $z_{i',k'} = v_{i'}$ need not be orthogonal; in this case, we make use of the tight-frame identity instead.

Claim 4. $\sum_{i=1}^{r} K_i^* K_i = I_a$ and $\sum_{i=1}^{r} K_i K_i^* = \frac{a}{b} I_b$.

Proof of Claim. From $K_i = \sum_{k=1}^{a} \lambda_{i,k} |z_{i,k}\rangle\langle e_k|$, we get

$$K_i^* K_i = \sum_{1 \leq k,k' \leq a} \lambda_{i,k}\lambda_{i,k'} \langle z_{i,k}|z_{i,k'}\rangle \, |e_k\rangle\langle e_{k'}|, \tag{15}$$

$$K_i K_i^* = \sum_{1 \leq k,k' \leq a} \lambda_{i,k}\lambda_{i,k'} \langle e_k|e_{k'}\rangle \, |z_{i,k}\rangle\langle z_{i,k'}|. \tag{16}$$

In the first sum, the previous claim gives $\langle z_{i,k}, z_{i,k'}\rangle = 0$ for $k \neq k'$. Since $\langle z_{i,k}, z_{i,k}\rangle = 1$, for $1 \leq i \leq r$ we have,

$$K_i^* K_i = \sum_{k=1}^{a} \lambda_{i,k}^2 \, |e_k\rangle\langle e_k|.$$

By interchanging the order of summation, we observe that

$$\sum_{i=1}^{r} K_i^* K_i = \sum_{i=1}^{r}\sum_{k=1}^{a} \lambda_{i,k}^2 \, |e_k\rangle\langle e_k| = \sum_{k=1}^{a} \Big(\sum_{i=1}^{r} \lambda_{i,k}^2 \Big) |e_k\rangle\langle e_k| = \sum_{k=1}^{a} |e_k\rangle\langle e_k| = I_a.$$

In the second sum, using $\langle e_k, e_{k'}\rangle = \delta_{kk'}$, we have

$$K_i K_i^* = \sum_{k=1}^{a} \lambda_{i,k}^2 \, |z_{i,k}\rangle\langle z_{i,k}|.$$

As before, by interchanging the order of summation, we observe that,

$$\begin{aligned} \sum_{i=1}^{r} K_i K_i^* &= w_a \sum_{(i,k)\in\Omega} |f_{\sigma(i,k)}\rangle\langle f_{\sigma(i,k)}| \; + \; w_p \sum_{i=1}^{a} |v_i\rangle\langle v_i| \\ &= w_a E_V + w_p \cdot \frac{a}{p} E_W = \frac{a}{b} E_V + \frac{a}{b} E_W = \frac{a}{b} I_b. \end{aligned}$$

Claim 5. For each $k \in \{1, \ldots, a\}$, the vectors $K_1 e_k, \ldots, K_r e_k$ are linearly independent.

Proof of Claim. Let $1 \le k \le a$. By Claim 3, $z_{1,k}, \dots, z_{r,k}$ are mutually orthogonal. Since $K_i e_k = \lambda_{i,k} z_{i,k}$ with $\lambda_{i,k} > 0$, the vectors $K_1 e_k, \dots, K_r e_k$ are non-zero and mutually orthogonal, hence linearly independent.

Now that the marginal constraints have been established, it remains to verify the hypotheses of Lemma 5.6. Let $j \in \{1, \dots, r\}$. Since $a \ge 2$, there is an index $k_j \ne j$ with $1 \le k_j \le a$, so that $(j, k_j) \in \Omega$, and we define $\xi_j := z_{j,k_j}$. By Claim 3, ξ_j is orthogonal to $z_{n,k}$ whenever $(n,k) \ne (j,k_j)$. Since $K_n^* = \sum_{k=1}^{a} \lambda_{n,k} |e_k\rangle\langle z_{n,k}|$, we have

$$K_n^* \xi_j = \sum_{k=1}^{a} \lambda_{n,k} \langle z_{n,k} | z_{j,k_j} \rangle e_k = \begin{cases} 0, & n \ne j, \\ \lambda_{j,k_j} e_{k_j}, & n = j. \end{cases}$$

Note that $\lambda_{j,k_j} = \sqrt{w_a} \ne 0$ as $k_j \ne j$. Thus hypothesis (a) of Lemma 5.6 is satisfied, and hypothesis (b) is precisely the assertion of Claim 5. From Lemma 5.6, we conclude that the Choi state of $\{K_i\}$ is an extreme point of $\mathcal{C}(I_a/a, I_b/b)$ of rank $r = \lceil \frac{b}{a} \rceil$. □

6. Concluding remarks

In this article, we have settled the question of KRP-tightness throughout the region, $b \ge \frac{1}{2}(a^2 - 1)$, and that of ES-tightness for $\mathrm{ES}(a,b) = 2$ (that is, $a < b \le 2a$), and throughout the region $b > a(a-1)$ (see Theorems 4.1, 5.13, 5.10, and 5.15). We end this article with two conjectures and two open problems.

Conjecture 6.1. *For every (a,b) with $a, b \ge 2$ and $(a,b) \notin \{(2,2),(3,3),(4,4)\}$, there exists a transversal pair of FUNTFs of length $r = \mathrm{KRP}(a,b)$ in $\mathbb{C}^a$ and $\mathbb{C}^b$.*

If Conjecture 6.1 holds, then the question of KRP-tightness would be settled for every pair other than $(2,2)$, which motivates the following conjecture (see also [DDD26]).

Conjecture 6.2. *$R_{\max}(a,b) = \mathrm{KRP}(a,b)$ for every $(a,b) \ne (2,2)$ with $a, b \ge 2$.*

In the context of the Schmidt bound, for $\mathrm{ES}(a,b) = 2$ (that is, $a < b \le 2a$), Theorem 5.13 gives a complete characterization, namely, the Schmidt bound is attained if and only if $b - a = \gcd(a,b)$. The following two problems remain open.

First, for $r := \mathrm{ES}(a,b) \ge 3$, in Theorem 5.10 we have shown that the Schmidt bound is attained whenever $b - (r-1)a$ divides a, and in Theorem 5.15, that this condition is not needed once $b > a(a-1)$. Thus, for a fixed a, the dimension pairs (a,b) for which the question of ES-tightness remains open are precisely those with $2a < b \le a(a-1)$ such that $b - (r-1)a$ does not divide a. Note that there are only finitely many such pairs for each a, and none for $a \le 3$; the first such pair is $(4, 11)$. Is the divisibility condition necessary in this intermediate range, as is the case when $r = 2$?

Second, Ohno's constructions show that $(3,3)$ and $(4,4)$ are KRP-tight, whereas from Corollary 4.9, we know that no transversal pair of FUNTFs reaches them. Note that Ohno's extreme points are built from Kraus operators of rank greater than one. Might rank-one Kraus operators with unequal weights yield maximal-rank extremal tracial couplings at these two pairs? Or is there a systematic extension of the transversality approach to Kraus operators of rank greater than one which accounts for these pairs, and any others at which equal-weight rank-one pairs fail?

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