Thermal processes and state achievability

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The resource theory of thermal operations aims at describing possible transitions of microscale systems interacting with a macroscale environment under the fundamental assumption of energy conservation. For initial quantum states diagonal in the basis of the local Hamiltonian, these transitions are completely described by thermal processes (TPs), which form a convex set. In this paper, we give a complete characterization of the set of states that can be achieved through TPs, by describing the boundary of the allowed set of states using the so-called thermomajorization curves as a tool. We address the problem of achieving a certain transition through a convex combination of products of extremal TPs. We characterize all extremal TPs by associating them with transportation matrices. It becomes evident that there are extremal TPs that are not required in the implementation of any transition allowed by TPs. The statement holds for every dimension $d \geqslant 4$ of the state space. A property of the associated graphs, biplanarity, is identified as the distinguishing feature of these extremal TPs that are required for the arbitrary transition allowed by TPs.

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I. INTRODUCTION

One of the approaches to a quantum description of microscale systems interacting with a macroscale environment is through the so-called resource theories, with thermal operations (TOs) [1,2] being one of the most fruitful. Within TOs one is not constrained to a specific type of system-environment interaction. Instead, it is only assumed that the resulting operation commutes with the sum of the local Hamiltonians of the system and of the environment, and that the environment is in a thermal (Gibbs) state with respect to some temperature. Any state of the system that is not thermal with respect to this temperature constitutes a resource that can exhibit a nontrivial transition under TOs. All these transitions have been fully characterized for initial system states diagonal in the eigenbasis of a local Hamiltonian [1,3,4]. In this case, under the assumption that work is stored deterministically on a selected qubit subsystem, formulas for maximal work extraction and minimal work cost of state formation [4,5] have been given, along with microscale second laws of thermodynamics constituting a set of necessary and sufficient conditions for state transitions. The latter are expressed as the nondecreasing of generalized free energies of the system [6].

Thermal processes (TPs) enter the picture in this specific case of diagonality of the initial state of the system. Due to the fact that TOs commute with the local evolution of the system, coherences in the basis of the local Hamiltonian cannot be created by TOs acting on initially diagonal states [7]. Therefore, it is only the vector on the diagonal of the density matrix of the system that can be modified, and an associated action on this vector can be described by a thermal process, i.e., a left-stochastic matrix that preserves the Gibbs distribution with respect to temperature of the environment (see Preliminaries section for details). Thermal processes form a convex set. On the other hand, the set of states that can be achieved by TPs from a given initial state, characterized by the so-called thermomajorization condition [4], is known to be convex as well. Nevertheless, relations between the two sets remain unknown, as well as the characterization of the set of states achievable by TPs by their extremal points.

This lack of knowledge makes it difficult to address one of the basic problems of TOs: achievability of their predictions in a realistic experimental setting. In such a case, one does not have full control over the system-environment interaction, and therefore possibly cannot perform the unitary commuting with the total Hamiltonian that leads to the optimal performance. Efforts have been undertaken to show which predictions of TOs can be saturated, that is, which state transitions are possible in practice. On one hand, in [8] the authors showed that all TPs can be implemented as a sequence of operations involving partial thermalizations (which require only weak coupling between the system and the environment [9]) and manipulation of the system Hamiltonian, though at the cost of using an ancilla. However, this sequence can be highly nontrivial, and it is tempting to ask which transitions can be achieved with only a selected subset of extremal points of TPs at our disposal, with possible convex combinations of their products.

The first candidate for this subset was the set of TPs acting nontrivially only on two-dimensional subspaces of the system, as such TPs can be implemented with high fidelity within the Jaynes-Cummings model of interaction with a single mode of bosonic environment [10]. Nevertheless, it has been shown [10,11] that a set of states achievable by convex combinations of products of two-dimensional TPs, $\rho_{\mathrm{init}}^{\mathrm{TP(2)}}$, is strictly smaller than the set of $\rho_{\mathrm{init}}^{\mathrm{TP(d)}}$ for local dimension $d > 2$ and some

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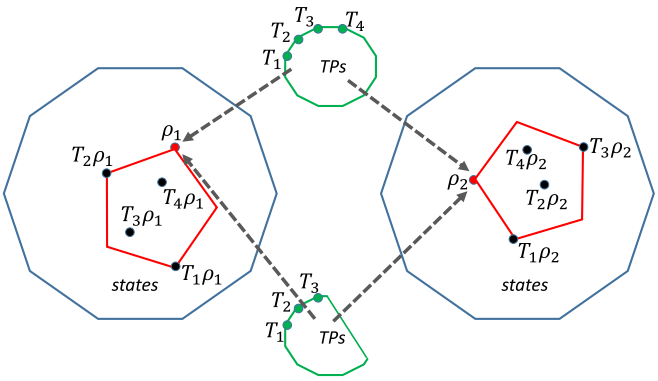

FIG. 1. Sets of diagonal states (blue polygons) and thermal processes (upper green polygon) for a system in a space of dimension d (not directly manifested in the picture). For different initial states ρ_1 and ρ_2, different sets of states achievable by TPs can be obtained: ρ_1^{TP} and ρ_2^{TP}, respectively (red polygons). Some extremal points of TPs, T_2 and T_3, map onto an extremal or nonextremal point of ρ^{TP}, depending on the initial state ρ. Non-biplanar extremal TPs, like T_4, never map onto an extremal point of ρ^{TP}, no matter which initial state ρ from the blue polygon is selected. When convex combinations of products of TPs are allowed, these extremal TPs can be discarded with no harm to the attainable set of states (lower green polygon). Non-biplanar extremal TPs exist for all $d \geqslant 4$.

initial state ρ_{init}. Furthermore, there always exists a state ρ_{init} for which the same relation holds between $\rho_{\mathrm{init}}^{\mathrm{TP(d-1)}}$ and $\rho_{\mathrm{init}}^{\mathrm{TP(d)}}$ for arbitrary $d \geqslant 3$ [11]. Even in the restricted scenario of TP(2) transformations, the length of TP(2) sequences required for all allowed transitions is not known for general d; only an upper bound has been derived [10].

In this paper, we address the problem of state achievability with limited resources, establishing a connection between the set of extremal TPs and the extremal points of the achievable states, $\rho_{\mathrm{init}}^{\mathrm{TP}}$. First, exploiting the thermomajorization condition, we obtain a complete characterization of the set of $\rho_{\mathrm{init}}^{\mathrm{TP}}$ by determining its extremal points, edges, and hyperfaces for arbitrary dimension d of an arbitrary initial system state ρ_{init}. Afterwards, we show that all extremal TPs, for arbitrary dimension d, possess a structure inherited from the set of transportation matrices, and therefore can be calculated using known algorithms for the determination of extremal points of the latter [12]. Finally, by exploiting properties of their associated graphs, we uniquely describe extremal TPs based on properties of extremal states in $\rho_{\mathrm{init}}^{\mathrm{TP}}$, whenever a given TP maps one of these extremal states into another.

Contrary to the intuition developed through studies of decomposability of TPs on 3-dimensional spaces, we show that for $d \geqslant 4$ there always exist extremal TPs that do not map between extremal states in $\rho_{\mathrm{init}}^{\mathrm{TP}}$, no matter which nontrivial ρ_{init} is chosen (see Fig. 1). Consequently, these maps do not need to be implemented in an experiment aiming at performing all transitions allowed by TPs. We call such TPs non-biplanar, motivated by the property of their associated bipartite graphs: they cannot be driven into a plane form by isometric transformations acting separately within two disjoint sets of vertices constituting the bipartite structure. We show a construction of such thermal processes, proving their existence for arbitrary finite, nonzero temperature.

Interestingly, the characterization of the set of extremal TPs may be useful for other than determining the set $\rho_{\mathrm{init}}^{\mathrm{TP}}$ of achievable states for decohered initial states of the system. For coherences present in the initial state, the analogous set $\rho_{\mathrm{init}}^{TO}$ that can be obtained through TO is only fully characterized for qubit systems [13]. Upper bounds on the evolution of system coherences were proposed for a general qudit case [7,13], but it was immediately shown that for some transitions they cannot be saturated. These bounds depend on a TP that a given thermal operation effectively applies to the diagonal of the system, and therefore the established knowledge about the structure of extremal points and the boundary of TPs may give insights into necessary and sufficient conditions for general transitions allowed by thermal operations in a fully quantum scenario.

We will proceed to the main part of the paper after introducing definitions and basic properties of thermal processes and transportation matrices.

II. PRELIMINARIES

A. Thermal processes

We start with a brief description of the resource theory of thermal operations. A d-dimensional system in a state $\rho \in \mathcal{B}(\mathcal{H}_S)$, $\mathcal{H}_S \cong \mathbb{C}^d$, is associated with a Hamiltonian $H_S = \sum_{i=0}^{d-1} E_i |E_i\rangle\langle E_i|$. For an environment $\mathcal{B}(\mathcal{H}_B)$ with a Hamiltonian H_B we define the Gibbs state $\mathcal{B}(\mathcal{H}_B) \ni \rho_\beta^B = e^{-\beta H_B}/\mathrm{Tr}[e^{-\beta H_B}]$, where $\beta = \frac{1}{kT}$; k is the Boltzmann constant, and T is temperature.

For a given β, we define a set of thermal operations (TOs) as all maps $\mathcal{E} : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S)$ that can be constructed by the following operations:

(1) One can perform an arbitrary unitary U on $\mathcal{H}_S \otimes \mathcal{H}_B$ that commutes with the total Hamiltonian: $[U, H_S + H_B] = 0$.

(2) One can extend the system by adding an arbitrary ancilla $\mathcal{B}(\mathcal{H}_A)$, $\mathcal{H}_A \cong \mathbb{C}^{d'}$, with a Hamiltonian H_A, in the Gibbs state $\rho_A = e^{-\beta H_A}/\mathrm{Tr}[e^{-\beta H_A}]$.

(3) One can trace out an arbitrary subsystem.

This leads to a set of trace-preserving, completely positive maps on a system, defined as $\rho \to \mathcal{E}(\rho) = \mathrm{Tr}_B(U[\rho \otimes \rho_\beta^B]U^\dagger)$.

Under the assumption that H_S has a nondegenerated spectrum, a TO acting on a state that is diagonal in the basis of its Hamiltonian ($[\rho_S, H_S] = 0$) cannot lead to creation of coherences in this basis. This follows from the fact that the evolution of nondiagonal elements of the density matrix is independent of the diagonal [7]. Moreover, it is easy to see that TOs conserve the Gibbs state of the system, ρ_β^S. Therefore, the action $\mathcal{E}(\rho)$ of the TO $\mathcal{E}$ on the state ρ diagonal in H_S, represented by the vector $\boldsymbol{p}$ comprising its eigenvalues, $\rho = \mathrm{diag}[\boldsymbol{p}]$, can be associated with the action $T\boldsymbol{p}$ of the left-stochastic matrix T preserving the Gibbs vector $\boldsymbol{g}$, $g_i = q_{i,0}/\sum_{j=0}^{d-1} q_{j,0}$, where we take $q_{m,n} = e^{-\beta(E_m - E_n)}$, with E_i being the eigenvalues of H_S.

We call this matrix a thermal process (TP):

Definition 1. The set of thermal processes $TP(d)_{\beta,H_S}$ is the set of $d \times d$ matrices T satisfying $\mathbf{1}^T T = \mathbf{1}^T$ and $T\boldsymbol{g} = \boldsymbol{g}$, where $\mathbf{1}^T = [1, \ldots, 1]$.

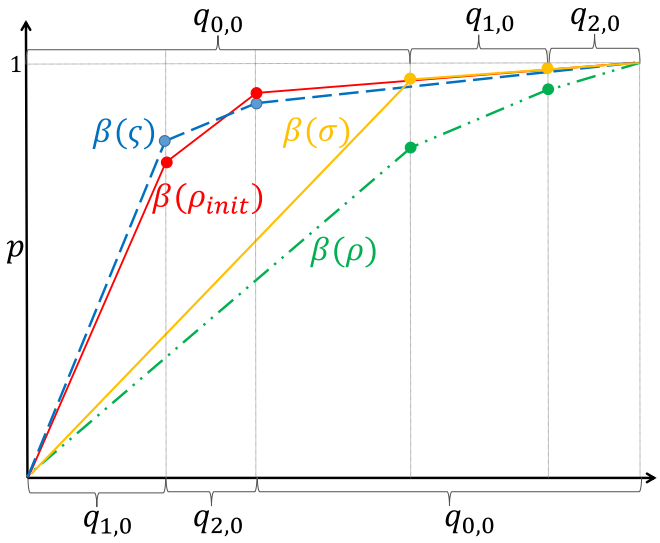

FIG. 2. Thermomajorization diagram for a $d = 3$ system, and certain H_S and β defining $q_{00} = 1$, q_{10}, and q_{20}. According to Lemma 1, $\rho, \sigma \in \rho_{\text{init}}^{\text{TP}}$, but $\zeta \notin \rho_{\text{init}}^{\text{TP}}$ and $\rho_{\text{init}} \notin \zeta^{\text{TP}}$. Elbows of curves are indicated by circles. Curves $\beta(\sigma)$ and $\beta(\rho)$ are *thermomajorized* by curve $\beta(\rho_{\text{init}})$. Curve $\beta(\sigma)$ is *tightly thermomajorized* by curve $\beta(\rho_{\text{init}})$. States ρ_{init} and ζ have β order (2,3,1), while states σ, ρ have β order (1,2,3).

In what follows, we will omit the indices d, β, H_S when this does not lead to confusion, assume that $E_0 = 0$, and assume that all states ρ satisfy $[\rho, H_S]$ for a nondegenerated Hamiltonian H_S and therefore can be represented by vectors $\boldsymbol{p}$ carrying information about their occupations on energy levels of H_S.

Above we showed that for every given TO, one can define its associated TP. On the other hand, for every TP there exists a TO on the environment and a system diagonal with respect to H_S that performs this TP on the system [4]. Therefore, all transformations allowed for diagonal states within thermal operations resource theory can be equivalently characterized by TPs.

Definition 2. $\rho_{\text{init}}^{\text{TP}}$ is the set of states that can be obtained through thermal processes from a state ρ_{init}.

From the fact that thermal processes form a convex polytope one can easily see that $\rho_{\text{init}}^{\text{TP}}$ is a convex polytope as well (cf. Remark 6 in Appendix A). Moreover, $\rho_{\text{init}}^{\text{TP}}$ is fully characterized by a criterion exploiting the representation of a vector $\boldsymbol{p}$ on the so-called thermomajorization diagram (see Fig. 2).

Definition 3 (thermomajorization curve). Define a vector $\boldsymbol{s} = (q_{00}, q_{10}, q_{20}, \ldots, q_{d-1,0})$. For every state ρ of the system commuting with H_S, let the vector $\boldsymbol{p}$ represent occupations p_i of energy levels E_i, $i = 0, 1, \ldots, d-1$. Choose a permutation π on $\boldsymbol{p}$ and $\boldsymbol{s}$ such that it leads to a nonincreasing order of elements in the vector $\boldsymbol{d}$, $d_k = \frac{\sum_{i=0}^{k}(\pi \boldsymbol{p})_i}{\sum_{i=0}^{k}(\pi \boldsymbol{s})_i}$, $k = 0, \ldots, d-1$. The set of points $\{\sum_{i=0}^{k}(\pi \boldsymbol{p})_i, \sum_{i=0}^{k}(\pi \boldsymbol{s})_i\}_{k=0}^{d-1} \cup \{0, 0\}$, connected by straight lines, defines a curve associated with the state ρ. We denote it by $\beta(\rho)$ and call it the thermomajorization curve of the state ρ represented by $\boldsymbol{p}$.

The points $\{\sum_{i=0}^{k}(\pi \boldsymbol{p})_i, \sum_{i=0}^{k}(\pi \boldsymbol{s})_i\}_{k=0}^{d-1}$ will be called elbows of the curve $\beta(\boldsymbol{p})$. The curve is concave due to the nonincreasing order of elements in $\boldsymbol{d}$. Let us note that there might be more than one permutation leading to a concave curve $\beta(\rho)$. The vector $\pi(1, \ldots, d)^T$ will be called a β order of ρ. It shows the order of segments assuring convexity of $\beta(\rho)$.

Thermomajorization curves are used to characterize possible transitions between states under TPs [4]:

Lemma 1. A transition from $\rho_{\text{init}} \in \mathcal{B}(\mathcal{H}_S)$, $\mathcal{H}_S \cong \mathbb{C}^d$, to $\rho_{\text{out}} \in \mathcal{B}(\mathcal{H}_S)$ under TPs is possible if and only if $\beta(\rho_{\text{init}})$ thermomajorizes $\beta(\rho_{\text{out}})$; i.e., all elbows of $\beta(\rho_{\text{out}})$ lie on $\beta(\rho_{\text{init}})$ or below it.

For the sake of characterization of the set of extremal points of $\rho_{\text{init}}^{\text{TP}}$ (Sec. III), we single out a specific relation between two curves:

Definition 4 (tight thermomajorization). If the curve $\beta(\rho)$ has all elbows on the curve $\beta(\sigma)$, then $\beta(\sigma)$ tightly thermomajorizes $\beta(\rho)$.

B. Transportation matrices

Below we introduce the notion of transportation matrices, whose properties will be useful in characterizing the connection between sets of states achievable by thermal processes, $\rho_{\text{init}}^{\text{TP}}$, and the set of thermal processes itself.

Definition 5 (transportation matrix). A transportation matrix M is an $m \times n$ matrix with non-negative entries determined by two vectors $\boldsymbol{c}$ and $\boldsymbol{r}$ of lengths m and n, respectively, in a way that all entries from the ith row (column) of M sum to r_i (c_i), and $\sum_i c_i = \sum_j r_j = C$.

For all pairs of non-negative vectors $\boldsymbol{c}$ and $\boldsymbol{r}$ satisfying the summation condition, an associated transportation matrix always exists: if $C = 0$, it is a matrix with all entries equal 0; for other cases we can construct M as $M_{i,j} = r_i c_j / C$.

For every pair of vectors the set of transportation matrices is a convex polytope, called a transportation polytope. The set of its extremal points is fully characterized by the following constructive algorithm ([12], Theorem 4.1), cf. Fig. 3(a):

Theorem 1 (extremal points of transportation polytope). A transportation matrix with defining vectors $\boldsymbol{c}$, $\boldsymbol{r}$, $\sum_i c_i = \sum_i r_i = C$ is extremal if and only if it can be constructed by repeating the following step, starting with a matrix with no values assigned:

(1) Pick a position (i, j) in the matrix that has no assigned value, and fill it with $\min(r_i, c_j)$. If $r_i \leqslant c_j$ ($r_i \geqslant c_j$), fill all remaining entries within the ith row (jth column) of the matrix with 0. (This implies that if $r_i = c_j$, all the remaining entries within the ith row and jth column will be filled with 0.) Update the values $r_i \to r_i - \min(r_i, c_j)$, $c_j \to c_j - \min(r_i, c_j)$. The updated vectors are non-negative and satisfy the summation criterion; therefore they define a transportation matrix.

(2) If $\boldsymbol{r} = \boldsymbol{0}$ and $\boldsymbol{c} = \boldsymbol{0}$, abort. All entries of the matrix have been determined, with at most $n + m - 1$ positive ones.

We define an important class of extremal transportation matrices in the following way:

Definition 6 (biplanar extremal transportation matrix). An extremal transportation matrix with defining vectors $\boldsymbol{c}$, $\boldsymbol{r}$,

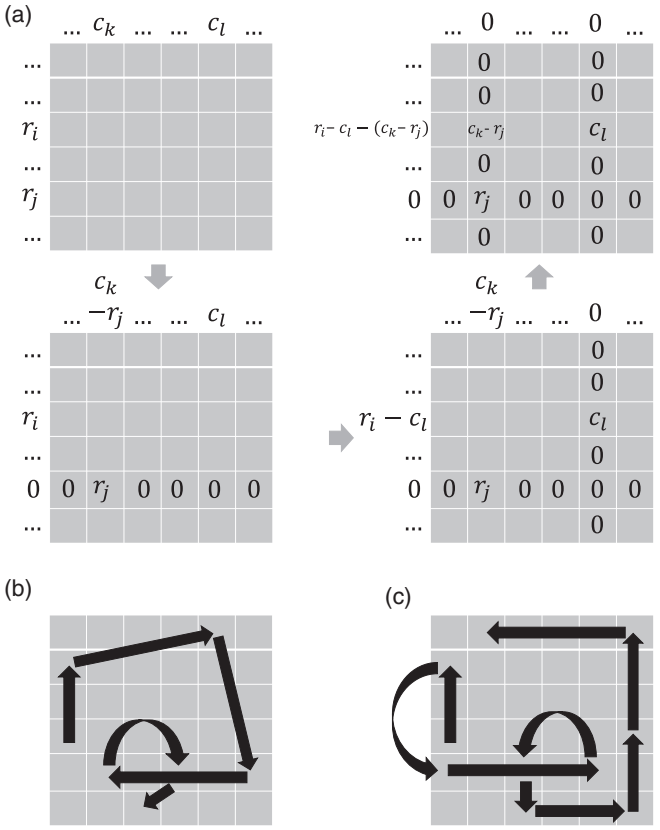

FIG. 3. (a) First three steps of procedure in Theorem 1 determining three nonzero matrix elements of an extremal point of a transportation polytope set by vectors $\boldsymbol{c}$ and $\boldsymbol{r}$ such that $c_k > r_j$, $r_i > c_l$, $r_i - c_l > c_k - r_j$. Entries of the vectors $\boldsymbol{r}$ and $\boldsymbol{c}$ are listed along the corresponding rows and columns, and are updated with each step. (b) Arrows joining nonzero matrix entries fixed in the consecutive steps of procedure in Theorem 1. An arbitrary element with nondetermined value can be fixed in the next step. (c) Arrows joining nonzero matrix entries fixed in the consecutive steps of procedure in Definition 6. Only elements with nondetermined values that lie on the same row or column as the previously picked element can be fixed in the next step.

$\sum c_i = \sum r_i = C$ is biplanar if it can be constructed by the following procedure:

(1) Pick a position (i, j) in the matrix and fill it with $\min(r_i, c_j)$. If $r_i \leqslant c_j$ ($r_i \geqslant c_j$), fill all the remaining entries within the ith row (jth column) of the matrix with 0. (This implies that if $r_i = c_j$, all the remaining entries within the ith row and jth column will be filled with 0.) Update the values $r_i \to r_i - \min(r_i, c_j)$, $c_j \to c_j - \min(r_i, c_j)$. The updated vectors are non-negative and satisfy the summation criterion; therefore they define a transportation matrix.

(2) If for indices i and j from step 1 the updated vector $\boldsymbol{r}(\boldsymbol{c})$ satisfies $r_i \neq 0$ ($c_j \neq 0$), choose a position without assigned value from the ith row (jth column) as a starting position of step 1, and execute it. If both $r_i = c_j = 0$, pick another position in the matrix that has no assigned value, (i', j'), and return to step 1 by substituting $i' \to i$, $j' \to j$.

(3) If $\boldsymbol{r} = \boldsymbol{0}$ and $\boldsymbol{c} = \boldsymbol{0}$, abort. All entries of the matrix have been determined, with at most $n + m - 1$ positive ones.

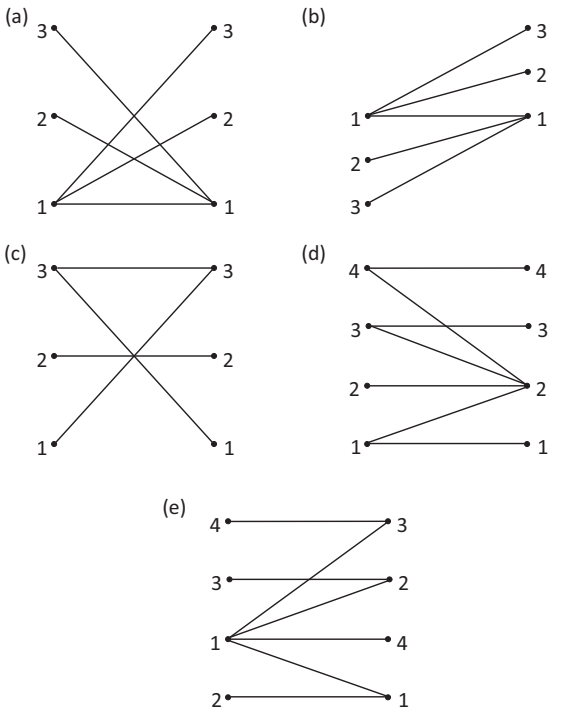

FIG. 4. Forests with no isolated vertices on bipartite graphs for chosen extremal transportation matrices: (a) $\left(\begin{smallmatrix}1&3&4\\2&0&0\\5&0&0\end{smallmatrix}\right)$, with $\boldsymbol{r} = (8, 2, 5)$, $\boldsymbol{c} = (8, 3, 4)$; (b) the same as in (a); (c) $\left(\begin{smallmatrix}0&0&2\\0&7&0\\5&0&1\end{smallmatrix}\right)$, with $\boldsymbol{r} = (2, 7, 6)$, $\boldsymbol{c} = (5, 7, 3)$; (d) $\left(\begin{smallmatrix}4&0&0&0\\5&3&6&7\\0&0&2&0\\0&0&0&1\end{smallmatrix}\right)$, with $\boldsymbol{r} = (4, 21, 2, 1)$, $\boldsymbol{c} = (9, 3, 8, 8)$; (e) $\left(\begin{smallmatrix}1&1&0&0\\1&0&1&0\\1&0&0&1\\1&0&0&0\end{smallmatrix}\right)$, with $\boldsymbol{r} = (2, 2, 2, 1)$, $\boldsymbol{c} = (4, 1, 1, 1)$. Notice that the graph in (b) is the plane version of the biplanar graph in (a). Graphs in (d) and (e) cannot be driven into plane forms by isomorphisms that do not switch vertices between sides of the bipartite structure. The graph in (c) can be driven into such form, and, as opposed to the rest of the graphs, is a forest composed of two trees instead of one tree. Labels of the vertices on the left (right) side of the graphs correspond to columns (rows) of the respective extremal transportation matrix.

The difference between the procedures of Theorem 1 and Definition 6, i.e., between constructing an arbitrary extremal transportation matrix and a bipartite one, is visible in Fig. 3(b) and Fig. 3(c).

The name of biplanar extremal transportation matrices comes from the property of the graphs associated with their adjacency matrices (see Fig. 4). To every extremal matrix we can assign its adjacency matrix. It is a matrix of the same size as the transportation matrix, with 0 entries except where its corresponding transportation matrix has a positive entry, where the adjacency matrix entry is 1. We construct the associated graph in the following way: associate the rows of an adjacency matrix with graph vertices on the right side of a bipartite graph, and the columns of the adjacency matrix with graph vertices on the left side of a bipartite graph, and connect vertices by edges whenever the corresponding entry of the

adjacency matrix is 1. For biplanar extremal transportation matrices, all the vertices of such a graph are assigned to disjoint subgraphs in a way that, within a selected subgraph, every vertex is connected to another vertex by a single path on edges.

In the graph-theoretic language, this means that extremal points of transportation matrices correspond to forests (sets of trees) on bipartite graphs with no isolated vertices [14]. This property is also visible directly from the construction of Theorem 1, which enforces that every vertex of the bipartite graph is included in some subgraph if vectors $\boldsymbol{r}$ and $\boldsymbol{c}$ are positive, and also sets these subgraphs to be trees. If they were not trees, the procedure would have to allow for the subgraphs to have cycles, which is forbidden by the fact that at every step we put 0 elements at nondetermined entries of a matrix along some column or row, and therefore we cannot assign to entries of this column or row positive entries in further steps, so cycles cannot be formed.

Biplanar extremal matrices are characterized by the property that for their associated graphs one can perform an isometric transformation on the vertices that preserves the bipartite structure (i.e., one can change positions of the vertices within each side of the bipartite graph without changing nearest neighbors within the graph), such that none of the edges cross (the graph becomes plane). This property justifies the name; while the existence of an isometric form of a graph with no edges crossing is a defining property of a planar graph, here we restrict isomorphic maps to those that preserve the bipartite structure. This property characterizes matrices from the biplanar class, because picking an initial element in step 1 of Definition 6 fixes the initial column and row numbers, as well as defines an edge connecting the corresponding vertices on the associated bipartite graph. If in step 2 we decide to continue the procedure on the same column, we would add an edge to a new vertex on the right side of the graph. In contrast, if we were to define a new element in the same row as the previous one, it would be equivalent to adding an edge starting from a selected vertex on the right side of the graph. The selection of a new, independent element starts the construction of a new tree.

What will be crucial in our applications is that the above implies that there exists an order of vertices (determined in the direction from the bottom to the top) of the bipartite graph such that the graph is plane. On the other hand, if such an order exists, then the extremal transportation matrix can be created by the procedure from Definition 6; thus the transportation matrix belongs to the class of biplanar extremal matrices. Note that in general this does not have to be the case; i.e., there exist bipartite graphs with forests of edges and no isolated vertices, such that they cannot be driven to a plane form by isomorphic transformations conserving the bipartite structure. Yet, these graphs can be associated with extremal transportation matrices [see Fig. 4(d)].

Note that a transportation matrix does not mix between elements belonging to different trees [Fig. 4(c)]. For rectangular transportation matrices of size $n \times n$, the maximal number of trees is achieved by a diagonal extremal transportation matrix (if it exists for given $\boldsymbol{c}$ and $\boldsymbol{r}$). Such a matrix has also the smallest possible number of positive elements (n).

III. GEOMETRY OF THE SET OF STATES ACHIEVABLE BY TPs

In this section we present our results concerning characterization of extremal points and the boundary of the set of states achievable through TPs from a given initial diagonal state ρ_{init}. This characterization is vital for the next section, where we address the problem of finding the minimal set of maps on the system required in performing all transitions allowed by TOs for initially diagonal states.

Let us denote by Extr[A] the set of extremal points of a convex set A.

Theorem 2 (extremal states achievable from ρ_{init} by thermal processes). A state ρ belongs to Extr[$\rho_{\text{init}}^{\text{TP}}$] if and only if $\beta(\rho)$ is tightly thermomajorized by $\beta(\rho_{\text{init}})$.

The proof of sufficiency of tight thermomajorization for extremality is based on Lemma 1, and is presented below. To prove necessity, in Appendix B we present a procedure for finding a representation of every state in $\rho_{\text{init}}^{\text{TP}}$ as a convex combination of states with curves tightly thermomajorized by $\beta(\rho_{\text{init}})$. This also shows that every state with a curve that is thermomajorized, but not tightly thermomajorized by $\beta(\rho_{\text{init}})$, cannot be an extremal point of $\rho_{\text{init}}^{\text{TP}}$.

Proof (*if part*). If $\beta(\rho)$ is (tightly) thermomajorized by $\beta(\rho_{\text{init}})$, then ρ belongs to $\rho_{\text{init}}^{\text{TP}}$ due to Lemma 1. Moreover, ρ is an extremal point of this set: if it were not true, then there would exist two different states σ_1, σ_2 belonging to $\rho_{\text{init}}^{\text{TP}}$, such that ρ could be created as their nontrivial convex combination. But this would imply that the thermomajorization curve of at least one of these states is not thermomajorized by $\beta(\rho_{\text{init}})$, therefore contradicting the fact that $\sigma_1 \in \rho_{\text{init}}^{\text{TP}}$. This implication is visible from the following reasoning: for a thermomajorization curve $\beta(\rho)$, by $\beta_i(\rho)$ we will denote the slope of the segment of length given by s_i. $\rho = a\sigma_1 + (1-a)\sigma_2$ implies $\beta_i(\rho) = a\beta_i(\sigma_1) + (1-a)\beta_i(\sigma_2)$ for every $i = 0, \ldots, d-1$. Therefore, if we choose i such that $\beta_i(\rho)$ is the highest slope of $\beta(\rho)$, from the fact that $\beta(\rho)$ is *tightly thermomajorized* by $\beta(\rho_{\text{init}})$ we see that $\beta_i(\rho)$ is the maximal slope that the segment of length s_i can take, such that $\beta(\rho)$ is *thermomajorized* by $\beta(\rho_{\text{init}})$. But from the convex combination relation we have that either $\beta_i(\sigma_1) > \beta_i(\rho)$, $\beta_i(\sigma_2) > \beta_i(\rho)$, or $\beta_i(\sigma_1) = \beta_i(\sigma_2) = \beta_i(\rho)$. Therefore, in the first two cases $\sigma_1 \notin \rho_{\text{init}}^{\text{TP}}$ or $\sigma_2 \notin \rho_{\text{init}}^{\text{TP}}$, and we arrive at the thesis. In the third case, we proceed to the segment characterized by i such that it has the second-highest slope of $\beta(\rho)$. Again, as $\beta(\rho)$ is tightly thermomajorized by $\beta(\rho_{\text{init}})$, $\beta_i(\rho)$ is the highest possible slope of the segment of length s_i, provided the slope of the segment of the highest slope is fixed according to the previous step. Again, creating ρ as a mixture of σ_1 and σ_2 would lead to a conclusion that either $\beta_i(\sigma_1) > \beta_i(\rho)$, $\beta_i(\sigma_2) > \beta_i(\rho)$, or $\beta_i(\sigma_1) = \beta_i(\sigma_2) = \beta_i(\rho)$. By iterating this procedure for consecutive segments, according to descending order of the slopes of $\beta(\rho)$, we see that the only allowed decomposition of ρ that is tightly thermomajorized by ρ_{init} into $\sigma_{1,2} \in \rho_{\text{init}}^{\text{TP}}$ is for $\sigma_{1,2} = \rho$. Therefore, $\rho \in \text{Extr}[\rho_{\text{init}}^{\text{TP}}]$. ■

Remark 1. The state ρ_{init} is a vertex of the set $\rho_{\text{init}}^{\text{TP}}$.

Proof. This trivially follows from Theorem 2 and the fact that for all states ρ, $\beta(\rho)$ is tightly thermomajorized by itself. ■

Having characterized the vertices of $\rho_{\text{init}}^{\text{TP}}$ in terms of thermomajorization curves, we can give a similar description of the faces of the set:

Remark 2. A state $\rho \in \rho_{\text{init}}^{\text{TP}}$ lies on a face of $\rho_{\text{init}}^{\text{TP}}$ if and only if at least one of the elbows of $\beta(\rho)$ lies on $\beta(\rho_{\text{init}})$.

We refer the reader to Appendix B 2 for the proof. Natural observations follow:

Remark 3. The interior of the set $\rho_{\text{init}}^{\text{TP}}$ is composed by states ρ such that $\beta(\rho)$ has all elbows below $\beta(\rho_{\text{init}})$.

Remark 4. For $\rho_{\text{init}} \neq \rho_\beta$ [i.e., for $\beta(\rho_{\text{init}})$ with segments of different slopes], the Gibbs state $\rho_\beta = e^{-\beta H}/\operatorname{Tr}[e^{-\beta H}]$ lies in the interior of the set $\rho_{\text{init}}^{\text{TP}}$.

In the most general case, for a d-dimensional system, we can obtain a description of the boundary of $\rho_{\text{init}}^{\text{TP}}$ in terms of its hyperfaces.

Definition 7 (hyperface). A hyperface of a polytope $\rho_{\text{init}}^{\text{TP}}$ is a convex subset H of states $\rho \in \rho_{\text{init}}^{\text{TP}}$ that cannot be expressed as a nontrivial convex combination of states from $\rho_{\text{init}}^{\text{TP}}/H$.

For $d = 3$, the set $\rho_{\text{init}}^{\text{TP}}$ is a polygon (see Fig. 5), with all its nontrivial hyperfaces (i.e., different from $\rho_{\text{init}}^{\text{TP}}$ itself) being its edges and vertices. For $d = 4$, $\rho_{\text{init}}^{\text{TP}}$ belongs to a tetrahedron of all possible diagonal states, and can have as its nontrivial hyperfaces both edges and vertices, as well as faces of dimension 2.

For a given ρ_{init}, let us denote by $\mathbb{S}_{\rho_{\text{init}}}$ the set of all possible nonempty sets of elbows of curves tightly thermomajorized by $\beta(\rho_{\text{init}})$. For every $S \in \mathbb{S}_{\rho_{\text{init}}}$, we define H_S as the set of all states ρ such that their thermomajorization curves $\beta(\rho)$ coincide with $\beta(\rho_{\text{init}})$ exactly on S. Every element of the set $\mathbb{S}_{\rho_{\text{init}}}$ then defines a hyperface:

Theorem 3. H_S is a hyperface of $\rho_{\text{init}}^{\text{TP}}$. We refer the reader to Appendix B 3 for the proof.

If we take $S_1, S_2, \ldots, S_k \in \mathbb{S}_{\rho_{\text{init}}}$ such that $S_1 \subseteq S_2 \subseteq \cdots \subseteq S_k$, then $H_{S_1} \supseteq H_{S_2} \supseteq \cdots \supseteq H_{S_k}$. In particular, we see that every extremal point ρ of $\rho_{\text{init}}^{\text{TP}}$, such that $\beta(\rho)$ has an elbow on $\beta(\rho_{\text{init}})$ on a given point, belongs to all hyperfaces of $\rho_{\text{init}}^{\text{TP}}$ that are composed by states with thermomajorization curves overlapping with ρ_{init} on this point. Moreover, the characterization of hyperfaces of the set of achievable states in terms of nonempty sets S is complete:

Remark 5. Every hyperface of $\rho_{\text{init}}^{\text{TP}}$ is H_S for some $S \in \mathbb{S}_{\rho_{\text{init}}}$.

If this was not true, then there would be some hyperface containing a state ρ with $\beta(\rho)$ such that it has no elbows on ρ_{init}. From Remark 2 it follows that such a state belongs to the interior of $\rho_{\text{init}}^{\text{TP}}$, and therefore does not belong to any hyperface of $\rho_{\text{init}}^{\text{TP}}$.

Let us denote by P_{ab} a permutation of a and b elements in a given sequence. Then we can identify all nearest neighbors of every extremal point by the following lemma (proof can be found in Appendix B 4):

Lemma 2. For a state ρ_{init} with all slopes of $\beta(\rho_{\text{init}})$ different, two distinct extremal states $\epsilon_1, \epsilon_2 \in \rho_{\text{init}}^{TO}$, with orders of thermomajorization curves π_1 and π_2, respectively, are connected by an edge iff $\pi_1 = P_{d-i,d-i+1}\pi_2$, for some $i \in \{2, \ldots, d\}$.

IV. GEOMETRY OF THE SET OF TPs

In this section we are going to use properties of biplanar transportation matrices. Every thermal process T acting on a d-level system can be turned into a transformation matrix P by the transformation $P = T\,\text{diag}[1, q_{10}, \ldots, q_{d-1,0}]$. P is characterized by the vectors $\boldsymbol{r} = \boldsymbol{c} = [1, q_{10}, \ldots, q_{d-1,0}]$. P and T have identical adjacency matrices, and therefore the same graph representation. Therefore, all extremal TPs can be

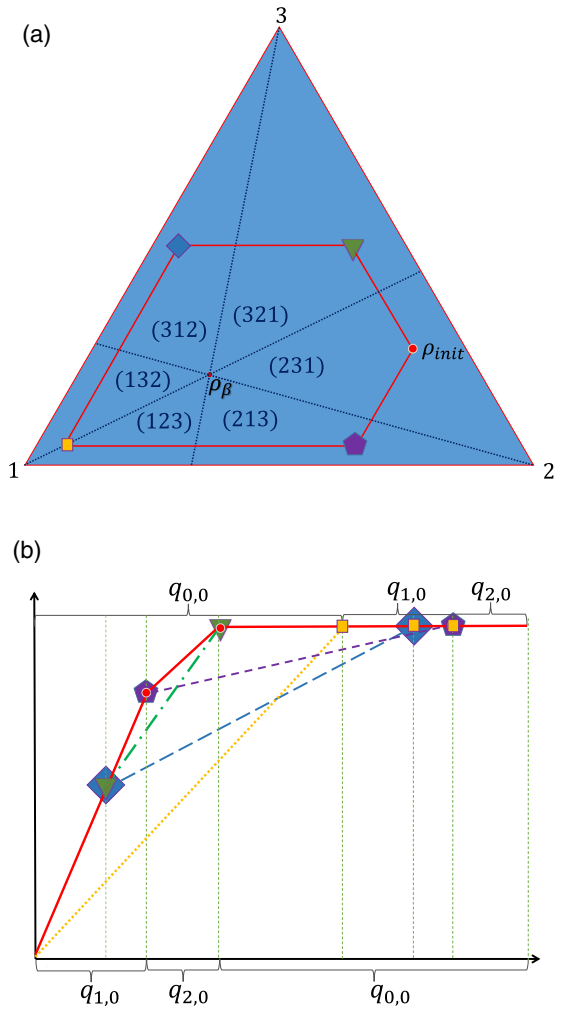

FIG. 5. Geometry of the set of achievable states for $d = 3$ and β and H_S such that $q_{10} + q_{20} \leqslant 1$. (a) Set $\rho_{\text{init}}^{\text{TP}}$ (solid-lined red polygon) for some state ρ_{init} with thermomajorization curve with β order (231). Regions of states with different β orders are separated by dotted black lines. Vertices 1,2,3 correspond to states diag[1, 0, 0], diag[0, 1, 0], and diag[0, 0, 1], respectively. (b) Thermomajorization curves of extremal points of $\rho_{\text{init}}^{\text{TP}}$. Shape and color of elbows within a curve correspond to shape of points in (a). Note that β order of the state represented by a yellow square is not determined uniquely, so its rightmost elbow can be placed both on pentagon and diamond elbows. In particular, the yellow rectangle state is achieved by an extremal thermal process $\begin{pmatrix} 1-q_{10}-q_{20} & 1 & 1 \\ q_{10} & 0 & 0 \\ q_{20} & 0 & 0 \end{pmatrix}$ on the diagonal elements of ρ_{init}. One can check that this thermal process has a graph representation as in Fig. 4(a) and Fig. 4(b), and therefore has associated orders $\pi_{\text{init}} = (231)$ and $\pi_{\text{out}} = (123)$ or $\pi_{\text{out}} = (132)$. Theorem 4 implies then that it is the only process mapping ρ_{init} into the yellow rectangle state. Green triangle, blue diamond, and purple pentagon extremal states can be obtained uniquely from ρ_{init} by the extremal TPs $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-q_{21} & 1 \\ 0 & q_{21} & 0 \end{pmatrix}$, $\begin{pmatrix} 1-q_{10} & 1-q_{21} & 1 \\ q_{10} & 0 & 0 \\ 0 & q_{21} & 0 \end{pmatrix}$, $\begin{pmatrix} 1-q_{20} & 0 & 1 \\ 0 & 1 & 0 \\ q_{20} & 0 & 0 \end{pmatrix}$, respectively.

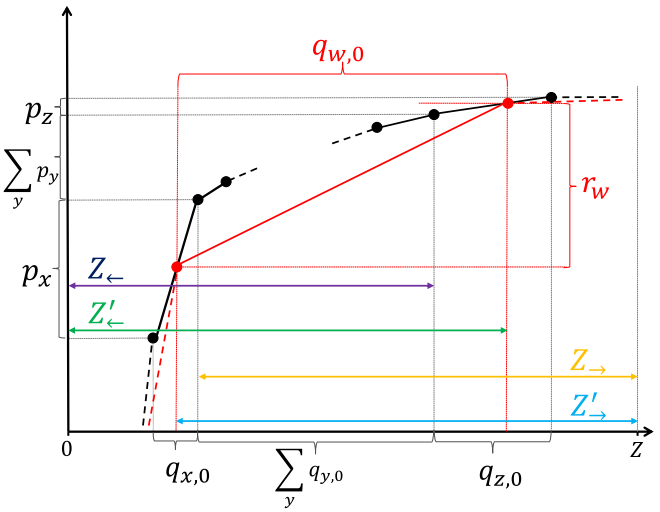

FIG. 6. Construction of an extremal thermal process from thermomajorization diagram.

associated with forests with no isolated vertices on bipartite graphs, having at most $2d-1$ positive entries (note, however, that some forests with isolated vertices may exist only for a specific choice of $\boldsymbol{r}$ and $\boldsymbol{c}$, so not all of them lead to extremal thermal processes). Moreover, extremal TPs that correspond to biplanar extremal transportation matrices play a special role in the characterization of transitions allowed by thermal operations. Below we show that every such TP can be attributed two quantities: an order $\pi_{in}(T)$, which is a sequence of labels on the left side of the bipartite graph of the associated transportation matrix P, and $\pi_{\text{out}}(T)$, which is a sequence of labels on the right side of the bipartite graph of the associated transportation matrix P, such that for these sequences the graph is plane. Note that these orders may not be given uniquely.

A. Biplanar extremal thermal processes

Lemma 3 (tight thermomajorization relation on states defines a biplanar extremal thermal process). Every pair of states $\rho_{\text{out}}, \rho_{\text{init}}$, such that $\boldsymbol{p} := \beta(\rho_{\text{init}})$ tightly thermomajorizes $\boldsymbol{r} := \beta(\rho_{\text{out}})$, determines a biplanar extremal thermal process T such that $T\rho_{\text{init}} = \rho_{\text{out}}$, $\pi_{in}(T) = \pi(p)$, and $\pi_{\text{out}}(T) = \pi(r)$. If all slopes of $\boldsymbol{p}$ are different, then T is the only TP that transforms ρ_{in} into ρ_{out}.

Please note that with a slight abuse of notation, we represent here the state and its thermomajorization curve by the same symbol. We will also denote the slope of the segment i on the curve associated with $\boldsymbol{p}$ as $\partial \boldsymbol{p}_i$.

Proof. Thermal process: Gibbs state preservation. Every β fixes values of $q_{k,0}$ coefficients that determine lengths of segments of curves $\boldsymbol{p}$ and $\boldsymbol{r}$ on a thermomajorization diagram, and the association between states and TPs is done on the basis of thermomajorization curves $\boldsymbol{p}$ and $\boldsymbol{r}$. If $\boldsymbol{r}$ is tightly thermomajorized by $\boldsymbol{p}$, then from the thermomajorization diagram we propose a procedure that determines all components of the transformation.

In the case presented in Fig. 6, $\boldsymbol{r}_w$ receives contributions from multiple segments of $\boldsymbol{p}$. It is visible that for every w, $\boldsymbol{r}_w$ can be formed from complete contributions from some levels of $\boldsymbol{p}$ (we will label these levels by y), and at most two partial contributions from segments x and z of $\boldsymbol{p}$. These two partial contributions are a product of slopes $\partial \boldsymbol{p}_x$ and $\partial \boldsymbol{p}_z$ of respective segments of the curve $\boldsymbol{p}$ and the lengths of these segments. These lengths can be calculated as differences in components of the partition function. We will denote them by $Z_{\rightarrow} = \sum q_{i,0}/Z$ for a sum over lengths of segments situated to the right from the point where the first segment included in $\sum \boldsymbol{p}_y$ originates, while $Z_{\leftarrow} = \sum q_{i,0}/Z$ is a sum over lengths of segments situated to the left from the point which the last segment included in $\sum \boldsymbol{p}_y$ has reached. $Z'_{\rightarrow}$ and $Z'_{\leftarrow}$ are defined analogously, but now with reference points changed to be initial and end points of the segment w of the curve $\boldsymbol{r}$. From the definition, the length of this segment is $q_{w,0}$, while its height is $\boldsymbol{r}_w$. We arrive at the following formula describing the map transforming state $\boldsymbol{p}$ into $\boldsymbol{r}$ which is tightly thermomajorized by $\boldsymbol{p}$: $\boldsymbol{r}_w = \partial \boldsymbol{p}_x(Z'_{\rightarrow} - Z_{\rightarrow}) + \sum_y \boldsymbol{p}_y + \partial \boldsymbol{p}_z(Z'_{\leftarrow} - Z_{\leftarrow})$. We have to show that this transformation is Gibbs preserving. In general we have $\partial \boldsymbol{p}_x = p_x q_{0,x}$. If we start from a Gibbs state curve $\boldsymbol{p}_x = q_{x,0}/Z$, then we arrive at $\boldsymbol{r}_w = q_{x,0}q_{0,x}/Z(Z'_{\rightarrow} - Z_{\rightarrow}) + \sum_y q_{y,0}/Z + q_{z,0}q_{0,z}/Z(Z'_{\leftarrow} - Z_{\leftarrow}) = (Z'_{\rightarrow} - Z_{\rightarrow} + \sum_y q_{y,0} + Z'_{\leftarrow} - Z_{\leftarrow})/Z$. But from Fig. 6 it is visible that $-Z_{\rightarrow} - Z_{\leftarrow} + \sum_y q_{y,0} = -Z$. Therefore, we have $\boldsymbol{r}_w = (Z'_{\rightarrow} + Z'_{\leftarrow} - Z)/Z = (Z + q_{w,0} - Z)/Z = q_{w,0}/Z$, which is a coefficient of a Gibbs state.

The same holds for all other possible constructions of $\boldsymbol{r}_w$: if $Z'_{\rightarrow} = Z_{\rightarrow}$, then $\sum_y p_y = Z'_{\leftarrow} - Z_{\leftarrow}$, while for $Z'_{\leftarrow} = Z_{\leftarrow}$, we have $\sum_y p_y = Z'_{\rightarrow} - Z_{\rightarrow}$, and one reaches the same conclusion about Gibbs state preservation of the process. Moreover, for all elbows of $\boldsymbol{r}$ lying within one segment f of $\beta(\boldsymbol{p})$, we have $Z_{\leftarrow} + Z_{\rightarrow} = Z$ and have $\sum_y p_y = 0$, for which $\boldsymbol{r}_w = p_f q_{0f} q_{w0}$, which again equals $q_{w,0}$ for initial Gibbs state $\boldsymbol{p}_f = q_{f,0}/Z$. This exhausts the set of all possible geometrical relations between $\boldsymbol{p}$ and a selected segment $\boldsymbol{r}_w$ of the curve $\boldsymbol{r}$.

Thermal process: Stochasticity. Stochasticity of the transformation stems directly from the fact that $\boldsymbol{r}$ is a curve on a thermomajorization diagram corresponding to a state: therefore every element $\boldsymbol{p}_i$ is fully distributed into some set or $\{\boldsymbol{r}_j\}_j$ (elements of every column of $T : T\rho_{\text{init}} = \rho_{\text{out}}$ sum to 1).

Extremality and biplanarity. To show that T is extremal and biplanar, it is enough to find a graph associated with P that is plane, and to show that the graph is a forest with no isolated vertices. We will construct this graph by connecting a vertex a from the right and b from the left side of the graph whenever a segment b on $\boldsymbol{p}$ lies on the thermomajorization diagram above a segment a on $\boldsymbol{r}$, as it signifies the positive coefficient in P on the position (a, b) (and therefore a positive element in T). This leads to a graph of forests (because once a particular segment is considered, it does not reappear after we move to another segment on the same curve, so cycles are not possible) with no isolated vertices (because every segment lies below or above at least one segment). Furthermore, the graph is planar, with orders $\pi_{in}(T)$ and $\pi_{\text{out}}(T)$ fixed to be the same as orders $\pi(\boldsymbol{p})$

and $\pi(\boldsymbol{r})$, respectively. We see that this sequence of mappings is the one in which elements of the transportation matrix P are fixed according to the defining procedure in Definition 6.

Uniqueness. Notice that the order of $\pi(\boldsymbol{r})$ may not be given uniquely, as it is in principle possible to obtain a state with a curve $\boldsymbol{r}$ that has more than one segment with the same slopes. On the other hand, if more than one segment has the same slope in $\boldsymbol{p}$, this means that the transformation between the states may not be unique: In the extremal case, if all slopes of $\boldsymbol{p}$ are the same, every TP performs the mapping (as every TP preserves a Gibbs state ρ_β). Therefore, we demand that all slopes in $\boldsymbol{p}$ are different: this prohibits segments of $\boldsymbol{p}$ to be permuted and fixes the sequence of points (i, j) that the procedure in Definition 6 utilizes to construct an associated transportation matrix. For every thermal process T there is an associated matrix $T^s := \frac{1}{Z^2}\mathrm{diag}[1, q_{0,1}, \ldots, q_{0,d-1}]T\,\mathrm{diag}[1, q_{1,0}, \ldots, q_{d-1,0}]$ that transforms slopes of the thermomajorization curve $\boldsymbol{x}$ into slopes of $\boldsymbol{y}$: $T\boldsymbol{x} = \boldsymbol{y} \iff T^s\partial\boldsymbol{x} = \partial\boldsymbol{y}$. T^s has the same adjacency matrix as T, and therefore is associated with the same transportation matrix P as T is. Therefore, we see that the condition that $\boldsymbol{r}$ is tightly thermomajorized by $\boldsymbol{p}$ implies a map T^s that is unique for all slopes of $\boldsymbol{p}$ different, as only this map assures the curve $\boldsymbol{r}$ has each of its elbows as high as possible (i.e., on $\boldsymbol{p}$), given position of elbows to the left. Therefore, T is also set uniquely. The property of the map of pushing the elbows as high as possible is resembled by construction of the corresponding transportation matrix P (Definition 6), where we assign the value $\min(r_i, c_j)$ to a given row or column; this value is the biggest possible under constraints of $\boldsymbol{r}$ and $\boldsymbol{c}$ at a given step of the procedure. ■

On the other hand, every biplanar extremal thermal process is associated with a pair of β orders of states, which are connected by a tight thermomajorization relation of their corresponding curves:

Lemma 4 (every biplanar extremal thermal process defines tight thermomajorization relation on states). For an arbitrary biplanar extremal thermal process T at temperature β, characterized by orders $\pi_{in}(T)$ and $\pi_{\mathrm{out}}(T)$, and a state ρ_{init} such that $\pi(\beta(\rho_{\mathrm{init}})) = \pi_{in}(T)$, we have that $\rho_{\mathrm{out}} = T\rho_{\mathrm{init}} \in \mathrm{Extr}[\rho_{\mathrm{init}}^{\mathrm{TP}}]$ and $\pi(\beta(\rho_{\mathrm{out}})) = \pi_{\mathrm{out}}(T)$. If all slopes of $\beta(\rho_{\mathrm{init}})$ are different, then T is the unique transformation that maps ρ_{in} to ρ_{out}.

Proof. Every biplanar extremal thermal process T is characterized by sequences of $\pi_{in}(T)$ and $\pi_{\mathrm{out}}(T)$, which label the left and right side of the associated graph of a transportation matrix P, and for which the graph is planar. Therefore, for every initial state ρ_{init} with order $\pi(\beta(\rho_{\mathrm{init}})) = \pi_{in}(T)$, we obtain a state $\rho_{\mathrm{out}} = T\rho_{\mathrm{init}}$ with order $\pi(\beta(\rho_{\mathrm{out}})) = \pi_{\mathrm{out}}(T)$. Also, ρ_{out} is an extremal point of $\rho_{\mathrm{init}}^{\mathrm{TP}}$, because $\beta(\rho_{\mathrm{out}})$ provides the highest possible position for elbows for a given order $\pi(\beta(\rho_{\mathrm{out}}))$, and the latter follows from the proof of uniqueness from Lemma 3. The proof for uniqueness of the transformation T is the same as in Lemma 3. ■

To summarize, the relation between biplanar extremal TPs and states with a tightly thermomajorizable relation can expressed as follows:

Theorem 4. For a state ρ_{init} with $\beta(\rho_{\mathrm{init}})$ with all slopes different and β order $\pi(\beta(\rho_{\mathrm{init}}))$, ρ_{out} with β order $\pi(\beta(\rho_{\mathrm{out}}))$, and a biplanar extremal thermal process T with orders $\pi_{in}(T)$ and $\pi_{\mathrm{out}}(T)$, respectively, $\rho_{\mathrm{out}} = T\rho_{\mathrm{init}} \in \mathrm{Extr}[\rho_{\mathrm{init}}^{\mathrm{TP}}]$ if and only if $\pi(\beta(\rho_{\mathrm{init}})) = \pi_{in}(T)$ and $\pi(\beta(\rho_{\mathrm{out}})) = \pi_{\mathrm{out}}(T)$. T is the only TP that satisfies $T\rho_{\mathrm{init}} = \rho_{\mathrm{out}}$.

Proof. *If part* follows directly from Lemma 4. *Only if part* follows from Lemma 3. ■

The example of the relation between extremal TPs and extremal states in $\rho_{\mathrm{init}}^{\mathrm{TP}}$ is shown in Fig. 5 for a qutrit system and temperature low enough to allow for $q_{10} + q_{20} \leqslant 1$ for a given Hamiltonian H_S. From Theorem 4 is follows that, for a selected temperature β, one can calculate all biplanar extremal thermal processes from thermomajorization diagrams by investigating all possible β orders of initial and final states, where initial states have curves with all their slopes different, and they tightly thermomajorize the curves of output states. Note that any change of β influences the relations between the different q_{mn} determining the lengths of segments, which in turn influence possible β orders of curves associated with $\rho_{\mathrm{out}} \in \mathrm{Extr}[\rho_{\mathrm{init}}^{\mathrm{TP}}]$. In this way, the temperature-dependent geometry of $\rho_{\mathrm{init}}^{\mathrm{TP}}$ reflects the temperature-dependent geometry of the set of thermal processes.

B. Non-biplanar extremal thermal processes

We see that it is enough to be able to perform an arbitrary biplanar extremal TP, as it allows one to achieve an arbitrary extremal point of $\rho_{\mathrm{init}}^{\mathrm{TP}}$ for every ρ_{init}. Therefore, while extremal TPs that do not belong to the class of biplanar extremal TPs cannot be calculated from thermomajorization diagrams, they also seem to lack an operational meaning: when we allow for convex combinations of TPs, every state in the set of $\rho_{\mathrm{init}}^{\mathrm{TP}}$ can be achieved solely by the use of biplanar extremal TPs. Moreover, extremal TPs that are not biplanar cannot even lead to extremal points of $\mathrm{Extr}[\rho_{\mathrm{init}}^{\mathrm{TP}}]$ for the case of different slopes of $\beta(\rho_{\mathrm{init}})$, for any ρ_{init}. This follows from the uniqueness of T for states with curves that have all slopes different. Naturally, in a degenerated case with some slopes in $\beta(\rho_{\mathrm{init}})$ the same ($\rho_{\mathrm{init}} = \rho_\beta$ being an extreme case), many processes may lead to the same state, so non-biplanar and biplanar extremal TPs can effectively coincide for a subset of possible ρ_{init}.

The question arises as to whether non-bipartite extremal TPs exist for a given d. In fact, all extremal TPs for $d = 2, 3$ are biplanar (their list can be found in [11]). For $d = 4$, while we have shown a transportation matrix that is non-biplanar [Fig. 4(d)], this construction is not valid for $\boldsymbol{r} = \boldsymbol{c}$, as in this case, the link connecting vertices labeled by 1 on both sides implies that there should be no edge connecting vertex "1" on the left with vertex "2" on the right. Therefore, we cannot construct a corresponding thermal process, for which it is necessary that $\boldsymbol{r} = \boldsymbol{c} = [1, q_{10}, \ldots, q_{d-1,0}]$.

Extremal points of TPs have a very simple form for zero temperature. There, they have a vector $[1, 0, \ldots, 0]^T$ as the first column, and independent permutations of this vector in different columns, e.g., $\begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$. Therefore, they are transportation matrices. It is visible that these matrices are associated with graphs that are forests (each column has exactly one "1", so no loops are possible), but isolated vertices may be present (as there are some rows filled with "0"). Moreover, each of the rows of the matrix corresponds to an independent tree in a forest, so the graphs are biplanar. However, already for $d = 4$, when going from zero to small temperatures, while

all graphs become connected, some of them also become immediately non-biplanar. Consider the extremal TP:

$$T_{\text{non-biplanar}} = \begin{pmatrix} 1-q_{10} & 1 & 0 & 0 \\ q_{10}-q_{20} & 0 & 1 & 0 \\ q_{20}-q_{30} & 0 & 0 & 1 \\ q_{30} & 0 & 0 & 0 \end{pmatrix}. \tag{1}$$

This process has an associated transportation matrix

$$P(T_{\text{non-biplanar}}) = \begin{pmatrix} 1-q_{10} & q_{10} & 0 & 0 \\ q_{10}-q_{20} & 0 & q_{20} & 0 \\ q_{20}-q_{30} & 0 & 0 & q_{30} \\ q_{30} & 0 & 0 & 0 \end{pmatrix}, \tag{2}$$

described by a graph composed from a forest with no isolated vertices, shown in Fig. 4(e). Note that the construction can be trivially extended for arbitrary $d > 4$. Therefore, non-bipartite extremal TPs are present for an arbitrary nonzero temperature for $d \geqslant 4$, and absent for $d = 2, 3$.

V. CONCLUSIONS

The established link between all physically significant extremal thermal processes and thermomajorization curves gives a recipe for determining the form of relevant extremal TPs for systems of higher dimension. The complexity of the algorithm is the same as for determining the corresponding extremal transportation matrices. The number of extremal points of transportation polytopes is not known in general.

With the complete characterization of the set $\rho_{\text{init}}^{\text{TP(d)}}$ established, a similar description of $\rho_{\text{init}}^{\text{TP(n)}}$ for $n < d$ should allow for the solution of the decomposability problem ($n = 2$) by determining the length of sequences of two-level transformations needed to generate $\rho_{\text{init}}^{\text{TP(2)}}$ for an arbitrary initial state.

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APPENDIX A: PROOFS OF SECTION II

Below we show that a set $\rho_{\text{init}}^{\text{TP}}$ of states that can be achieved by thermal processes from an initial state ρ_{init} is a convex polytope.

Remark 6. $\rho_{\text{init}}^{\text{TP}}$ is a convex polytope.

Proof. From the definition of a thermal process we see that TP is a convex polytope. Now, take $\rho_1, \rho_2 \in \rho_{\text{init}}^{\text{TP}}$: $T_1\rho_{\text{init}} = \rho_1$, $T_2\rho_{\text{init}} = \rho_2$, where $T_1, T_2 \in TP$. For every $0 \leqslant \alpha \leqslant 1$, a state $\alpha\rho_1 + (1-\alpha)\rho_2$ belongs to $\rho_{\text{init}}^{\text{TP}}$ due to convexity of TP: $\alpha\rho_1 + (1-\alpha)\rho_2 = \alpha T_1\rho_{\text{init}} + (1-\alpha)T_2\rho_{\text{init}} = T_3\rho_{\text{init}}$, where $T_3 = [\alpha T_1 + (1-\alpha)T_2] \in TP$. Therefore, $\rho_{\text{init}}^{\text{TP}}$ is convex. Each of $\rho_{\text{out}} \in \rho_{\text{init}}^{\text{TP}}$ can be represented as $\rho_{\text{out}} = \sum \alpha_i T_i^{\text{ext}}\rho_{\text{init}}$, where $0 \leqslant \alpha_i \leqslant 1$ and $\sum_i \alpha_i = 1$ and $\{T_i^{\text{ext}}\}_i$ is a set of extremal points of TP. If ρ_{out} is extremal, then $T_k^{\text{ext}}\rho_{\text{init}} = T_l^{\text{ext}}\rho_{\text{init}}$ for all pairs of T_i^{ext} contributing with a nonzero coefficient to the decomposition of ρ_{out}. Therefore, the number of extremal points of $\rho_{\text{init}}^{\text{TP}}$ cannot be bigger than the number of extremal points of TP, and as the latter set is a convex polytope, the former one is a polytope as well. ■

APPENDIX B: PROOFS OF SECTION III

1. Theorem 2, Section III, *only if part* (procedure for constructing a convex decomposition of a state)

Let us recall that, according to Theorem 2, tight thermomajorization of a curve $\beta(\rho)$ by a curve $\beta(\rho_{\text{init}})$ is equivalent to ρ being an extremal point of $\rho_{\text{init}}^{\text{TP}}$. Below we present a proof that every state in $\rho_{\text{init}}^{\text{TP}}$ with a thermomajorization curve that is not tightly thermomajorized by $\beta(\rho_{\text{init}})$ cannot be an extremal point of $\rho_{\text{init}}^{\text{TP}}$.

We do this by representing every state $\rho \in \rho_{\text{init}}^{\text{TP}}$ as $\rho = \sum p_i\sigma_i$, where $\sum p_i = 1$, $0 < p_i$, and thermomajorization curves of σ_i, $\beta(\sigma_i)$, are all tightly thermomajorized by $\beta(\rho_{\text{init}})$; therefore, this set of extremal points is complete. First, we notice that for a 2-level system, every thermal process can be described with just two extremal TPs: $\mathcal{I} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ and $\mathcal{B} = \left(\begin{smallmatrix} 1-q_{10} & 1 \\ q_{10} & 0 \end{smallmatrix}\right)$. Therefore, if $\rho \in \rho_{\text{init}}^{\text{TP(2)}_{\beta,\text{H}_\text{S}}}$, then $\rho = [(1-\alpha)\mathcal{I} + \alpha\mathcal{E}]\rho_{\text{init}}$, for $0 \leqslant \alpha \leqslant 1$. The corresponding curve, $\beta(\rho(\alpha))$, has an elbow on two possible vertical lines (see Fig. 7). For $\alpha = 0$, the elbow is on the initial curve $\beta(\rho_{\text{init}})$; it goes down with increasing α to reach a line characterizing a Gibbs state $\beta(\rho_\beta)$, switches lines, and continues up, to reach $\beta(\rho_{\text{init}})$ again for $\alpha = 1$. In this way, we can achieve all states of $\rho_{\text{init}}^{\text{TP(2)}_{\beta,\text{H}_\text{S}}}$ characterized by curves with elbows lying between $\beta(\rho_{\text{init}})$ and $\beta(\rho_\beta)$ on two specified lines. In what follows, we will be using this to decompose a given d-level state belonging to $\rho_{\text{init}}^{\text{TP(d)}_{\beta,\text{H}_\text{S}}}$ into two states that have equal occupations on all

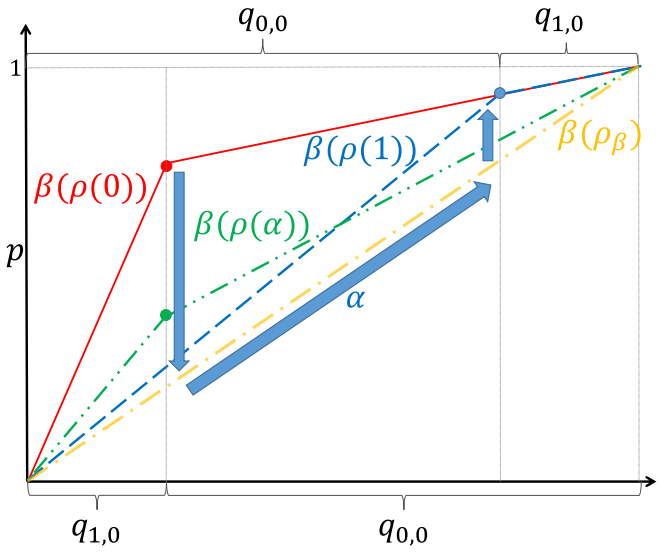

FIG. 7. All states $\rho \in \rho_{\text{init}}^{\text{TP(2)}_{\beta,\text{H}_\text{S}}}$ can be represented as $\rho(\alpha) = [(1-\alpha)\mathcal{I} + \alpha\mathcal{E}]\rho_{\text{init}}$, with value $\alpha \in [0, 1]$ determining the position of the only elbow of thermomajorization curve $\beta(\rho(\alpha))$. The movement of the elbow associated with continuous increase of α is marked by arrows. For $\alpha = 1/(1+q_{10})$ marking a transition to a Gibbs state ρ_β, the elbow disappears, to reemerge for higher α on a different vertical line.

$(d-2)$ levels, apart from the selected two. The difference in occupations on these two levels makes one of the elbows from each of corresponding β curves lie on a different position, as in Fig. 7 for $\beta(\rho(0))$ and $\beta(\rho(1))$, while the rest of the elbows from the two curves lie on the same positions.

First, decompose the curve $\beta(\rho) = c_{1,1}\gamma'_{1,1} + c_{1,2}\gamma'_{1,2}$ [see Fig. 8(a)] into a convex combination of curves $\gamma'_{1,1}$ and $\gamma'_{1,2}$ such that $\gamma'_{1,1}$ has the same β order as $\beta(\rho)$, i.e., $\pi(\gamma'_{1,1}) = \pi(\beta(\rho))$, and $\gamma'_{1,2}$ has the same β order as $\beta(\rho)$, except for the last two segments, which are permuted: $\pi(\gamma'_{1,2}) = P_{d-1,d}\pi(\beta(\rho))$, where $P_{d-1,d}$ marks the permutation between the segments that are at the position $d-1$ and d in the following vector. Demand also that the last elbows of $\gamma'_{1,1}$ and $\gamma'_{1,2}$ lie on $\beta(\rho_{\text{init}})$. Other elbows of $\gamma'_{1,1}$ and $\gamma'_{1,2}$ have the same positions as in $\beta(\rho)$. This decomposition corresponds to a decomposition of a state ρ into two states that differ by occupations only on two selected levels. As we see from the case of two-level systems, these requirements fix parameters $c_{1,1}$ and $c_{1,2}$, while preserving $c_{1,1} + c_{1,2} = 1$. At the end, whenever curves $\gamma'_{1,1}$ or $\gamma'_{1,2}$ are not concave, we change order of segments such that we obtain proper thermomajorization curves, $\gamma_{1,1}$ and $\gamma_{1,2}$, respectively [Fig. 8(b)]. Therefore, we have obtained $\rho = c_{1,1}\rho(\gamma_{1,1}) + c_{1,2}\rho(\gamma_{1,2})$, where $\rho(\gamma)$ marks a state ρ associated with thermomajorization curve γ, and $\rho(\gamma_{1,1})$, $\rho(\gamma_{1,2}) \in \rho^{\text{TP}}_{\text{init}}$.

In the second step, we decompose the curves $\gamma_{1,1}$ [Fig. 9(a)] and $\gamma_{1,2}$ [Fig. 9(b)] as $c_{1,1}\gamma_{1,1} = c_{2,1}\gamma'_{2,1} + c_{2,2}\gamma'_{2,2}$ and $c_{1,2}\gamma_{1,2} = c_{2,3}\gamma'_{2,3} + c_{2,4}\gamma'_{2,4}$, such that $\pi(\gamma'_{2,1}) = \pi(\gamma_{1,1})$, $\pi(\gamma'_{2,2}) = P_{d-2,d-1}\pi(\gamma_{1,1})$, $\pi(\gamma'_{2,3}) = \pi(\gamma_{1,2})$, $\pi(\gamma'_{2,4}) = P_{d-2,d-1}\pi(\gamma_{1,2})$, and such that the two last elbows of $\gamma'_{2,1}$, $\gamma'_{2,2}$, $\gamma'_{2,3}$, $\gamma'_{2,4}$ lie on $\beta(\rho_{\text{init}})$, while the position of the remaining elbows is like in the original lines, $\gamma_{1,1}$ and $\gamma_{1,2}$, respectively. Therefore, again we were using a decomposition of a given state into states with different occupations on just two energy levels; just now these two levels correspond to segments on a thermomajorization curve shifted towards the left.

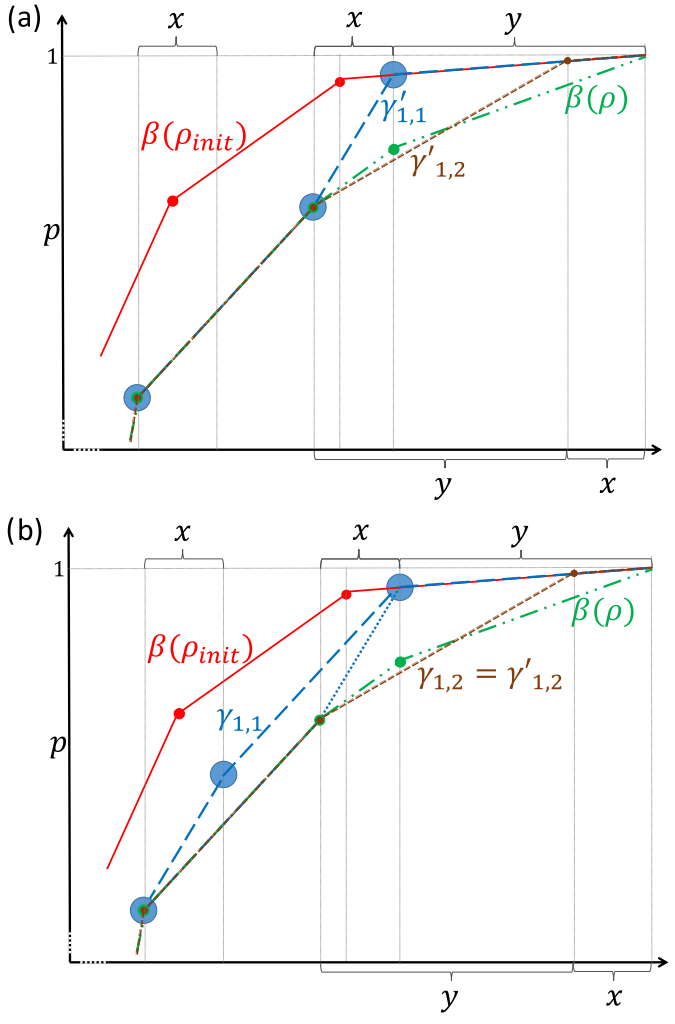

FIG. 8. Representing a state as a convex composition of extremal points (step 1). Decomposition of a state $\rho = c_{1,1}\rho(\gamma_{1,1}) + c_{1,2}\rho(\gamma_{1,2})$, with last elbows of $\gamma_{1,1}$ and $\gamma_{1,2}$ lying on $\beta(\rho_{\text{init}})$. (a) Validity of a construction comes from a decomposition of states of two-level systems (Fig. 7), trivially extended to states of higher dimension and equal occupations on the added levels. (b) Permuting the segments turns $\gamma'_{1,1}$ and $\gamma'_{1,2}$ into $\gamma_{1,1}$ and $\gamma_{1,2}$, respectively, and asserts that the curves are concave.

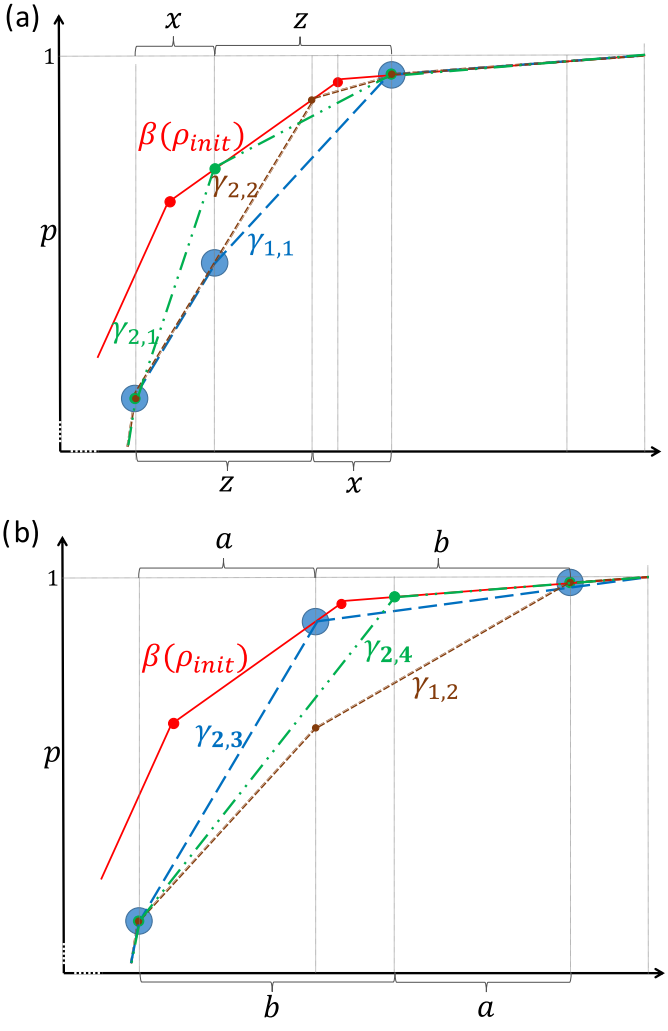

FIG. 9. Representing a state as a convex decomposition of extremal points (step 2). Decomposition of (a) $\rho(\gamma_{1,1})$ and (b) $\rho(\gamma_{1,2})$ into states represented by thermomajorization curves $\gamma_{2,i}$, $i = 1, 2, 3, 4$, with last 2 elbows lying on $\beta(\rho_{\text{init}})$.

Again, if necessary we permute segments to obtain concave curves $\gamma_{2,1}$, $\gamma_{2,2}$, $\gamma_{2,3}$, and $\gamma_{2,4}$,. In this way, parameters $c_{2,1}$, $c_{2,2}$, $c_{2,3}$, $c_{2,4}$, $\sum_{i=1,4} c_{2,i} = 1$ are fixed, and a decomposition $\rho = \sum_{i=1,4} c_{2,i}\rho(\gamma_{2,i})$ is obtained.

In general, we iterate this procedure for steps $j = 1, \ldots, d-1$, in each step dividing curves $c_{j-1,i}\gamma_{j-1,i} = c_{j,2i-1}\gamma'_{j,2i-1} + c_{j,2i}\gamma'_{j,2i}$ for all $i = 1, \ldots, 2^j$ such that $\pi(\gamma'_{j,2i-1}) = \pi(\gamma_{j-1,i})$, $\pi(\gamma'_{j,2i}) = P_{d-j,d-j+1}\pi(\gamma_{j-1,i})$, such that the last j elbows of $\gamma'_{j,2i-1}$ and $\gamma'_{j,2i}$ lie on $\beta(\rho_{\text{init}})$, and the remaining elbows lie on $\gamma_{j-1,i}$. We take $c_{0,1} = 1$ and $\gamma_{0,1} = \beta(\rho)$. We permute segments to obtain concave curves $\gamma_{j,2i-1}$ and $\gamma_{j,2i}$. As each step fixes one more elbow of curves to lie on $\beta(\rho_{\text{init}})$, after $j = d-1$ steps all curves in the decomposition $\beta(\rho) = \sum_{i=1,2^{d-1}} c_{d-1,i}\gamma_{d-1,i}$ are tightly thermomajorized by $\beta(\rho_{\text{init}})$. Also, as at each step we have $c_{j-1,i} = c_{j,2i-1} + c_{j,2i}$, this implies $\sum_{i=1,2^{d-1}} c_{d-1,i} = 1$. Therefore, after rewriting $c_{d-1,i} = p_i$ and $\rho(\gamma_{d-1,i}) = \sigma_i$, we arrive with the convex decomposition $\rho = \sum p_i\sigma_i$.

2. Remark 2, Section III

Proof (*if part*). It is enough to show that for every $\rho \in \rho^{\text{TP}}_{\text{init}}$, with at least one of the elbows of $\beta(\rho)$ lying on $\beta(\rho_{\text{init}})$, there is a state $\rho_1 \in \rho^{\text{TP}}_{\text{init}}$ such that there is no state $\rho_2 \in \rho^{\text{TP}}_{\text{init}}$ satisfying $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$, $\lambda \in [0, 1]$. Choose ρ_1 such that $\beta(\rho_1)$ has elbows on the same positions as $\beta(\rho)$, apart from the one lying on a vertical line that goes through a selected elbow of $\beta(\rho)$ lying on $\beta(\rho_{\text{init}})$; place this elbow δ distance below the elbow $\beta(\rho)$. We can always choose $\delta > 0$ to be small enough such that $\pi(\rho) = \pi(\rho_1)$. In this case, in order for $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$ to be satisfied, all elbows of $\beta(\rho_2)$ have to lie on elbows of $\beta(\rho_1)$, apart from the one that lies on a vertical line that goes through a selected elbow of $\beta(\rho)$ lying on $\beta(\rho_{\text{init}})$; this elbow has to lie $\epsilon > 0$ above the elbow of $\beta(\rho_{\text{init}})$. But this implies that $\rho_2 \notin \rho^{\text{TP}}_{\text{init}}$. ■

Proof (*only if part*). If a state ρ lies on a face of $\rho^{\text{TP}}_{\text{init}}$, then there exists some state $\rho_1 \in \rho^{\text{TP}}_{\text{init}}$ such that there is no state $\rho_2 \in \rho^{\text{TP}}_{\text{init}}$ that satisfies $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$, $\lambda \in [0, 1]$. Assume that all elbows of $\beta(\rho)$ lie below $\beta(\rho_{\text{init}})$. We will show that it leads to a contradiction, i.e., that for an arbitrary state $\rho_1 \in \rho^{\text{TP}}_{\text{init}}$ we can construct a state ρ_2 that satisfies $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$. For curves that have all elbows below an initial curve, we can always modify the procedure of decomposing a state ρ into extremal points of $\rho^{\text{TP}}_{\text{init}}$ (*only if part* of the proof of Theorem 2) by taking $\gamma'_{1,1}$ such that $\pi(\gamma'_{1,1}) = \pi(\beta(\rho_1))$ and $\gamma'_{1,2}$ such that $\pi(\gamma'_{1,2}) = P_{d-1,d}\pi(\beta(\rho_1))$ in the first step, and then carry on with the procedure. At the end, we have $c_{d-1,1} = \lambda$, $\rho(\gamma_{d-1,1}) = \rho_1$ and $\sum_{i=2,2^{d-1}} c_{d-1,i} = (1-\lambda)$, $\sum_{i=2,2^{d-1}} \rho(\gamma_{d-1,i}) = \rho_2$. ■

3. Theorem 3, Section III

Proof. Assume that H_S is not a hyperface. Therefore, there is ρ from H_S, which can be represented as a convex combination $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$, $\lambda \in [0, 1]$, $\rho_{1,2} \in \rho^{\text{TP}}_{\text{init}}$, such that at least one state, ρ_1, belongs to $\rho^{\text{TP}}_{\text{init}}/H_S$. This implies that on a vertical line passing through some point of $\beta(\rho_{\text{init}})$, being an elbow of some curve tightly thermomajorized by $\beta(\rho_{\text{init}})$ and belonging to S, $\beta(\rho_1)$ lies below this elbow (see Fig. 10).

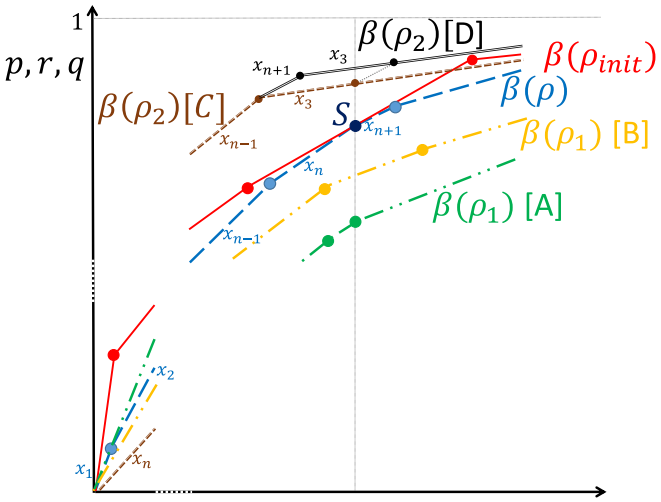

FIG. 10. A state ρ belongs to a facet H_S of $\rho^{\text{TP}}_{\text{init}}$ given by a set of points S. A point from this set defines a set of segments $\mathcal{X} = \{x_1, \ldots, x_n\}$ that lie to the left of it on $\beta(\rho)$. If $\rho_1 \notin H_S$, then $\beta(\rho_1)$ has an elbow below S (case [A]) or a segment below S (case [B]). Then, the state ρ_2 from the decomposition $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$, $\lambda \in [0, 1]$, has a curve that has to lie over S, both in the case [C] with all segments of $\beta(\rho_2)$ to the left from S being taken from the set $\mathcal{X}$, as well as for different arrangements (case [D]). Therefore, $\rho_2 \notin \rho^{\text{TP}}_{\text{init}}$.

Let us denote state populations by vectors $\boldsymbol{p}$, $\boldsymbol{r}$, and $\boldsymbol{q}$: $\rho_1 = \text{diag}[\boldsymbol{p}]$, $\rho_2 = \text{diag}[\boldsymbol{r}]$, $\rho = \text{diag}[\boldsymbol{q}]$. Assume that $\beta(\rho_1)$ has an elbow on this line (case [A]). If we denote by $\mathcal{X} = \{x_1, \ldots, x_n\}$ a set of segments lying to the left of the elbow on $\beta(\rho)$, it is clear that in order to have $\sum_{\mathcal{X}} q_x = \lambda \sum_{\mathcal{X}} p_x + (1-\lambda)\sum_{\mathcal{X}} r_x$, ρ_2 has to satisfy $\sum_{\mathcal{X}} q_x < \sum_{\mathcal{X}} r_x$ if the elbow of $\beta(\rho_1)$ lies below the elbow of S ($\sum_{\mathcal{X}} p_x < \sum_{\mathcal{X}} q_x$). This is because, if all segments of $\beta(\rho_1)$ that lie to the left from the elbow belong to $\mathcal{X}$, we have $\sum_{\mathcal{X}} p_x < \sum_{\mathcal{X}} q_x$. If some segments from $\mathcal{X}$ lie to the right from the elbow on $\beta(\rho_1)$, this means that $\sum_{\mathcal{X}} p_x$ is even smaller. Assume that segments from $\mathcal{X}$ of ρ_2 all lie to the left of the elbow (case [C]). Then, as $\sum_{\mathcal{X}} q_x < \sum_{\mathcal{X}} r_x$, we see that $\beta(\rho_2)$ is not thermomajorized by $\beta(\rho_{\text{init}})$, and therefore $\rho_2 \notin \rho^{\text{TP}}_{\text{init}}$. On the other hand, if some segments from the set $\mathcal{X}$ lie to the right of the elbow (case [D]), this implies that other segments in $\beta(\rho_2)$ have even higher slopes, and the curve $\beta(\rho_2)$ reaches even higher on a vertical line passing through the elbow; therefore $\rho_2 \notin \rho^{\text{TP}}_{\text{init}}$.

Now we will consider the case of $\beta(\rho_1)$ not having an elbow on the vertical line passing through an elbow belonging to S (case [B]). Again, this implies that $\sum_{\mathcal{X}} p_x < \sum_{\mathcal{X}} q_x$, as otherwise $\sum_{\mathcal{X}} q_x \leqslant \sum_{\mathcal{X}} p_x$ and the curve $\beta(\rho_1)$ would not be thermomajorized by $\beta(\rho_{\text{init}})$ or $\beta(\rho_1)$ would not lie below S [as before, for $\beta(\rho_1)$ to have some segments with higher slopes than segments from $\mathcal{X}$, this only increases the height of the $\beta(\rho_1)$ curve over the elbow from S on $\beta(\rho_{\text{init}})$]. Therefore, $\sum_{\mathcal{X}} p_x < \sum_{\mathcal{X}} q_x < \sum_{\mathcal{X}} r_x$ in order to have $\sum_{\mathcal{X}} q_x = \lambda \sum_{\mathcal{X}} p_x + (1-\lambda)\sum_{\mathcal{X}} r_x$, but this, as we showed before, leads to $\rho_2 \notin \rho^{\text{TP}}_{\text{init}}$ (a contradiction). ■

4. Lemma 2, Section III

Proof (*if part*). For two extremal points to share an edge means that for all states $\rho_\lambda = \lambda\epsilon_1 + (1-\lambda)\epsilon_2$, $\lambda \in (0,1)$, belonging to $\rho_{\text{init}}^{\text{TP}}$, and for every state $\sigma \in \rho_{\text{init}}^{\text{TP}}$ and $\sigma \notin \{\rho_\lambda\}_\lambda$, there is no state $\sigma' \in \rho_{\text{init}}^{\text{TP}}$ such that $\rho_\lambda = \gamma\sigma + (1-\gamma)\sigma'$ for $\gamma \in [0,1]$. For an arbitrary $\sigma \notin \{\rho_\lambda\}_\lambda$, there is at least one elbow of $\beta(\rho_\lambda)$ lying on $\beta(\rho_{\text{init}})$, such that $\beta(\sigma)$ lies below it.

Assume that, looking from the left side of the thermomajorization diagram, the first elbow of $\beta(\rho_\lambda)$ satisfies this property. This means that the segment of $\beta(\sigma)$ of the same length as the first segment of $\beta(\rho_\lambda)$ has to have smaller slope than the slope of this segment in $\beta(\rho_\lambda)$. Therefore, a corresponding segment in $\beta(\sigma')$ has to have bigger slope than the slope of this segment in $\beta(\rho_\lambda)$, as only in this way we can achieve $\rho_\lambda = \gamma\sigma + (1-\gamma)\sigma' \iff \forall_i \beta_i(\rho_\lambda) = \gamma\beta_i(\sigma) + (1-\gamma)\beta_i(\sigma')$. But this leads to a contradiction with the requirement that $\sigma \in \rho_{\text{init}}^{\text{TP}}$, as $\beta(\sigma')$ would not be thermomajorized by $\beta(\rho_{\text{init}})$.

If we assume that $\beta(\sigma)$ coincides with $\beta(\rho_\lambda)$ on its first elbow lying on $\beta(\rho_{\text{init}})$, but the second such elbow of $\beta(\rho_\lambda)$ lies above $\beta(\sigma)$, then this means that $\beta(\sigma)$ had to have an elbow on the first elbow of $\beta(\rho_\lambda)$; otherwise, $\beta(\rho_\lambda)$ would not be thermomajorized by $\beta(\rho_{\text{init}})$ for all of its slopes different. Therefore, we conclude that $\beta(\rho_\lambda)$, $\beta(\sigma)$ and $\beta(\sigma')$ are identical on their first segments. We can therefore treat the first elbow of $\beta(\rho_\lambda)$ as the effective start of a new thermomajorization diagram, and apply the argument from the last step again.

We continue doing so for all the segments of $\beta(\rho_\lambda)$, until we reach a segment $d-i$. If no elbow of $\beta(\rho_\lambda)$ is lying above $\beta(\sigma)$ on this side of the original thermomajorization diagram, we apply the same reasoning to the right side of the diagram, until we reach the segment $d-i+1$. In this way, we are guaranteed to find an elbow of $\beta(\rho_\lambda)$ that lies above $\beta(\sigma)$, as otherwise $\sigma \in \rho_\lambda$. At such event, we reach a conclusion $\sigma' \notin \rho_{\text{init}}^{\text{TP}}$, as shown above. ■

Proof (*only if part*). Assume that for two distinctive extremal states ϵ_1 and ϵ_2, their respective orders cannot be related via $\pi_1 \neq P_{d-i,d-i+1}\pi_2$, for any of $i \in \{2,\ldots,d\}$. This means that a construction $\rho_\lambda = \lambda\epsilon_1 + (1-\lambda)\epsilon_2$ for $\lambda \in (0,1)$ results in $\beta(\rho_\lambda)$ that has at least 2 elbows below $\beta(\rho_{\text{init}})$, as $P_{d-i,d-i+1}$ is the only relation between the orders of distinctive extremal states that leads to 1 elbow below $\beta(\rho_{\text{init}})$ for all slopes of $\beta(\rho_{\text{init}})$ different. According to the procedure for decomposing a given state into extremal states (only if part of the proof of Theorem 2), every elbow of ρ_λ leads to a generation of 2 extremal points in the convex decomposition of this state into extremal points of $\rho_{\text{init}}^{\text{TP}}$. Therefore, ρ_λ can be decomposed into at least 4 states, which contradicts the uniqueness of the decomposition $\rho_\lambda = \lambda\epsilon_1 + (1-\lambda)\epsilon_2$, $\lambda \in (0,1)$. ■

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