

A GEOMETRIC DESCRIPTION OF FEASIBLE SINGULAR VALUES
IN THE TENSOR TRAIN FORMAT*

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Abstract. Tree tensor networks such as the tensor train (TT) format are a common tool for high-dimensional problems. The associated multivariate rank and accordant tuples of singular values are based on different matricizations of the same tensor. While the behavior of such is as essential as in the matrix case, here questions about the *feasibility* of specific constellations arise: which prescribed tuples can be realized as singular values of a tensor, and what is this feasible set? We first show the equivalence of the *tensor feasibility problem* (TFP) to the *quantum marginal problem* (QMP). In higher dimensions, in case of the TT-format, the conditions for feasibility can be decoupled. By present results for three dimensions for the QMP, it then follows that the tuples of squared, feasible TT-singular values form polyhedral cones. We further establish a connection to eigenvalue relations of sums of Hermitian matrices, which in turn are described by sets of interlinked, so-called *honeycombs*, as they have been introduced by Knutson and Tao. Besides a large class of universal, necessary inequalities as well as the vertex description for a special, simpler instance, we present a linear programming algorithm to check feasibility and a simple, heuristic algorithm to construct representations of tensors with prescribed, feasible TT-singular values in parallel.

Key words. tensor, TT-format, singular value, honeycomb, eigenvalue, Hermitian matrix, linear inequality, quantum marginal problem

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1. Introduction. For $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$, let $A \in \mathbb{K}^{n_1 \times \dots \times n_d}$ be a d th-order tensor, such as in Figure 1. The tensor A can be reshaped into certain matricizations,

$$A^{(\{1, \dots, \mu\})} \in \mathbb{K}^{n_1 \times \dots \times n_\mu \times n_{\mu+1} \times \dots \times n_d}, \quad \mu = 1, \dots, d-1,$$

which are related to the so-called tensor train (TT) decomposition [12, 28]. The vectorization $\text{vec}(\cdot)^1$ in co-lexicographic order (columnwise) is to be an invariant to these reshapings, i.e.,

$$\text{vec}(A^{(\{1, \dots, \mu\})}) = \text{vec}(A) \in \mathbb{K}^{n_1 \times \dots \times n_d \times 1}, \quad \mu = 1, \dots, d-1,$$

such that they become uniquely defined.

We may also explicitly write $A^{(\{1, \dots, \mu\})}((i_1, \dots, i_\mu)_1, (i_{\mu+1}, \dots, i_d)_{\mu+1}) = A(i)$ with $(i_1, \dots, i_\mu)_\nu := 1 + \sum_{s=1}^\mu (\prod_{h=1}^{s-1} n_{\nu+h-1})(i_s - 1) \in \{1, \dots, n_\nu \dots n_{\nu+\mu-1}\} \subset \mathbb{N}$ (we will skip the index ν when context renders it obsolete). The $d-1$ tuples of TT-singular values $\sigma = (\sigma^{(1)}, \dots, \sigma^{(d-1)}) = \text{sv}_{\text{TT}}(A)$ and the according TT-rank(s) $r = (r_1, \dots, r_{d-1}) \in \mathbb{N}^{d-1}$ of $A \neq 0$ are given through the matrix singular values (sv) of its reshapings,

$$\sigma^{(\mu)} := \text{sv}(A^{(\{1, \dots, \mu\})}), \quad r_\mu := \text{rank}(A^{(\{1, \dots, \mu\})}), \quad \mu = 1, \dots, d-1,$$

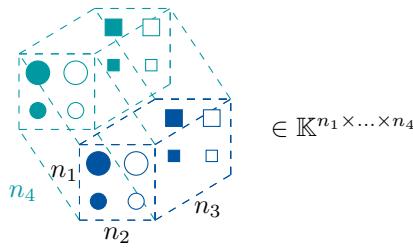
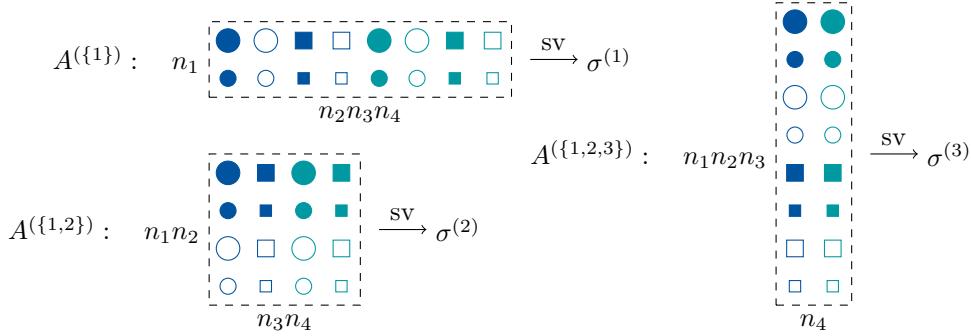
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¹In MATLAB syntax, $\text{vec}(A) = A(:)$.

FIG. 1. Visualization of a four-dimensional tensor A with mode sizes $n_1 = \dots = n_4 = 2$.FIG. 2. Matricizations (or reshapings, or unfoldings) of the 4th-order tensor A into the matrices $A^{(1)} \in \mathbb{K}^{n_1 \times n_2 n_3 n_4}$, $A^{(1,2)} \in \mathbb{K}^{n_1 n_2 \times n_3 n_4}$, and $A^{(1,2,3)} \in \mathbb{K}^{n_1 n_2 n_3 \times n_4}$ through which $\sigma = \text{sv}_{\text{TT}}(A)$ is obtained.

such as displayed in Figure 2. We require σ to be formally independent of the size of the tensor, so each of the singular values $\sigma^{(\mu)} = (\sigma_1^{(\mu)}, \sigma_2^{(\mu)}, \dots)$ is considered to be an infinite (weakly decreasing, nonnegative) sequence with finitely many nonzero entries—hence an element of the cone which we denote by $\mathcal{D}_{\geq 0}^{\infty}$ (cf. Definition 2.5). Being based on the same entries within A , the question about the *feasibility* of prescribed TT-singular value arises immediately.

DEFINITION 1.1 (TT-feasibility). *Let $\sigma = (\sigma^{(1)}, \dots, \sigma^{(d-1)}) \in (\mathcal{D}_{\geq 0}^{\infty})^{d-1}$. Then σ is called feasible for $n = (n_1, \dots, n_d)$ if there exists a tensor $A \in \mathbb{K}^{n_1 \times \dots \times n_d}$ giving rise to it in the form of its TT-singular values, i.e., $\sigma = \text{sv}_{\text{TT}}(A)$.*

In other words, we ask which σ are in the range of sv_{TT} . One necessary condition,

$$(1.1) \quad \|A\|_F = \|\sigma^{(\mu)}\|_2 = \|\sigma^{(\nu)}\|_2, \quad \mu, \nu = 1, \dots, d-1,$$

where $\|\cdot\|_F$ is the Frobenius norm, follows directly and is denoted as the *trace property*. Note that if σ is feasible for n , then it is also feasible for an increased value $\tilde{n} \in \mathbb{N}^d$, $\tilde{n}_\mu \geq n_\mu$, $\mu = 1, \dots, d$. One problem setting is hence to determine the smallest possible mode sizes n_μ for which a given σ is feasible.

Understanding the nature of this and related problems regarding low rank decompositions is essential, given that many methods rely on at least basic, if not rigorous, assumptions about these generalized singular values, just as in the matrix case. At the same time, they are a key tool to the (complexity) analysis of higher-order data, whether, for example, in signal processing, machine learning, or quantum chemistry, as presented in the extensive survey articles [3, 13, 25, 31].

As we will see in subsection 3.2, σ is feasible for n in the case $\mathbb{K} = \mathbb{C}$ if and only if it is already feasible for $\mathbb{K} = \mathbb{R}$. The choice of \mathbb{K} hence does not influence the range of sv_{TT} .

1.1. Equivalence of the tensor feasibility and the quantum marginal problem. Let $I = \{1, \dots, d-1\}$, and let $\mathcal{K} \subset \{J \mid \emptyset \neq J \subset I\}$ be a family of subsets. The quantum marginal problem (see, for example, [4, 21, 29]) and the tensor feasibility problem, as defined below, are equivalent in the sense of Theorem 1.4.

The mapping $\text{trace}_{I \setminus J} : \mathbb{K}^{n_I \times n_I} \rightarrow \mathbb{K}^{n_J \times n_J}$, $n_J := \prod_{i \in J} n_i$, $J \subset I$, is called the *partial trace*. For an elementary Kronecker product of matrices $A_i \in \mathbb{K}^{n_i \times n_i}$, it holds that

$$\text{trace}_{I \setminus J}(A_1 \otimes \cdots \otimes A_{d-1}) = \prod_{i \notin J} \text{trace}(A_i) \cdot \bigotimes_{i \in J} A_i \in \mathbb{K}^{n_J \times n_J}.$$

The map is then extended to the whole space $\mathbb{K}^{n_I \times n_I}$ by linearity. In the following, as for singular values, we also consider eigenvalues to be infinite (weakly decreasing) sequences.

DEFINITION 1.2 (quantum marginal problem (QMP)). *For each $J \in \mathcal{K}$, $J \subset I$, let $\lambda^{(J)} \in \mathcal{D}_{\geq 0}^\infty$ (potential eigenvalues). Then the collection $\{\lambda^{(J)}\}_{J \in \mathcal{K}}$ is called compatible (for (n_1, \dots, n_{d-1})) if there exists a Hermitian, positive semidefinite matrix $\rho_I \in \mathbb{C}^{n_I \times n_I}$ such that*

$$(1.2) \quad \text{eig}(\rho_J) = \lambda^{(J)}, \quad \rho_J = \text{trace}_{I \setminus J}(\rho_I) \in \mathbb{C}^{n_J \times n_J},$$

for all $J \in \mathcal{K}$.

DEFINITION 1.3 (tensor feasibility problem (TFP) for $\mathbb{K} = \mathbb{C}$). *For each $J \in \mathcal{K}$, $J \subset I$, let $\sigma^{(J)} \in \mathcal{D}_{\geq 0}^\infty$ (potential singular values). Then the collection $\{\sigma^{(J)}\}_{J \in \mathcal{K}}$ is called feasible (for $n = (n_1, \dots, n_d)$) if there exists a tensor $A \in \mathbb{C}^{n_1 \times \cdots \times n_d}$ such that*

$$(1.3) \quad \text{sv}(A^{(J)}) = \sigma^{(J)}, \quad A^{(J)} \in \mathbb{C}^{n_J \times n_{\{1, \dots, d\} \setminus J}},$$

for all $J \in \mathcal{K}$.

The matrices $A^{(J)}$ are reshapings² of the tensor A analogous to those given in the introduction, but for arbitrary $J \subset I$. For a formal definition, see [12]. Sets for which $d \in J$ need not be included in the definition of feasibility, since simply $\text{sv}(A^{(J)}) = \text{sv}(A^{\{1, \dots, d\} \setminus J})$, $\{1, \dots, d\} \setminus J \subset I$. The proof of Theorem 1.4 and the subsequent discussion give further insight into why one requires I to only have $d-1$ elements, and how the rank of ρ_I is related to n_d . Note that in the introduction, and all subsequent sections, we use the short notation $\sigma^{(\mu)} = \sigma^{\{1, \dots, \mu\}}$ for the TT-format.

THEOREM 1.4 (equivalence of TFP and QMP). *The feasibility of $\{\sigma^{(J)}\}_{J \in \mathcal{K}}$ is equivalent to the compatibility of the entrywise squared values $\{(\sigma^{(J)})^2\}_{J \in \mathcal{K}}$, where n_d may be chosen as large as necessary (although at most $n_d = \text{rank}(\rho_I)$ is required).*

Proof of Theorem 1.4. Equivalence is achieved by setting

$$(1.4) \quad A^{(I)} A^{(I)^H} = \rho_I,$$

²In MATLAB syntax, $A^{(J)} = \text{reshape}(\text{permute}(A, [J, \{1, \dots, d\} \setminus J]), [n_J, n_{\{1, \dots, d\} \setminus J}])$.

where \cdot^H is the conjugate (also called Hermitian) transpose. The rest follows by the simple fact that $\text{trace}_{I \setminus J}(A^{(I)} A^{(I)H}) = A^{(J)} A^{(J)H}$ and hence

$$(1.5) \quad \lambda^{(J)} = \text{eig}(\rho_J) = \text{eig}(\text{trace}_{I \setminus J}(A^{(I)} A^{(I)H})) = \text{sv}(A^{(J)})^2 = (\sigma^{(J)})^2$$

for all $J \subset \{1, \dots, d\}$: First, let $\{\sigma^{(J)}\}_{J \in \mathcal{K}}$ be feasible for $n \in \mathbb{N}^d$ by means of the tensor A as in (1.3). Then by (1.4) and (1.5) the family $\{(\sigma^{(J)})^2\}_{J \in \mathcal{K}}$ is compatible. Conversely, assume the family is compatible by means of ρ_I as in (1.2). Then we define the tensor $A \in \mathbb{C}^{n_1 \times \dots \times n_{d-1} \times \text{rank}(\rho_I)}$ via the Cholesky decomposition of ρ_I as in (1.4). Hence, via (1.5), the family $\{\sigma^{(J)}\}_{J \in \mathcal{K}}$ is feasible for any $n_d \geq \text{rank}(\rho_I)$. \square

The *pure* QMP adds the condition $\text{rank}(\rho_I) = 1$. To obtain the equivalent TFP, one sets $n_d = 1$. For $d - 1 = 2$, the problem is reduced to the ordinary matrix singular values by which $\sigma^{\{\{1\}\}} = \sigma^{\{\{2\}\}}$. For $d - 1 = 3$, the relation between the pure QMP and the TFP for $\mathcal{K} = \{\{1\}, \{2\}, \{3\}\}$ is commonly mentioned, e.g., in [21]. More generally, the pure QMP for $\mathcal{K} = \{\{1\}, \{2\}, \dots\}$ which is concerned with the spectra of $\rho_{\{1\}}, \rho_{\{2\}}, \dots$ (often denoted as density matrices ρ_A, ρ_B, \dots) is the same as the Tucker-feasibility problem (cf. [6]). Since $\mathbb{K}^{n_1 \times \dots \times n_d} \cong \mathbb{K}^{n_1 \times \dots \times n_{d-1}}$ for $n_d = 1$, we may substitute $d \leftarrow d - 1$ and use $\tilde{\mathcal{K}} = \{\{1\}, \dots, \{d-2\}, \{1, \dots, d-1\}\}$. This reveals that the pure QMP for \mathcal{K} is equivalent to the QMP for $\tilde{\mathcal{K}}$. For dimension 3, this equivalence is stated in [21] (using the notation $\rho_A, \rho_B, \rho_{AB}$ and ρ_A, ρ_B, ρ_C).

The TT-feasibility problem in turn is identified with the QMP for $\mathcal{K} = \{\{1\}, \{1, 2\}, \dots, \{1, \dots, d-1\}\}$, that is, the problem which is concerned with the spectra of $\rho_{\{1\}}, \rho_{\{1,2\}}, \dots, \rho_{\{1,\dots,d-1\}}$ (often denoted as density matrices ρ_A, ρ_{AB}, \dots). The feasibility problem may demand an additional constraint $n_d < \infty$, which, however, only restricts $\text{rank}(\rho_I) \leq n_d$.

1.2. The quantum marginal problem. Earlier articles have answered several special instances of the QMP, which suggest that sets of compatible values form convex, closed cones.

Pure QMP for $\mathcal{K} = \{\{1\}, \dots, \{d-1\}\}$ (Tucker-feasibility). For $n_i = 2$, $i = 1, \dots, d$, the physical interpretation of the pure QMP is related to an array of qubits. For every $d \in \mathbb{N}$, it is governed by the simple inequalities

$$(1.6) \quad \lambda_2^{(\{i\})} \leq \sum_{j(\neq i)} \lambda_2^{(\{j\})}, \quad i \in I,$$

as proven by [18] (cf. subsection 1.4). All constraints for the pure QMP with $n_i = 3$, $i = 1, \dots, d$ for $d-1 = 3$, have been derived in [8, 17]. Subsequently, [21] has presented a general solution to the pure QMP for $\mathcal{K} = \{\{1\}, \{2\}, \{3\}\}$ for arbitrary n , based on geometric invariant theory, and states that the cases $d-1 > 3$ are straightforward.

QMP for $\mathcal{K} = \{\{1\}, \{1, 2\}\}$ (TT-feasibility for $d-1 = 2$). Similarly, [4] has provided an elaborate answer to this QMP in the form of a relation between cohomologies of Grassmannians. For each specific n_1 and n_2 , a finite set of linear inequalities can thereby be derived which are equivalent (cf. [1]) to compatibility. Although the two latter solutions are in a certain sense complete (from an algebraic perspective), [4] could, for example, only conjecture that in the special case $n_1 \leq n_2$, compatibility of $(\lambda^{\{1\}}, \lambda^{\{1,2\}})$ is equivalent to just

$$(1.7) \quad \sum_{i=1}^k \lambda_i^{(\{1\})} \leq \sum_{i=1}^{n_2 k} \lambda_i^{(\{1,2\})}, \quad k = 1, \dots, n_1,$$

where equality must hold for $k = n_1$ (which relates to the trace property for feasibility). This instance was later confirmed by [26] (in again different notation).

QMP for hierarchically structured \mathcal{K} . Interestingly, other classes of families \mathcal{K} pose open problems, but may be approached through tensor format theory, such as for the TT-format. If the sets in \mathcal{K} fulfill the hierarchy condition (cf. [12])

$$(1.8) \quad J \cap \tilde{J} \in \{\emptyset, J, \tilde{J}\} \quad \text{for all } J, \tilde{J} \in \mathcal{K},$$

then the equivalent feasibility problem can be decoupled into three-dimensional subproblems using a hierarchical standard representation (for both $\mathbb{K} = \mathbb{C}$ and $\mathbb{K} = \mathbb{R}$) analogous to the one we define in Proposition 2.6. We will, however, restrict ourselves to the TT-format here, since the general tensor tree network case is beyond the scope of this paper. Also, the TT-format poses a certain special case as it corresponds to a tree graph in which each node is connected with at most two other ones.

1.3. Overview of results in this work. We show that if σ and τ are feasible for $n \in \mathbb{N}^d$ (in the sense of Definition 1.1), then $v := \sqrt{\sigma^2 + \tau^2}$, evaluated entrywise, is feasible for n as well (Corollary 5.2). This means that the set of squared feasible TT-singular values forms a convex cone, which is closed and finitely generated, as is to be expected from earlier QMP results on other families of matricizations. This result is based on a decoupling (Proposition 2.6), by which we prove that the single conditions for neighboring pairs $(\gamma, \theta) = (\sigma^{(\mu-1)}, \sigma^{(\mu)})$ of singular values already provide all conditions for the higher-dimensional case (Corollary 2.10). Further, these conditions are independent of $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ (cf. Theorem 3.6).

Our slightly different perspective on feasibility of pairs (that is, $d = 3$) leads to the investigation of sets of interconnected (Definition 4.3), so-called *honeycombs* [23]. Apart from a pleasant graphical depiction (e.g., Figure 7), these constructions are at the same time a universal linear programming tool (Algorithm 6.1) which can decide the feasibility of each single pair (γ, θ) with low-order polynomial computational complexity. Hence, we can thereby also decide the feasibility of TT-singular values σ . We further provide classes of necessary, linear inequalities (Corollary 5.5) for arbitrary $n \in \mathbb{N}$ and revisit the above-mentioned special case (1.7), providing a complete vertex description as well (Corollary 5.10). Last but not least, we provide algorithms to construct tensors with prescribed, feasible singular values in parallel (subsection 3.1 and Algorithm 6.2).

1.4. Other results on the feasibility problem. Although many results can be overtaken from the QMP (see subsection 1.2), we will here give a history of the thus far independently approached feasibility problem. For higher-order tensors, several notions of rank exist, of which the TT-format and Tucker format (or higher-order SVD (HOSVD)) [5, 32] capture two particular ones. The problem of feasibility was originally introduced and defined by [15] for the Tucker decomposition. Shortly afterwards, further steps were taken in [14], from which we have borrowed some notation. However, due to the difference between the two mentioned formats, no results could, so far, be transferred. Through matrix analysis and eigenvalue relations, [6] later introduced necessary and sufficient linear inequalities regarding feasibility mostly restricted to the largest Tucker singular values of tensors with one common mode size. Independently, [30] proved the same result for the Tucker format, provided $n_1 = \dots = n_d = 2$, using yet other approaches within algebraic geometry.

This article, on the other hand, is based on a reduction through gauge conditions to coupled, pairwise problems which are then linked to eigenvalue problems and so-

called honeycombs [23]. In our TT case, which to the best of our knowledge has not been dealt with before, the literature related to honeycombs as well as [4] fortunately provide both a theoretical and practical resolution to the simpler pairwise problem (see subsection 1.3). The connection of feasibility to the Horn conjecture has, to a smaller extent, also synchronously and again independently been investigated by the aforementioned article [6], as they deal with yet different eigenvalue problems. As already mentioned in subsection 1.2, an analogous way of decoupling can be applied to the Tucker case, and indeed any other hierarchical format, so that any such feasibility problem for a d th-order tensor can be reduced to the pairwise problems as in the TT-format and/or the Tucker format in three dimensions.

1.5. Organization of article. In section 2, we use the *standard representation*, an essentially unique representation which meets important gauge conditions, to reduce the problem of TT-feasibility to only pairs of tuples of singular values. In section 3, we show the relation to the Horn conjecture, giving a short overview of related results, and in section 4 apply these to our problem with the help of *honeycombs*. We thereby identify the topological structure of sets of squared TT-feasible singular values as cones, which we further investigate in section 5. Related algorithms can be found in section 6.

2. Reduction to modewise eigenvalues problems. For the sake of simplicity, in the remainder of the article, we set $r_0 = r_d = 1$ as well as $\sigma_+^{(0)} = \sigma_+^{(d)} = 1$. The set of all tensors with (TT-)rank r is denoted by $TT(r) \subset \mathbb{K}^{n_1 \times \dots \times n_d}$ (see [28]). This set is closely related to so-called *representations* (or decompositions) $G = (G_1, \dots, G_d)$, where each so-called *core*

$$G_\mu \in (\mathbb{K}^{r_{\mu-1} \times r_\mu})^{n_\mu} \cong \mathbb{K}^{r_{\mu-1} \times r_\mu \times n_\mu}$$

is an array of matrices $G_\mu(i_\mu) \in \mathbb{K}^{r_{\mu-1} \times r_\mu}$, $i_\mu = 1, \dots, n_\mu$. This emphasizing notation originally stems from the *matrix product states (MPS) format* [33], but is also used widely in TT literature. For now we call $r = (r_1, \dots, r_{d-1}) \in \mathbb{N}^{d-1}$ the size of G (cf. Theorem 2.3).

DEFINITION 2.1 (representation map). *For representations G of size $r \in \mathbb{N}^{d-1}$ as above, we define the representation map τ_r via*

$$\tau_r : \bigtimes_{\mu=1}^d (\mathbb{K}^{r_{\mu-1} \times r_\mu})^{n_\mu} \rightarrow \mathbb{K}^{n_1 \times \dots \times n_d}, \quad \tau_r(G) := A,$$

where each entry of the tensor A is a product of matrices in G ,

$$A(i_1, \dots, i_d) := G_1(i_1) \cdot \dots \cdot G_d(i_d)$$

for all $i_\mu = 1, \dots, n_\mu$, $\mu = 1, \dots, d$.

The product \boxtimes , which we define for cores in Definition 2.2, can be viewed as a generalization of the outer product \otimes for vectors in $\mathbb{K}^{n_\mu} \cong (\mathbb{K}^{1 \times 1})^{n_\mu}$.

DEFINITION 2.2 (TT-product). *For $k_1, k_2, k_3, \ell, s \in \mathbb{N}$, $1 \leq s < \ell$, and $m \in \mathbb{N}^\ell$, we define the product*

$$\begin{aligned} \boxtimes : (\mathbb{K}^{k_1 \times k_2})^{m_1 \times \dots \times m_s} \times (\mathbb{K}^{k_2 \times k_3})^{m_{s+1} \times \dots \times m_\ell} &\rightarrow (\mathbb{K}^{k_1 \times k_3})^{m_1 \times \dots \times m_\ell} \\ (H_1 \boxtimes H_2)(i_1, \dots, i_m) &:= H_1(i_1, \dots, i_s) \cdot H_2(i_{s+1}, \dots, i_\ell) \in \mathbb{K}^{k_1 \times k_3} \end{aligned}$$

for all $i_\mu = 1, \dots, m_\mu$. We may skip the symbol \boxtimes in products of a core and matrix (interpreting matrices as arrays of length one).

For example, the product of two single cores is a two-dimensional array of matrices. This then extends to $A = G_1 \boxtimes \cdots \boxtimes G_d$ (having implicitly used the isomorphism $\mathbb{K}^{1 \times 1} \cong \mathbb{K}$). The TT-SVD,³ a generalization of the matrix SVD, provides the following theorem.

THEOREM 2.3 (see [28]). *It holds that $\text{range}(\tau_r) = \bigcup_{\tilde{r} \leq r} TT(\tilde{r})$, where $\tilde{r} \leq r \in \mathbb{N}^{d-1}$ is to be read entrywise.*

Hence, for every tensor with (TT-)rank r , $A \in TT(r)$, there is a representation G of size r for which $A = \tau_r(G)$. One therefore also says G has rank r . These representations will allow us to change the perspective on feasibility and reduce the problem from a $(d-1)$ -tuple to local, pairwise problems.

DEFINITION 2.4 (left and right unfoldings). *For a (product of) cores $H \in (\mathbb{K}^{k_1 \times k_2})^{m_1 \times \cdots \times m_s}$ (cf. Definition 2.2), the left unfolding $\mathfrak{L}(H) \in \mathbb{K}^{k_1 \cdot (m_1 \cdots m_s) \times k_2}$ is obtained by stacking the matrices $H(i_1, \dots, i_s) \in \mathbb{K}^{k_1 \times k_2}$ on top of each other in one column, and, likewise, the right unfolding $\mathfrak{R}(H) \in \mathbb{K}^{k_1 \times k_2 \cdot (m_1 \cdots m_s)}$ is formed by stacking the same matrices, but side by side, in one row (in co-lexicographic order). Explicitly,*

$$\begin{aligned}\mathfrak{L}(H) &:= [H(1, 1, \dots, 1)^T \quad H(2, 1, \dots, 1)^T \quad \dots \quad H(m_1, \dots, m_s)^T]^T, \\ \mathfrak{R}(H) &:= [H(1, 1, \dots, 1) \quad H(2, 1, \dots, 1) \quad \dots \quad H(m_1, \dots, m_s)].\end{aligned}$$

H is called left-unitary if $\mathfrak{L}(H)$ is column-unitary, and right-unitary if $\mathfrak{R}(H)$ is row-unitary.⁴ For a representation G , we correspondingly define the interface matrices

$$\begin{aligned}G^{\leq \mu} &= \mathfrak{L}(G_1 \boxtimes \cdots \boxtimes G_\mu) \in \mathbb{K}^{n_1 \cdots n_\mu \times r_\mu}, \\ G^{\geq \mu} &= \mathfrak{R}(G_\mu \boxtimes \cdots \boxtimes G_d) \in \mathbb{K}^{r_{\mu-1} \times n_\mu \cdots n_d}, \quad \mu = 1, \dots, d.\end{aligned}$$

We also use $G^{<\mu} := G^{\leq \mu-1}$ and $G^{>\mu} := G^{\geq \mu+1}$.

For any tensor $A = \tau_r(G)$ it thus holds that $A^{(\{1, \dots, \mu\})} = G^{\leq \mu} G^{> \mu}$, $\mu = 1, \dots, d$. If we for a moment interpret H as tensor $H \in \mathbb{K}^{k_1 \times k_2 \times m_1 \times \cdots \times m_s}$, then $\mathfrak{L}(H)^T = H^{(\{2\})}$ and $\mathfrak{R}(H) = H^{(\{1\})}$ (cf. [12]).

DEFINITION 2.5 (set of weakly decreasing tuples/sequences). *For $n \in \mathbb{N}$, let $\mathcal{D}^n \subset \mathbb{R}^n$ be the cone of weakly decreasing n -tuples, and let $\mathcal{D}_{\geq 0}^n := \mathcal{D}^n \cap \mathbb{R}_{\geq 0}^n$ be its restriction to nonnegative numbers. Further, let $\mathcal{D}_{\geq 0}^\infty \subset \mathbb{R}^\mathbb{N}$ be the cone of weakly decreasing, nonnegative sequences with finitely many nonzero entries.*

The positive part $v_+ \in \mathcal{D}_{>0}^{\deg(v)}$ is defined as the positive elements of v , where $\deg(v) := \max_{i: v_i > 0} i$ is its degree. For $n \neq \infty$, the negation $-v \in \mathcal{D}_{\leq 0}^n$ of $v \in \mathcal{D}_{\geq 0}^n$ is defined via $-v := (-v_n, \dots, -v_1)$ (cf. [23]).

For example, for $\gamma = (2, 2, 1, 0, 0, \dots) \in \mathcal{D}_{\geq 0}^\infty$, we have $\deg(\gamma) = 3$ and $\gamma_+ = (2, 2, 1) \in \mathcal{D}_{>0}^3$ as well as $-\gamma_+ = (-1, -2, -2)$. Similarly to before, we will denote $\Gamma := \text{diag}(\gamma_+) = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. With a tilde, we will emphasize that a tuple may contain zeros, that is, $\tilde{\gamma} \in \{v \in \mathcal{D}_{\geq 0}^n \mid v_+ = \gamma_+, n \geq \deg(\gamma)\}$. For example, we may have $\tilde{\gamma} = (2, 2, 1, 0) \in \mathcal{D}_{\geq 0}^4$.

³Although called SVD, the singular values do not explicitly appear in the decomposition as in the matrix SVD.

⁴For $\mathbb{K} = \mathbb{R}$, unitary is just orthonormal.

The map τ_r is not injective. However, there is an essentially unique *standard representation* (in terms of uniqueness of the truncated matrix SVD⁵). In the context of matrix product states, it has previously appeared in [33] and is frequently referred to as *canonical MPS*. Instead of just d cores, this extended representation also contains the tuple of TT-singular values. For that matter, it is easy to verify that if both H and N are left- or right-unitary, then $H \boxtimes N$ is left- or right-unitary, respectively.

PROPOSITION 2.6 (standard representation). *Let $A \in \mathbb{K}^{n_1 \times \dots \times n_d}$ be a tensor, and let $\Sigma^{(1)} = \text{diag}(\sigma_+^{(1)}), \dots, \Sigma^{(d-1)} = \text{diag}(\sigma_+^{(d-1)})$ be square diagonal matrices which contain the positive TT-singular values of A . Then there exists an essentially unique (extended) representation*

$$\mathcal{G}^\sigma := (\mathcal{G}, \sigma) := (\mathcal{G}_1, \sigma^{(1)}, \mathcal{G}_2, \sigma^{(2)}, \dots, \mathcal{G}_{d-1}, \sigma^{(d-1)}, \mathcal{G}_d),$$

with cores $\mathcal{G}_\mu \in (\mathbb{K}^{r_{\mu-1} \times r_\mu})^{n_\mu}$, $r_\mu = \deg(\sigma^{(\mu)})$, $\mu = 1, \dots, d$, for which the following property holds:

- (1) For each $\mu = 1, \dots, d-1$,

$$(2.1) \quad \mathfrak{L}(\mathcal{G}_1 \boxtimes \Sigma^{(1)} \mathcal{G}_2 \boxtimes \dots \boxtimes \Sigma^{(\mu-1)} \mathcal{G}_\mu) = \Sigma^{(\mu)} = \mathfrak{R}(\mathcal{G}_{\mu+1} \Sigma^{(\mu+1)} \boxtimes \dots \boxtimes \mathcal{G}_d)$$

is a (truncated) matrix SVD of $A^{\{1, \dots, \mu\}}$.

Essentially unique here means that for any other such representation $\tilde{\mathcal{G}}^\sigma$, it holds that $\tilde{\mathcal{G}}_\mu = w_{\mu-1}^H \mathcal{G}_\mu w_\mu$, $\mu = 1, \dots, d$, where each w_μ is a unitary matrix that commutes with $\Sigma^{(\mu)}$ (and $w_0 = w_d = 1$).

COROLLARY 2.7. *Property (1) in Proposition 2.6 is equivalent to the following:*

- (2) It holds that

$$(2.2) \quad A = \mathcal{G}_1 \boxtimes \Sigma^{(1)} \boxtimes \mathcal{G}_2 \boxtimes \Sigma^{(2)} \boxtimes \dots \boxtimes \mathcal{G}_{(d-2)} \boxtimes \Sigma^{(d-1)} \boxtimes \mathcal{G}_d$$

and $\mathcal{G}_1, \Sigma^{(\mu-1)} \mathcal{G}_\mu, \mu = 2, \dots, d-1$, are left-unitary and $\mathcal{G}_\mu \Sigma^{(\mu)}, \mu = 2, \dots, d-1, \mathcal{G}_d$ are right-unitary (cf. Definition 2.4).

Hence also this property provides essential uniqueness.

Proof of Proposition 2.6.

Uniqueness: In the following, each w_μ denotes some unitary matrix that commutes (therefore the lowercase letter) with $\Sigma^{(\mu)}$. Let there be two such representations, $\tilde{\mathcal{G}}^\sigma$ and \mathcal{G}^σ . First, $\mathfrak{L}(\mathcal{G}_1) = \mathfrak{L}(\tilde{\mathcal{G}}_1)w_1$ since both left-unfoldings contain the left-singular vectors of $A^{\{1\}}$ due to (2.1). By induction hypothesis (*IH*), let $\tilde{\mathcal{G}}_s = w_{s-1}^H \mathcal{G}_s w_s$ for $s < \mu$. Analogously, we have

$$\begin{aligned} (\mathcal{G}_1 \boxtimes \dots \boxtimes \Sigma^{(\mu-1)} \mathcal{G}_\mu) &\stackrel{(2.1)}{=} (\tilde{\mathcal{G}}_1 \boxtimes \Sigma^{(1)} \tilde{\mathcal{G}}_2 \boxtimes \dots \boxtimes \Sigma^{(\mu-2)} \tilde{\mathcal{G}}_{\mu-1} \boxtimes \Sigma^{(\mu-1)} \tilde{\mathcal{G}}_\mu) w_\mu^H \\ &\stackrel{(\text{IH})}{=} (\mathcal{G}_1 w_1 \boxtimes \Sigma^{(1)} w_1^H \mathcal{G}_2 w_2 \boxtimes \dots \boxtimes \Sigma^{(\mu-2)} w_{\mu-2}^H \mathcal{G}_{\mu-1} w_{\mu-1} \boxtimes \Sigma^{(\mu-1)} \tilde{\mathcal{G}}_\mu) w_\mu^H \\ &\stackrel{w_\mu \Sigma^{(\mu)} w_\mu^H = \Sigma^{(\mu)}}{=} \mathcal{G}_1 \boxtimes \Sigma^{(1)} \mathcal{G}_2 \boxtimes \dots \boxtimes \Sigma^{(\mu-2)} \mathcal{G}_{\mu-1} \boxtimes \Sigma^{(\mu-1)} (w_{\mu-1} \tilde{\mathcal{G}}_\mu w_\mu^H). \end{aligned}$$

Since $T := \mathcal{G}_1 \boxtimes \dots \boxtimes \Sigma^{(\mu-2)} \mathcal{G}_{\mu-1}$ is left-unitary by (2.1), the map $H \mapsto T \boxtimes \Sigma^{(\mu-1)} H$ is injective, and it follows that $\tilde{\mathcal{G}}_\mu = w_{\mu-1}^H \mathcal{G}_\mu w_\mu$. This completes the inductive argument.

⁵Both $U\Sigma V^H$ and $\tilde{U}\Sigma\tilde{V}^H$ are truncated SVDs of A if and only if there exists a unitary matrix w that commutes with Σ and for which $\tilde{U} = Uw$ and $\tilde{V} = Vw$. For any subset of pairwise distinct nonzero singular values, the corresponding submatrix of w needs to be diagonal with entries in $\{z \in \mathbb{K} \mid |z| = 1\}$.

Existence (constructive): Let G be a representation of $A = \tau_r(G)$, where G_μ , $\mu = 2, \dots, d$, are right-unitary (this can always be achieved using the degrees of freedom within a representation) as well as $V_0 := 1$, $\Sigma^{(0)} := 1$. For $\mu = 1, \dots, d-1$, let the cores \mathcal{G}_μ , U_μ and the matrix V_μ be defined via

$$\mathfrak{L}(U_\mu) \Sigma^{(\mu)} V_\mu^H \stackrel{\text{SVD}}{:=} \mathfrak{L}(\Sigma^{(\mu-1)} V_{\mu-1}^H G_\mu), \quad \mathcal{G}_\mu := (\Sigma^{(\mu-1)})^{-1} U_\mu.$$

as well as $\mathcal{G}_d := V_{d-1}^H G_d$. By construction, (2.2) holds and each $\Sigma^{(\mu-1)} \mathcal{G}_\mu = U_\mu$ is left-unitary. Since further each $\mathfrak{L}(U^{\leq \mu}) \Sigma^{(\mu)} \mathfrak{R}(V_\mu^H G^{>\mu})$ is an SVD of $A^{(\{1, \dots, \mu\})}$, $\mu = 1, \dots, d-1$, also (2.1) holds true. \square

It is also possible to construct the standard representation directly from A by defining $\mathfrak{L}(U_\mu) \Sigma^{(\mu)} B_\mu^{(\{1\})} \stackrel{\text{SVD}}{:=} B_{\mu-1}^{(\{1,2\})}$, $B_\mu \in \mathbb{K}^{r_\mu \times n_{\mu+1} \times \dots \times n_d}$, $\mathcal{G}_\mu := (\Sigma^{(\mu-1)})^{-1} U_\mu$ for $\mu = 1, \dots, d-1$ as well as $\mathfrak{R}(\mathcal{G}_d) := B_{d-1}^{(\{1\})}$, and the starting value $B_0^{(\{1,2\})} := A^{(\{1\})}$.

Proof of Corollary 2.7. “(2) \Rightarrow (1)”: This follows directly by transitivity of left- or right-unitary.

“(1) \Rightarrow (2)”: In the previous construction in the proof of Proposition 2.6, the core $\mathcal{G}_\mu \Sigma^{(\mu)} = (\Sigma^{(\mu-1)})^{-1} U_\mu \Sigma^{(\mu)} = V_{\mu-1}^H G_\mu V_\mu$ is right-unitary ($V_0 := 1$, $\Sigma^{(0)} := 1$) and $\Sigma^{(\mu-1)} \mathcal{G}_\mu$ is left-unitary. Due to Proposition 2.6, property (1) provides the (essential) uniqueness of that \mathcal{G}^σ . Hence, these constraints hold independently of the construction. \square

COROLLARY 2.8. *Let $\mathcal{G}^\sigma = (\mathcal{G}_1, \sigma^{(1)}, \mathcal{G}_2, \dots, \sigma^{(d-1)}, \mathcal{G}_d)$ such that property (2) in Corollary 2.7 is fulfilled. Then A is a tensor in $TT(r)$ with TT-singular values σ and standard representation \mathcal{G}^σ .*

By basic linear algebra, a left-unitary core $H \in (\mathbb{K}^{1 \times k})^m$ (analogously a right-unitary core $H \in (\mathbb{K}^{k \times 1})^m$) exists if and only if $k \leq m$. In three dimensions, the decoupling through the standard representation (Corollary 2.7 for $d = 3$) yields the following.

COROLLARY 2.9. *For $m \in \mathbb{N}$, a pair $(\gamma, \theta) \in \mathcal{D}_{\geq 0}^\infty \times \mathcal{D}_{\geq 0}^\infty$ is feasible for the triplet $(\deg(\gamma), m, \deg(\theta))$ if and only if there exists a core $H \in (\mathbb{K}^{\deg(\gamma) \times \deg(\theta)})^m$ for which ΓH is left-unitary and $H\Theta$ is right-unitary, $\Gamma = \text{diag}(\gamma_+)$, $\Theta = \text{diag}(\theta_+)$.*

Proof. Let⁶ (γ, θ) be feasible for $(\deg(\gamma), m, \deg(\theta))$. Then by Corollary 2.7 there exists an (extended) standard representation $\mathcal{G}^\sigma = (\mathcal{G}_1, \gamma, \mathcal{G}_2, \theta, \mathcal{G}_3)$ for which $H := \mathcal{G}_2$ fulfills the unitary conditions as required. For the other direction, let H be given. There exist some left-unitary core $H_{\text{left}} \in (\mathbb{K}^{1 \times \deg(\gamma)})^{\deg(\gamma)}$ as well as some right-unitary core $H_{\text{right}} \in (\mathbb{K}^{\deg(\theta) \times 1})^{\deg(\theta)}$. These, together with γ and θ , then form the (extended) standard representation of $B := H_{\text{left}} \boxtimes \Gamma \boxtimes H \boxtimes \Theta \boxtimes H_{\text{right}} \in \mathbb{K}^{\deg(\gamma) \times m \times \deg(\theta)}$. By Corollaries 2.7 and 2.8, this tensor provides the feasibility of (γ, θ) as required. \square

COROLLARY 2.10 (decoupling). $\sigma \in (\mathcal{D}_{\geq 0}^\infty)^{d-1}$ is feasible for $n \in \mathbb{N}^d$ if and only if $\deg(\sigma^{(1)}) \leq n_1$, $\deg(\sigma^{(d-1)}) \leq n_d$ and for each $\mu = 2, \dots, d-1$, the pair $(\sigma^{(\mu-1)}, \sigma^{(\mu)})$ is feasible for $(\deg(\sigma^{(\mu-1)}), n_\mu, \deg(\sigma^{(\mu)}))$.

⁶In this case, the statement can also be derived via [5], as the HOSVD provides the equivalence of the feasibility to the existence of an *all-unitary* tensor S . If we reshape this tensor into a core $S \in (\mathbb{K}^{\deg(\gamma) \times \deg(\theta)})^m$, then the core $H := \Gamma^{-1} S \Theta^{-1}$ fulfills the required unitary conditions.

Proof. Let σ be feasible. Then this is equivalent (cf. Corollaries 2.7 and 2.8) to the existence of an extended representation \mathcal{G}^σ , such that each \mathcal{G}_μ fulfills the unitary conditions as in Corollary 2.7. For each fixed $\mu \in \{2, \dots, d-1\}$, Corollary 2.9 for $H := \mathcal{G}_\mu$, $\gamma := \sigma^{(\mu-1)}$, $\theta := \sigma^{(\mu)}$ provides the equivalence of the unitary conditions to the feasibility of the pair $(\sigma^{(\mu-1)}, \sigma^{(\mu)})$ for $(\deg(\sigma^{(\mu-1)}), n_\mu, \deg(\sigma^{(\mu)}))$. As remarked before, \mathcal{G}_1 can only be left-unitary if $\deg(\sigma^{(1)}) \leq n_1$, and \mathcal{G}_d can only be left-unitary if $\deg(\sigma^{(d-1)}) \leq n_d$. \square

Note that feasibility for $(\deg(\gamma), m, \deg(\theta))$ of (γ, θ) (cf. Corollary 2.9) implies feasibility for (n_1, m, n_3) , provided $\deg(\gamma) \leq n_1$, $\deg(\theta) \leq n_3$. Additionally, Corollary 2.10 for $d = 3$ provides the other direction, showing equivalence.

THEOREM 2.11 (equivalence to an eigenvalue problem). *Let $m \in \mathbb{N}$. A pair $(\gamma, \theta) \in \mathcal{D}_{\geq 0}^\infty \times \mathcal{D}_{\geq 0}^\infty$ is feasible for $(\deg(\gamma), m, \deg(\theta))$ if and only if the following holds: There exist m pairs of Hermitian,⁷ positive semidefinite matrices $(A^{(i)}, B^{(i)}) \in \mathbb{K}^{\deg(\theta) \times \deg(\theta)} \times \mathbb{K}^{\deg(\gamma) \times \deg(\gamma)}$, each with identical (multiplicities of) eigenvalues up to zeros, such that $A := \sum_{i=1}^m A^{(i)}$ has eigenvalues θ_+^2 and $B := \sum_{i=1}^m B^{(i)}$ has eigenvalues γ_+^2 .*

Proof (constructive). We show both directions separately.

“ \Rightarrow ”: Let (γ, θ) be feasible for m . Then by Corollary 2.9, for $\Gamma = \text{diag}(\gamma_+)$, $\Theta = \text{diag}(\theta_+)$, and a single core \widehat{N} , we have both $\sum_{i=1}^m \widehat{N}(i)^H \Gamma^2 \widehat{N}(i) = I$ as well as $\sum_{i=1}^m \widehat{N}(i) \Theta^2 \widehat{N}(i)^H = I$. By substitution of $\widehat{N} = \Gamma^{-1} N \Theta^{-1}$, this is equivalent to

$$(2.3) \quad \sum_{i=1}^m N(i)^H N(i) = \Theta^2, \quad \sum_{i=1}^m N(i) N(i)^H = \Gamma^2.$$

Now, for $A^{(i)} := N(i)^H N(i)$ and $B^{(i)} := N(i) N(i)^H$, we have found matrices as desired, since the eigenvalues of $A^{(i)}$ and $B^{(i)}$ are each the same (up to zeros).

“ \Leftarrow ”: Let $A^{(i)}$ and $B^{(i)}$ be matrices as required. Then, by eigenvalue decompositions, $A = Q_A \Theta^2 Q_A^H$, $B = Q_B \Gamma^2 Q_B^H$ for unitary Q_A , Q_B , and thereby $\sum_{i=1}^m Q_A^H A^{(i)} Q_A = \Theta^2$ and $\sum_{i=1}^m Q_B^H B^{(i)} Q_B = \Gamma^2$. Then again, by truncated eigenvalue decompositions of these summands, we obtain

$$Q_A^H A^{(i)} Q_A = V_i S_i V_i^H, \quad Q_B^H B^{(i)} Q_B = U_i S_i U_i^H, \quad S_i \in \mathbb{R}^{r \times r},$$

for $r = \min(\deg(\gamma), \deg(\theta))$, unitary (eigenvectors) V_i, U_i , and shared (positive eigenvalues) S_i . With the choice $N(i) := U_i S_i^{1/2} V_i^H$, we arrive at (2.3), which is equivalent to the desired statement. \square

Remark 2.12 (diagonalization). Since the condition regarding the sums of Hermitian matrices in Theorem 2.11 remains true under conjugation, we may assume, without loss of generality, that $A = \Theta^2$ and $B = \Gamma^2$.

3. Feasibility of pairs. We have shown in the previous section, i.e., Corollary 2.10, that we only have to consider the feasibility of pairs (γ, θ) for mode sizes $(\deg(\gamma), m, \deg(\theta))$. In order to avoid the redundant entries $\deg(\gamma)$ and $\deg(\theta)$, we will from now on abbreviate as follows.

DEFINITION 3.1 (feasibility of pairs). *For $m \in \mathbb{N}$, we say a pair (γ, θ) is feasible for m if and only if it is feasible for $(\deg(\gamma), m, \deg(\theta))$ (cf. Definition 1.1).*

⁷For $\mathbb{K} = \mathbb{R}$, Hermitian is just symmetric and the conjugate transpose $.^H$ is just the transpose $.^T$.

As outlined in subsection 1.1, the property is equivalent to the compatibility of (γ^2, θ^2) for $(\deg(\gamma), m)$ given $\mathcal{K} = \{\{1\}, \{1, 2\}\}$. In fact, there exist several results on this topic as discussed in subsection 1.2, e.g., that compatible pairs form a cone. In the following, we analyze the problem from the different perspective provided by Theorem 2.11.

3.1. Constructive, diagonal feasibility. The feasibility of pairs is a reflexive and symmetric relation, but it is not transitive. In some cases, verification can be easier.

LEMMA 3.2 (diagonally feasible pairs). *Let $(\gamma, \theta) \in \mathcal{D}_{\geq 0}^\infty \times \mathcal{D}_{\geq 0}^\infty$ as well as $a^{(1)}, \dots, a^{(m)} \in \mathbb{R}_{\geq 0}^r$, $r = \max(\deg(\gamma), \deg(\theta))$, and permutations $\pi_1, \dots, \pi_m \in S_r$ such that*

$$a_i^{(1)} + \dots + a_i^{(m)} = \gamma_i^2, \quad a_{\pi_1(i)}^{(1)} + \dots + a_{\pi_m(i)}^{(m)} = \theta_i^2, \quad i = 1, \dots, r.$$

Then (γ, θ) is feasible for m (we write diagonally feasible in that case). For $m, r_1, r_2 \in \mathbb{N}$, $\gamma_+^2 = (1, \dots, 1)$ of length r_1 and $\theta_+^2 = (k_1, \dots, k_{r_2}) \in \mathcal{D}_{\geq 0}^{r_2} \cap \{1, \dots, m\}^{r_2}$, with $\|k\|_1 = r_1$, the pair (γ, θ) is diagonally feasible for m .

Proof. The given criterion is just the restriction to diagonal matrices in Theorem 2.11. All sums of zero-eigenvalues can be ignored; i.e., we also find diagonal matrices of actual sizes $\deg(\gamma) \times \deg(\gamma)$ and $\deg(\theta) \times \deg(\theta)$. The subsequent explicit set of feasible pairs follows immediately by restricting $a_i^{(\ell)} \in \{0, 1\}$ and by using appropriate permutations. \square

For example, to show that (γ, θ) , $\gamma_+^2 = (1, 1, 1, 1)$, $\theta_+^2 = (2, 2)$, is feasible for $m = 2$, we can set $a^{(1)} = (1, 1, 0, 0)$, $a^{(2)} = (0, 0, 1, 1)$, and $\pi_1 = \text{Id}$, $\pi_2 = (1, 3, 2, 4)$. The resulting matrices in Theorem 2.11 then are $B^{(1)} = \text{diag}((1, 1, 0, 0))$, $B^{(2)} = \text{diag}((0, 0, 1, 1))$ as well as $A^{(1)} = A^{(2)} = \text{diag}((1, 1))$. Following the procedure in Theorem 2.11, we obtain the single core N , for which ΓN , $N\Theta$ are left- and right-unitary, respectively:

$$N(1) = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \\ 0 & 0 \end{bmatrix}, \quad N(2) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}.$$

Although for $m = 2$, $r \leq 3$, each feasible pair happens to be diagonally feasible, this does not hold in general. For example, the pair (γ, θ) ,

$$(3.1) \quad \gamma_+^2 = (7.5, 5) \quad \text{and} \quad \theta_+^2 = (6, 3.5, 2, 1),$$

is feasible (cf. (1.7) or Figure 6) for $m = 2$, but it is quite easy to verify that it is not diagonally feasible.

DEFINITION 3.3 (set of feasible pairs). *Let $\mathcal{F}_{m,(r_1,r_2)}$ be the set of pairs $(\tilde{\gamma}, \tilde{\theta}) \in \mathcal{D}_{\geq 0}^{r_1} \times \mathcal{D}_{\geq 0}^{r_2}$ for which $(\gamma, \theta) = ((\tilde{\gamma}, 0, \dots), (\tilde{\theta}, 0, \dots))$ is feasible for m (cf. Definition 3.1), and*

$$\mathcal{F}_{m,(r_1,r_2)}^2 := \{(\gamma_1^2, \dots, \gamma_{r_1}^2, \theta_1^2, \dots, \theta_{r_2}^2) \mid (\tilde{\gamma}, \tilde{\theta}) \in \mathcal{F}_{m,(r_1,r_2)}\}.$$

The following theorem is a special case of (1.7) and features a constructive proof as outlined below.

THEOREM 3.4. Let $m \in \mathbb{N}$. If $r_1, r_2 \leq m$, then

$$\mathcal{F}_{m,(r_1,r_2)} = \mathcal{D}_{\geq 0}^{r_1} \times \mathcal{D}_{\geq 0}^{r_2} \cap \{(\tilde{\gamma}, \tilde{\theta}) \mid \|\tilde{\gamma}\|_2 = \|\tilde{\theta}\|_2\},$$

that is, any pair $(\gamma, \theta) \in \mathcal{D}_{\geq 0}^{\infty} \times \mathcal{D}_{\geq 0}^{\infty}$ with $\deg(\gamma), \deg(\theta) \leq m$, for which the trace property holds true, is (diagonally) feasible for m .

Proof. We give a proof by contradiction. Set $\tilde{\gamma} = (\gamma_+, 0, \dots, 0)$ as well as $\tilde{\theta} = (\theta_+, 0, \dots, 0)$ such that both have length m . Let the permutation $\tilde{\pi}$ be given by the cycle $(1, \dots, m)$ and $\pi_\ell := \tilde{\pi}^{\ell-1}$. For each k , let $R_k := \{(i, \ell) \mid \pi_\ell(k) = i\}$. Now, let the nonnegative (eigen)values $a_i^{(\ell)}$, $\ell, i = 1, \dots, m$, form a minimizer of $w := \|A(1, \dots, 1)^T - \tilde{\gamma}^2\|_1$, subject to

$$\sum_{(i,\ell) \in R_k} a_i^{(\ell)} = a_{\pi_1(k)}^{(1)} + \dots + a_{\pi_m(k)}^{(m)} = \theta_k^2, \quad k = 1, \dots, m,$$

where $A = \{a_i^{(\ell)}\}_{(i,\ell)}$ (the minimizer exists since the allowed values form a compact set). For $m = 3$, for example, we aim at the following, where R_3 has been highlighted.

$$\begin{pmatrix} a_{\pi_1(1)}^{(1)} & a_{\pi_2(3)}^{(2)} & a_{\pi_3(2)}^{(3)} \\ a_{\pi_1(2)}^{(1)} & a_{\pi_2(1)}^{(2)} & a_{\pi_3(3)}^{(3)} \\ a_{\pi_1(3)}^{(1)} & a_{\pi_2(2)}^{(2)} & a_{\pi_3(1)}^{(3)} \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \rightarrow \begin{pmatrix} \gamma_1^2 \\ \gamma_2^2 \\ \gamma_3^2 \end{pmatrix}.$$

Further, let

$$\#\gtrless := \{i \mid a_i^{(1)} + \dots + a_i^{(m)} \gtrless \gamma_i^2, i = 1, \dots, m\}.$$

As $\|\gamma\|_2 = \|\theta\|_2$ by assumption, either $\#>$ and $\#<$ are both empty or both not empty. In the first case, we are finished. Assume, therefore, that there is an $(i, j) \in \#> \times \#<$. Then there is an index ℓ_1 such that $a_i^{(\ell_1)} > 0$ as well as indices k and ℓ_2 such that $(i, \ell_1), (j, \ell_2) \in R_k$. This is, however, a contradiction, since replacing $a_i^{(\ell_1)} \leftarrow a_i^{(\ell_1)} - \varepsilon$ and $a_j^{(\ell_2)} \leftarrow a_j^{(\ell_2)} + \varepsilon$ for some small enough $\varepsilon > 0$ is valid, but yields a lower minimum w . Hence it already holds that $a_i^{(1)} + \dots + a_i^{(m)} = \gamma_i^2, i = 1, \dots, m$. Due to Lemma 3.2, the pair (γ, θ) is feasible. \square

The entries $a_i^{(\ell)}$ can be found via a linear programming algorithm, since they are given through linear constraints. A corresponding core can easily be calculated subsequently, as the proof of Theorem 2.11 is constructive.

In the following section, we address related theory that was subject to nearly a century of development. Fortunately, many results in that area can be transferred—last but not least because of the work of Knutson and Tao and their illustrative theory of *honeycombs* [23].

3.2. Weyl's problem and the Horn conjecture. In 1912, Weyl posed a problem [34] that asks for an analysis of the following relation.

DEFINITION 3.5 (eigenvalues of a sum of two Hermitian matrices [23]). *Let $\lambda, \mu, \nu \in \mathcal{D}^n$. Then the relation*

$$(3.2) \quad \lambda \boxplus \mu \sim_c \nu$$

is defined to hold if there exist Hermitian matrices $A, B \in \mathbb{C}^{n \times n}$ and $C := A + B$ with eigenvalues λ, μ , and ν , respectively. This definition is straightforwardly extended to more than two summands.⁸

The relation (3.2) may equivalently be written as $\lambda \boxplus \mu \boxplus (-\nu) \sim_c 0$ (cf. [23] and Definition 2.5). A result that was discovered much later by Fulton [10], which we want to pull forward, states that there is no difference when restricting oneself to real matrices.

THEOREM 3.6 (see [10, Theorem 3]). *A triplet (λ, μ, ν) occurs as eigenvalues for an associated triplet of real symmetric matrices if and only if it appears as one for Hermitian matrices.*

Assuming without loss of generality $\deg(\gamma) \leq \deg(\theta)$, the condition (cf. Theorem 2.11) for the feasibility of a pair (γ, θ) for m can now be restated as follows: There exist $a_1, \dots, a_m \in \mathcal{D}_{\geq 0}^{\deg(\gamma)}$ with $a_1 \boxplus \dots \boxplus a_m \sim_c \gamma_+^2$ and $(a_1, 0, \dots) \boxplus \dots \boxplus (a_m, 0, \dots) \sim_c \theta_+^2$. Theorem 4.8 below uses Theorem 3.6 to confirm that the initial choice $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ is also irrelevant regarding the conditions for feasibility.

Weyl and Fan [7] were among the first ones to give necessary, linear inequalities to the relation (3.2). We refer to the (survey) article “Honeycombs and Sums of Hermitian Matrices”⁹ [23] by Knutson and Tao, which has been the main point of reference for the remaining part and serves as historical survey as well (see also [2]). We use parts of their notation as long as we remain within this topic. Therefore, m remains the number of matrices ($m = 2$ in Definition 3.5), but n denotes the size of the Hermitian matrices and r is used as the index. Horn introduced the famous *Horn conjecture* in 1962.

THEOREM 3.7 ((verified) Horn conjecture [19]). *There is a specific set $T_{r,n}$ (defined, for example, in [2]) of triplets of monotonically increasing r -tuples such that the following holds: The relation $\lambda \boxplus \mu \sim_c \nu$ is satisfied if and only if for each $(i, j, k) \in T_{r,n}$, $r = 1, \dots, n - 1$, the inequality*

$$(3.3) \quad \nu_{k_1} + \dots + \nu_{k_r} \leq \lambda_{i_1} + \dots + \lambda_{i_r} + \mu_{j_1} + \dots + \mu_{j_r}$$

holds, as well as the trace property $\sum_{i=1}^n \lambda_i + \sum_{i=1}^n \mu_i = \sum_{i=1}^n \nu_i$.

As already indicated, the conjecture is correct, as proven through the contributions of Knutson and Tao (cf. section 4) and Klyachko [20]. Fascinatingly, the quite inaccessible, recursively defined set $T_{r,n}$ can in turn be described by eigenvalue relations themselves, as stated by Fulton [10].

THEOREM 3.8 (description of $T_{r,n}$ [10, 19, 23]). *Let $\Delta\ell := (\ell_r - r, \ell_{r-1} - (r - 1), \dots, \ell_2 - 2, \ell_1 - 1) \in \mathcal{D}_{\geq 0}^r$ for any set or tuple ℓ of r increasing natural numbers. The triplet (i, j, k) of such is in $T_{r,n}$ if and only if for the corresponding triplet it holds that $\Delta i \boxplus \Delta j \sim_c \Delta k$.*

Even with just diagonal matrices, one can thereby derive various (possibly all) triplets. For example, Ky Fan’s inequality [7], $\sum_{i=1}^k \nu_i \leq \sum_{i=1}^k \lambda_i + \sum_{i=1}^k \mu_i$, relates to the simple $0 \boxplus 0 \sim_c 0 \in \mathbb{R}^k$, $k = 1, \dots, n$. A further interesting property, as already shown by Horn, is given if (3.3) holds as equality.

⁸The symbol \boxplus used in [23] only appears within such relations and hints at the addition of A and B . There is no relation to the earlier used \boxtimes .

⁹To the best of our knowledge, in Conjecture 1 (Horn conjecture) on page 176 of the AMS publication, the relation \geq needs to be replaced by \leq . This is a mere typo without any consequences, and the authors are most likely aware of it by now.

LEMMA 3.9 (see [19, 23]). Let $(i, j, k) \in T_{r,n}$ and $\lambda \boxplus \mu \sim_c \nu$. Further, let i^c, j^c, k^c be their complementary indices with respect to $\{1, \dots, n\}$. Then the following statements are equivalent:

- $\nu_{i_1} + \dots + \nu_{i_r} = \lambda_{i_1} + \dots + \lambda_{i_r} + \mu_{j_1} + \dots + \mu_{j_r}$.
- Any associated triplet of Hermitian matrices (A, B, C) is block diagonalizable into two parts, which contain eigenvalues indexed by (i, j, k) and (i^c, j^c, k^c) , respectively.
- $\lambda|_i \boxplus \mu|_j \sim_c \nu|_k$.
- $\lambda|_{i^c} \boxplus \mu|_{j^c} \sim_c \nu|_{k^c}$.

The relation is in that sense split in two with respect to the triplet (i, j, k) .

4. Honeycombs and hives. The following result by Knutson and Tao poses a complete resolution to Weyl's problem and is based on preceding breakthroughs [16, 20, 22, 24]. This problem has since then also been generalized; see, for example, [9, 11].

4.1. Honeycombs and eigenvalues of sums of Hermitian matrices. While we can only give a quick introduction, the article [23] provides a good understanding of *honeycombs*—a central tool in the verification of the Horn conjecture. They allow graph theory as well as linear programming to be applied to Weyl's problem. A honeycomb h (cf. Figure 3) is a two-dimensional object, embedded into $h \subset \mathbb{R}_{\sum=0}^3 := \{x \in \mathbb{R}^3 \mid x_1 + x_2 + x_3 = 0\}$, consisting of line segments (edges or rays), each parallel to one of the cardinal directions $(0, 1, -1)$ (northwest), $(-1, 0, 1)$ (northeast), or $(1, -1, 0)$ (south), as well as vertices, where those join. Thereby, each segment has exactly one constant coordinate, the collection of which we formally denote with $\text{edge}(h) \in \mathbb{R}^N$, $N = \frac{3}{2}n(n+1)$ (including the boundary rays). Nondegenerate n -honeycombs follow one identical topological structure and are identifiable through linear constraints: The constant coordinates of three edges meeting at a vertex add up to zero, and every edge has strictly positive length. This leads to one archetype, as displayed in Figure 3 (for $n = 3$). The involved eigenvalues appear as *boundary values* $\delta(h) := (\mathfrak{w}(h), \mathfrak{e}(h), \mathfrak{s}(h)) := (\lambda, \mu, -\nu) \in (\mathcal{D}^n)^3$ (west, east, and south), i.e., the constant coordinates of the outer rays.

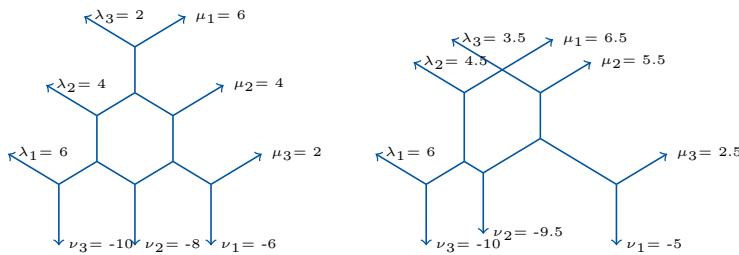


FIG. 3. Left: The archetype of nondegenerate ($n = 3$)-honeycombs as described in section 4. The rays pointing in directions northwest, northeast, and south have constant coordinates $\mathfrak{w}(h)_i = \lambda_i$, $\mathfrak{e}(h)_i = \mu_i$, and $\mathfrak{s}(h)_i = -\nu_i$, respectively. The remaining line segments contribute to the total edge length of the honeycomb. Right: A degenerate honeycomb, where the line segment at the top has been completely contracted. Here, only eight line segments remain to contribute to the total edge length.

The set HONEY_n of all n -honeycombs is identified as the closure of the set of nondegenerate ones, allowing edges of length zero as well. Thereby, $C = \{\text{edge}(h) \mid h \in \text{HONEY}_n\} \subset \mathbb{R}^N$ is a closed, convex, polyhedral cone.

THEOREM 4.1 (relation to honeycombs [23]). *The relation $\lambda \boxplus \mu \sim_c \nu$ is satisfied if and only if there exists a honeycomb h with boundary values $\delta(h) = (\lambda, \mu, -\nu)$.*

The set of triplets $\{(\lambda, \mu, -\nu) \in (\mathcal{D}^n)^3 \mid \lambda \boxplus \mu \sim_c \nu\}$ thus equals $\text{BDRY}_n := \{\delta(h) \mid h \in \text{HONEY}_n\}$, which is at the same time the orthogonal projection of the cone C to the coordinates associated with the boundary (the rays)—and, as shown in its verification, the very same cone described by the (in)equalities in Theorem 3.7.

There is also a related statement implicated by those in Lemma 3.9. If a triplet $(i, j, k) \in T_{r,n}$ yields an equality as in (3.3), then for the associated honeycomb h , $\delta(h) = (\lambda, \mu, -\nu)$, it holds that

$$(4.1) \quad h = h_1 \otimes h_2, \quad \delta(h_1) = (\lambda|_i, \mu|_j, -\nu|_k), \quad \delta(h_2) = (\lambda|_{i^c}, \mu|_{j^c}, -\nu|_{k^c}),$$

which means that h is a literal overlay of two smaller honeycombs. Conversely, if a honeycomb is an overlay of two smaller ones, then it yields two separate eigenvalue relations; however, the splitting does not necessarily correspond to a triplet in $T_{r,n}$ [23].

4.2. Hives and feasibility of pairs.

DEFINITION 4.2 (positive semidefinite honeycomb). *We define a positive semidefinite honeycomb h as a honeycomb with boundary values $\mathbf{w}(h), \mathbf{e}(h) \geq 0$ and $\mathbf{s}(h) \leq 0$.*

A honeycomb can connect three matrices. In order to connect m matrices, chains or systems of honeycombs are put in relation to each other through their boundary values. Although the phrase *hive* occurs in related literature with other meanings, we use the term to emphasize that a collection of honeycombs is given.¹⁰ Considerations for simple chains of honeycombs (cf. Lemma 4.6) have also been made in [22, 24], but we need to rephrase these ideas for our own purposes.

DEFINITION 4.3 (hives). *Let $n, M \in \mathbb{N}$. We define a (positive semidefinite) (n, M) -hive H as a collection of M (positive semidefinite) n -honeycombs $h^{(1)}, \dots, h^{(M)}$.*

DEFINITION 4.4 (structure of hives). *Let H be an (n, M) -hive, and let $B := \{(i, \mathbf{b}) \mid i = 1, \dots, M, \mathbf{b} \in \{\mathbf{w}, \mathbf{e}, \mathbf{s}\}\}$. Further, let $\sim_S \in B \times B$ be an equivalence relation. We say H has structure \sim_S if the following holds:*

Provided $(i, \mathbf{b}) \sim_S (j, \mathbf{p})$, then if both \mathbf{b} and \mathbf{p} or neither of them equal \mathbf{s} , it holds that $\mathbf{b}(h^{(i)}) = \mathbf{p}(h^{(j)})$, or otherwise $\mathbf{b}(h^{(i)}) = -\mathbf{p}(h^{(j)})$.

We define the hive set $\text{HIVE}_{n,M}(\sim_S)$ as the set of all (n, M) -hives H with structure \sim_S .

In order to specify a structure \sim_S , we will only list generating sets of equivalences (with respect to reflexivity, symmetry, and transitivity).

DEFINITION 4.5 (boundary map of structured hives). *Let H be an (n, M) -hive with structure \sim_S . Further, let $P := \{(i, \mathbf{b}) \mid |[(i, \mathbf{b})]_{\sim_S}| = 1\}$ be the set of singletons. We define the boundary map $\delta_P : \text{HIVE}_{n,M}(\sim_S) \rightarrow (\mathcal{D}^n)^P$ to map any hive $H \in \text{HIVE}_{n,M}(\sim_S)$ to the function $f_P : P \rightarrow \mathcal{D}^n$ defined as follows:*

For all $(i, \mathbf{b}) \in P$, if \mathbf{b} equals \mathbf{s} , it holds that $f_P(i, \mathbf{b}) = -\mathbf{b}(h^{(i)})$, or otherwise $f_P(i, \mathbf{b}) = \mathbf{b}(h^{(i)})$.

A single n -honeycomb h with boundary values $(\lambda, \mu, -\nu)$ can hence be identified as $(n, 1)$ -hive H with trivial structure \sim_S generated by the empty set, singleton set $P = \{(1, \mathbf{w}), (1, \mathbf{e}), (1, \mathbf{s})\}$, and boundary $\delta_P(H) = \{(1, \mathbf{w}) \mapsto \lambda, (1, \mathbf{e}) \mapsto$

¹⁰In absence of further bee related vocabulary.

$\mu, (1, \mathfrak{s}) \mapsto \nu\}.$ ¹¹ In this sense, it holds that $\text{HONEY}_n \cong \text{HIVE}_{n,1}(\emptyset)$, and we regard honeycombs as hives as well. Another example is illustrated in Figure 4, where \sim_S is generated by $(1, \mathfrak{s}) \sim_S (2, \mathfrak{w})$ and $(2, \mathfrak{s}) \sim_S (3, \mathfrak{w})$, such that the singletons are $P = \{(1, \mathfrak{w}), (1, \mathfrak{e}), (2, \mathfrak{e}), (3, \mathfrak{e}), (3, \mathfrak{s})\}$.

LEMMA 4.6 (eigenvalues of a sums of matrices). *The relation $a^{(1)} \boxplus \dots \boxplus a^{(m)} \sim_c c$ is satisfied if and only if there exists a hive H of size $M = m - 1$ (cf. Figure 4) with structure \sim_S , generated by $(i, \mathfrak{s}) \sim_S (i + 1, \mathfrak{w})$, $i = 1, \dots, M - 1$, and $\delta_P(H) = \{(1, \mathfrak{w}) \mapsto a^{(1)}, (1, \mathfrak{e}) \mapsto a^{(2)}, (2, \mathfrak{e}) \mapsto a^{(3)}, \dots, (M, \mathfrak{e}) \mapsto a^{(m)}, (M, \mathfrak{s}) \mapsto c\}$.*

Proof. “ \Rightarrow ”: The relation $a^{(1)} \boxplus \dots \boxplus a^{(m)} \sim_c c$ is equivalent to the existence of Hermitian (or real symmetric; cf. Theorem 3.6) matrices $A^{(1)}, \dots, A^{(m)}$, $C = A^{(1)} + \dots + A^{(m)}$ with eigenvalues $a^{(1)}, \dots, a^{(m)}, c$, respectively. For $A^{(1, \dots, k+1)} := A^{(1, \dots, k)} + A^{(k+1)}$, $k = 1, \dots, m - 1$, with accordant eigenvalues $a^{(1, \dots, k)}$, the relation can equivalently be restated as $a^{(1, \dots, k)} \boxplus a^{(k+1)} \sim_c a^{(1, \dots, k+1)}$, $k = 1, \dots, m - 1$. This in turn is equivalent to the existence of honeycombs $h^{(1)}, \dots, h^{(m-1)}$ with boundary values $\delta(h^{(1)}) = (a^{(1)}, a^{(2)}, -a^{(1,2)})$, $\delta(h^{(2)}) = (a^{(1,2)}, a^{(3)}, -a^{(1,2,3)})$, \dots , $\delta(h^{(m-1)}) = (a^{(1, \dots, m-1)}, a^{(m)}, -c)$. This depicts the structure \sim_S and boundary function $\delta_P(H)$.

“ \Leftarrow ”: If in reverse the hive H is assumed to exist, then we know, via the single honeycombs, that there exist matrices $\tilde{A}^{(1, \dots, k+1)} = A^{(1, \dots, k)} + A^{(k+1)}$, $k = 1, \dots, m - 1$, with corresponding eigenvalues. Although we only know that $\tilde{A}^{(1, \dots, k+1)}$ and $A^{(1, \dots, k+1)}$ share eigenvalues, the remaining, reverse construction is done via an inductive diagonalization argument (cf. Remark 2.12). \square

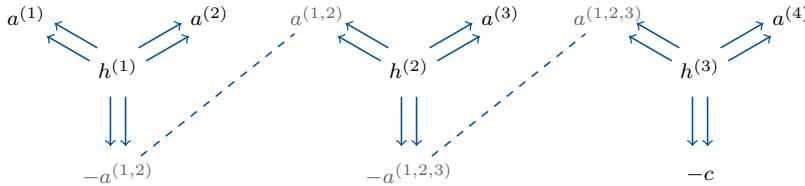


FIG. 4. The schematic display of an $(n, 3)$ -hive H with structure \sim_S as in Lemma 4.6. Northwest, northeast, and south rays correspond to the boundary values $\mathfrak{w}(h_i)$, $\mathfrak{e}(h_i)$, and $\mathfrak{s}(h_i)$, respectively. Coupled boundaries are in gray and connected by dashed lines.

The idea behind honeycomb overlays (cf. (4.1)) can be extended to hives as well.

LEMMA 4.7 (zero eigenvalues). *If the relation $a^{(1)} \boxplus \dots \boxplus a^{(m)} \sim_c c$ is satisfied for $a^{(i)} \in \mathcal{D}_{\geq 0}^n$, $i = 1, \dots, m$, and $c_n = 0$, then $a_n^{(1)} = \dots = a_n^{(m)} = 0$ and already $a^{(1)}|_{\{1, \dots, n-1\}} \boxplus \dots \boxplus a^{(m)}|_{\{1, \dots, n-1\}} \sim_c c|_{\{1, \dots, n-1\}}$.*

Proof. The first statement follows by basic linear algebra, since $a^{(1)}, \dots, a^{(m)}$ are nonnegative. For the second part, Lemma 4.6 and (4.1) are used. Inductively, in each honeycomb of the corresponding hive H , a separate 1-honeycomb with boundary values $(0, 0, 0)$ can be found. Hence, each honeycomb is an overlay of such a 1-honeycomb and an $(n - 1)$ -honeycomb. All remaining $(n - 1)$ -honeycombs then form a new hive with identical structure \sim_S . \square

We arrive at an extended version of Theorem 2.11.

¹¹This denotes $f_P(1, \mathfrak{w}) = \lambda$, $f_P(1, \mathfrak{e}) = \mu$, $f_P(1, \mathfrak{s}) = \nu$ for $f_P = \delta_P(H)$.

THEOREM 4.8 (equivalence to existence of a hive). *Let $(\gamma, \theta) \in \mathcal{D}_{\geq 0}^\infty \times \mathcal{D}_{\geq 0}^\infty$ and $n \geq \deg(\gamma), \deg(\theta)$. Further, let $\tilde{\theta} = (\theta_+, 0, \dots, 0)$, $\tilde{\gamma} = (\gamma_+, 0, \dots, 0)$ be n -tuples. The following statements are equivalent, independent of the choice $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$:*

- The pair (γ, θ) is feasible for $m \in \mathbb{N}$.
- There are m pairs of Hermitian, positive semidefinite matrices $(A^{(i)}, B^{(i)}) \in \mathbb{C}^{n \times n} \times \mathbb{C}^{n \times n}$, each with identical (multiplicities of) eigenvalues, such that $A := \sum_{i=1}^m A^{(i)}$ has eigenvalues $\tilde{\theta}^2$ and $B := \sum_{i=1}^m B^{(i)}$ has eigenvalues $\tilde{\gamma}^2$, respectively.
- There exist $a^{(1)}, \dots, a^{(m)} \in \mathcal{D}_{\geq 0}^n$ such that $a^{(1)} \boxplus \dots \boxplus a^{(m)} \sim_c \tilde{\gamma}^2$ as well as $a^{(1)} \boxplus \dots \boxplus a^{(m)} \sim_c \tilde{\theta}^2$.
- There exists a positive semidefinite (n, M) -hive H of size $M = 2(m - 1)$ (cf. Figure 5) with structure \sim_S , where $(i+u, \mathfrak{s}) \sim_S (i+1+u, \mathfrak{w}), i = 1, \dots, M/2 - 1, u \in \{0, M/2\}$, as well as $(1, \mathfrak{w}) \sim_S (1 + M/2, \mathfrak{w})$ and $(i, \mathfrak{e}) \sim_S (i + M/2, \mathfrak{e}), i = 1, \dots, M$. Further, $\delta_P(H) = \{(M/2, \mathfrak{s}) \mapsto \tilde{\gamma}^2, (M, \mathfrak{s}) \mapsto \tilde{\theta}^2\}$.

Proof. The existence of matrices with actual size $\deg(\gamma)$, $\deg(\theta)$, respectively, follows by repeated application of Lemma 4.7. The hive essentially consists of two rows of honeycombs as in Lemma 4.6. Therefore, the same argumentation holds, but instead of prescribed boundary values $a^{(i)}$, these values are coupled between the two hive parts. Due to Theorem 3.6, there is no difference whether we consider real or complex matrices and tensors. \square

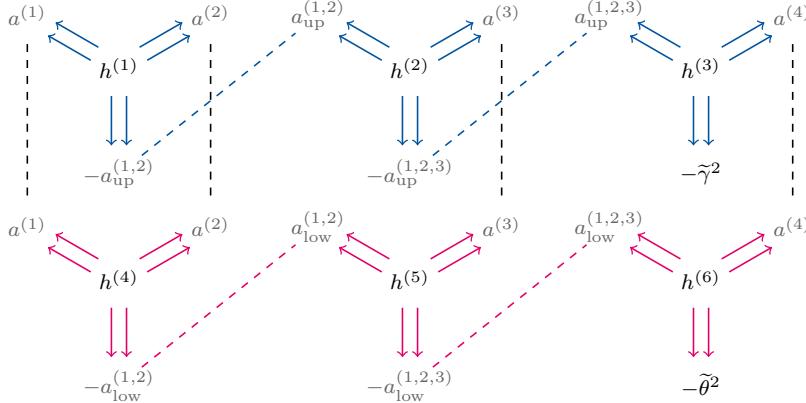


FIG. 5. The schematic display of an $(n, 6)$ -hive H (upper part in blue, lower part in magenta) with structure \sim_S as in Lemma 4.6. Northwest, northeast, and south rays correspond to the boundary values $\mathfrak{w}(h_i)$, $\mathfrak{e}(h_i)$, and $\mathfrak{s}(h_i)$, respectively. Coupled boundaries are in gray and connected by dashed lines. (Color available online.)

The feasibility of (γ, θ) as in (3.1) is provided by the hive in Figure 6. Even though not diagonally feasible, the pair can be disassembled, as later shown in subsection 5.2, into multiple, diagonally feasible pairs, which then as well prove its feasibility. As another example serves $\gamma_+^2 = (10, 2, 1, 0.25, 0.25)$ and $\theta_+^2 = (4, 3, 2.5, 2, 2)$. According to (1.7), the pair (γ, θ) is not feasible for $m = 2, 3$, but may be feasible for $m = 4$. The hive in Figures 7 and 8 (having been constructed with Algorithm 6.1) provides that this is indeed the case. We further know that the pair is diagonally feasible for $m = 5$ (due to the constructive Theorem 3.4).

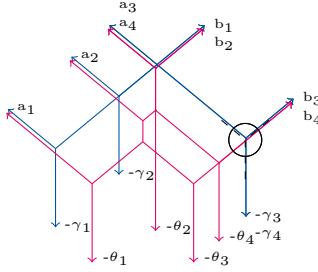


FIG. 6. A $(4, 2)$ -hive consisting of two coupled honeycombs (blue for γ , magenta for θ), which are slightly shifted for better visibility, generated by Algorithm 6.1. Note that some lines have multiplicity 2. The coupled boundary values are given by $a = (4, 1.5, 0, 0)$ and $b = (3.5, 3.5, 0, 0)$. It proves the feasibility of the pair (γ, θ) , $\tilde{\gamma}^2 = (7.5, 5, 0, 0)$, $\tilde{\theta}^2 = (6, 3.5, 2, 1)$ for $m = 2$, since $\tilde{\gamma}^2, \tilde{\theta}^2 \sim_c a \boxplus b$ (the exponent 2 has been skipped for better readability). Only due to the short, vertical line segment in the middle does the hive not provide diagonal feasibility. (Color available online.)

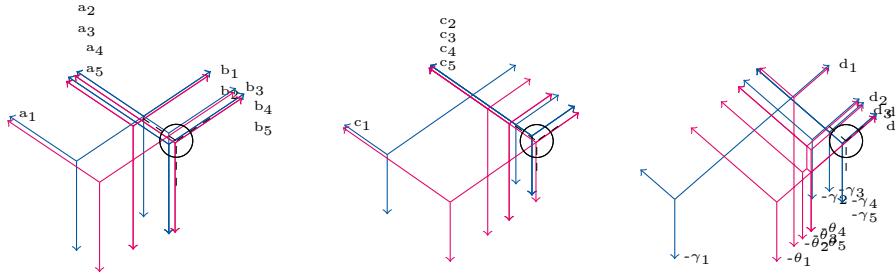


FIG. 7. A $(5, 4)$ -hive consisting of six coupled honeycombs (blue for γ , magenta for θ), which are slightly shifted for better visibility, generated by Algorithm 6.1. Note that some lines have multiplicity larger than 1. Also, in each second pair of honeycombs, the roles of boundaries λ and μ have been switched (which we can do due to the symmetry regarding \boxplus), such that the honeycombs can be combined to a single diagram as in Figure 8. This means that the south rays of an odd-numbered pair are always connected to the northeast (instead of northwest) rays of the consecutive pair. The boundary values are given by $a = (2, 0.25, 0.25, 0, 0)$, $b = (1, 1, 0.25, 0, 0)$, $c = (4, 0, 0, 0, 0)$, and $d = (3, 1, 0.75, 0, 0)$. It proves the feasibility of the pair (γ, θ) , $\tilde{\gamma}^2 = (10, 2, 1, 0.25, 0.25)$, $\tilde{\theta}^2 = (4, 3, 2.5, 2, 2)$ for $m = 4$, since both $\tilde{\gamma}^2, \tilde{\theta}^2 \sim_c a \boxplus b \boxplus c \boxplus d$ (the exponent 2 has been skipped for better readability). (Color available online.)

4.3. Hives are polyhedral cones. As previously done for honeycombs, we also associate hives with certain vector spaces.

DEFINITION 4.9 (hive sets and edge image). *Let H be an (n, M) -hive consisting of honeycombs $h^{(1)}, \dots, h^{(M)}$. We define*

$$\text{edge}(H) = (\text{edge}(h^{(1)}), \dots, \text{edge}(h^{(M)})) \in \mathbb{R}^{N \times M}$$

as the collection of constant coordinates of all edges appearing in the honeycombs within the hive H . Although defined via the abstract set B (in Definition 4.3), we let \sim_S act on the related edge coordinates as well. For $H \in \text{HIVE}_{n,M}(\sim_S)$, we then define the edge image as $\text{edge}_S(H) \in \mathbb{R}^{N \times M} / \sim_S \cong \mathbb{R}^{N^*}$, in which coupled boundaries are assigned the same coordinate.

THEOREM 4.10 (hive sets are described by polyhedral cones).

- The hive set $\text{HIVE}_{n,M}(\sim_S)$ is a closed, convex, polyhedral cone, i.e., there

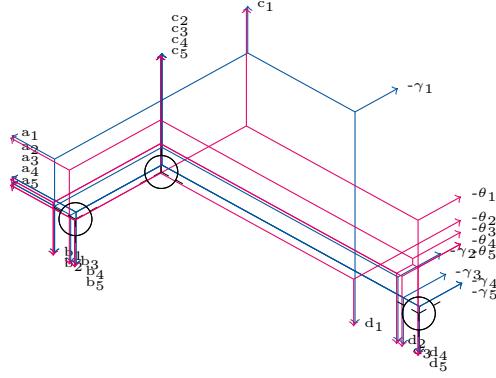


FIG. 8. The three overlaid honeycomb pairs in Figure 7 put together with respect to their coupling (the exponent 2 for γ, θ has been skipped for better readability). (Color available online.)

exist matrices L_1, L_2 such that $\text{edge}_S(\text{HIVE}_{n,M}(\sim_S)) = \{x \mid L_1x \leq 0, L_2x = 0\}$.

- Each fiber of δ_P (i.e., a set of hives with structure \sim_S and boundary f_P) forms a closed, convex polyhedron, i.e., there exist matrices L_1, L_2, L_3 and a vector b such that $\text{edge}_S(\delta_P^{-1}(f_P)) = \{x \mid L_1x \leq 0, L_2x = 0, L_3x = b\}$.

Proof. Each honeycomb of a hive follows its linear constraints. The hive structure and identification of coordinates as one and the same by \sim_S only imposes additional linear constraints. The rest is elementary geometry. \square

COROLLARY 4.11. *The boundary set*

$$\text{BDRY}_{n,M}(\sim_S) := \{\text{image}(f_P) \in (\mathcal{D}^n)^P \mid f_P = \delta_P(H), H \in \text{HIVE}_{n,M}(\sim_S)\}$$

forms a closed, convex, polyhedral cone. This hence also holds for any intersection with or projection to a lower-dimensional subspace.

Proof. The boundary set is given by the projection of $\text{edge}_S(\text{HIVE}_{n,M}(\sim_S))$ to the subset of coordinates associated to the ones in P . The proof is finished, since projections to fewer coordinates of closed, convex, polyhedral cones are again such cones. The same holds for intersections with subspaces. \square

5. Cones of squared feasible values. The following fact has already been established in [4] but also follows from Corollary 4.11.

COROLLARY 5.1 (squared feasible pairs form cones). *Let $m, r_1, r_2 \in \mathbb{N}$. The set of squared feasible pairs $\mathcal{F}_{m,(r_1,r_2)}^2$ (cf. Definition 3.3) is a closed, convex, polyhedral cone embedded into $\mathbb{R}^{r_1+r_2}$. If $r_1 \leq mr_2$ and $r_2 \leq mr_1$, then its dimension is $r_1 + r_2 - 1$. Otherwise, $\mathcal{F}_{m,(r_1,r_2)}^2 \cap \mathcal{D}_{>0}^{r_1} \times \mathcal{D}_{>0}^{r_2}$ is empty.*

Proof. By Corollary 4.11 and Theorem 4.8 it directly follows that $\mathcal{F}_{m,(r_1,r_2)}^2$ is a closed, convex, polyhedral cone. For the first case, it only remains to show that the cone has dimension $r_1 + r_2 - 1$, or, equivalently, it contains as many linearly independent vectors. These are, however, already given by the examples carried out in Lemma 3.2. From Corollary 2.9, it directly follows that if (γ, θ) is feasible for m , then it must hold that $\deg(\gamma) \leq m \deg(\theta)$ and $\deg(\theta) \leq m \deg(\gamma)$, which provides the second case. \square

The implication for the original TT-feasibility then is as follows.

COROLLARY 5.2 (cone property for higher order tensors). *For $d \in \mathbb{N}$, let both $\sigma, \tau \in (\mathcal{D}_{\geq 0}^{\infty})^{d-1}$ be feasible for $n \in \mathbb{N}^d$ (in the sense of Definition 1.1). Then $v, (v^{(\mu)})^2 := (\sigma^{(\mu)})^2 + (\tau^{(\mu)})^2$, $\mu = 1, \dots, d-1$, is feasible for n as well.*

More generally, squared feasible TT-singular values form a closed, convex, polyhedral cone. Its H -description is the collection of linear constraints for the pairs $(\sigma^{(\mu-1)}, \sigma^{(\mu)})$.

Proof. Due to Corollary 2.10, it only remains to show that each pair $(v^{(\mu-1)}, v^{(\mu)})$ is feasible for n_{μ} , $\mu = 1, \dots, d$. For each single μ , this follows directly from Corollary 5.1. \square

5.1. Necessary inequalities. While for each specific m and r_1 , the results in [4] allow us to calculate the H -description of the cone $\mathcal{F}_{m,(r_1,mr_1)}^2$ (i.e., a set of necessary and sufficient inequalities), we will concern ourselves with possibly weaker but generalized statements for arbitrary m in this section. In subsection 5.2, we will derive a V -description of $\mathcal{F}_{m,(m,m^2)}^2$ (i.e., a set of generating vertices).

LEMMA 5.3. *For $n, m \in \mathbb{N}$, let $T^{(j)}, I^{(j)} \subset \{1, \dots, n\}$ be sets of equal cardinality, $j = 1, \dots, m$, with $T^{(1)} = I^{(1)}$ and $\Delta T^{(j)} \sim_c \Delta T^{(j-1)} \boxplus \Delta I^{(j)}$ (cf. Theorem 3.8) for $j = 2, \dots, m$. Then, provided $\zeta \sim_c a^{(1)} \boxplus \dots \boxplus a^{(m)}$, the inequality*

$$(5.1) \quad \sum_{i \in T^{(m)}} \zeta_i \leq \sum_{j=1}^m \sum_{i \in I^{(j)}} a_i^{(j)}$$

holds true for every $a^{(j)}, \zeta \in \mathcal{D}^n$, $j = 1, \dots, m$. If (5.1) holds as equality, then already $\zeta|_{T^{(m)}} \sim_c a^{(1)}|_{I^{(1)}} \boxplus \dots \boxplus a^{(m)}|_{I^{(m)}}$ and $\zeta|_{(T^{(m)})^c} \sim_c a^{(1)}|_{(I^{(1)})^c} \boxplus \dots \boxplus a^{(m)}|_{(I^{(m)})^c}$. (cf. Lemma 3.9).

Proof. Statement (5.1) follows inductively if, for each $j = 2, \dots, m$,

$$(5.2) \quad \sum_{i \in T^{(j)}} \nu_i \leq \sum_{i \in T^{(j-1)}} \lambda_i + \sum_{i \in I^{(j)}} \mu_i$$

is true whenever $\nu \sim_c \lambda \boxplus \mu$. By Theorem 3.8, this holds since by assumption $\Delta T^{(j)} \sim_c \Delta T^{(j-1)} \boxplus \Delta I^{(j)}$ for $j = 2, \dots, m$. If (5.1) holds as equality, then all single inequalities (5.2) must hold as equality, and hence Lemma 3.9 can be applied inductively as well. \square

THEOREM 5.4. *In the situation of Lemma 5.3, let \widehat{T} and \widehat{I} fulfill the same assumptions as T and I . Further, let $I^{(j)} \cap \widehat{I}^{(j)} = \emptyset$, $j = 1, \dots, m$. If the pair $(\gamma, \theta) \in \mathcal{D}_{\geq 0}^{\infty} \times \mathcal{D}_{\geq 0}^{\infty}$ is feasible for m , then*

$$(5.3) \quad \sum_{i \in T^{(m)}} \gamma_i^2 \leq \sum_{i \in \{1, \dots, \deg(\theta)\} \setminus \widehat{T}^{(m)}} \theta_i^2$$

must hold true. If (5.3) holds as equality, then $((\gamma|_{T^{(m)}}, 0, \dots), (\theta|_{(\widehat{T}^{(m)})^c}, 0, \dots))$ and $((\gamma|_{(T^{(m)})^c}, 0, \dots), (\theta|_{\widehat{T}^{(m)}}, 0, \dots))$ are already feasible.

Together with (4.1), this also implies that the corresponding hive is an overlay of two smaller hives, modulo zero boundaries.

Proof. Let $n \geq \max(T^{(m)}, \deg(\gamma), \deg(\theta))$. As (γ, θ) is feasible, due to Lemma 5.3, inequality (5.1) holds for some joint eigenvalues $a^{(1)}, \dots, a^{(m)} \in \mathcal{D}_{\geq 0}^n$ for both $\zeta :=$

$\tilde{\gamma}^2 = (\gamma_1^2, \dots, \gamma_n^2)$, T , I and $\hat{\zeta} = \tilde{\theta}^2 := (\theta_1^2, \dots, \theta_n^2)$, \hat{T} , \hat{I} . Furthermore, we have $\sum_{i=1}^n \theta_i^2 = \sum_{i=1}^n a_i^{(1)} + \dots + \sum_{i=1}^n a_i^{(m)}$. Subtracting (5.1) for $\hat{\zeta}$ from this equality yields

$$(5.4) \quad \sum_{i \notin \hat{T}^{(m)}} \theta_i^2 \stackrel{n \geq \deg(\theta)}{=} \sum_{i \in \{1, \dots, n\} \setminus \hat{T}^{(m)}} \theta_i^2 \stackrel{(5.1) \text{ for } \hat{\zeta}}{\geq} \sum_{j=1}^m \sum_{i \in \{1, \dots, n\} \setminus \hat{T}^{(j)}} a_i^{(j)}$$

$$(5.5) \quad \stackrel{a_i^{(j)} \geq 0}{\geq} \sum_{j=1}^m \sum_{i \in I^{(j)}} a_i^{(j)} \stackrel{(5.1) \text{ for } \zeta}{\geq} \sum_{i \in T^{(m)}} \gamma_i^2.$$

This finishes the first part. In case of an equality, since the second “ \geq ” must hold as equality, we have $a^{(j)}|_{\{1, \dots, n\} \setminus \hat{T}^{(j)}} = (a^{(j)}|_{I^{(j)}}, 0, \dots)$ and $a^{(j)}|_{\{1, \dots, n\} \setminus I^{(j)}} = (a^{(j)}|_{\hat{T}^{(j)}}, 0, \dots)$ for each $j = 1, \dots, m$. Furthermore, the first and third “ \geq ” in (5.5) must hold as equality as well. Hence, the latter statement in Lemma 5.3 can be applied to inequalities (5.1) for both ζ and $\hat{\zeta}$, such that we can conclude the latter statement in this corollary. \square

COROLLARY 5.5 (a set of inequalities for feasible pairs). *Let $p^{(1)} \dot{\cup} p^{(2)} = \mathbb{N}$ be two disjoint sets, with $p^{(1)}$ finite of size r . If $(\gamma, \theta) \in \mathcal{D}_{\geq 0}^\infty \times \mathcal{D}_{\geq 0}^\infty$ is feasible for $m \in \mathbb{N}$, then it holds ($p_i^{(u)}$ being the i th smallest element) that*

$$\sum_{i \in P_m^{(1)}} \gamma_i^2 \leq \sum_{i \notin P_m^{(2)}} \theta_i^2, \quad P_m^{(u)} := \{m(p_i^{(u)} - i) + i \mid i = 1, 2, \dots\}, \quad u = 1, 2.$$

Proof. Let $n \geq \max(P_m^{(1)}, \deg(\gamma), \deg(\theta))$. Further, let $\tilde{P}_j^{(2)}$ contain the \hat{k} smallest elements of $P_j^{(2)}$, where \hat{k} is the number of elements in $P_m^{(2)} \cap \{1, \dots, n\}$, and let $\tilde{P}_j^{(1)} = P_j^{(1)}$, $j = 1, \dots, m$. Thereby $\tilde{P}_1^{(1)} = p^{(1)} = P_1^{(1)}$ and $\tilde{P}_1^{(2)} \subset p^{(2)} = P_1^{(2)}$. We have the following (diagonal) matrix identities:

$$\begin{aligned} \text{diag}(\tilde{P}_j^{(u)}) - \text{diag}(1, \dots, \ell) &= \text{diag}(\tilde{P}_{j-1}^{(u)}) + \text{diag}(\tilde{P}_1^{(u)}) - 2 \text{diag}(1, \dots, \ell) \\ \Leftrightarrow j(p_i^{(u)} - i) &= (j-1)(p_i^{(u)} - i) + (p_i^{(u)} - i), \quad i = 1, \dots, \ell, \quad \ell = |\tilde{P}_j^{(u)}|, \end{aligned}$$

where the diagonal elements are placed in ascending order. Hence, $\Delta \tilde{P}_j^{(u)} \sim_c \Delta \tilde{P}_{j-1}^{(u)} \boxplus \Delta \tilde{P}_1^{(u)}$ for $j = 2, \dots, m$, $u \in \{1, 2\}$. For $T^{(j)} := \tilde{P}_j^{(1)}$, $I^{(j)} := \tilde{P}_1^{(1)}$ and $\hat{T}^{(j)} := \tilde{P}_j^{(2)}$, $\hat{I}^{(j)} := \tilde{P}_1^{(2)}$, we can apply Theorem 5.4 to obtain the desired statement. \square

Among the various inequalities contained in Corollary 5.5, the following two correspond to earlier mentioned inequalities for Weyl’s problem. The first case is (1.7) and is also referred to as the *basic inequalities* in [4].

COROLLARY 5.6 (Fan analogue for feasible pairs). *The choice $a^{(1)} = \{1, \dots, r\}$ in Corollary 5.5 yields the inequality $\sum_{i=1}^r \gamma_i^2 \leq \sum_{i=1}^{mr} \theta_i^2$.*

COROLLARY 5.7 (Weyl analogue for feasible pairs). *The choice $a^{(1)} = \{r+1\}$ in Corollary 5.5 yields the inequality $\gamma_{rm+1}^2 \leq \sum_{i=r+1}^{r+m} \theta_i^2$.*

The QMP article [4] explicitly provides the derivation for the case $\deg(\gamma) \leq 3$ and $m = 2$. Thereby, the necessary (and sufficient) inequalities for the feasibility of (γ, θ) , apart from the trace property, are as follows: Corollary 5.6 for $r = 1, 2$; Corollary 5.7 for $r = 1$ and $\gamma_2^2 + \gamma_3^2 \leq \theta_1^2 + \theta_2^2 + \theta_3^2 + \theta_6^2$. The last inequality is not included in

Corollary 5.5, but can be derived from Theorem 5.4 and generalized in different ways. For example, for $I^{(1)} = I^{(2)} = \{1, 3\}$, $T^{(2)} = \{2, 3\}$, $\widehat{I}^{(1)} = \widehat{I}^{(2)} = \{2, 4, 5, 6, \dots\}$, $\widehat{T}^{(2)} = \{4, 5, 7, 8, \dots\}$ and $I^{(j)} = \{1, 2\}$, $T^{(j)} = \{2, 3\}$, $\widehat{I}^{(j)} = \{3, 4, 5, 6, \dots\}$, $\widehat{T}^{(j)} = \{2j, 2j+1, 2j+3, 2j+4, \dots\}$, $j = 3, \dots, m$ (where we add the same amount of arbitrarily many consecutive numbers in $\widehat{I}^{(j)}$ and $\widehat{T}^{(j)}$), one can conclude that $\gamma_2^2 + \gamma_3^2 \leq \sum_{i=1}^{2m-1} \theta_i^2 + \theta_{2m+2}^2$ whenever (γ, θ) is feasible for m . Theorem 5.4 does not, however, reveal when this generalized inequality is redundant to other necessary ones.

The right sum in Corollary 5.5 has always m -times as many summands as the left sum. For these inequalities, it further holds that $\sum_{i \notin P_m^{(2)}} i - \sum_{i \in P_m^{(1)}} i = \sum_{i=k+1}^{mk} i = \frac{k(m-1)(m+1)k+1}{2}$, where $k = |P_m^{(1)}|$. We can, however, only conjecture that this holds in general for every inequality in the H -description of $\mathcal{F}_{m, (r_1, mr_1)}^2$.

5.2. Vertex description of $\mathcal{F}_{m, (m, m^2)}^2$. We revisit the special case (1.7) and derive the vertex description of the corresponding cone $\mathcal{F}_{m, (m, m^2)}^2$ (cf. Definition 3.3). In this section, for $a, b \in \mathbb{N} \cup \{0\}$, we therefore let $(a \# b) = (a, \dots, a) \in \mathcal{D}_{\geq 0}^b$ (length b).

LEMMA 5.8. *Let $\alpha, \beta, m \in \mathbb{N}$, $\beta \leq m$, $\alpha \leq \beta m$, $\gamma_+^2 = (\alpha \# \beta)$, and $\theta_+^2 = (\beta \# \alpha)$. Then (γ, θ) is feasible for m .*

Proof. We prove by induction over m . Without loss of generality, we may assume $\alpha > \beta$ by which $\alpha = k\beta + t$ for unique natural numbers $k < m, t < \beta$. Considering Remark 2.12, it suffices to show that for $\tilde{\gamma}^2 := \gamma_+^2 - (t, \beta \# \beta - 1) = (k\beta, (\alpha - \beta) \# \beta - 1)$ and $\tilde{\theta}^2 := \theta_+^2 - (0, \dots, 0, t, \beta \# \beta - 1) = (\beta \# \alpha - \beta, \beta - t, 0 \# \beta - 1)$ the pair $((\tilde{\gamma}, 0, \dots), (\tilde{\theta}, 0, \dots))$ is feasible for $m - 1$. In order to show this, we split $\tilde{\gamma} = (\tilde{\gamma}_{(1)}, \tilde{\gamma}_{(2)})$, $\tilde{\theta} = (\tilde{\theta}_{(1)}, \tilde{\theta}_{(2)})$ into two pairs, $\tilde{\gamma}_{(1)}^2 := (k\beta)$, $\tilde{\gamma}_{(2)}^2 := (\beta \# k)$ and $\tilde{\theta}_{(1)}^2 := ((\alpha - \beta) \# \beta - 1, 0, \dots, 0)$, $\tilde{\theta}_{(2)}^2 := (\beta \# v, \beta - t, 0, \dots, 0)$ with $v = \alpha - \beta - k = (k - 1)(\beta - 1) + (t - 1)$. We can then, considering overlays of honeycombs, treat both pairs independently. While $((\tilde{\gamma}_{(1)}, 0, \dots), (\tilde{\theta}_{(1)}, 0, \dots))$ is feasible for $k \leq m - 1$, in the second case, $(\tilde{\gamma}_{(2)}^2, \theta_{(2)}^2)$ is a convex combination of $((v + 1) \# \beta - 1)$, $((\beta - 1) \# v + 1)$ and $(v \# \beta - 1)$, $((\beta - 1) \# v)$. Since $\beta - 1 \leq m - 1$ and $v \leq v + 1 \leq (m - 1)(\beta - 1)$, the proof is finished by induction. \square

The following theorem was previously conjectured by [4] and proven by [26]. We prove it in a way which allows us to identify all vertices as in Corollary 5.10.

THEOREM 5.9. *Let $(\gamma, \theta) \in \mathcal{D}_{\geq 0}^\infty \times \mathcal{D}_{\geq 0}^\infty$ and $m \in \mathbb{N}$. If $\deg(\gamma) \leq m$ and if all Ky Fan inequalities (Corollary 5.6) as well as the trace property $\|\gamma\|_2 = \|\theta\|_2$ hold, then the pair is feasible for m .*

Proof. Here, we denote the Ky Fan inequality (Corollary 5.6) for r with K_r , and in case of an equality we say E_r holds. Due to K_m , $\deg(\gamma) \leq m$, and the trace property, E_m and $\deg(\theta) \leq m \deg(\gamma)$ must be true. For fixed m , we prove by induction over $\deg(\gamma) + \deg(\theta)$. Let $0 \leq k < m$ be the largest number for which E_k is fulfilled, and let $\alpha = \deg(\theta) - mk$ as well as $\beta = \deg(\gamma) - k$. We define $(\widehat{\gamma}^2 \mid \widehat{\theta}^2) := (\gamma_+^2 \mid \theta_+^2) - f \cdot (m\beta \# k, \alpha \# \beta \mid \beta \# mk, \beta \# \alpha)$, $f > 0$. Then E_k and K_j , $j < k$, are true for $(\widehat{\gamma} \mid \widehat{\theta})$ for all $f > 0$. Further, as long as K_{k+1} holds for $(\widehat{\gamma} \mid \widehat{\theta})$ (which it does for any $f > 0$ if $k = m - 1$), then due to K_{k-1} and E_k it follows that $\widehat{\gamma}_{k+1} \leq \widehat{\gamma}_k$. Hence, f can be chosen such that K_i , $i = 1, \dots, m - 1$, and $(\widehat{\gamma} \mid \widehat{\theta}) \in \mathcal{D}_{\geq 0}^\beta \times \mathcal{D}_{\geq 0}^\alpha$ as well as either (i) E_j for at least one j , $k < j < m$, or (ii) $\widehat{\gamma}_\beta = 0 \vee \widehat{\theta}_\alpha = 0$. In case of (i), we can repeat the above construction for increased k until $k = m - 1$, and hence (ii) remains the sole option. In that case, we are finished by induction. \square

COROLLARY 5.10. *A complete vertex description of $\mathcal{F}_{m,(m,m^2)}$ is given by*

$$\begin{aligned} \mathcal{V} = \{(\tilde{\gamma}, \tilde{\theta}) \in \mathcal{F}_{m,(m,m^2)} \mid & \tilde{\gamma}_+^2 = (m\beta_{\#k}, \alpha_{\#\beta}), \tilde{\theta}_+^2 = (\beta_{\#mk}, \beta_{\#\alpha}), \\ & k \in \{0, \dots, m - \beta\}, \alpha, \beta \in \mathbb{N}, \beta \leq m, \alpha \leq \beta m; \text{ and } k = 0 \text{ if } \alpha = \beta m\}. \end{aligned}$$

A short calculation shows that the number of vertices $|\mathcal{V}|$ is given by a polynomial with leading monomial $m^4/6$.

Proof. The proof of Theorem 5.9 is constructive and decomposes a squared feasible pair into a convex combination of squared feasible pairs in \mathcal{V} . It hence remains to show that the elements of \mathcal{V} are vertices. Given any two elements $v = v(k_1, \alpha_1, \beta_1)$, $w = w(k_2, \alpha_2, \beta_2)$, $v^2, w^2 \in \mathcal{V}$, let $y_f^2 = v^2 - f \cdot w^2$, $f > 0$. For $y_f \in \mathcal{D}_{\geq 0}^m \times \mathcal{D}_{\geq 0}^{m^2}$ to be true, we must have $mk_1 + \alpha_1 = mk_2 + \alpha_2$ as well as either (i) $k_1 = k_2$ and $\beta_1 = \beta_2$ or (ii) $k_2 = 0$ and $\beta_1 + k_1 = \beta_2$. In the second case, y_f would violate K_{k_1} if $k_1 \neq 0$. If y_f^2 is again a convex combination of elements in \mathcal{V} , then y_f must be feasible. Due to the above, it then follows, however, that $v = w$, $y^2 = (1 - f)v^2$. In other words, v^2 cannot be a convex combination of other elements in \mathcal{V} . \square

For example, all 7 vertices v_1^2, \dots, v_7^2 of $\mathcal{F}_{2,(2,4)}^2$ ($m = 2$) are given through

$$\begin{bmatrix} 1 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 2 & 1 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 2 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 2 & 1 \\ 1 & 1 \\ 0 & 0 \end{bmatrix}, \begin{bmatrix} 3 & 2 \\ 3 & 2 \\ 0 & 0 \end{bmatrix}, \text{ and } \begin{bmatrix} 2 & 1 \\ 2 & 1 \\ 1 & 1 \end{bmatrix}.$$

For $m = 3$, we already have 27 vertices. Although all these vertices happen to be diagonally feasible, this is not the case in general. For example, $(5_{\#3} \mid 3_{\#5}, 0_{\#4}) \in \mathcal{F}_{3,(3,9)}^2$ is a vertex, but it is easy to show that it is not diagonally feasible. For (γ, θ) as in (3.1), $\gamma_+^2 = (7.5, 5)$, $\theta_+^2 = (6, 3.5, 2, 1)$, we have $(\gamma_+, \theta_+) = 1.5v_1^3 + 0.5v_2^3 + 1.5v_4^2 + v_5^2 + v_7^2$.

6. TFP algorithms. MATLAB implementations of algorithms mentioned in this work can be found under the name **TT-feasibility-toolbox** or directly at

<https://git.rwth-aachen.de/sebastian.kraemer1/TT-feasibility-toolbox>.

The description in Theorem 4.10 yields the straightforward Algorithm 6.1 to determine the minimal value m for which some pair $(\gamma, \theta) \in \mathcal{D}_{\geq 0}^\infty \times \mathcal{D}_{\geq 0}^\infty$ is feasible. The summed up length of all (inner) edges is minimized, since then the algorithm tends to return a hive from which diagonal feasibility can be read off (cf. Lemma 3.2). Algorithm 6.1 always terminates for at most $m = \max(\deg(\gamma), \deg(\theta))$ due to Lemma 3.2. In practice, a slightly different coupling of boundaries is used (cf. Figure 7), since then the entire hive can be visualized in \mathbb{R}^2 . For that, it is required to rotate and mirror some of the honeycombs (cf. Figure 8). Depending on the linear programming algorithm, the input may be too badly conditioned to allow a verification with satisfying residual. The simple and heuristic Algorithm 6.2 can be more reliable. As we have seen, we can restrict ourselves to $\mathbb{K} = \mathbb{R}$ (cf. Theorem 3.6). Fixed points of the iteration are cores $H \in (\mathbb{R}^{r_1 \times r_2})^{\{1, \dots, m\}}$ for which $H\Theta^{-1}$ is left-orthonormal and $\Gamma^{-1}H$ is right-orthonormal. Hence $H^* = \Gamma^{-1}H\Theta^{-1}$ is a core for which ΓH^* is left-orthonormal and $H^*\Theta$ is right-orthonormal, as required by Corollary 2.9. Furthermore, the iterates cannot diverge in the following sense.

LEMMA 6.1 (behavior of Algorithm 6.2). *For every $k > 1$ it holds that $\|\gamma^{(k)} - \gamma_+\|_2 \leq \|\theta^{(k)} - \theta_+\|_2$ as well as $\|\theta^{(k)} - \theta_+\|_2 \leq \|\gamma^{(k-1)} - \gamma_+\|_2$.*

Algorithm 6.1. Linear programming check for feasibility.

Require: $(\tilde{\gamma}, \tilde{\theta}) \in \mathcal{D}_{\geq 0}^r \times \mathcal{D}_{\geq 0}^r$ with $\|\tilde{\gamma}\|_2 = \|\tilde{\theta}\|_2$ for some $r \in \mathbb{N}$

- 1: **for** $m = 2 \dots$ **do**
- 2: as in Theorem 4.10, set L such that $\text{edge}_S(\delta_P^{-1}(f_P)) = \{x \mid L_1x \leq 0, L_2x = 0, L_3x = b\}$ for the hive H as in Theorem 4.8
- 3: use a linear programming algorithm to minimize Fx subject to $x \in \text{edge}_S(\delta_P^{-1}(f_P))$, where F is the vector for which $Fx \in \mathbb{R}_{\geq 0}$ is the summed up length of all (inner) edges in H
- 4: **if** no solution exists **then**
- 5: continue with $m + 1$
- 6: **else**
- 7: **return** minimal number $m \in \mathbb{N}$ for which (γ, θ) is feasible and a corresponding $(r, 2(m - 1))$ -hive H with minimal total edge length
- 8: **end if**
- 9: **end for**

Algorithm 6.2. Heuristic check for numerical feasibility.

Require: $(\gamma_+, \theta_+) \in \mathcal{D}_{>0}^{r_1} \times \mathcal{D}_{>0}^{r_2}$ for some $r_1, r_2 \in \mathbb{N}$ and a natural number m
(as well as $\text{tol} > 0$, $\text{iter}_{\max} > 0$)

- 1: initialize a core $H_1^{(1)}$ of length m and size (r_1, r_2) randomly
- 2: set $\gamma^{(0)}, \theta^{(0)} \equiv 0$, $\text{relres} = 1$ and $k = 0$
- 3: **while** $\text{relres} > \text{tol}$ and $k \leq \text{iter}_{\max}$ **do**
- 4: $k = k + 1$
- 5: calculate the SVD and set $U_1 \Theta^{(k)} V_1^T = \mathfrak{L}(H_1^{(k-1)})$
- 6: set $H_2^{(k)}$ via $\mathfrak{L}(H_2^{(k)}) = U_1 \Theta$
- 7: calculate the SVD and set $U_2 \Gamma^{(k)} V_2^T = \mathfrak{R}(H_2^{(k)})$
- 8: set $H_1^{(k)}$ via $\mathfrak{R}(H_1^{(k)}) = \Gamma V_2^T$
- 9: $\text{relres} = \max \left(\max_{i=1, \dots, r_1} (|\gamma_i^{(k)} / \gamma_i - 1|), \max_{i=1, \dots, r_2} (|\theta_i^{(k)} / \theta_i - 1|) \right)$
- 10: **end while**
- 11: **if** $\text{relerr} \leq \text{tol}$ **then**
- 12: **return** $H^* = \Gamma^{-1} H_1^{(k)} \Theta^{-1}$
- 13: (γ, θ) is (numerically) feasible for m
- 14: **else**
- 15: (γ, θ) is *likely* to not be feasible for m
- 16: **end if**

Proof. We only consider the first case, since the other one is analogous. Let $k > 1$ be arbitrary, but fixed. Then in line 5 of Algorithm 6.2 we have

$$\underbrace{\|U_1 \Theta^{(k)} V_1^T - U_1 \Theta V_1^T\|_F}_{A:=} = \|\Theta^{(k)} - \Theta\|_F.$$

$\mathfrak{R}(A)$ has singular values γ_+ , inherited from the last iteration, and $\mathfrak{R}(B)$ has the same singular values as $\mathfrak{R}(B) \text{diag}(V_1, \dots, V_1) = \mathfrak{R}(BV_1) = \mathfrak{R}(H_2^{(k)})$, which are given by $\gamma^{(k)}$. It follows by Mirsky's inequality about singular values [27] that $\|\gamma^{(k)} - \gamma_+\|_2 \leq \|A - B\|_F = \|\theta^{(k)} - \theta_+\|_2$. \square

Convergence is hence not assured but likely in the sense that the perturbation of

matrices usually leads to a fractional amount of perturbation of its singular values. To construct an entire tensor, the algorithm may be run in parallel for each single core.

7. Conclusions and outlook. The simple equivalence between the tensor feasibility problem (TFP) and the quantum marginal problem (QMP) allows for an interesting interaction between the different perspectives on either side. Through the standard representation, the tensor train (TT) feasibility problem can be decoupled into pairwise problems, by which, first, results from the QMP can be applied. Thereby, the full H -description of the cone of squared TT-feasible values can be calculated in any specific instance. At the same time, through our alternative consideration of orthogonality constraints on cores, one can derive universal classes of necessary inequalities for the feasibility of pairs, whereas the concept of hives yields a corresponding linear programming algorithm. Further on the practical side, we have introduced simple ways to construct tensors with prescribed singular values in parallel, based only on the sufficient construction of feasible pairs. Given that the concept of a standard representation is transferable to any hierarchical format, implications for both the TFP and QMP are subject to future research.

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