Exploring the Limits of Controlled Markovian Quantum Dynamics with Thermal Resources

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Abstract. Our aim is twofold: First, we rigorously analyse the generators of quantum-dynamical semigroups of thermodynamic processes. We characterise a wide class of GKSL-generators for quantum maps within thermal operations and argue that every infinitesimal generator of (a one-parameter semigroup of) Markovian thermal operations belongs to this class. We completely classify and visualise them and their non-Markovian counterparts for the case of a single qubit.

Second, we use this description in the framework of bilinear control systems to characterise reachable sets of coherently controllable quantum systems with switchable coupling to a thermal bath. The core problem reduces to studying a hybrid control system ("toy model") on the standard simplex allowing for two types of evolution: (i) instantaneous permutations and (ii) a one-parameter semigroup of d-stochastic maps. We generalise upper bounds of the reachable set of this toy model invoking new results on thermomajorisation. Using tools of control theory we fully characterise these reachable sets as well as the set of stabilisable states as exemplified by exact results in qutrit systems.

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Dedicated to the memory of Andrzej Kossakowski.

It is a pleasure to contribute to honour Andrzej Kossakowski as key figure in laying and triggering the now classical groundwork (around [54, 55, 35, 34, 33], see [17]) that completely characterises the infinitesimal generators of (Markovian) quantum maps in finite dimensions. His towering work continues to be a well of inspiration. With the recent focus in quantum dynamics now taking "the bath" as quantum thermodynamical resource, here we try to carry on somewhat in his spirit, in particular when characterising the generators of Markovian thermal quantum operations[0a] *in a Lie-semigroup frame.*

1. Introduction

Linking the well established field of quantum control [21, 26, 32, 51] with the emerging subject of quantum thermodynamics [9, 61] is quite a novel and important line of research. Thus in this article we focus on framing and studying *quantum-dynamical control problems with coherent controls and thermal resources as additional controls*[1a] [7, 28], where the time evolution of controlled systems is taken to be defined by a controlled GKSL-equation. We build on recent progress in interfacing (non-)Markovian[1b] processes with quantum thermodynamics in general [83, 14, 1, 22, 81, 15, 18], and with its resource-theory approach in particular [36, 8, 64, 72].

To this end, (Lie-)semigroup techniques [40, 42, 44, 58] lend themselves as a common frame naturally extending to concepts of (i) classical majorisation and of (ii) thermomajorisation [66] as well as (iii) Markovianity of quantum maps [27, 78]. Moreover, (iv) the set of reachable states related to a given initial state of a (Markovian) quantum control system takes the form of a Lie-semigroup orbit [27, 78].

Studying reachable sets of such control systems is paramount, e.g., to ensure well-posedness of many (optimal) control tasks. The main question is whether a desired target state can be prepared given an equation of motion (plus some control variables) and an initial condition, and how to characterise feasible state transfers in general. Interestingly, the core problem of

[0a]see Thm. 2 in Sec. 3.1.

[1a]i.e. with non-unitary controls chosen from the set of thermal operations [48, 46, 11]

[1b]In accordance with [92] the (time-dependent) Markovian quantum maps are taken as those which are infinitesimal CPTP-divisible.

the resource approach to quantum thermodynamics (as initially sparked by Brandão et al. [10], Horodecki & Oppenheim [46], as well as Renes [73], and further pursued in [31, 38, 62, 76, 67, 2, 85]) is similar—namely: given a fixed background temperature as well as initial and target states of a quantum system, can the former be mapped to the latter in a "thermodynamically consistent" [53] manner? Here the admissible quantum maps are "thermal operations" which form the fundamental building block of the resource theory approach to quantum thermodynamics. Roughly speaking, they comprise operations (assumed to be) performable in arbitrary number without cost. A precise definition is given in Sec. 3.1., and for a comprehensive introduction to the general topic see, e.g., the review by Lostaglio [61].

As teasers for the power of combining control theory with "thermal resources" in the sense of allowing for (non-)Markovian processes consider the following two (known) examples:

(1) Take any closed quantum system with non-trivial Hamiltonian which can be fully unitarily controlled. Then there always exists a *non-Markovian thermal operation* (known as β-SWAP [62]) such that adding it to the setup as an additional control allows to generate the ground state up to arbitrary precision [2], [87, Prop. 4.12] (and thus *every* state: use the Schur-Horn theorem to generate the eigenvalues of the target state on the diagonal, followed by a full dephasing via the β-swap[1c]).

(2) n-qubit systems with full coherent control plus switchable amplitude damping (coupling to a bath of temperature $T = 0$) for one of the qubits act (up to closure) transitively on the set of all density operators [7]. The result generalises from qu*b*its to arbitrary qu*d*its and m-level systems [28].

Hence in these two instances reachability is settled. However, for controlled *Markovian* dynamics with thermal resources (e.g., coupling to a bath of temperature $0 < T < \infty$) the reachability problem is open and subject of this work. Here, a fundamental property of thermal processes will be central: Under thermal operations, diagonal density matrices (in the eigenbasis of the system Hamiltonian) remain diagonal, meaning diagonal elements (populations) evolve independently from off-diagonal ones (coherences), refer also to Cor. 2. This greatly simplifying property lends itself for studying the restricted control system on diagonal states, later called "toy model". Gen-

[1c]This only holds unconditionally if $e^{-1/T} \geq \frac{1}{2}$. For temperatures lower than that the β-swap has to be implemented as a two-step dephasing thermalisation (i.e. one needs to be able to implement the dephasing independent of the diagonal action of the β-swap) in order to get from the ground state to a ball around the maximally mixed state. See also the Worked Example at the end of Sec. 3.1.

eral results and numerical illustrations, as well as analytic results in a low-dimensional setting will be presented in Secs. 4.1. and 4.2., respectively.

Structure and Main Results. Sec. 2. sets the stage for discussing the dynamics of open Markovian systems as incarnations of *bilinear control systems* with two types of controls: coherent Hamiltonian ones as well as incoherent dissipative ones such as switchable thermal operations as brought about by coupling the quantum system to a thermal bath.

Sec. 3. paves the semigroup background for introducing general concepts of majorisation (such as d-majorisation, a special case of thermomajorisation) needed in the context of describing reachability under thermal operations. Within this framework, *Markovian* quantum maps come with the particular structure of *Lie* semigroups [27, 78], which allows for putting majorisation and Markovianity on a common ground.

In particular, we give the respective Lie wedges to certain sets of quantum maps such as Gibbs-preserving ones (Gibbs) as well as thermal ($\overline{\mathsf{TO}}$) and enhanced thermal operations (EnTO); the corresponding generated Lie semigroups thus define the respective Markovian counterparts MGibbs, MTO, and MEnTO. By giving set-inclusions, in Sec. 3.1. we interrelate them all. As another important result (Thm. 2) one gets an explicit construction for (possibly all) generators of Markovian thermal operations via temperature-weighted projections out of a total Hamiltonian (preserving energy of system and bath) in the Stinespring dilation. With regard to reachable sets of diagonal states under such controlled Markovian dynamics, in Sec. 3.3. we recall the d-majorisation polytope and its properties.

Sec. 4. illustrates the theory of bilinear open quantum control systems, where the incoherent controls are brought about by Markovian thermal operations. Reachable sets for diagonal states under such operations are characterised by extreme points of the d-majorisation polytope. More precisely, in n-level systems, the enclosure of the reachable set by a convex set is given by the convex hull over the permuted extreme points of the d-majorisation polytope (Thm. 7). Sec. 4.2. discusses three-level systems in detail. By reformulating the control system as a differential inclusion, we find an analytic expression for the set of stabilisable states. Moreover we compute the set of reachable states for arbitrary initial states, and we deduce the structure of control sets and their reachability order.

2. Control Setting of Markovian Quantum Dynamics

To fix notations, we write $\mathfrak{pos}_1(n)$ for the convex set of all $n \times n$ density matrices (i.e. all positive semi-definite $n \times n$-matrices of trace one), $\mathcal{L}(\mathbb{C}^{n\times n})$

for the space of all linear operators acting on complex $n \times n$-matrices, and $\mathsf{CPTP}(n)$ for the convex subset of $\mathcal{L}(\mathbb{C}^{n\times n})$ which consists of all completely positive and trace-preserving maps, also known as quantum channels, quantum maps, or Kraus maps. We prefer to use the term "quantum maps".

Consider the usual Markovian master equation

$$\dot\rho(t) = -i[H_0, \rho(t)] - \mathbf{\Gamma}(\rho(t))\,, \quad \rho(0) = \rho_0 \in \mathfrak{pos}_1(n) \tag{1}$$

with $\mathbf{\Gamma} \in \mathcal{L}(\mathbb{C}^{n\times n})$ of GKSL-form [35, 60], i.e.

$$\mathbf{\Gamma}(\rho) := \sum_k \left(\tfrac{1}{2}\big(V_k^\dagger V_k \rho + \rho V_k^\dagger V_k\big) - V_k \rho V_k^\dagger \right) \tag{2}$$

and $V_k \in \mathbb{C}^{n\times n}$ arbitrary to ensure the evolution $\rho(t) = e^{-t(i\,\mathrm{ad}_{H_0} + \mathbf{\Gamma})}\rho_0$ solving (1) remains in $\mathfrak{pos}_1(n)$ for all $t \in \mathbb{R}_+ := [0, \infty)$. Recall $(e^{-t(i\,\mathrm{ad}_{H_0} + \mathbf{\Gamma})})_{t\in\mathbb{R}_+}$ is CPTP, hence a (trace norm-)contraction semigroup [71] leaving $\mathfrak{pos}_1(n)$ invariant.

In this work, an overarching goal is to characterise control systems Σ extending Eq. (1) by coherent controls (generated by Hermitian H_j and (piecewise constant) $u_j(t) \in \mathbb{R}$) and by making dissipation bang-bang switchable in the sense

$$\dot\rho(t) = -i\Big[H_0 + \sum_{j=1}^m u_j(t) H_j, \rho(t)\Big] - \gamma(t)\mathbf{\Gamma}(\rho(t)) \tag{3}$$

with $\gamma(t) \in \{0, 1\}$. This setting is a typical incarnation of the wide class of *bilinear control systems* [49, 29]

$$\dot{\mathbf{x}}(t) = -\Big(A + \sum_j u_j(t) B_j\Big)\mathbf{x}(t)\,, \quad \mathbf{x}(0) = \mathbf{x}_0\,, \tag{4}$$

where A denotes an uncontrolled drift, while the control terms[2a] consist of (piecewise constant) control amplitudes $u_j(t) \in \mathbb{R}$ and linear control operators B_j. Here the state $\mathbf{x}(t)$ should be thought of as density operator.

A paramount notion in such control systems is the *reachable set* of $\mathbf{x}_0$ at time $\tau \geq 0$, denoted $\mathfrak{reach}(\mathbf{x}_0, \tau)$. It is defined as the collection of all $\mathbf{x}(\tau)$, where $t \mapsto \mathbf{x}(t)$ is any solution of (4). Likewise, the reachable set until time τ is defined as $\mathfrak{reach}_{[0,\tau]}(\mathbf{x}_0) := \bigcup_{\tau'\in[0,\tau]} \mathfrak{reach}(\mathbf{x}_0, \tau')$, and the overall reachable set as $\mathfrak{reach}(\mathbf{x}_0) := \bigcup_{\tau'\geq 0} \mathfrak{reach}(\mathbf{x}_0, \tau')$. The latter is mostly used in this work, where analogously, we write $\mathfrak{reach}(\rho_0)$ for the entire reachable set of Eq. (3). The system Lie algebra of (4), which provides the crucial tool

[2a]The bilinearity of the control terms w.r.t u and x entails the terminology of Eq. (4).

for analyzing controllability, accessibility, and reachability questions, reads $\mathfrak{k} := \langle A, B_j \,|\, j = 0, \dots, m \,\rangle_{\mathsf{Lie}}$.

In particular for closed quantum systems, i.e. systems which do not interact with their environment ($\mathbf{\Gamma}$=0=B_0) one would choose A as $i\,\mathrm{ad}_{H_0}$ and B_j as $i\,\mathrm{ad}_{H_j}$, $j = 1, \dots, m$ to recover the right-hand side of (3). Then it is known [50, 12, 49, 26] that $\mathfrak{reach}(\mathbf{x}_0)$ is given by the orbit of the initial state under the action of the dynamical systems group $\mathbf{K} := \langle \exp \mathfrak{k} \rangle$, provided $\mathbf{K}$ is a closed and thus compact subgroup[2b] of $\mathrm{Ad}_{\mathrm{SU}(n)} \cong \{\bar{U} \otimes U : U \in \mathrm{SU}(n)\} \subseteq \mathrm{SU}(n^2)$. More generally, for open systems undergoing Markovian dissipation which are driven by coherent controls $B_j = i\,\mathrm{ad}_{H_j}$ for $j = 1, \dots, m$ one sets the operator $B_0 = \mathbf{\Gamma}$ to include the environmental interaction. This operator takes the form of a GKSL-dissipator as given in Eq. (2). If B_0 is *bang-bang switchable* it acts as additional control, and if it is uncontrolled it contributes to the drift term $A = i\,\mathrm{ad}_{H_0}$. Motivated by recent experimental progress [43, 95, 16, 93] as described in [7] here we address the first case and refer to it as **Scenario BB** in the sequel.

In general, a concise description of reachable sets of Eq. (3) is challenging in particular in higher-dimensional cases. Although it is known that it always takes the form of a (Lie-)semigroup orbit, see, e.g., [27] this is usually not enough to obtain explicit characterisations. Currently there are only a few scenarios for which reachability is settled: (a) In the unital case $\mathbf{\Gamma}(\mathbb{1}_n) = 0$, one has [4, 96]

$$\mathfrak{reach}_\Sigma(\rho_0) \subseteq \{\rho \in \mathbb{C}^{n\times n} \,|\, \rho \prec \rho_0\}\,. \tag{5}$$

(b) If in addition $\mathbf{\Gamma}$ is generated by a single normal V, one gets (up to closure) equality in (5) provided the unitary part of Eq. (3) is *controllable* and the switching function $\gamma(t)$ gives extra control (cf. [7], [84, Prop. 5.2.1] for finite and [90] for infinite dimensions).

Under the scenario **BB** above plus the invariance of diagonal states imposed by thermal processes (see [61] and Cor. 2 below) as, e.g., implemented by the GKSL-generators V_1 and V_2 of Eqs. (19) and (20), the closure of the unitary orbit of $\mathrm{diag}\big(\mathfrak{reach}_\Lambda(x_0)\big)$ sits in the closure of $\mathfrak{reach}_\Sigma(U\,\mathrm{diag}(x_0)U^\dagger)$. Here Λ denotes a simplified version of Σ—later called "toy model"—which will be introduced in Sec. 4.1. Settings beyond thermal relaxation are pursued with similar techniques, e.g., by [74] at the expense of arriving at conditions that are hard to verify for higher-dimensional systems.

[2b] According to the above definition, in closed systems the system Lie algebra $\mathfrak{k}$ is a Lie subalgebra of the adjoint representation of the special unitary Lie algebra, i.e. $\mathfrak{k} \subseteq \mathrm{ad}_{\mathfrak{su}(n)}$. Yet the commutator identity $[\mathrm{ad}_H, \mathrm{ad}_{H'}] = \mathrm{ad}_{[H,H']}$ allows for identifying $\mathfrak{k}$ with the Lie subalgebra of $\mathfrak{su}(n)$ generated by $iH_0, \dots, iH_m$. In generic open systems, however, the GKSL-term $\mathbf{\Gamma}$ precludes any similar a-priori simplification of the system Lie algebra $\mathfrak{k}$.

3. Semigroups, Majorisation, and Markovian Quantum Dynamics

In this section, we introduce background and terminology for unifying several existing and seemingly different notions in the literature.

Majorisation via Semigroups. First, let us have a closer look at "the" concept of majorisation from the point-of-view of semigroups. Let $\mathcal{Z}$ be a real or complex finite-dimensional[3a] vector space and let $\mathcal{C} \subseteq \mathcal{Z}$ be a closed and convex subset. Moreover, let $\mathcal{B}(\mathcal{Z})$ denote the set of all linear operators acting on $\mathcal{Z}$ and let $S(\mathcal{C})$ be the set of operators in $\mathcal{B}(\mathcal{Z})$ which leave $\mathcal{C}$ invariant. Obviously, $S(\mathcal{C})$ is a subsemigroup of $\mathcal{B}(\mathcal{Z})$, i.e. $S(\mathcal{C})$ is closed under multiplication and contains the identity. Finally, let $S_0 \subseteq S(\mathcal{C})$ be any subsemigroup of $S(\mathcal{C})$. Then $x \in \mathcal{Z}$ is said to be S_0-*majorised* by $y \in \mathcal{Z}$ (denoted by $x \prec_{S_0} y$) if there exists a transformation $A \in S_0$ such that $Ay = x$ holds. This concept was first introduced by Parker and Ram [70] and is known as semigroup majorisation [66, Ch. 14.C]. A well-studied example of S_0-majorisation is classical vector-majorisation on $\mathbb{R}^n$, where $\mathcal{C} := \{x \in \mathbb{R}^n_+ : \sum_{j=1}^n x_j = 1\} \subset \mathbb{R}^n$ is the standard simplex and S_0 is chosen as the set of all real doubly-stochastic matrices of size $n \times n$ [66, Ch. 1 & 2]. Further physically relevant examples are discussed in the following sections; here we summarise some basic properties which result from the above definition.

Proposition 1. *Let $S(\mathcal{C})$ be the subsemigroup of $\mathcal{B}(\mathcal{Z})$ which leaves $\mathcal{C}$ invariant and let S_0 be any subsemigroup of $S(\mathcal{C})$. Then the following hold:*

(i) $S(\mathcal{C})$ is (topologically) closed and convex, and thus simply connected.

(ii) If $\mathcal{C}$ is compact and the convex cone $\mathcal{C}_0 := \mathbb{R}_+ \cdot \mathcal{C}$ generated by $\mathcal{C}$ has non-empty interior, then $S(\mathcal{C})$ is compact.

(iii) Given any $y \in \mathcal{Z}$, if S_0 is convex or compact, then so is the set $M_{S_0}(x) := \{y \in \mathcal{C} : y \prec_{S_0} x\} = S_0 \cdot x$.

Proof. (i) and (iii) are obvious so we only prove (ii). If $\mathcal{C}$ is compact, then so is $\mathcal{C}' := [0,1] \cdot \mathcal{C}$; in particular $\mathcal{C}' \subseteq B_K(0)$ for some $K > 0$. Moreover, $\mathcal{C}'$ is invariant under $S(\mathcal{C})$ by linearity. Now, by assumption on $\mathcal{C}_0$ there exist $x_0 \in \mathcal{C}'$ and $r > 0$ such that $B_r(x_0) \subseteq \mathcal{C}'$. Thus—given any $A \in S(\mathcal{C})$—for all $\Delta \in B_r(0)$ we obtain the estimate

$$\|A\Delta\| = \|A(\Delta + x_0) - Ax_0\| \leq \|A(\Delta + x_0)\| + \|Ax_0\| \leq 2K\,,$$

[3a] This is just to avoid further technicalities; in principle this approach works in arbitrary dimensions.

where we used the invariance of $\mathcal{C}'$ and its boundedness. This shows that $S(\mathcal{C})$ is bounded by $2Kr$ (with respect to the operator norm). Together with closedness from (i) we conclude that $S(\mathcal{C})$ is compact. □

The relation $\prec_{S_0}$ induced by S_0 is always reflexive and transitive and thus a preorder on $\mathcal{C}$. In general, however, $\prec_{S_0}$ fails to be anti-symmetric and hence a partial order, e.g., if S_0 contains a subgroup which acts non-trivially on $\mathcal{C}$. This can always be resolved by a suitable equivalence relation[3b] such that the corresponding quotient space provides a natural domain on which $\prec_{S_0}$ becomes an order. In the above example of classical vector-majorisation such a "natural domain" can be identified with a fixed "Weyl chamber".

Lie Theory for Semigroups, e.g., Quantum Maps. Next, we elucidate Markovianity of quantum maps from the perspective of Lie-semigroup theory. To this end let S be any closed (sub-)semigroup of $\mathcal{B}(\mathcal{Z})$ or $\mathsf{GL}(\mathcal{Z})$, where $\mathsf{GL}(\mathcal{Z})$ denotes the set of all invertible elements of $\mathcal{B}(\mathcal{Z})$. For what follows, recall that $\mathcal{B}(\mathcal{Z})$ is the Lie algebra of $\mathsf{GL}(\mathcal{Z})$. Then one defines the concept of a *Lie wedge of S* via

$$\mathsf{L}(S) := \{A \in \mathcal{B}(\mathcal{Z}) \,:\, e^{tA} \in S \text{ for all } t \geq 0\}\,. \tag{6}$$

Obviously this construction generalises the notion of a Lie (sub-)algebra for Lie (sub-)groups[3c] of $\mathsf{GL}(\mathcal{Z})$. The natural example of a *Lie wedge* in relation to quantum control is the set of all GKSL-generators [35, 60] which constitutes the Lie wedge to the semigroup $\mathsf{CPTP}(n)$ of *all* quantum maps [27] (of dimension n). Here, $\mathcal{Z}$ can be taken to be $i\mathfrak{u}(n)$, the set of all Hermitian $n \times n$-matrices, and $\mathcal{C}$ to be $\mathfrak{pos}_1(n)$. Then $\mathsf{CPTP}(n)$ is a compact convex subsemigroup of $S(\mathfrak{pos}_1(n)) \subset \mathcal{B}(i\mathfrak{u}(n))$.

The following proposition and corollary summarise elementary properties of the above construction. In particular, part (iv) below justifies calling $\mathsf{L}(S)$ the "tangent cone" of S at the identity.

Proposition 2. *Let S be a closed semigroup in $\mathcal{B}(\mathcal{Z})$ or $\mathsf{GL}(\mathcal{Z})$ and let $\mathsf{L}(S)$ be its Lie wedge. Then the following properties hold:*

- *(i) $\mathsf{L}(S)$ is a closed convex cone of $\mathcal{B}(\mathcal{Z})$.*
- *(ii) $\mathsf{L}(S)$ is invariant under conjugation by arbitrary edge elements, that is, $e^{A}\mathsf{L}(S)e^{-A} = \mathsf{L}(S)$ for all $A \in \mathsf{E}(\mathsf{L}(S))$, where the edge $\mathsf{E}(\mathsf{L}(S))$ is defined as largest subspace contained in $\mathsf{L}(S)$.*
- *(iii) $\mathsf{E}(\mathsf{L}(S))$ is a Lie subalgebra of $\mathcal{B}(\mathcal{Z})$. More precisely, it is the Lie algebra of $\mathsf{E}(S)$, where $\mathsf{E}(S)$ denotes the largest subgroup[3d] of S.*

[3b] $x \sim y :\Longleftrightarrow x \prec_{S_0} y$ and $y \prec_{S_0} x$

[3c] For simplicity, we drop the prefix "sub" whenever the corresponding superset is obvious.

[3d] Note that $\mathsf{E}(S)$ is also called edge—yet edge of S instead of $\mathsf{L}(S)$.

(iv) The operator $A \in \mathcal{B}(\mathcal{Z})$ belongs to $\mathsf{L}(S)$ if and only if there exists a C^1-curve $\gamma : [0,\varepsilon] \to S$ for some $\varepsilon > 0$ with $\gamma(0) = \mathrm{id}$, $\dot\gamma(0) = A$, i.e.

$$\mathsf{L}(S) = \{\dot\gamma(0) \,:\, \gamma \in C^1([0,\varepsilon], S) \text{ and } \gamma(0) = \mathrm{id}\}\,. \tag{7}$$

For the statements (i), (ii), and (iii) we refer to [42, Prop. 1.14] and [58, Thm. 4.4]. Statement (iv) can be found in [58, Def. 4.2] (without proof) and in [40, Prop. V.1.7] (yet under a much more general setting). For completeness, a sketch of a proof is given in App. A. Due to Prop. 2 any subset of $\mathcal{B}(\mathcal{Z})$ featuring property (i) and (ii) (and thus also (iii)) will be called an (abstract) *Lie wedge*.

Later we will encounter a scenario where the first derivative of a certain family of curves is not only in the Lie wedge but rather in its edge. In this case one can extract further information from higher derivatives:

Corollary 1. *Let $\varepsilon > 0$, a closed, convex semigroup $S \subseteq \mathcal{B}(\mathcal{Z})$, and a C^2-curve $\gamma : [0,\varepsilon] \to S$ with $\gamma(0) = \mathrm{id}$, $\dot\gamma(0) \in \mathsf{E}(\mathsf{L}(S))$ be given. Then $\ddot\gamma(0) \in \mathsf{L}(S)$.*

Proof. Let us assume, by way of contradiction, that $A_0 := \dot\gamma(0) \in \mathsf{E}(\mathsf{L}(S))$ and $B_0 := \ddot\gamma(0) \notin \mathsf{L}(S)$. Since $\mathsf{L}(S)$ is closed and convex there exists a separating linear functional $\alpha : \mathcal{B}(\mathcal{Z}) \to \mathbb{R}$, i.e. $\alpha(B_0) < 0$ and $\alpha(A) \geq 0$ for all $A \in \mathsf{L}(S)$ [75, Thm. 3.4]. Because $A_0 \in \mathsf{E}(\mathsf{L}(S))$ we know $\mathbb{R}A_0 \in \mathsf{L}(S)$ which forces $\alpha(A_0) = 0$. Moreover, convexity of S together with Prop. 2 (iv) implies $S - \mathrm{id} \subseteq \mathsf{L}(S)$: to see this, simply consider the curve $t \mapsto tA + (1-t)\mathrm{id} \in S$ where $A \in S$ is arbitrary. With this we obtain the estimate

$$\begin{aligned}\alpha(\mathrm{id}) \leq \alpha(\mathrm{id}) + \alpha(\gamma(t) - \mathrm{id}) &= \alpha\big(\gamma(t)\big) = \alpha\Big(\gamma(0) + tA_0 + \frac{B_0}{2}t^2 + \mathcal{O}(t^2)\Big)\\ &= \alpha(\mathrm{id}) + \frac{\alpha(B_0)}{2}t^2 + \mathcal{O}(t^2)\end{aligned}$$

leading to the contradiction $\alpha(B_0) + \mathcal{O}(1) \geq 0$. Thus $B_0 \in \mathsf{L}(S)$ which concludes the proof. □

Now, trivial examples of closed (and path-connected) semigroups of $\mathcal{B}(\mathcal{Z})$ reveal that, in general, semigroups cannot be recovered via the exponential map from their Lie wedge—in contrast to path-connected subgroups of $\mathcal{B}(\mathcal{Z})$ which are fully characterised by their Lie subalgebras, cf. [94] or [41, Thm. 9.6.1]. Therefore, the above concept of a Lie wedge naturally suggests the notion of a *Lie semigroup* for those closed semigroups S which can be reconstructed from their Lie wedge in the following sense:

$$S = \overline{\langle \exp\big(\mathsf{L}(S)\big)\rangle_{\mathrm{SG}}}\,. \tag{8}$$

Here, the overbar denotes the topological closure[3e] and $\langle \exp\big(\mathsf{L}(S)\big)\rangle_{\mathrm{SG}}$ is the semigroup generated by the set $\exp\big(\mathsf{L}(S)\big)$. Notably, the operation $\langle\ \cdot\ \rangle_{\mathrm{SG}}$ cannot be avoided as $\exp\big(\mathsf{L}(S)\big)$ is in general not closed under multiplication.

Conversely, given an (abstract) Lie wedge $\mathfrak{w}$ in $\mathcal{B}(\mathcal{Z})$ does there exist a Lie semigroup[3f] $S \subseteq \mathsf{GL}(\mathcal{Z})$ such that $\mathfrak{w} = \mathsf{L}(S)$? Again, contrary to Lie algebras, the answer is in general no. Therefore, Lie wedges which do allow for such a representation are called *global* (in $\mathsf{GL}(\mathcal{Z})$) in the following theorem. We collect some key results on globality, which will be important for constructing Markovian counterparts to (enhanced) thermal operations and Gibbs preserving maps in Eqs. (13), see also Rem. 4. For technical details and more sophisticated characterisations see [40, Ch. V & VI], [42, Ch. 1], and [58, Prop. 6.2].

Theorem 1. *Given any Lie wedge $\mathfrak{w} \subseteq \mathcal{B}(\mathcal{Z})$ the following statements hold.*

(a) If there exists a closed semigroup S of $\mathcal{B}(\mathcal{Z})$ or of $\mathsf{GL}(\mathcal{Z})$ such that $\mathsf{L}(S) = \mathfrak{w}$, then there exists a unique closed Lie semigroup $S_0 \subseteq S$ such that $\mathsf{L}(S_0) = \mathfrak{w}$, i.e. $\mathfrak{w}$ is global. In particular, $S_0 = \overline{\langle \exp\big(\mathsf{L}(S)\big)\rangle_{\mathrm{SG}}}$. Moreover, S_0 can be characterised

(i) either as the largest Lie semigroup in S

(ii) or as (the closure of) the reachable set of the identity id *of the bilinear control system*[3g]

$$\dot{\Phi}(t) = L(t)\Phi(t)\,, \tag{9}$$

where $L(t) \in \mathsf{L}(S)$ acts as control and the set of admissible controls can be any set of locally integrable functions which contains at least all piecewise constant ones.

(b) If there exists a Lie wedge $\mathfrak{w}_0$ which is global in $\mathcal{B}(\mathcal{Z})$ or $\mathsf{GL}(\mathcal{Z})$ and $\mathfrak{w}$ satisfies $\mathfrak{w} \subseteq \mathfrak{w}_0$ as well as $\mathfrak{w} \setminus \mathsf{E}(\mathsf{L}(\mathfrak{w})) \subseteq \mathfrak{w}_0 \setminus \mathsf{E}(\mathsf{L}(\mathfrak{w}_0))$, then $\mathfrak{w}$ is global in $\mathcal{B}(\mathcal{Z})$ or $\mathsf{GL}(\mathcal{Z})$.

The proof is given in App. B.

Remark 1. As $\mathsf{L}(S)$ is a convex cone, any "time"-scaling $\tau \mapsto \Phi(\mu\tau)$, $\mu > 0$ of a solution $\tau \mapsto \Phi(\tau)$ of (9) is again a solution of (9). Thus one has $\overline{\mathfrak{reach}(\mathrm{id},\tau)} = S_0$ for all $\tau > 0$. Yet, a distinction $\overline{\mathfrak{reach}_{[0,\tau]}(\mathrm{id})} \neq S_0$ (for τ sufficiently small) is brought about for example by restricting $L(t)$ to a bounded

[3e] In Eq. (8), one can consider either the closure with respect to $\mathcal{B}(\mathcal{Z})$ or with respect to $\mathsf{GL}(\mathcal{Z})$ or an even finer topology. The latter case is only of interest if S is not assumed to be closed in $\mathcal{B}(\mathcal{Z})$ or in $\mathsf{GL}(\mathcal{Z})$, cf. [40].

[3f] Strictly speaking, one has to relax the concept of a Lie semigroup slightly by admitting subgroups which are not necessarily closed with respect to $\mathsf{GL}(\mathcal{Z})$, cf. [40] Def. V.1.11 and footnote 3e .

[3g] Here (9) can be regarded as the operator lift of system (4).

spanning set (e.g., $\mathsf{L}(S) \cap B_K(0)$ for $K > 0$), cf. [58]. This allows for introducing a non-arbitrary physical time parameter: imposing appropriate restrictions on the global energy-conserving Hamiltonian (for system and bath in Stinespring dilation, see Eq. (11)) concomitantly and consistently restricts the generators of (Markovian) thermal operations to a bounded spanning set via the constructive projection of Thm. 2. — For qubit thermal operations, this is explicitly carried out in the Worked Example[3h] in Sec. 3.1..

Relation to Markovianity of Quantum Maps [27, 78]. These abstract ideas have concrete implications and a direct link to Kossakowski's work. They provide the tools for constructing Markovian counterparts to various types of quantum maps. Following [27], the well-established GKSL-results can be recast to a characterisation of the Lie wedge of the semigroup CPTP of *all* quantum maps (of fixed finite dimension): the set of *all* infinitesimal generators $-(i\,\mathrm{ad}_H + \mathbf{\Gamma})$ of GKSL-form (2) constitutes the (global) Lie wedge $\mathfrak{w}_{\mathsf{GKSL}}$ of CPTP. It generates the largest *Lie semigroup* S_{GKSL} contained in CPTP. Thus S_{GKSL} is given by the closure of all maps which can be written as finite product of maps $\mathrm{e}^{-t(i\,\mathrm{ad}_H + \mathbf{\Gamma})}$, $t \geq 0$. Equivalently, one may see S_{GKSL} as the set of quantum maps which can be obtained as solutions to the operator lifts of (possibly time-dependent) GKSL-master equations, cf. (9). This is why—in anticipation of the proper definitions given in (13) below—we identify S_{GKSL} with the set of all *(time-dependent) Markovian quantum maps* MCPTP. To sum up, one gets

$$S_{\mathsf{GKSL}} = \overline{\langle \exp \mathfrak{w}_{\mathsf{GKSL}} \rangle}_{\mathrm{SG}} = \mathsf{MCPTP} \quad \text{from} \quad \mathfrak{w}_{\mathsf{GKSL}} = \mathsf{L}(S_{\mathsf{GKSL}}) = \mathsf{L}(\mathsf{CPTP})\,.$$

The remaining quantum maps which do *not* belong to the Lie semigroup S_{GKSL} are called *non-Markovian*: they cannot be obtained by solutions to the operator lifts of (possibly time-dependent) GKSL-master equations and hence they are not infinitesimal CPTP-divisible in the sense of [92].

The connection to *time-independent Markovian quantum maps* is revealing: Although the set of all time-*in*dependent Markovian quantum maps (i.e. the collection $\exp(\mathfrak{w}_{\mathsf{GKSL}})$ of all one-parameter Lie semigroups) generates up to closure the entire *Lie semigroup* S_{GKSL}, the concatenation of two time-*in*dependent Markovian quantum maps does in general *not* give yet another time-*in*dependent Markovian quantum map[3i]. These results are summarised in Tab. 1, further details can be found in [27, 78].

[3h] Once a timescale of interest is fixed, such as the dephasing of the off-diagonals (in the example denoted by x), then the only parameter in the scaled global Hamiltonian $\frac{1}{\sqrt{x}} H_{\mathsf{tot}}$ is the *bounded* ratio of thermalisation of diagonal elements to dephasing $\frac{u}{x} \in [0, \frac{2}{1+\varepsilon}]$.

[3i] More precisely, close to the identity the concatenation of two time-*in*dependent Marko-

Table 1: Lie-semigroup properties decide Markovianity type of quantum maps (QMs) in terms of their infinitesimal generators as detailed in [27, 78].

Markovianity Type	structure of QMs	inf. generators
time-*in*dependent[a]	collection of 1-par. semigroups[d]	GKSL-Lie wedge
time-*de*pendent[b]	largest Lie semigroup S_{GKSL}	GKSL-Lie wedge
non-Markovian[c]	QMs outside Lie semigroup S_{GKSL}	—

[a]: infinitely resp. [b]: infinitesimal (and not just infinitely) CP-divisible [92]
[c]: *not* infinitesimal CP-divisible [92]
[d]: generally not closed under concatenation, cf. footnote 3i

3.1. Application to Thermomajorisation

Having settled the foundations, let us apply above semigroup theory to explicit sets of quantum maps. For understanding how to "use thermal resources to enhance control systems" we make the notion of thermal resources precise and specify which resources fit into the (Markovian) dynamical picture of the control framework. As mentioned in the introduction this is the goal of the resource theory approach to quantum thermodynamics: it formalises which operations can be carried out at no cost (e.g., work) by defining a set of operations "allowed" under some basic thermodynamic assumptions. One set commonly used is the following: given an n-level system with Hamiltonian H_0 and some fixed background temperature $T \in (0, \infty]$ the *thermal operations* $\mathsf{TO}(H_0, T)$ are defined to be [61, 85]

$$\Big\{ \operatorname{tr}_B \Big(U \Big((\cdot) \otimes \frac{e^{-H_B/T}}{\operatorname{tr}(e^{-H_B/T})} \Big) U^\dagger \Big) : \substack{m \in \mathbb{N}, H_B \in i\mathfrak{u}(m), U \in \mathsf{U}(mn) \\ U(H_0 \otimes \mathbb{1}_B + \mathbb{1} \otimes H_B) U^\dagger = H_0 \otimes \mathbb{1}_B + \mathbb{1} \otimes H_B} \Big\}. \quad (10)$$

Here $\mathsf{U}(m)$ is the unitary group in m dimensions with its Lie algebra $\mathfrak{u}(m)$ being the set of all $m \times m$ skew-Hermitian matrices and tr_B is the partial trace over the bath, i.e. the unique linear map $\operatorname{tr}_B : \mathbb{C}^{n\times n} \otimes \mathbb{C}^{m \times m} \to \mathbb{C}^{n \times n}$ which satisfies $\operatorname{tr}(X \operatorname{tr}_B(\rho)) = \operatorname{tr}((X \otimes \mathbb{1})\rho)$ for all $X \in \mathbb{C}^{n\times n}$, $\rho \in \mathbb{C}^{n\times n} \otimes \mathbb{C}^{m\times m}$.

Using the short-hand notation $\rho_B^{(T)} := e^{-H_B/T}/\operatorname{tr}(e^{-H_B/T})$ for the Gibbs state of the bath and restricting the global unitaries U to the commutant of

vian quantum maps is again a time-*in*dependent Markovian quantum map if their generators are part of a Lie subwedge $\mathfrak{w}$ of $\mathfrak{w}_{\mathsf{GKSL}}$ taking the special form of a Lie semialgebra: A Lie wedge $\mathfrak{w}$ is called *Lie semialgebra*, if it is locally (i.e. near the origin) closed under Baker-Campbell-Hausdorff (BCH) multiplication $X, Y \in \mathfrak{w} \mapsto X \star Y := \log(e^X e^Y)$. This requires an open BCH neighbourhood B of the origin such that $(\mathfrak{w} \cap B) \star (\mathfrak{w} \cap B) \subseteq \mathfrak{w}$ [40].

$(H_0 \otimes \mathbb{1}_B + \mathbb{1} \otimes H_B)$ to preserve the total energy of system (S) and bath (B), quantum maps brought about by thermal operations of the form of Eq. (10) can be envisaged in the spirit of a Stinespring dilation as

$$\begin{array}{ccc} \rho_S(0) \otimes \rho_B^{(T)} & \xrightarrow[(2)]{\mathrm{Ad}_U} & \rho_{SB}(U) \\ \iota_B \Big\uparrow (1) & & (3) \Big\downarrow \mathrm{tr}_B \\ \rho_S(0) & \xrightarrow[\mathsf{TO}(H_0,T)]{} & \rho_S(U)\,. \end{array} \qquad (11)$$

Thus $\mathsf{TO}(H_0, T)$ collects all quantum maps Φ which model a three-step procedure: (1) coupling the system to an arbitrary finite-dimensional bath with Hamiltonian H_B (and temperature T), followed (2) by a unitary transformation on the full system which leaves the global energy invariant, and finally (3) discarding the bath by projecting back onto the system via tr_B.

Up to now, the description has been "thermostatic" with no explicit continuous time-parameter involved. When introducing time evolutions by constructing quantum maps as curves $\Phi(t) \in \mathsf{TO}(H_0, T)$ (see Lem. 2 and Thm. 2), one may adopt above diagram to a Schrödinger picture by taking one-parameter groups of time evolutions $U(t)$ [again from the commutant of $(H_0 \otimes \mathbb{1}_B + \mathbb{1} \otimes H_B)$ to preserve energy of system and bath] as global unitaries in (11) to arrive at quantum maps $\Phi(t) \in \mathsf{TO}(H_0, T) : \rho_S(0) \mapsto \rho_S(t)$ describing the time evolutions of the system by curves of thermal operations. As mentioned in Rem. 1 above, the time scaling itself can then be induced by the choice of global Hamiltonian, see again Thm. 2 below.

Key topological properties of $\mathsf{TO}(H_0, T)$ are collected in the following:

Proposition 3. *Given $H_0 \in i\mathfrak{u}(n)$, $T \in (0, \infty]$ the following statements hold:*

(i) $\mathsf{TO}(H_0, T)$ *is a bounded, path-connected semigroup with identity.*

(ii) $\overline{\mathsf{TO}(H_0, T)}$ *is a convex, compact semigroup with identity.*

(iii) $\overline{\mathsf{TO}(H_0, T)}$ *is a subset of* $\mathsf{Gibbs}(H_0, T)$ *which is defined to be the collection of all* CPTP *maps which leave $e^{-H_0/T}$ invariant.*

(iv) One has $[\Phi, \mathrm{ad}_{H_0}] = 0$ for all $\Phi \in \overline{\mathsf{TO}(H_0, T)}$.

Statements (i) through (iii) can be found in Sec. II of [85] while statement (iv) is Thm. 1 in [63]. Some intuition as to whence condition (iv) can be gained from the following basic observation: given any system with Hamiltonian $H_0 = \sum_{j=1}^n E_j |g_j\rangle\langle g_j|$ in state $\rho = (\langle g_j, \rho g_k \rangle)_{j,k=1}^n$ there exists a thermal operation which mixes ρ_{ij} and ρ_{kl} if and only if $E_i - E_j = E_k - E_l$ [85, Rem. 3]. But $E_i - E_j, E_k - E_l \in \sigma(\mathrm{ad}_{H_0})$ so the action of any thermal operation is restricted by the degeneracies of ad_{H_0}. In particular, choosing

$i = j$ or $k = l$ shows that a thermal operation can mix diagonal and off-diagonal elements only if H_0 is degenerate. This turns out to be a special case of the following (well-known and readily verified) result:

Corollary 2. *If H_0 has non-degenerate spectrum, then the diagonal and the off-diagonal (w.r.t any eigenbasis of H_0) action of any* CPTP *map satisfying the covariance law from Prop. 3 (iv) are strictly separated.*

This symmetry is the defining property of what is called the set of *enhanced thermal operations* (sometimes *thermal processes*) [20]:

$$\mathsf{EnTO}(H_0, T) := \{S \in \mathsf{Gibbs}(n) \,:\, [S, \mathrm{ad}_{H_0}] = 0\}\,.$$

Note that the enhanced thermal operations—just like the closure of the thermal operations—form a convex, compact semigroup with identity.

Now a central task in this framework is characterising if some initial state can be transformed into a given target state by a thermal operation. Thus one naturally defines *thermomajorisation* as the majorisation induced by the semigroup $\overline{\mathsf{TO}(H_0, T)}$ (the latter sometimes denoted $\mathsf{CTO}(H_0, T)$ [37]), and the set of all states thermomajorised by some $\rho \in \mathfrak{pos}_1(n)$ is defined as

$$M_{H_0,T}(\rho) := M_{\overline{\mathsf{TO}(H_0,T)}}(\rho) = \left\{\Phi(\rho) : \Phi \in \overline{\mathsf{TO}(H_0, T)}\right\}. \tag{12}$$

This is also known as *(future) thermal cone* [63, 52, 24] or, in the case of quasi-classical states (i.e. states ρ which satisfy $[\rho, H_0] = 0$) as thermal polytope [2] or thermomajorisation polytope [91]. Note that in (12) we did not choose $\mathsf{TO}(H_0, T)$ but its closure (which is known to make a difference [63]) because this guarantees "reasonable" mathematical structure: combining Prop. 1 and 3 shows that $M_{H_0,T}(\rho)$ is a convex compact subset of $\mathfrak{pos}_1(n)$. Similarly one can define the semigroup majorisation induced by $\mathsf{EnTO}(H_0, T)$ and $\mathsf{Gibbs}(H_0, T)$, respectively. While $\overline{\mathsf{TO}(H_0, T)} \subseteq \mathsf{EnTO}(H_0, T) \subseteq \mathsf{Gibbs}(H_0, T)$ for all $H_0 \in i\mathfrak{u}(n)$, $T \in (0, \infty]$ (Prop. 3) it is known that—although the action of these sets coincides on the diagonal (cf. Sec. 3.3.)—the corresponding notions of majorisation are strictly different (as long as $n > 2$ [20, 89]) due to an explicit counterexample by Ding et al. [25]. Therefore it makes a conceptual difference whether one defines thermomajorisation via thermal operations, enhanced thermal operations, or the Gibbs-preserving quantum maps [31].

In a recent approach to unify *dynamics* of open quantum systems with quantum thermodynamics, Lostaglio and Korzekwa [64] studied the intersection of enhanced thermal operations with (time-dependent) Markovian quantum maps: they characterised which states can be generated by such maps in case the initial state ρ is quasi-classical. Their approach was to consider Markovian dynamics $(e^{-tL})_{t\geq 0}$ (i.e. $L = i\,\mathrm{ad}_{H_0} + \mathbf{\Gamma}$ with $\mathbf{\Gamma}$ as in (2)) and study the thermodynamic restraints the condition $(e^{-tL})_{t\geq 0} \subseteq \mathsf{EnTO}(H_0,T)$ imposes on the generator of the system-environment-interaction $\mathbf{\Gamma}$ (which until now was arbitrary except its GKSL-form). They found that such dynamics are in $\mathsf{EnTO}(H_0,T)$ at all times if and only if[3j] $[L,\mathrm{ad}_{H_0}] = 0$ and $L(e^{-H_0/T}) = 0$, cf. also [53].

Cast into the framework of Lie semigroups what they did translates into characterising the Lie wedge of $\mathsf{EnTO}(H_0,T)$. Accordingly this motivates us to introduce the following constructive *definitions* for the *Markovian* counterparts of the sets above:

$$\begin{aligned} \mathsf{MTO}(H_0,T) &:= \overline{\langle \exp\big(\mathsf{L}(\overline{\mathsf{TO}(H_0,T)})\big)\rangle_{\mathrm{SG}}} \\ \mathsf{MEnTO}(H_0,T) &:= \overline{\langle \exp\big(\mathsf{L}(\mathsf{EnTO}(H_0,T))\big)\rangle_{\mathrm{SG}}} \\ \mathsf{MGibbs}(H_0,T) &:= \overline{\langle \exp\big(\mathsf{L}(\mathsf{Gibbs}(H_0,T))\big)\rangle_{\mathrm{SG}}} \end{aligned} \tag{13}$$

As before, the overbar denotes the closure and $\langle\,\cdot\,\rangle_{\mathrm{SG}}$ is the semigroup generated by the set in question. In other words $\mathsf{MEnTO}(H_0,T)$ is the collection of all enhanced thermal operations that are time-dependent Markovian, which likewise holds for $\mathsf{MTO}(H_0,T)$ and $\mathsf{MGibbs}(H_0,T)$. Translated to this language Lostaglio and Korzekwa studied the semigroup majorisation induced by $\mathsf{MEnTO}(H_0,T)$ in the quasi-classical realm. We provide a sketch of the sets introduced in this section in Fig. 1.

Remark 2. By definition $\mathsf{MTO}(H_0,T)$, $\mathsf{MEnTO}(H_0,T)$, $\mathsf{MGibbs}(H_0,T)$ contain all propagators of bilinear control systems (Sec. 2.) under the corresponding thermodynamic constraints. This connection allows us to translate results from quantum control theory into this majorisation framework: for example Prop. 5.2.1 in [84] implies that if $e^{-H_0/T}$ is a multiple of the identity, then the semigroup majorisation induced by $\mathsf{Gibbs}(H_0,T)$ and by $\mathsf{MGibbs}(H_0,T)$ coincide. In other words each unital state transfer can also be realised by unital (time-dependent) *Markovian* maps.

In the remainder of this section we generalise the result of Lostaglio and Korzekwa [64] to the more physically motivated set of thermal operations. We begin studying its *Lie semigroup structure* by specifying the edge of the sets defined above:

Lemma 1. *Given $H_0, H \in i\mathfrak{u}(n)$ and $T \in (0,\infty]$ the following statements are equivalent:*

(i) $[H,H_0] = 0$

[3j] The straightforward identity $[B^m,A] = \sum_{k=1}^m B^{m-k}[B,A]B^{k-1}$ $(m\in\mathbb{N})$ shows that $[B,A]=0$ if and only if $[B^m,A]=0$ for all m if and only if $[e^{tB},A]=0$ for all $t\geq 0$.

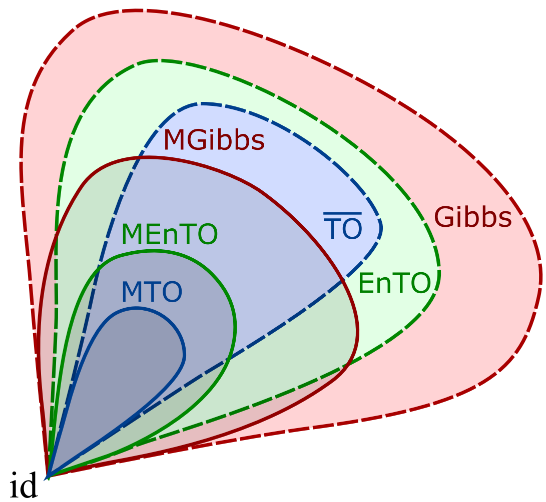

Fig. 1: (Colour online). Sketch of the semigroups $\mathsf{(En)TO}$ and Gibbs, as well as their Markovian counterparts $\mathsf{M(En)TO}$ and MGibbs defined as *Lie semigroups* generated by their corresponding Lie wedges, see also the qubit example in Fig. 2 . Note that Markovianity depends on the semigroup, i.e. there might be elements in $\mathsf{EnTO} \cap \mathsf{MGibbs}$ outside of MEnTO. A similar set-inclusion for *elementary* thermal operations (ETOs, which in general are a proper subset of $\overline{\mathsf{TO}}$s) can be found in [62, Fig. 3].

(ii) $(\mathrm{Ad}_{e^{-itH}})_{t\geq 0} \subseteq \mathsf{TO}(H_0, T)$

(iii) $(\mathrm{Ad}_{e^{-itH}})_{t\geq 0} \subseteq \overline{\mathsf{TO}(H_0, T)}$

(iv) $(\mathrm{Ad}_{e^{-itH}})_{t\geq 0} \subseteq \mathsf{EnTO}(H_0, T)$

Moreover, if $T \in (0, \infty)$, then all of the above statements are equivalent to:

(v) $\mathrm{Ad}_{e^{-itH}}(e^{-H_0/T}) = e^{-H_0/T}$ *for all* $t \geq 0$.

Proof. "(i) $\Rightarrow$ (ii)": In the definition of the thermal operations (10) choose $m = 1$ and $U = e^{-itH}$. Doing so is allowed as $[H, H_0] = 0$ by assumption. "(ii) $\Rightarrow$ (iii) $\Rightarrow$ (iv)": Obvious from $\mathsf{TO}(H_0, T) \subseteq \overline{\mathsf{TO}(H_0, T)} \subseteq \mathsf{EnTO}(H_0, T)$ [63]. "(iv) $\Rightarrow$ (i)": Evidently, the generator of $(\mathrm{Ad}_{e^{-itH}})_{t\geq 0}$ is $-i\,\mathrm{ad}_H$. By our previous considerations $-i\,\mathrm{ad}_H \in \mathsf{L}(\mathsf{EnTO}(H_0, T))$ implies $[\mathrm{ad}_H, \mathrm{ad}_{H_0}] \equiv 0$. Using $[\mathrm{ad}_H, \mathrm{ad}_{H_0}] = \mathrm{ad}_{[H,H_0]}$ this is equivalent to $[H, H_0] = \lambda\mathbb{1}$ for some $\lambda \in \mathbb{C}$; but this λ has to vanish as $0 = \mathrm{tr}([H, H_0]) = \lambda\,\mathrm{tr}(\mathbb{1}) = \lambda n$.

Now assume that $T < \infty$. "(iv) $\Rightarrow$ (v)": By definition of $\mathsf{EnTO}(H_0, T)$. "(v) $\Rightarrow$ (i)": Differentiating (v) at zero gives $[H, e^{-H_0/T}] = 0$ so there exists $U \in \mathbb{C}^{n\times n}$ unitary such that $UHU^\dagger$ and $Ue^{-H_0/T}U^\dagger$ are both diagonal [45, Thm. 2.5.5]. But $Ue^{-H_0/T}U^\dagger = e^{-UH_0U^\dagger/T}$ so using functional calculus, the matrix $(-T)\ln\left(e^{-UH_0U^\dagger/T}\right) = UH_0U^\dagger$ has to be diagonal due to $T \in (0,\infty)$. Thus $U[H,H_0]U^\dagger = [UHU^\dagger, UH_0U^\dagger] = 0$, hence (i) follows. □

As the inverse of a bijective CPTP map is again CPTP if and only if it is a unitary map[3k] [13, Thm. III.2], $\mathsf{E}(\mathsf{L}(\mathsf{CPTP}(n))) = \{i\mathrm{ad}_H : H \in i\mathfrak{u}(n)\}$. But the edge of any subsemigroup of $\mathsf{CPTP}(n)$ has to be a subspace of $\mathsf{E}(\mathsf{L}(\mathsf{CPTP}(n)))$, and the condition for one-parameter groups $(\mathrm{Ad}_{e^{-itH}})_{t\geq 0}$ to live in the corresponding semigroup—depending on the temperature T—is precisely condition (i) from Lem. 1. This immediately yields the following:

Corollary 3. *Given $H_0 \in i\mathfrak{u}(n)$, $T \in (0,\infty]$ one finds that $\mathsf{E}(\mathsf{L}(\mathsf{TO}(H_0,T)))$, $\mathsf{E}(\mathsf{L}(\overline{\mathsf{TO}(H_0,T)}))$, and $\mathsf{E}(\mathsf{L}(\mathsf{EnTO}(H_0,T)))$ equal $\{i\mathrm{ad}_H : H \in i\mathfrak{u}(n), [H,H_0] = 0\}$, and if $T \in (0,\infty)$ the same holds true for $\mathsf{E}(\mathsf{L}(\mathsf{Gibbs}(H_0,T)))$.*

The next step is to specify the *Lie wedge* of the semigroups in question. This turns out to be almost trivial for the Gibbs-preserving maps and the enhanced thermal operations:

Lemma 2. *Given $H_0, H \in i\mathfrak{u}(n)$ and $T \in (0,\infty]$ one has:*

$$\begin{aligned}\mathsf{L}(\mathsf{Gibbs}(H_0,T)) &= \{L \in \mathcal{L}(\mathbb{C}^{n\times n}) : L \textit{ is of } \textsc{gksl}\textit{-form and } L(e^{-H_0/T}) = 0\}\\ \mathsf{L}(\mathsf{EnTO}(H_0,T)) &= \{L \in \mathcal{L}(\mathbb{C}^{n\times n}) : L \in \mathsf{L}(\mathsf{Gibbs}(H_0,T)) \textit{ and } [L,\mathrm{ad}_{H_0}] = 0\}\end{aligned}$$

One can see this by taking the condition in Eq. (6) and differentiating at zero to get back the generator L.

In contrast, specifying the Lie wedge of $\overline{\mathsf{TO}(H_0,T)}$ is more involved. This is where we make use of Prop. 2 (iv) as well as Cor. 1 which state that elements of $\mathsf{L}(S)$ are characterised via derivatives of certain curves in S starting at the identity. Thereby introducing a "time" parameter, an obvious way to specify such curves for the case of $\mathsf{TO}(H_0,T)$ is by interpreting the energy-preserving unitary as endpoint of a curve of unitaries starting at zero in the sense of the diagram Eq. (11). This is done by choosing H_{tot} such that $U = e^{-iH_{\mathsf{tot}}}$ in

$$\mathrm{tr}_B\left(U\big((\cdot)\otimes\rho_B^{(T)}\big)U^\dagger\right) = \mathrm{tr}_B\left(e^{-itH_{\mathsf{tot}}}\big((\cdot)\otimes\rho_B^{(T)}\big)e^{itH_{\mathsf{tot}}}\right)\Big|_{t=1}\,.$$

By definition this curve is in $\mathsf{TO}(H_0,T)$ at all times. Such curves and their first and second derivative have been studied recently by one of us: for all $m\in\mathbb{N}$, $H \in i\mathfrak{u}(mn)$, $\omega \in \mathfrak{pos}_1(m)$

$$\begin{aligned}&\mathrm{tr}_{\mathbb{C}^m}\left(e^{-itH}((\cdot)\otimes\omega)e^{itH}\right)\equiv\\ &\qquad\equiv \mathrm{id} - it\big[\,\mathrm{tr}_\omega(H),\,\cdot\,\big] - \frac{t^2}{2}\sum_{j,k=1}^m \mathbf{\Gamma}_{\sqrt{2r_k}\,\mathrm{tr}_{|g_k\rangle\langle g_j|}(H)} + \mathcal{O}(t^3)\end{aligned}\tag{14}$$

[3k]Actually the map is unitary iff the inverse is positive, cf. [92, Cor. 3] & [88, Prop. 1].

if $\omega = \sum_{i=1}^m r_i |g_i\rangle\langle g_i|$ for $r_i \geq 0$ and an orthonormal basis $\{g_i\}_{i=1}^m$ of $\mathbb{C}^m$. Here, given matrices $X \in \mathbb{C}^{m\times m}$, $B \in \mathbb{C}^{mn\times mn}$ the expression $\operatorname{tr}_X(B)$ is called "partial trace of B with respect to X" [31]. A proof can be found in [86, Eq. (5)] or, for the reader's convenience, in App. C.

Now applying Prop. 2 (iv) to these curves yields the Hamiltonian generator $i[\operatorname{tr}_{\rho_B^{(T)}}(H_{\mathsf{tot}}), \cdot\,]$ which by Cor. 3 and Eq. (14) is in $\mathsf{E}(\mathsf{L}(\overline{\mathsf{TO}(H_0,T)}))$. However, we are interested in the dissipative action of the curve which is locked away behind the second derivative. This is where we apply Cor. 1:

Theorem 2. *Let $m \in \mathbb{N}$, $H_B \in i\mathfrak{u}(m)$, as well as $H_{\mathsf{tot}} \in i\mathfrak{u}(mn)$ be given such that $[H_{\mathsf{tot}}, H_0 \otimes \mathbb{1} + \mathbb{1} \otimes H_B] = 0$. If Φ is the solution to*

$$\dot\Phi(t) = \big(-i\,\mathrm{ad}_H - \mathbf{\Gamma}_{B,\mathsf{tot}}\big)\Phi(t)\,, \quad \Phi(0) = \mathrm{id}$$

with H any element of $i\mathfrak{u}(n)$ such that $[H, H_0] = 0$ and

$$\mathbf{\Gamma}_{B,\mathsf{tot}} := \sum_{j,k=1}^m \Big(\tfrac12\big(V_{jk}^\dagger V_{jk}(\cdot) + (\cdot)V_{jk}^\dagger V_{jk}\big) - V_{jk}(\cdot)V_{jk}^\dagger\Big)\,,$$

$V_{jk} = e^{-E_k'/(2T)}\operatorname{tr}_{|g_k\rangle\langle g_j|}(H_{\mathsf{tot}})$ for all $j,k = 1,\ldots,m$ where $\sum_{j=1}^m E_j'|g_j\rangle\langle g_j|$ is any spectral decomposition of the bath Hamiltonian H_B, then $(\Phi(t))_{t\geq 0}$ is a continuous one-parameter semigroup in $\overline{\mathsf{TO}(H_0,T)}$.

Proof. Consider $\gamma : [0,\infty) \to \overline{\mathsf{TO}(H_0,T)}$, $t \mapsto \operatorname{tr}_B(e^{-itH_{\mathsf{tot}}}((\cdot)\otimes\rho_B^{(T)})e^{itH_{\mathsf{tot}}})$ and note that γ is well-defined by assumption on H_B, H_{tot}. Also $\gamma(0) = \mathrm{id}$ and $\dot\gamma(0) \in \mathsf{E}(\mathsf{L}(\overline{\mathsf{TO}(H_0,T)}))$ by Eq. (14) & Cor. 3. Thus—because $\overline{\mathsf{TO}(H_0,T)}$ is a compact, convex semigroup (Prop. 3 (ii))—we may apply Cor. 1 to γ which shows that $\ddot\gamma(0) \in \mathsf{L}(\overline{\mathsf{TO}(H_0,T)})$. If $H_B = \sum_{j=1}^m E_j'|g_j\rangle\langle g_j|$, then $e^{-H_B/T} = \sum_{j=1}^m e^{-E_j'/T}|g_j\rangle\langle g_j|$ so, again using Eq. (14)

$$\ddot\gamma(0) = -\frac{2}{\operatorname{tr}(e^{-H_B/T})}\sum_{j,k=1}^m \mathbf{\Gamma}_{\sqrt{e^{-E_k'/T}}\operatorname{tr}_{|g_k\rangle\langle g_j|}(H_{\mathsf{tot}})}$$

is in $\mathsf{L}(\overline{\mathsf{TO}(H_0,T)})$. But the latter is a convex cone (Prop. 2 (i)) so for all $H \in i\mathfrak{u}(n)$, $[H, H_0] = 0$

$$\mathsf{L}(\overline{\mathsf{TO}(H_0,T)}) \ni -i\,\mathrm{ad}_H + \frac{\operatorname{tr}(e^{-H_B/T})}{2}\ddot\gamma(0) = -i\,\mathrm{ad}_H - \mathbf{\Gamma}_{B,\mathsf{tot}} \qquad (15)$$

which concludes the proof. ∎

[31] More precisely, $\operatorname{tr}_X(B)$ is set to be the unique $n\times n$-matrix which satisfies $\operatorname{tr}(A\operatorname{tr}_X(B)) = \operatorname{tr}((A\otimes X)B)$ for all $A \in \mathbb{C}^{n\times n}$ [23, Ch. 9, Lem. 1.1]. Note that this recovers the "usual" partial trace when setting $X = \mathbb{1}$.

Remark 3. Though $(\mathrm{tr}_{|g_k\rangle\langle g_j|}(H_{\mathsf{tot}}))^\dagger = \mathrm{tr}_{|g_j\rangle\langle g_k|}(H_{\mathsf{tot}})$, note the "asymmetry" in the V_{jk} induced by temperature via the factor $e^{-E'_k/(2T)}$. Assuming $T<\infty$ prevents the dynamics from automatically being unital (i.e. identity-preserving). It is worth stressing that the temperature-independent projection $\mathrm{tr}_{|g_j\rangle\langle g_k|}(H_{\mathsf{tot}})$ also preserves the time scaling chosen for the global energy conserving one-parameter unitary time evolution $e^{-itH_{\mathsf{tot}}}$ and takes it over into scaling the generators of the semigroup $\overline{\mathsf{TO}(H_0,T)}$ to be *consistent* with the same time parameter—as anticipated in Rem. 1.

At this point, Andrzej Kossakowski would have insisted that Thm. 2 does not provide a complete characterisation yet—and rightly so: we have to leave the converse open for now, but do so at the level of a well supported conjecture.

Conjecture 1. *The converse of Thm. 2 holds true, up to taking the closure of the collection of all these generators.*

This conjecture is supported by the following two observations:

- Conjecture 1 holds for general quantum maps, that is, after getting rid of the commutator relation $[H_{\mathsf{tot}}, H_0\otimes\mathbb{1}+\mathbb{1}\otimes H_B]=0$ as well as replacing $\overline{\mathsf{TO}}$ with $\mathsf{CPTP}(n)$. The only difference here is that only full-rank ancilla states are allowed whereas [86, Thm. 2] uses arbitrary ancilla states. This difference, however, vanishes in the closure.
- For any $H_0\in i\mathfrak{u}(n)$, $T\in(0,\infty]$ the collection of all generators described in Thm. 2 is invariant under conjugation by arbitrary edge elements (i.e. the necessary condition from Prop. 2 (ii)). Indeed given any $H'\in i\mathfrak{u}(n)$ with $[H',H_0]=0$—hence $i\mathrm{ad}_{H'}\in\mathsf{E}(\mathsf{L}(\overline{\mathsf{TO}(H_0,T)}))$ by Cor. 3—one finds

$$\begin{aligned}
&\mathrm{Ad}_{e^{-iH'}}\circ\big(-i\,\mathrm{ad}_H-\mathbf{\Gamma}_{B,\mathsf{tot}}\big)\circ\mathrm{Ad}_{e^{iH'}}\\
&\quad=-i[e^{-iH'}He^{iH'},\,\cdot\,]-\sum_{j,k=1}^m\mathbf{\Gamma}_{e^{-E'_k/(2T)}e^{-iH'}\mathrm{tr}_{|g_k\rangle\langle g_j|}(H_{\mathsf{tot}})e^{iH'}}\\
&\quad=-i[e^{-iH'}He^{iH'},\,\cdot\,]-\sum_{j,k=1}^m\mathbf{\Gamma}_{e^{-E'_k/(2T)}\mathrm{tr}_{|g_k\rangle\langle g_j|}((e^{-iH'}\otimes\mathbb{1})H_{\mathsf{tot}}(e^{-iH'}\otimes\mathbb{1})^\dagger)}\,.
\end{aligned}$$

  But this generator is of the form described in Thm. 2 as can be seen by replacing H_{tot} by $(e^{-iH'}\otimes\mathbb{1})H_{\mathsf{tot}}(e^{-iH'}\otimes\mathbb{1})^\dagger$, replacing H by $e^{-iH'}He^{iH'}$, and keeping H_B as is. One readily verifies that the new H (H_{tot}) commutes with H_0 ($H_0\otimes\mathbb{1}+\mathbb{1}\otimes H_B$), and thus is a valid generator; this follows from $e^{-iH'}H_0e^{iH'}=e^{-i\,\mathrm{ad}_{H'}}(H_0)=0$ which is a direct consequence of $[H',H_0]=0$.

Remark 4. To sum up, we emphasise that the Lie wedges to the quantum maps Gibbs, EnTO (Lem. 2) and to $\overline{\mathsf{TO}}$ (Thm. 2 and Eq. (15)) are *global*, as by Thm. 1 they generate the corresponding Lie semigroups, which in turn *define* the respective Markovian counterparts MGibbs, MEnTO, and MTO via the construction of Eqs. (13). The set inclusions are illustrated in Fig. 1.

Explicitly scrutinising and visualising the above sets and relations in the case of qubits will elucidate the concepts introduced in this section concretely.

3.2. Worked Example: Markovian Thermal Operations in Qubits

Let us demonstrate how to arrive from a general non-Markovian (enhanced) thermal operation via the GKSL-generator in its Lie wedge at the corresponding Lie semigroup giving the desired *Markovian* counterpart to the given (enhanced) thermal operation as in Eq. (13). We study the simple case of a single qubit. What is special about two-dimensional systems is twofold: first, time-independent and time-dependent Markovianity coincide (as explained at the end of this example), and secondly the thermal operations and the enhanced thermal operations approximately coincide [47], [85, Thm. 10]. Thus, every thermal operation for $H_0 := \frac{1}{2}\operatorname{diag}(-1,1)$ acts like

$$\begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} \mapsto \begin{pmatrix} (1-w\varepsilon)\rho_{11} + w\rho_{22} & z\rho_{12} \\ z^*\rho_{21} & w\varepsilon\rho_{11} + (1-w)\rho_{22} \end{pmatrix}$$

for some $w \in [0,1]$, $z \in \mathbb{C}$ such that $|z| \leq \sqrt{(1-w)(1-w\varepsilon)}$ [85, Sec. IV] with the short-hand $\varepsilon := e^{-1/T}$ used henceforth.

Parameterising the Elements in the Lie Wedge

With these stipulations, Lem. 2 then allows to specify the elements in the Lie wedge of the (enhanced) thermal operations: a linear map L on $\mathbb{C}^{2\times 2}$ is a generator of a one-parameter semigroup in $\mathsf{EnTO}(H_0, T)$ if and only if

(i) L preserves Hermiticity,

(ii) L is trace-annihilating,

(iii) L is conditionally completely positive ([60, Cor. 1] & [30, Thm. 14.7]),

$$(\mathbb{1} - |\Omega\rangle\langle\Omega|)\big((\mathrm{id}\otimes L)(|\Omega\rangle\langle\Omega|)\big)(\mathbb{1} - |\Omega\rangle\langle\Omega|) \geq 0$$

where $\Omega = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & 1 \end{pmatrix}^\top$,

(iv) $L(e^{-H_0/T}) = 0$, and

(v) $[L, \mathrm{ad}_{H_0}] = 0$.

Property (v) is equivalent to

$$L\begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} = \begin{pmatrix} x\rho_{11} + u\rho_{22} & z\rho_{12} \\ y\rho_{21} & v\rho_{11} + w\rho_{22} \end{pmatrix}$$

for some $u, v, w, x, y, z \in \mathbb{C}$ (cf. also Cor. 2). Thereby (i), (ii), and (iv) combined are equivalent to $v = -x = ue^{-1/T}$, $w = -u$, and $y = z^*$ where

$u \in \mathbb{R}$. Finally, evaluating conditional complete positivity yields $u \geq 0$ and $2\,\mathrm{Re}\, z \leq -u(1+\varepsilon)$. Altogether this shows $L \in \mathsf{L}(\mathsf{EnTO}(H_0, T))$ if and only if

$$L \begin{pmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{pmatrix} = \begin{pmatrix} u(\rho_{22} - \rho_{11}\varepsilon) & (-x + i\omega)\rho_{12} \\ (-x - i\omega)\rho_{21} & u(\rho_{11}\varepsilon - \rho_{22}) \end{pmatrix}$$

for some $u \geq 0$, $x, \omega \in \mathbb{R}$ such that $2x \geq u(1+\varepsilon)$. Casting this into the Markovian GKSL master equation (1) yields (in superoperator representation)

$$L = -i\,\mathrm{ad}_{\mathrm{diag}(-\omega,\omega)/2} - \mathbf{\Gamma}_{\text{GKSL}} \mathrel{\widehat{=}} \begin{pmatrix} -\varepsilon u & 0 & 0 & u \\ 0 & -x - i\omega & 0 & 0 \\ 0 & 0 & -x + i\omega & 0 \\ \varepsilon u & 0 & 0 & -u \end{pmatrix}.$$

where the (by assumption well-defined) generators of $\mathbf{\Gamma}_{\text{GKSL}}$ are

$$V_{11} = \frac{\sqrt{2x - u(1+\varepsilon)}}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \; V_{12} = \sqrt{u} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \; V_{21} = \sqrt{u\varepsilon} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Setting $V_{22} = 0$, in the language of Thm. 2 this corresponds to $H_B := \mathrm{diag}(-1, 1)/2 = H_0$ and a global Hamiltonian (with $u \geq 0$ playing the role of a scaling parameter later used for fixing the time scale t)

$$H_{\mathsf{tot}} := \begin{pmatrix} \frac{1}{2}\sqrt{2x - u(1+\varepsilon)} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{u} & 0 \\ 0 & \sqrt{u} & -\frac{1}{2}\sqrt{2x - u(1+\varepsilon)} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \in i\mathfrak{u}(4)\,.$$

Characterising One-Parameter Semigroups in $\mathsf{MEnTO}(H_0, T)$

For the one-parameter semigroup of time evolutions ($t \geq 0$) one finds

$$\begin{aligned} S(t) \;=\; e^{tL} \;&\widehat{=}\; \begin{pmatrix} \frac{1+\varepsilon e^{-tu(1+\varepsilon)}}{1+\varepsilon} & 0 & 0 & \frac{1-e^{-tu(1+\varepsilon)}}{1+\varepsilon} \\ 0 & e^{-(x+i\omega)t} & 0 & 0 \\ 0 & 0 & e^{-(x-i\omega)t} & 0 \\ \frac{\varepsilon(1-e^{-tu(1+\varepsilon)})}{1+\varepsilon} & 0 & 0 & \frac{\varepsilon+e^{-tu(1+\varepsilon)}}{1+\varepsilon} \end{pmatrix} \\ &= \begin{pmatrix} 1 - \varepsilon\mu_t & 0 & 0 & \mu_t \\ 0 & e^{-xt}e^{-i\omega t} & 0 & 0 \\ 0 & 0 & e^{-xt}e^{i\omega t} & 0 \\ \varepsilon\mu_t & 0 & 0 & 1 - \mu_t \end{pmatrix}, \end{aligned} \tag{16}$$

where the last identity uses another short-hand $\mu_t := (1 - e^{-tu(1+\varepsilon)})/(1+\varepsilon)$ with non-negative times enforcing $0 \leq \mu_t \leq 1/(1+\varepsilon)$. For the action on just the vector of diagonal elements of the density operator one gets

$$G(t) = \begin{pmatrix} 1-\varepsilon\mu_t & \mu_t \\ \varepsilon\mu_t & 1-\mu_t \end{pmatrix},$$

which resembles the β-swap for a two-level system: Note that $S(t)$ and $G(t)$ are both Gibbs-stochastic for the entire fictitious parameter range[a] $\mu_t \in [0,1]$ exploited in the β-swap (then including “complex times”[b]), whereas they are *Markovian* only in the positive-time segment $\mu_t \in [0, 1/(1+\varepsilon)]$, whence $G(t)$ derives from a one-parameter semigroup $S(t) \in \mathsf{MEnTO}(H_0, T)$ of the form of Eq. (16) and has itself a non-negative determinant.

How the Markovian MTO*s Sit in General* TO*s*

More generally, (the superoperator of) any map $\Phi \in \overline{\mathsf{TO}(H_0,T)}$ is of the form

$$\begin{pmatrix} 1-\varepsilon\mu & 0 & 0 & \mu \\ 0 & e^{-x}e^{-i\omega} & 0 & 0 \\ 0 & 0 & e^{-x}e^{i\omega} & 0 \\ \varepsilon\mu & 0 & 0 & 1-\mu \end{pmatrix} \tag{17}$$

for $\mu \in [0,1]$, $x \geq 0$ so that $e^{-2x} \leq (1-\varepsilon\mu)(1-\mu) = 1-\mu(1+\varepsilon)+\varepsilon\mu^2$, and it is again in $\mathsf{MTO}(H_0,T)$ if and only if $\mu \in [0, \frac{1}{(1+\varepsilon)}]$ (see [2, 72]) plus $e^{-2x} \leq 1-\mu(1+\varepsilon)$. Since $\varepsilon = e^{-1/T} \to 0$ for temperatures $T \to 0^+$ it is obvious that—in the case of a single qubit—Markovianity becomes no longer a restriction and $\mathsf{MTO}(H_0,T) \to \overline{\mathsf{TO}(H_0,T)}$ as $T \to 0^+$ (e.g., in the Hausdorff metric [56, §21.VII]). Not only are these two scenarios equivalent in terms of *state conversion* as $T \to 0^+$ (as was known for arbitrary finite dimensions [28, Thm. 1]), but equality also holds on the level of *quantum maps*—in the case of qubits, which is new. Whether this holds for qutrits and higher dimensions is an open question.

Visualisation

By Eqs. (16) & (17) one can visualise the set of (Markovian) qubit thermal operations. The main tool is the semigroup homomorphism Ψ_T from the Hermiticity-preserving linear maps on $\mathbb{C}^{2\times 2}$ to $(\mathbb{R}\times\mathbb{C}, \circ_T)$[c] which acts like $\Psi_T : \Phi \mapsto (\langle e_1, \Phi(|e_2\rangle\langle e_2|)e_1\rangle, \langle e_1, \Phi(|e_1\rangle\langle e_2|)e_2\rangle)^\top$, cf. [85, Sec. IV]. One finds

$$\Psi_T\big(\overline{\exp\big(\mathsf{L}(\overline{\mathsf{TO}(H_0,T)})\big)}\big) = \Big\{ \begin{pmatrix} \mu_t \\ e^{2\pi i\phi}\, r\sqrt{1-\mu_t(1+\varepsilon)} \end{pmatrix} : r,\phi \in [0,1];\ t \in [0,\infty] \Big\}.$$

This set turns out to be a subsemigroup of $(\mathbb{R}\times\mathbb{C},\circ_T)$ which implies that the closure of $\exp\big(\mathsf{L}(\overline{\mathsf{TO}(H_0,T)})\big)$ is a subsemigroup of $\overline{\mathsf{TO}(H_0,T)}$. One gets

$$\mathsf{MTO}(H_0,T) = \overline{\langle \exp\big(\mathsf{L}(\overline{\mathsf{TO}(H_0,T)})\big)\rangle_{\mathrm{SG}}} = \overline{\exp\big(\mathsf{L}(\overline{\mathsf{TO}(H_0,T)})\big)},$$

which shows that $\mathsf{MTO}(H_0,T)$ is *weakly exponential* [d]. Actually, commutativity of $\circ_T$ for *fixed temperature* [e] immediately implies that $\mathsf{MTO}(H_0,T)$ is *locally* as well as *(weakly) exponential* and its Lie wedge takes the special form of a Lie semialgebra, cf. [44, Ch. 1, Thm. A & Ch. 2, Ex. 1.6] and [27, Thm. 2.2]. So—here in the qubit case—the two notions of time-dependent and time-independent Markovianity coincide. Taking the union of $\mathsf{MTO}(H_0,T)$ over *all temperatures* one obtains a semigroup $\mathsf{MTO}(H_0) := \overline{\bigcup_{T\in(0,\infty)}\mathsf{MTO}(H_0,T)}$ which turns out to be both, weakly exponential and locally exponential as shown in App. E.

Finally let us actually visualise how $\mathsf{MTO}(H_0,T)$ sits inside $\overline{\mathsf{TO}(H_0,T)}$ in Fig. 2 (cf. [85, Fig. 2]) for the case of a single qubit. Its upper left panel also illustrates how for small times $\mu_t\to 0$ the non-Markovian blue cone extends to the identity map including an infinitesimal region *outside* the connected component of the (orange) Markovian Lie semigroup.
Now this becomes obvious by the shapes determined by the outer curves of the blue (orange) cone in the time direction μ_t which—up to rotational symmetry—follow $\sqrt{1-\mu_t(1+\varepsilon)+\mu_t^2\varepsilon}$ where $\mu_t \in [0,1]$ (resp. $\sqrt{1-\mu_t(1+\varepsilon)}$ in the Markovian case where $\mu_t\in[0,1/(1+\varepsilon)]$).

In the lower panel of Fig. 2 the time dependence in $\mu_t = (1-e^{-tu(1+\varepsilon)})/(1+\varepsilon)$ formally leads to a time in multiples of the scaling factor $u>0$ reading $t[u] = -\ln(1-\mu_t(1+\varepsilon))/(1+\varepsilon)$. Taking "the" preimage of the interval $[0,1]$ under this function yields a (partially) complex set: $t(\mu_t)$ is real (orange) for $0\le\mu_t\le 1/(1+\varepsilon) =: \mu_*$, i.e. up to its pole at the Markovian limit μ_*, whence it becomes complex (blue) with constant imaginary part $\pm\pi/(1+\varepsilon)$ in the non-Markovian segment $\mu_* < \mu_t \le 1$.

[a] in which $S(t)$ resp. $G(t)$ stabilise the Gibbs state $\frac{1}{1+\varepsilon}\,\mathrm{diag}(1,\varepsilon)$ resp. $\frac{1}{1+\varepsilon}(1,\varepsilon)^\top$

[b] Formally $t = -\ln(1-\mu_t(1+\varepsilon))/u(1+\varepsilon)$; recall that for complex $\ell = |\ell|e^{i\lambda}$ one has $\ln(\ell) = \ln(|\ell|)+i\lambda$, as used in Fig. 2.

[c] The operation $\circ_T$ is defined via $(\mu_1,c_1)\circ_T(\mu_2,c_2) := (\mu_1+\mu_2-\mu_1\mu_2(1+\varepsilon), c_1c_2)$.

[d] A closed subsemigroup $\mathbf{S}\subseteq\mathcal{B}(\mathcal{Z})$ with Lie wedge $\mathsf{L}(\mathbf{S})$ is *exponential* and *weakly exponential* if $\mathbf{S} = \exp(\mathsf{L}(\mathbf{S}))$ and $\mathbf{S} = \overline{\exp(\mathsf{L}(\mathbf{S}))}$, respectively. It is *locally exponential* if there exists a id-neighbourhood basis w.r.t. $\mathbf{S}$ consisting of exponential subsets, both being detailed in [44, 27], refer also to footnote 3e. Note that $\mathsf{MTO}(H_0,T)$ is actually exponential once the closure in Eq. (8) is taken with respect to $\mathsf{GL}(\mathcal{Z})$.

[e] Commutativity is lost for different temperatures, see the comment in App. E.

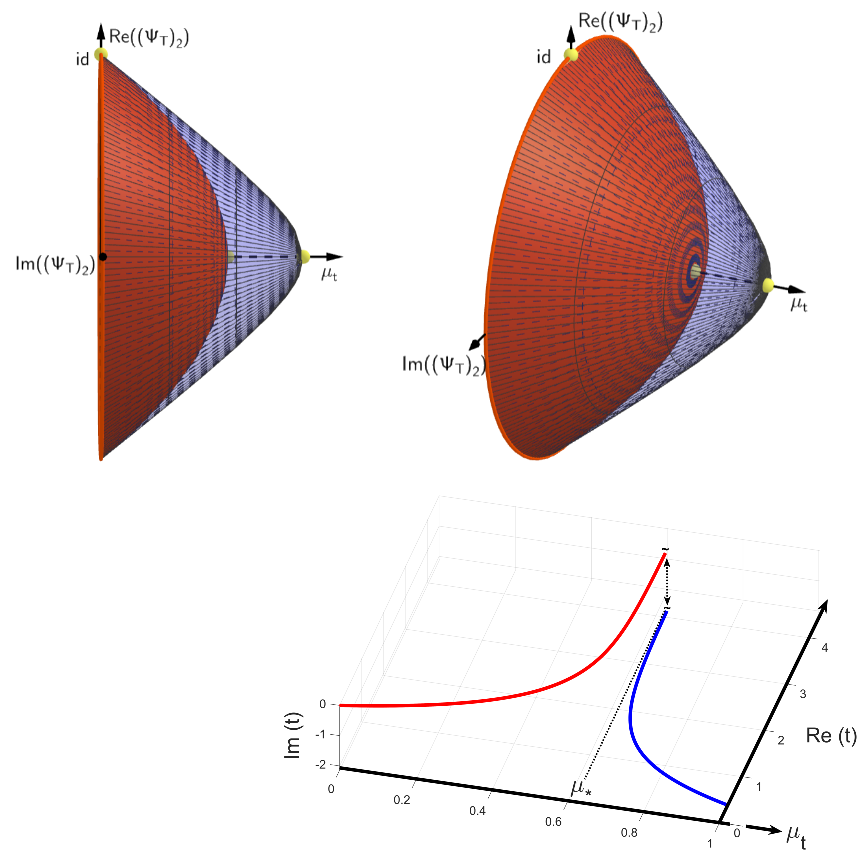

Fig. 2: (Colour online). Upper panels: Two aspect angles for the graphs of Ψ_T (with $\varepsilon = 0.6$) when restricting the domain to $\overline{\mathsf{TO}(H_0, T)}$ (blue cone), and its Markovian counterpart $\mathsf{MTO}(H_0, T)$ (orange cone), respectively. The yellow "tip" of the blue (orange) cone corresponds to the respective β-swaps (the "thermal reset" map $\rho \mapsto \rho_{\mathsf{Gibbs}}(H_0, T)$). — Lower panel: The time dependence in μ_t formally leads to a time in multiples of the scaling factor $u > 0$ of $t[u]$, which is real in the Markovian segment $0 \leq \mu_t \leq \mu_*$, i.e. up to the pole at μ_* and complex in the non-Markovian segment $\mu_* < \mu_t \leq 1$ as detailed in the text. The critical $\mu_* \in [\frac{1}{2}, 1]$ tends to one as $T \to 0^+$, thus illustrating $\mathsf{MTO}(H_0, T) \to \overline{\mathsf{TO}(H_0, T)}$ in the zero-temperature limit.

To sum up, the worked example discussed here also elucidated that the *single-qubit case* is special in as much as

(1) For fixed temperature T (and for the union over all T) $\mathsf{MTO}(H_0, T)$ (resp. $\mathsf{MTO}(H_0)$) are generated by Lie semialgebras, respectively.

(2) So here time-independent and time-dependent Markovianity coincide.

(3) In the zero-temperature limit, Markovian thermal operations even exhaust all thermal operations: $\mathsf{MTO}(H_0, T) \to \overline{\mathsf{TO}(H_0, T)}$ as $T \to 0^+$.

Due to statement (2) throughout this example we have been using the term "Markovian" without further specification.

To avoid misunderstandings, let us emphasise that in the *general case* (i.e. beyond single qubits) one has the following: (1) For fixed temperature T (and for the union over all T) $\mathsf{MTO}(H_0, T)$ (resp. $\mathsf{MTO}(H_0)$) need *not* be generated by Lie semialgebras. (2) Hence time-independent and time-dependent Markovianity need *not* coincide in general. (3) In the zero-temperature limit, the relation between Markovian thermal operations $\mathsf{MTO}(H_0, T)$ and thermal operations $\overline{\mathsf{TO}(H_0, T)}$ is an open problem.

3.3. The Role of d-Majorisation and the Associated Polytope

Let us return to the characterisation of state transitions via (enhanced) thermal operations for the case of non-degenerate H_0 and quasi-classical initial states ρ, i.e. $[\rho, H_0] = 0$. In this case ρ is diagonal in some basis which diagonalises H_0 so w.l.o.g. $\rho = \operatorname{diag}(y)$, $H_0 = \operatorname{diag}(E_i)_{i=1}^n$. It follows

$$M_{H_0,T}(\operatorname{diag}(y)) = \big\{ \operatorname{diag}(Ay) : A \in \mathbb{R}^{n\times n} \text{ Gibbs-stochastic} \big\} ,$$

where $\subseteq$ is due to Cor. 2 and $\supseteq$ is shown in [79] (cf. also [91]). Recall that $A \in \mathbb{R}^{n\times n}$ is called *Gibbs-stochastic* if A is column-stochastic ($a_{ij} \geq 0$ for all i, j and all columns of A sum up to 1) and the Gibbs-vector $d := (e^{-E_i/T})_{i=1}^n$ is a fixed point of A, that is $Ad = d$ [61]. In the mathematics literature such a matrix is called *d-stochastic* [66, Ch. 14.B] which motivates defining

$$M_d(y) := \big\{ Ay : A \in \mathbb{R}^{n\times n} \; d\text{-stochastic} \big\}$$

as *all diagonals of states* one can thermodynamically generate (i.e. by $\overline{\mathsf{TO}}$ and hence by EnTO or of course by Gibbs) starting from $\operatorname{diag}(y)$. In other words the diagonal action of every Gibbs-preserving map (when projecting onto the diagonal) is a d-stochastic matrix, and every d-stochastic matrix is the diagonal action of some element of $\overline{\mathsf{TO}}$. The object $M_d(y)$ is known as *d-majorisation polytope* [89]. Note that in the high-temperature limit d becomes the vector of equal weights $\frac{1}{n}(1, \ldots, 1)^\top$ which recovers the concept of doubly stochastic matrices, leading back to classical majorisation [66, Ch. 2.B].

There are several ways to characterise the conditions for a d-stochastic matrix to exist so that it maps one real vector to another. Thus let us start with the most common one in the physics literature originally defined by Horodecki and Oppenheim [46]: given any vector of Gibbs weights $d \in \mathbb{R}^n$

with $d > 0$ as well as some $y \in \mathbb{R}^n$, the *thermomajorisation curve of* y is defined to be the piecewise linear, continuous curve fully characterised by the elbow points $\{\big(\sum_{i=1}^j d_{\pi(i)}, \sum_{i=1}^j y_{\pi(j)}\big)\}_{j=0}^n$. Here, $\pi \in S_n$ is any permutation such that $\frac{y_{\pi(1)}}{d_{\pi(1)}} \geq \ldots \geq \frac{y_{\pi(n)}}{d_{\pi(n)}}$. Equivalently [89, Rem. 7], this map—which we denote by $\mathsf{th}_{d,y} : [0, \mathbb{e}^\top d] \to \mathbb{R}$ where $\mathbb{e} := (1, \ldots, 1)^\top$—satisfies

$$\mathsf{th}_{d,y}(c) = \min_{\{i=1,\ldots,n\,:\,d_i>0\}} \Big(\Big(\sum_{j=1}^n \max\Big\{y_j - \frac{y_i}{d_i}d_j, 0\Big\}\Big) + \frac{y_i}{d_i}c\Big)$$

for all $c \in [0, \mathbb{e}^\top d]$. Together with [89, Prop. 1] one thus gets:

Proposition 4. *Let $x, y, d \in \mathbb{R}^n$ with $d > 0$ be given. The following statements are equivalent:*

(i) There exists a d-stochastic matrix $A \in \mathbb{R}^{n\times n}$ such that $Ay = x$. We denote this by $x \prec_d y$ and say that x is d-majorised *by y.*

(ii) $\mathbb{e}^\top x = \mathbb{e}^\top y$ and $\mathsf{th}_{d,x}(c) \leq \mathsf{th}_{d,y}(c)$ for all $c \in [0, \mathbb{e}^\top d]$.

(iii) $\mathbb{e}^\top x = \mathbb{e}^\top y$, and for all $j = 1, \ldots, n-1$

$$\sum_{i=1}^j x_{\pi(i)} = \mathsf{th}_{d,x}\Big(\sum_{i=1}^j d_{\pi(i)}\Big) \leq \mathsf{th}_{d,y}\Big(\sum_{i=1}^j d_{\pi(i)}\Big)$$

if $\pi \in S_n$ is any permutation such that $\frac{x_{\pi(1)}}{d_{\pi(1)}} \geq \ldots \geq \frac{x_{\pi(n)}}{d_{\pi(n)}}$.

(iv) $\mathbb{e}^\top x = \mathbb{e}^\top y$ and $\|d_i x - y_i d\|_1 \leq \|d_i y - y_i d\|_1$ for all $i = 1, \ldots, n$ where $\|\cdot\|_1$ is the usual vector 1-norm.

Moreover, if $H_0 \in i\mathfrak{u}(n)$, $T \in (0, \infty]$ are such that H_0 is non-degenerate and d is the vector of Gibbs weights w.r.t. H_0 and T, then the above conditions are equivalent to $\operatorname{diag}(y)$ *thermomajorising* $\operatorname{diag}(x)$ *w.r.t. H_0 and T.*

Interestingly, above characterisations extend to the case where entries of the d-vector are allowed to be zero[3m]. While (iv) $\Rightarrow$ (i) is usually proven indirectly via Farkas' Lemma [77, Cor. 7.1.d] there also exists a constructive algorithm which translates two comparable thermomajorisation curves into a d-stochastic transition matrix [79]. Notably this procedure simplifies considerably if the final state is an extreme point of the d-majorisation polytope induced by the initial state [2, 91]. Either way this leads to the following characterisation of the thermomajorisation polytope [89, Thm. 10]:

$$M_d(y) = \big\{x \in \mathbb{R}^n : \mathbb{e}^\top x = \mathbb{e}^\top y \quad \wedge \quad \forall_{m\in\{0,1\}^n}\ m^\top x \leq \mathsf{th}_{d,y}(m^\top d)\big\}$$

[3m]More precisely Prop. 4 continues to hold if the background temperature equals zero and if the system's ground state energy is non-degenerate [91].

This finally justifies calling $M_d(y)$ a polytope because any bounded set which is the intersection of finitely many halfspaces is a convex polytope. From a geometric point of view, the facets of the polytope $M_d(y)$ have universal orientation given by $m^\top$, whereas their location defined by $\mathsf{th}_{d,y}(m^\top d)$ depends on y and d. In particular, $M_d(y)$ being a convex polytope means it has a finite number of extreme points which in turn generate $M_d(y)$ via the convex hull, cf. [39, Ch. 3]. Remarkably, these can even be computed analytically [62, 2, 89]: given $d, y \in \mathbb{R}^n$ with $d \geq 0$ define the extreme point map $E_{d,y} : S_n \to \mathbb{R}^n$ on the permutation group S_n via

$$E_{d,y}(\sigma) := \Big(\mathsf{th}_{d,y}\Big(\sum_{i=1}^{\sigma^{-1}(j)} d_{\sigma(i)}\Big) - \mathsf{th}_{d,y}\Big(\sum_{i=1}^{\sigma^{-1}(j)-1} d_{\sigma(i)}\Big)\Big)_{j=1}^{n}.$$

For computing the corners of $M_d(y)$, in practice one has to go through all permutations $\sigma \in S_n$, find the value of the thermomajorisation curve for the inputs $d_{\sigma(1)}, d_{\sigma(1)} + d_{\sigma(2)}, \ldots, \sum_{i=1}^{n-1} d_{\sigma(i)}$, and finally arrange the consecutive differences into a vector ordered according to σ. This procedure turns out to be quite simple as is nicely illustrated by a straightforward qutrit example, cf. [91, Example 1]. Interestingly, said example also shows that there exists an extreme point (corresponding to the trivial permutation) which is maximal in the polytope in the sense that it majorises all other (extreme) points *classically.* For physical systems, this turns out to be a general property which will be the key to upper bounding the reachable sets in Sec. 4.

Theorem 3. *Let $y, d \in \mathbb{R}^n$ with $d > 0$ be given. If $y \geq 0$, then $x \prec E_{d,y}(\sigma)$ for all $x \in M_d(y)$ where $\sigma \in S_n$ is any permutation which orders d decreasingly, that is, $d_{\sigma(1)} \geq \ldots \geq d_{\sigma(n)}$. Moreover d and $\frac{E_{d,y}(\sigma)}{d}$ are ordered likewise*[3n]*, and if $y > 0$ then $E_{d,y}(\sigma) > 0$.*

A proof can be found in [89, Thm. 16 & Rem. 3]. Note that the assumption $y \geq 0$ is necessary as a simple counterexample shows [89, Example 4]. Either way, these extreme point techniques break down as soon as one goes beyond quasi-classical states, regardless of whether one considers the action of (enhanced) thermal operations or of general Gibbs-preserving maps. The latter leads to the theory of D-matrix majorisation [87]—where D plays the role of the Gibbs state of the physical system—which is a generalisation of classical majorisation. However, requiring maps to only preserve the Gibbs state dismisses intrinsic thermodynamic symmetries (Prop. 3 (iv)) which is why we will focus on (enhanced) thermal operations in the sequel.

[3n]This means that there exists a permutation $\pi \in S_n$ such that $d_{\pi(1)} \geq \ldots \geq d_{\pi(n)}$ and $\frac{(E_{d,y}(\sigma))_{\pi(1)}}{d_{\pi(1)}} \geq \ldots \geq \frac{(E_{d,y}(\sigma))_{\pi(n)}}{d_{\pi(n)}}$.

4. Thermal Operations in Quantum Control by Example

In this section we specify Markovian control problems (3) by explicitly using Markovian thermal operations as additional control resource in the sense $-\mathbf{\Gamma} \in \mathsf{L}(\overline{\mathsf{TO}(H_0,T)})$. Given a Hamiltonian $H_0 \in i\mathfrak{u}(n)$ with increasing eigenvalues E_k, the corresponding equilibrium state resulting from coupling to a bath of temperature T is $\rho_{\mathsf{Gibbs}} = \frac{e^{-H_0/T}}{\operatorname{tr}(e^{-H_0/T})} \in \mathfrak{pos}_1(n)$ where the eigenvalues of the Gibbs state are collected in the *Gibbs vector*

$$d := \frac{(e^{-E_k/T})_{k=1}^n}{\sum_{k=1}^n e^{-E_k/T}} \in \Delta^{n-1}\,. \tag{18}$$

Here, $\Delta^{n-1} := \{x \in \mathbb{R}^n_+ \,|\, \sum_{i=1}^n x_i = 1\}$ is the collection of all probability vectors, called standard simplex. As shown in [28], ρ_{Gibbs} can then be obtained as the unique fixed point of (1) when choosing the GKSL-terms as

$$V_1 = \sigma_+^d := \sum_{k=1}^{n-1} \sqrt{k(n-k)}\cos(\theta_k)\,|k\rangle\langle k+1| \tag{19}$$

$$V_2 = \sigma_-^d := \sum_{k=1}^{n-1} \sqrt{k(n-k)}\sin(\theta_k)\,|k+1\rangle\langle k|\,, \tag{20}$$

where $|k\rangle$ is "the" eigenvector of H_0 to the eigenvalue E_k and

$$\theta_k := \arccos\Big(\big(1+\frac{d_{k+1}}{d_k}\big)^{-\frac12}\Big) \in \Big(0, \frac{\pi}{4}\Big]. \tag{21}$$

Assuming non-degenerate spectrum of H_0, the limiting cases of zero and infinite temperature can be included:

- Taking the limit $T \to 0^+$ yields $d = (1,0,\ldots,0)^\top$, $\theta_k \to \arccos(1) = 0$ for all k, as well as $\sigma_+^d \to \sigma_+ = \sum_{k=1}^{n-1}\sqrt{k(n-k)}|k\rangle\langle k+1|$ and $\sigma_-^d \to 0$.
- The limit $T \to \infty$ yields $d = \frac{1}{n}(1,\ldots,1)^\top$ so $\theta_k = \frac{\pi}{4}$, i.e. $\cos(\theta_k) = \sin(\theta_k) = \frac{1}{\sqrt{2}}$.

Confining ourselves to σ_+^d and σ_-^d with their non-zero entries on the first off-diagonals is in accordance with the common dipolar selection rules allowing for "one-quantum transitions" (as governed by Wigner's $3j$-symbol) [97, p. 185 ff.]. This is further motivated by the fact that for spin systems these generators yield dynamics within the thermal operations:

Corollary 4. *Let $\Delta E > 0$, $n \in \mathbb{N}$, and $T > 0$ be given. Defining the system's Hamiltonian $H_0 := \operatorname{diag}(0,\ldots,n-1)\cdot\Delta E$ as well as $\mathbf{\Gamma}_d := \mathbf{\Gamma}_{\sigma_+^d} + \mathbf{\Gamma}_{\sigma_-^d}$ the generator induced by Eqs. (19) & (20) via Eq. (2), one finds the inclusion $(e^{-t(i\,\mathrm{ad}_H + \mathbf{\Gamma}_d)})_{t\ge 0} \subseteq \overline{\mathsf{TO}(H_0,T)}$ for all $H \in i\mathfrak{u}(n)$ such that $[H,H_0]=0$.*

Proof. We apply Thm. 2 with $m = 2$, $H_B = \mathrm{diag}(0, 1) \cdot \Delta E$, and

$$H_{\mathsf{tot}} := \sum_{j=1}^{n-1} \sqrt{\frac{j(n-j)}{1+e^{-\Delta E/T}}} \big(|e_j\rangle\langle e_{j+1}| \otimes |e_2\rangle\langle e_1| + |e_{j+1}\rangle\langle e_j| \otimes |e_1\rangle\langle e_2|\big)\,.$$

We may do so because H_{tot} commutes with $H_0 \otimes \mathbb{1} + \mathbb{1} \otimes H_B$ as can be seen easily. Now, said theorem guarantees that the dynamical semigroup generated by $-i\,\mathrm{ad}_H - \sum_{j,\ell=1}^{2} \mathbf{\Gamma}_{V_{j\ell}}$ with $V_{j\ell} = \sqrt{e^{-E'_j/T}}\,\mathrm{tr}_{|g_j\rangle\langle g_\ell|}(H_{\mathsf{tot}})$ is in $\overline{\mathsf{TO}(H_0, T)}$. But $V_{11} = V_{22} = 0$ and

$$V_{12} = \mathrm{tr}_{|e_1\rangle\langle e_2|}(H_{\mathsf{tot}}) = \sum_{j=1}^{n-1} \sqrt{\frac{j(n-j)}{1+e^{-\Delta E/T}}} |e_j\rangle\langle e_{j+1}|$$

$$V_{21} = \sqrt{e^{-\Delta E/T}}\,\mathrm{tr}_{|e_2\rangle\langle e_1|}(H_{\mathsf{tot}}) = \sum_{j=1}^{n-1} \sqrt{\frac{j(n-j)e^{-\Delta E/T}}{1+e^{-\Delta E/T}}} |e_{j+1}\rangle\langle e_j|\,,$$

that is, $V_{12} = \sigma_+^d$ and $V_{21} = \sigma_-^d$. This concludes the proof. □

Remark 5. The assumption in Cor. 4 that H_0 has equidistant eigenvalues is necessary since otherwise the generator $\mathbf{\Gamma}_d$ building simply on Eqs. (19) and (20) is no longer in $\mathsf{L}(\overline{\mathsf{EnTO}(H_0, T)})$ for any $T > 0$ (due to $[\mathbf{\Gamma}_d, \mathrm{ad}_{H_0}] \neq 0$)[4a] so it in particular cannot be in $\mathsf{L}(\overline{\mathsf{TO}(H_0, T)})$ anymore. — In the non-equidistant case one just has to replace the simple uniform σ_+^d of Eq. (19) accordingly by a family $\sigma_{+,1}^d, \ldots, \sigma_{+,l}^d$ ($l \geq 2$) such that the non-zero entries of $V_{+,l}$ correspond to the neighbouring levels of H_0 of a certain energy distance (and similarly for σ_-^d) to ensure the resulting $-\mathbf{\Gamma}$ is again in $\mathsf{L}(\overline{\mathsf{TO}(H_0, T)})$.

Considering the standard control system (3) with dissipator $\mathbf{\Gamma}_d$, Cor. 4 shows that if all coherent controls are compatible with the thermodynamic framework from Sec. 3.1., i.e. $[H_0, H_j] = 0$ for all $j = 1, \ldots, m$ (cf. Lem. 1), then the reachable set of this control problem is automatically upper bounded by the future thermal cone defined by Eq. (12). Now the richness thermodynamic control systems have to offer comes from the interplay between thermodynamic dissipation (i.e. $-\mathbf{\Gamma} \in \mathsf{L}(\overline{\mathsf{TO}(H_0, T)})$) and general unitary controls which become an asset due to *not* stabilising H_0. However, this overlap of different categories comes at the expense of making it more difficult to study.

Recalling from Sec. 3.1. that diagonal elements evolve separately from off-diagonal ones under (enhanced) thermal operations, in the next section we study a modified version of control system (3) (with $\mathbf{\Gamma} = \mathbf{\Gamma}_d$ from Cor. 4) focussing on *diagonal states* represented by the standard simplex Δ^{n-1}.

[4a]To see this, let $n \geq 3$ and let $H_0 = \mathrm{diag}(E_1, \ldots, E_n) \in i\mathfrak{u}(n)$, $E_1 \leq \ldots \leq E_n$ such that $E_i - E_{i+1} \neq E_j - E_{j+1}$ for some $i, j \in \{1, \ldots, n-1\}$, $i \neq j$ (i.e. H_0 does not have equidistant eigenvalues). A straightforward computation shows $\langle e_{i+1}, [\mathbf{\Gamma}_d, \mathrm{ad}_{H_0}](|e_i\rangle\langle e_j|)e_{j+1}\rangle \neq 0$.

4.1. Toy Models by Diagonal States

The idea for reducing reachability problems of (finite-dimensional) Markovian open quantum systems to hybrid control systems on the standard simplex of $\mathbb{R}^n$ will be to *only* include unitary controls in the model which do not mix the diagonal and the off-diagonal of any state $\rho(t)$— as the same holds for all thermal operations (Cor. 2). This means we have to restrict the coherent controls to generators of (unitary channels induced by) permutation matrices.

Recalling the bilinear control system (4), now we confine the discussion to $\mathbf{x}(t)$ denoting the vector of diagonal elements of $\rho(t)$ in "the" eigenbasis of H_0. We address a scenario with coherent controls $\{B_j\}_{j=1}^m$ and a *bang-bang switchable* dissipator $B_0 \in \mathsf{L}(\overline{\mathsf{TO}(H_0, T)})$ as motivated by recent experimental progress [43, 95, 16, 93] and used in [7]. The controls of the toy model shall amount to permutation matrices acting instantaneously on the entries of $x(t)$ and a continuous-time one-parameter semigroup $(e^{-tB})_{t\in\mathbb{R}^+}$ of stochastic maps with a unique fixed point d in Δ^{n-1}. As $(e^{-tB})_{t\in\mathbb{R}^+}$ results from the restriction of the bang-bang switchable dissipator B_0, with abuse of notation we will denote its infinitesimal generator by B. The "*equilibrium state*" d is defined in (18) by system parameters and the absolute temperature $T \geq 0$ of an external bath.

These stipulations suggest the following hybrid/impulsive scenario to define the *toy model* Λ_B on $\Delta^{n-1} \subset \mathbb{R}^n$ by

$$\begin{aligned} &\dot{x}(t) = -Bx(t)\,, \quad x(t_k) = \pi_k x_k\,, \quad t \in [t_k, t_{k+1})\,, \\ &x_0 \in \Delta^{n-1}\,, \quad x_{k+1} = e^{-(t_{k+1}-t_k)B} x(t_k)\,, \quad k \geq 0\,. \end{aligned} \tag{22}$$

Furthermore, $0 =: t_0 \leq t_1 \leq t_2 \leq \ldots$ is an arbitrary switching sequence and π_k are arbitrary permutation matrices. Both the switching points and the permutation matrices are regarded as controls for (22). For simplicity, we assume that the switching points do not accumulate on finite intervals. For more details on hybrid/impulsive control systems see, e.g., [57, 59, 3]. The reachable sets of (22)

$$\mathfrak{reach}_{\Lambda_B}(x_0) := \{x(t)\,|\,x(\cdot) \text{ is a solution of (22), } t \geq 0\}$$

allow for the characterisation $\mathfrak{reach}_{\Lambda_B}(x_0) = \mathcal{S}_{\Lambda_B} x_0$, where $\mathcal{S}_{\Lambda_B} \subseteq \mathsf{GL}(n, \mathbb{R})$ is the (1-norm-)contraction semigroup generated by $(e^{-tB})_{t\in\mathbb{R}_+}$ and the set of all permutation matrices π.

Recent Results. For the scenario just specified, the state-of-the-art [28] can be sketched as follows. Take the n-level toy model where the infinitesimal generator results from coupling to a bath of temperature $T \in [0,\infty]$, i.e. one has $B = B(\mathbf{\Gamma}_d)$ with $\mathbf{\Gamma}_d$ from Cor. 4. We denote this particular toy model by $\Lambda_d := \Lambda_{B(\mathbf{\Gamma}_d)}$.

Theorem 4. *The closure of the reachable set of any initial vector $x_0 \in \Delta^{n-1}$ under the dynamics of Λ_{e_1} exhausts the full standard simplex, i.e.*

$$\overline{\mathfrak{reach}_{\Lambda_{e_1}}(x_0)} = \Delta^{n-1}\,.$$

Moving from a single n-level system (qu*d*it) with $x_0 \in \Delta^{n-1}$ to a tensor product of m such n-level systems gives $x_0 \in \Delta^{n^m-1} \subset (\mathbb{R}^n)^{\otimes m}$. If the bath of temperature $T = 0$ is coupled to just one (say the last) of the m qu*d*its, $\mathbf{\Gamma}$ is generated by $V := \mathbb{1}_{n^{m-1}} \otimes \sigma_+$ and one obtains the following generalisation.

Theorem 5. *The statement of Thm. 4 holds analogously for all m-qudit states $x_0 \in \Delta^{n^m-1}$.*

In a first step to generalise the findings from the extreme case $T = 0$ to $T \in (0,\infty]$ we found that general statements about the reachable set of Λ_d can only be made under the following assumption

Assumption A: H_0 has equidistant energy eigenvalues.

In this case we obtained:

Theorem 6. *Assuming **A**, the reachable set of the thermal state d under the dynamics of the toy model Λ_d satisfies $\mathfrak{reach}_{\Lambda_d}(d) \subseteq \{x \in \Delta^{n-1} \,|\, x \prec d\}$, where '$\prec$' refers to classical majorisation. In particular, this is the smallest convex upper bound for the reachable set one can find.*

There are counterexamples to Thm. 6 as soon as H_0 no longer has equidistant eigenvalues [28, Example 3]. This is because assumption **A** is necessary for the dynamics of Λ_d to be thermal operations (see the generalising Rem. 5).

The recent toy-model results of [28] thus extend the diagonal part of the qu*b*it picture (previously analysed in [7]) to n-level systems, and even more generally to systems of m qu*d*its. — Next we explore further generalisations to non-zero temperatures, e.g., by allowing for general initial states x_0 instead of the thermal state d in Thm. 6.

Generalisations. To generalise previous reachability characterisations we use deeper results on d-majorisation (Sec. 3.3.). For the toy-model dynamics one gets:

(1) $e^{-tB}x_0 \in M_d(x_0)$ for all $t \geq 0$;

(2) $M_d(x_0)$ is a convex subset within the simplex Δ^{n-1},

which means the *dissipative time evolution* of any x_0 remains within the convex set of states d-majorised by x_0. Beyond pure dissipative evolution the toy model also allows for permutations π, so one naturally obtains $\mathfrak{reach}_{\Lambda_d}(x_0) = \mathfrak{reach}_{\Lambda_d}(\pi(x_0))$ for all $\pi \in S_n$. Clearly, the simplex region $M_d(x_0)$ intertwines overall permutations π (in the symmetric group S_n) in the sense $\pi\, M_d(x_0) = M_{\pi(d)}(\pi(x_0))$. For the maximally mixed state ($d \simeq \mathbb{e}$) it boils down to permutation invariance under classical majorisation $\pi\, M_{\mathbb{e}}(x_0) = M_{\mathbb{e}}(\pi(x_0)) = M_{\mathbb{e}}(x_0)$. This immediately entails a first generalisation:

Corollary 5 (generalising Thm. 6)**.** *Assuming* ***A*** *those initial states x_0 classically majorised by d (i.e. $x_0 \in M_{\mathbb{e}}(d)$) remain within $M_{\mathbb{e}}(d)$ under the dynamics of the toy model Λ_d. In other words $\overline{\mathfrak{reach}_{\Lambda_d}(x_0)} \subseteq M_{\mathbb{e}}(d)$.*

In turn, this is but a special case of the following generalisation to arbitrary initial states building on some deeper results on d-majorisation (Sec. 3.3.):

Theorem 7. *Invoke assumption* ***A****. For the toy model Λ_d with Gibbs state d corresponding to coupling to a bath of temperature $T \in (0, \infty]$, the reachable set of any $x_0 \in \Delta^{n-1}$ is included in the following convex hull:*

$$\overline{\mathfrak{reach}_{\Lambda_d}(x_0)} \subseteq \operatorname{conv}\big\{\pi(z)\,|\,\pi \in S_n\big\} = M_{\mathbb{e}}(z)\,. \tag{23}$$

Here, z is any element from the "ordered past cone"[4b]

$$\big\{z \in \Delta^{n-1} \,:\, x_0 \prec z \;\wedge\; d \text{ and } \tfrac{z}{d} \text{ are ordered likewise}\big\} \tag{24}$$

which, most importantly, contains an element $z > 0$ whenever $x_0 > 0$.

The idea of the proof of Eq. (23) is to show that the vector field driving the dynamics of Λ_d points *inside* the classical majorisation polytope $M_{\mathbb{e}}(z)$ at each of its $n!$ extreme points $\pi(z)$ with $\pi \in S_n$, see also Fig. 3. Finally, if $x_0 > 0$ then the existence of a vector $z > 0$ in Eq. (24) is due to Thm. 3 (as detailed in the first author's PhD thesis [84, Thm. 5.1.15]).

We emphasise that—while Thm. 6 becomes trivial in the limit $T \to \infty$—Thm. 7 reproduces the known result that in the high-temperature limit the reachable set for unital dynamics is upper bounded by all states classically majorised by the initial state.

Remark 6. One can show that the set (24) of possible extreme points from Thm. 7 used for an upper bound forms a convex polytope. Thus by means of convex optimisation one can find an "optimal" majorisation bound in the sense that z is closest to the fixed point of the dynamics, i.e.[4c] $\|z - d\|_1 =$

[4b]By definition [24, Def. 3] the (unordered) past cone of a vector x_0 is the set of all states *starting from which* one can generate x_0 via doubly-stochastic matrices.

[4c]Of course the 1-norm can be replaced by any other function $f : \Delta^{n-1} \to \mathbb{R}_+$ of interest.

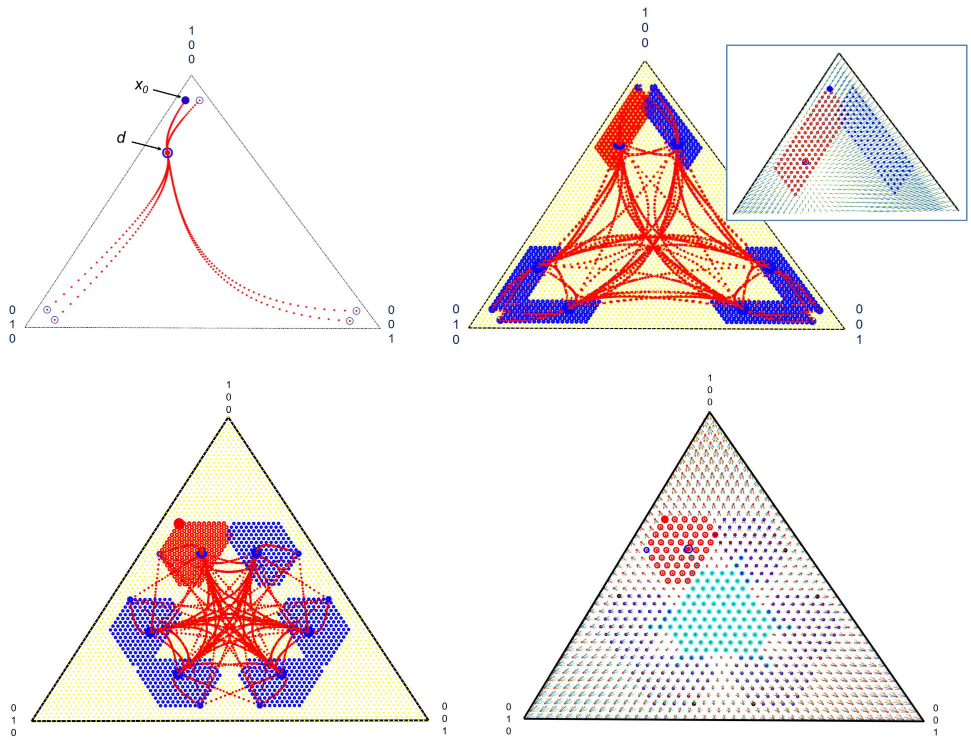

Fig. 3: (Colour online). Upper left: Evolutions of initial $x_0 = (0.9, 0.07, 0.03)^\top$ and permutations $\pi(x_0)$ under $\mathbf{\Gamma}_d$ with V_1, V_2, $\theta = \frac{\pi}{6}$ of Eqs. (19)-(21) drive to fixed point d; upper right panel includes all permutations of trajectories starting with permutations of d, i.e. $x_0 = \pi(d)$; the red region shows states d-majorised by x_0, blue regions are their permutations; the convex hull over red and blue regions contains entire reachable set $\mathfrak{reach}_{\Lambda_d}(x_0)$; inset gives the vector field to the dissipative part of the dynamics.
Lower left: For $\theta = \frac{\pi}{5}$ in (21), as generically, the extreme point $z = (0.65, 0.30, 0.05)^\top$ in red differs from $x_0 = (0.55, 0.40, 0.05)^\top$ as well as from $d = (0.55, 0.29, 0.16)^\top$. The lower right shows the vector fields under the full dynamics Λ_d of dissipation and permutation control with stabilisable points (cp. Sec. 4.2., Fig. 7) in turkish blue.

$\min_{y \in (24)} \|y - d\|_1$. While this is unambiguous if $x_0 \prec d$ or if x_0 is in its own ordered past cone[4d], note that for general $x_0 \in \Delta^{n-1}$ the convex hull of $\overline{\mathfrak{reach}_{\Lambda_d}(x_0)}$ need not be a majorisation polytope anymore.

Fig. 3 illustrates these general findings for the special case of three-level systems (again assuming the drift term H_0 has equidistant eigenvalues).

[4d] If $x_0 \prec d$, then the "optimal" z is d, in the sense that $\operatorname{conv}(\overline{\mathfrak{reach}_{\Lambda_d}(x_0)}) = M_{\mathbb{e}}(d)$: on the one hand $\operatorname{conv}(\overline{\mathfrak{reach}_{\Lambda_d}(x_0)}) \subseteq \operatorname{conv}(M_{\mathbb{e}}(d)) \subseteq M_{\mathbb{e}}(d)$ by Thm. 7 because d is in the ordered past cone of x_0; also $M_{\mathbb{e}}(d) = \operatorname{conv}(\{\pi d : \pi \in S_n\}) \subseteq \operatorname{conv}(\overline{\mathfrak{reach}_{\Lambda_d}(x_0)})$. Similarly one sees that if x_0 is in its own ordered past cone, i.e. d and $\frac{x_0}{d}$ are ordered likewise, then the "optimal" z (as def. above) is x_0 itself.

4.2. Explicit Results and Examples for Qutrits

So far, we have given upper bounds for reachable sets of the toy model. In this section we will explicitly determine the shape of the reachable set and of the set of stabilisable states for the three-dimensional case $d \in \mathbb{R}^3$, $d > 0$. For this we first introduce some general notions.

It pays off to approach the toy model (22) from a different, but equivalent[4e], perspective: instead of letting the permutations act on the states, leading to discontinuous paths, we let the permutations act on the drift vector field, leading to the following differential inclusion[4f], where—in analogy to $\mathfrak{reach}_B(x)$—we write $\mathfrak{derv}(x)$ for the *set of achievable derivatives at* x:

$$\dot{x}(t) \in \operatorname{conv}(\mathfrak{derv}(x(t))), \quad \mathfrak{derv}(x) := \{-\pi B \pi^{-1} x : \pi \in S_n\}, \tag{25}$$

cf. [80][4g] for an introduction to this topic. Many ideas work for any matrix $-B$ which generates a one-parameter semigroup of stochastic matrices and has unique fixed point d, but for some results we will restrict B to the case where the generator is of the form given in Eqs. (19) & (20) and the corresponding Hamiltonian has equidistant energies. This ensures that we obtain sensible formulas, and it is physically motivated, see Rem. 5. As above we call this Assumption **A**.

Stabilisable States. The set of *stabilisable states* $\mathfrak{stab}_B$ is defined to be all $x \in \Delta^{n-1}$ such that $0 \in \operatorname{conv}(\mathfrak{derv}(x))$. Intuitively, these are the points in Δ^{n-1} that, when taken as starting point, one can remain arbitrarily close to. More precisely we have the following result:

Lemma 3. *A state $x_0 \in \Delta^{n-1}$ is stabilisable if and only if for every $\varepsilon > 0$ and $\tau > 0$ there is a solution $x : [0, \tau] \to \Delta^{n-1}$ to* (25) *with $x(0) = x_0$ which remains inside of the ε-ball $B_\varepsilon(x_0) \cap \Delta^{n-1}$.*

Proof. If x_0 is stabilisable, then the constant path $x \equiv x_0$ is a solution to (25). Conversely, assume that x_0 is not stabilisable. Then, by continuity, there is some $\delta > 0$ and some linear functional β on $\mathbb{R}^n$ such that β is less than $-\delta$ on $\mathfrak{derv}(y)$ for all y in some neighborhood of x_0. Hence there is some time $\tau > 0$ where any solution must leave $B_\varepsilon(x_0)$ for some ε small enough. □

[4e]The systems are equivalent in the sense that every solution of one system has a corresponding solution in the other system differing only by some (time-dependent) permutation. Note however that we allow more general controls in the differential inclusion, so that this equivalence is only approximate in general.

[4f]By abuse of notation, $\pi \in S_n$ also denotes the induced permutation matrix.

[4g]In particular Thm. 2.3 therein shows the equivalence of control systems and the corresponding differential inclusions. Note that taking the convex hull leads to a relaxation of the differential inclusion, which is still approximately equivalent to the original control system, see [5, Ch. 2.4, Thm. 2].

Remark 7. It is possible to define a control system on the simplex Δ^{n-1} similar to the toy model (i.e. by projecting (3) onto "the" diagonal) but allowing for the full unitary control of the system given by Eq. (3). In this case there is a characterisation of stabilisability in basic Lie-algebraic terms: Every point in the simplex Δ^{n-1} is stabilisable if and only if all GKSL-terms V_k can be simultaneously (upper) triangularised [65]. By Lie's Theorem, this is equivalent to the V_k generating a solvable Lie algebra. Also be aware of the special cases if all V_k commute, or one just has a single V_k, such as σ_+^d of Eq. (19) in the case $T = 0$ (i.e. $\theta_k = 0$ in (21)). As soon as $T > 0$, however, the situation gets more involved, as the qutrit example below shows.

If zero is not contained in the convex hull of achievable derivatives at x, then there must exist some linear functional α on $\mathbb{R}^n$ which is negative on $\mathfrak{derv}(x)$. Note that while α lives on $\mathbb{R}^n$, only the part parallel to the simplex Δ^{n-1} matters. Based on this observation, the idea is to consider the "permuted" functionals $\alpha_\pi(x) := -\alpha(\pi B \pi^{-1} x)$ because, given any $x \in \Delta^{n-1}$, if there exists α such that $\alpha_\pi(x) < 0$ for all $\pi \in S_n$, then x cannot be stabilisable. Conversely, if x is not stabilisable, then there exists some α for which $\alpha_\pi(x) < 0$ for all $\pi \in S_n$. Obviously, d as well as all permutations of d are stabilisable.

Let us now focus on the three-dimensional case. We will compute a closed curve connecting all these points, which will turn out to be the boundary of the set of stabilisable states: everything (on or) inside the curve will be stabilisable and everything outside will be non-stabilisable—refer to Fig. 5 below for two examples. Let us, e.g., focus on the part of the boundary curve between d and $\tau_{23}\, d$, where τ_{23} is the transposition acting on the second and third element. Note that d and $\tau_{23}\, d$ are located in neighbouring Weyl chambers since the elements in d are always increasing or decreasing. The idea for determining its shape is: for every functional α (in a certain range) one can compute a point $\ker(\alpha_{\mathrm{id}}) \cap \ker(\alpha_{\tau_{23}}) \cap \Delta^2$ with the property that all points in the simplex "above" it cannot be stabilisable as shown in Fig. 4. Moreover, due to Assumption **A**, the curve will always be part of a conic section. To motivate this approach, note that any point x with $\alpha_\pi(x) < 0$ for some α and for all $\pi \in S_n$ in contained in an open neighborhood of non-stabilisable points and hence cannot lie on the boundary. Thus we are looking for points lying in the kernel of at least one of the $\alpha_\pi(x)$. Moreover, we really need to find points lying in the intersection of two such kernels, since otherwise a small perturbation applied to α shows that the point has a non-stabilisable neighborhood.

Let us now invoke Assumption **A** so, w.l.o.g., $H_0 := \mathrm{diag}(-1, 0, 1) \cdot \Delta E$ for some $\Delta E \in \mathbb{R}$, and thus $d = (1, a, a^2)/(1 + a + a^2)$ with $a = e^{-\Delta E/T}$. The generators of our dissipative dynamics (19) & (20) are fully characterised by the (constant) angle $\theta = \arccos(\frac{1}{\sqrt{1+a}})$ in (21). With this, the generator of

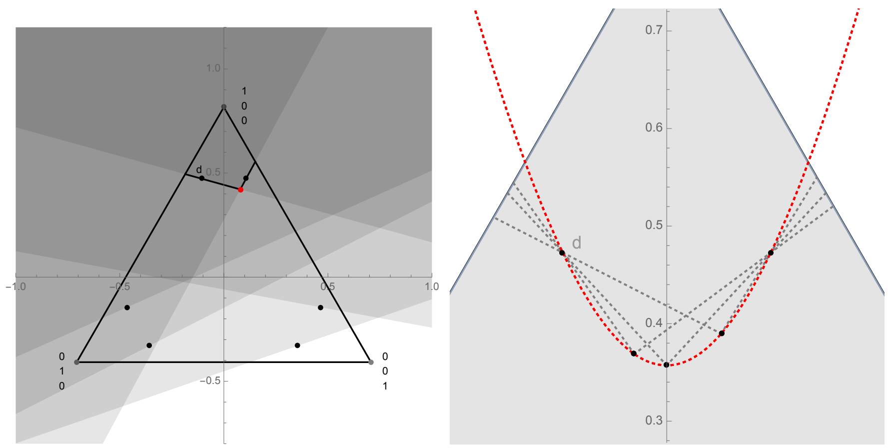

Fig. 4: (Colour online). Illustration of how to construct the boundary curves of the set of stabilisable points in the case of $a = 0.3$. Left: For $\alpha = \begin{pmatrix} 0 & -0.4 & -0.6 \end{pmatrix}$ the shaded regions comprise the points where the functionals α_π are negative; highlighted is the intersection of all the negative regions with the simplex. The points in this region are certainly not stabilisable. In particular the intersection point of $\ker(\alpha_{\mathrm{id}})$ and $\ker(\alpha_{\tau_{23}})$ is marked in red. Right: For three different values of α, parts of $\ker(\alpha_{\mathrm{id}})$ and $\ker(\alpha_{\tau_{23}})$ and their intersections are shown. Taken together, these intersections form the curve given in red, which constitutes a part of the boundary of the set of stabilisable points.

the toy model takes the form (cf. also [28])

$$-B = \frac{2}{1+a} \begin{pmatrix} -a & 1 & 0 \\ a & -1-a & 1 \\ 0 & a & -1 \end{pmatrix} .$$

Let us go through the construction of the curve for the special (parabolic) case[4h] where $a = \frac{1}{4}$. It will turn out that the boundary curve between d and $\tau_{23} d$ is fully determined by the family of functionals[4i] α^λ, $\lambda \in [-\frac{1}{7}, \frac{1}{7}]$ where

$$\alpha^\lambda := -(\tfrac{1}{2} + \lambda) \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} - (\tfrac{1}{2} - \lambda) \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} , \tag{26}$$

[4h] This is the case where the energy gap $|\Delta E| = \ln(4) k_B T$, where we explicitly write the Boltzmann constant k_B.

[4i] Since we only care about the component of the functional parallel to the simplex and since the normalisation does not matter, it suffices to consider a one-parameter family of functionals. The exact parametrisation and parameter range are chosen for ease of computation.

so $\alpha^\lambda(x) = \lambda(x_2 - x_3) - \frac{1}{2}(x_2 + x_3)$ for all $x \in \mathbb{R}^3$. In order to compute $\ker(\alpha^\lambda_{\mathrm{id}}) \cap \ker(\alpha^\lambda_{\tau_{23}}) \cap \Delta^2$ we find that $\alpha^\lambda_{\mathrm{id}} = \alpha^\lambda \circ (-B)$ (up to a global factor, which we may omit because we have to normalise later on anyway) equals

$$-(\tfrac{1}{2} + \lambda)\begin{pmatrix}0 & \tfrac{1}{2} & -2\end{pmatrix} - (\tfrac{1}{2} - \lambda)\begin{pmatrix}\tfrac{1}{2} & -\tfrac{5}{2} & 2\end{pmatrix} = \begin{pmatrix}\tfrac{\lambda}{2} - \tfrac{1}{4} & 1 - 3\lambda & 4\lambda\end{pmatrix}.$$

Also $\alpha^\lambda_{\tau_{23}} = \alpha^{-\lambda}_{\mathrm{id}} \circ \tau_{23}$ is generated by $\begin{pmatrix}-\frac{\lambda}{2} - \frac{1}{4} & -4\lambda & 3\lambda + 1\end{pmatrix}$. With this we compute $\ker(\alpha^\lambda_{\mathrm{id}}) \cap \ker(\alpha^\lambda_{\tau_{23}})$ to be spanned by "the" vector which is orthogonal to the normal vector of both $\alpha^\lambda_{\mathrm{id}}$ and $\alpha^\lambda_{\tau_{23}}$, that is,

$$\begin{pmatrix}\frac{\lambda}{2} - \frac{1}{4} \\ 1 - 3\lambda \\ 4\lambda\end{pmatrix} \times \begin{pmatrix}-\frac{\lambda}{2} - \frac{1}{4} \\ -4\lambda \\ 3\lambda + 1\end{pmatrix} = \begin{pmatrix}1 + 7\lambda^2 \\ -\frac{7}{2}\lambda^2 - \frac{3}{4}\lambda + \frac{1}{4} \\ -\frac{7}{2}\lambda^2 + \frac{3}{4}\lambda + \frac{1}{4}\end{pmatrix}$$

Intersecting the line generated by this vector with the standard simplex only introduces a normalising factor since we have: $\ker(\alpha^\lambda_{\mathrm{id}}) \cap \ker(\alpha^\lambda_{\tau_{23}}) \cap \Delta^2 = \frac{1}{6}(4 + 28\lambda^2, -14\lambda^2 - 3\lambda + 1, -14\lambda^2 + 3\lambda + 1)^\top$. Finally, we reduce the dimensionality of the problem by isometrically embedding[4j] the simplex Δ^2 in $\mathbb{R}^2$; this leads to the (parabolic) boundary curve $(\frac{\lambda}{\sqrt{2}}, \frac{1+14\lambda^2}{\sqrt{6}})$ where $\lambda \in [-\frac{1}{7}, \frac{1}{7}]$.

If $a \neq \frac{1}{4}$ we modify the family of functionals α^λ introduced previously by multiplying λ in (26) by $\frac{1}{2}\sqrt{1 + 2a}|(3 + 2a)(1 - 4a)|^{-1/2}$; however, the idea and the calculations are analogous. In the hyperbolic[4k] case $a > \frac{1}{4}$ the boundary curve can be parametrised via

$$\left(w\frac{-2\lambda}{\lambda^2 - 1}, u\frac{\lambda^2 + 1}{\lambda^2 - 1} + v\right)$$

where

$$v - u = \sqrt{\frac{2}{3}}\frac{1 - a}{1 + 2a}\,,\; u + v = \sqrt{\frac{2}{3}}\frac{1 - a}{1 - 4a}\,,\; w = \frac{\sqrt{2}(1 - a)a}{\sqrt{|(1 + 2a)(3 + 2a)(1 - 4a)|}}\,.$$

For the elliptic case $a \in (0, \frac{1}{4})$ one finds

$$\left(w\frac{2\lambda}{\lambda^2 + 1}, u\frac{\lambda^2 - 1}{\lambda^2 + 1} + v\right).$$

This covers the segment of the curve which connects d and $\tau_{23}d$. For the rest of the boundary curve note that—due to the permutation symmetry—there are only two different curve segments, cf. Fig. 5. We have just computed one of them. The other one is obtained by re-arranging the elements of d in

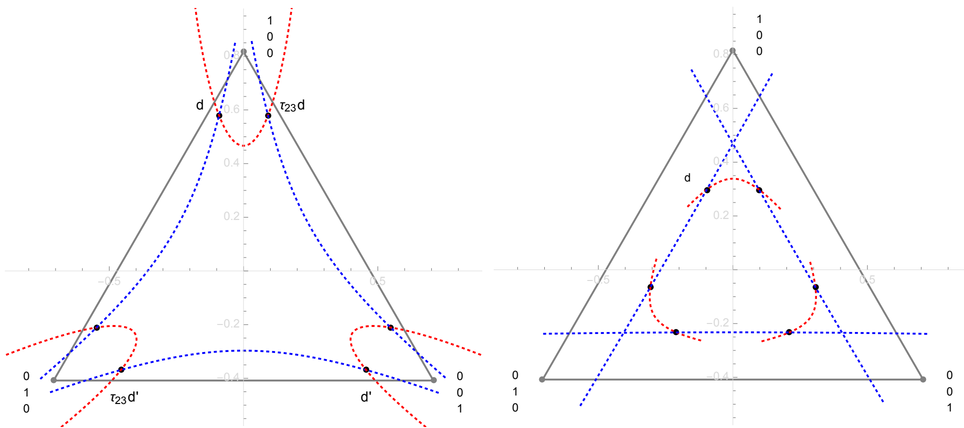

Fig. 5: (Colour online). Left: The set of stabilisable states for the equidistant energy case with $a = \frac{1}{5}$. The set is bounded by six conics and contains the permutations of d. This is the elliptic case, and part of the ellipse is drawn in red, together with its permuted copies. The blue curve is obtained analogously by taking the hyperbolic case $a = 5$ whose fixed point we denote d'. Right: The same approach gives the boundary of the set of stabilisable states for a random generator B numerically. NB: In general the bounding curves need not be conic sections, and one may obtain a convex shape.

reverse order and repeating the calculation. One obtains the same formulas with a replaced by a^{-1}.

We have seen that for each α we obtain an open (convex) region which is certainly not stabilisable. Parametrising α in a circular fashion—i.e. $\alpha \in S^2 \cap \{\mathbb{e}\}^\perp$ in accordance with footnote 4i—shows that this region moves continuously around the simplex, and its closure always touches our closed curve in such a way that each point outside of the curve is part of this region at some point, implying that all these points outside are non-stabilisable.

It remains to be shown that every point on the boundary or enclosed within the boundary curve we just computed can in fact be stabilised. We will only give a hand-wavy explanation; again, each α yields a convex region which is not stabilisable, and which touches our curve in some point. Two cases may occur: Either one of the halfplanes on which some α_π is negative lies outside of the majorisation polytope of d, in which case no point inside our curve is in this halfplane. Otherwise, we are in the case illustrated in

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[4j] As usual this is done using the partial isometry $P = \begin{pmatrix} 0 & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \sqrt{\frac{2}{3}} & \frac{-1}{\sqrt{6}} & \frac{-1}{\sqrt{6}} \end{pmatrix}$.

[4k] The unital scenario $a = 1$ is a special case because then $d = \frac{\mathbb{e}}{3}$, so the set of stabilisable points collapses to $\{\frac{\mathbb{e}}{3}\}$.

Fig. 4. Here the convex region of non-stabilisable points given by α, when intersected with the majorisation polytope of d, is a triangle with vertices given by two permutations of d and some point on our curve. Since the curve is always concave, again no point enclosed by the curve lies in the triangle of non-stabilisable points. The case for arbitrary admissible generators $-B$ in the qutrit case is analogous, but the large number of parameters makes the formulas unwieldy. In higher dimensions, the idea of using the functionals α_π to determine non-stabilisable points still applies, but it is unclear how to analytically compute the resulting shapes of the stabilisable set.

Reachable States. Let us now turn towards the set of reachable states (or, more precisely, its closure) for some given initial state and any stochastic generator matrix $-B$ with unique fixed point $d \in \Delta^{n-1}$, $d > 0$. Let us use the notation $y \twoheadleftarrow x$ to denote that $y \in \overline{\mathfrak{reach}_B(x)}$. Then $\twoheadleftarrow$ is a preorder and so it induces an equivalence relation $\sim$ on which it becomes a partial order. In other words, $x \sim y$ if and only if $x \in \overline{\mathfrak{reach}_B(y)}$ and $y \in \overline{\mathfrak{reach}_B(x)}$ meaning there exists an approximately periodic solution through x and y. Note that up to a viability condition, the equivalence classes $[x]$ of this equivalence relation correspond to *control sets* as defined in [19, Def. 3.1.2], and the induced partial order corresponds to the *reachability order* [19, Def. 3.1.7].

First we observe that the maximally mixed state can always be reached:

Lemma 4. *For all $x \in \Delta^{n-1}$, the vectors d and $\frac{1}{n}\mathbb{e}$ are in $\overline{\mathfrak{reach}_B(x)}$.*

Proof. Since d is the unique fixed point of e^{-tB} for $t > 0$, and since it is attractive[41], $d \twoheadleftarrow x$ for all $x \in \Delta^{n-1}$. Similarly, consider $\hat{B} = \frac{1}{n!}\sum_{\pi\in S_n} \pi B \pi^{-1}$. Then $\hat{B}$ is invariant under permutations, which implies that $\hat{B}\mathbb{e} = 0$. Moreover $\frac{1}{n}\mathbb{e}$ is the unique fixed point in Δ^{n-1} since otherwise, by permutation symmetry there would be an open set of fixed points in Δ^{n-1}, and hence $\hat{B} \equiv 0$. This would imply that $B \equiv 0$ as one can check by considering the value of $\hat{B}$ at the vertices of Δ^{n-1}. As before, the fixed point $\frac{1}{n}\mathbb{e}$ of $\hat{B}$ is attractive. □

This lemma shows $d \sim \frac{1}{n}\mathbb{e}$, and that the equivalence class $[d] = [\frac{1}{n}\mathbb{e}]$ is an invariant control set as defined in [19, Def. 3.1.3].

Let us now, again, restrict to the three-dimensional case. It turns out that this equivalence class is the only one that contains more than a single point: the idea is that equivalence classes with at least two points lead to

[41]This follows from a basic result on continuous-time Markov chains. Here $-B$ is the transition rate matrix. It is irreducible (in the sense of [69, p. 111]) since $d > 0$ is the unique fixed point. Then [69, Thm. 3.6.2] shows that the corresponding Markov chain is ergodic, i.e. the unique fixed point is attractive.

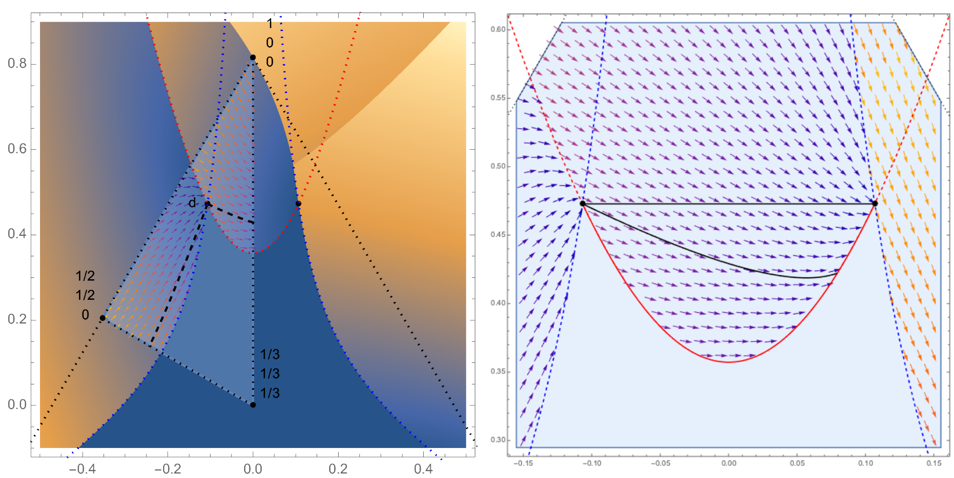

Fig. 6: (Colour online). Left: The left extremal vector field in the case $a = 0.3$ depicted in the indicated Weyl chamber. The vector field is undefined on the stabilisable set, and hence this yields another way to compute the set of stabilisable points. We plotted again the bounding conics of the stabilisable set and the trajectories bounding the reachable set $\overline{\mathfrak{reach}_B(d)}$. In this case the boundary trajectories are obtained by starting at d and permuting B such that one of the neighbours of d is the unique fixed point. The background colors show the norm of the left extremal vector field, and its discontinuities are clearly visible. Right: A zoomed-in picture of the "D"-shaped region considered in the proof of Lem. 7 again with parameter $a = 0.3$.

(approximately) periodic solutions which must enclose a stabilisable point. Since the set of non-stabilsable points is simply connected, when restricting to a Weyl chamber the periodic solution intersects the set of stabilisable states, which are all equivalent to $\frac{1}{3}\mathbb{e}$. A proof can be found in App. D.

For any non-stabilisable state x, it holds that the convex cone generated by $\mathfrak{derv}(x)$ is pointed (i.e. its edge is a point). Hence there are two extremal derivatives at the boundary of the cone, which we will call the left and right extremal derivatives, as seen from x. The resulting extremal vector fields are depicted in Fig. 6. More precisely we have the following result.

Lemma 5. *On the set* $\Delta^2 \setminus \operatorname{int}(\mathfrak{stab}_B)$ *there exist left and right extremal vector fields. The norm of these vector fields might not be continuous, but the direction field is locally Lipschitz continuous, except possibly at* d *(and its permutations).*

Proof. As already mentioned, for any non-stabilisable point x, the convex cone generated by $\mathfrak{derv}(x)$ is pointed. On the other hand, if for some x

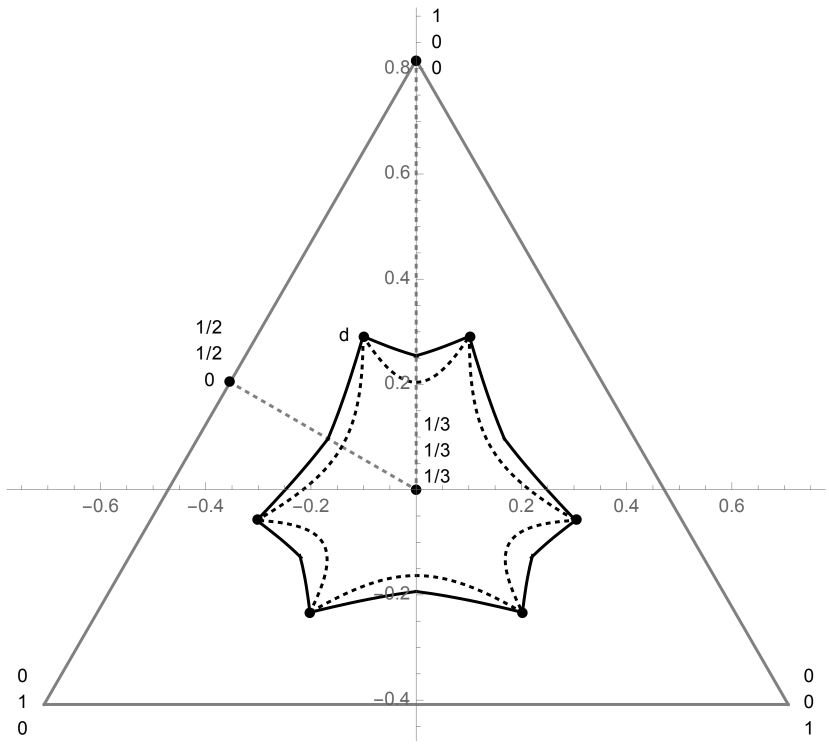

Fig. 7: The boundary of the reachable set $\overline{\mathfrak{reach}_B(d)}$ in the case $a = 0.5$ is shown with solid lines, and the boundary of the stabilisable set $\mathfrak{stab}_B$ is shown using dotted lines (cp. Fig. 3). NB: The curve segments of the boundary of the reachable set are not straight, though the curvatures are hardly visible.

the convex cone is the plane, then x is in the interior of the stabilisable set. Hence on the boundary of the stabilisable set, the convex cone is either pointed or a half space. Either way there is a well defined left and right extremal derivative, and so the corresponding vector fields are well-defined. Locally, for $x \neq \pi d$ the direction field can be seen as a maximum of finitely many smooth functions, and hence it is locally Lipschitz continuous. □

The discontinuities in the norm are important, as they tell us when the control permutation has to be applied. The shapes of these discontinuities are non-trivial, and we show an example in Fig. 6.

Now the boundary of the reachable set can be computed using solutions following the left and right extremal derivatives. By the previous lemma these solutions exist and are unique. See again Fig. 6 as well as Fig. 7. Note that the extremal vector fields never vanish where they are defined, and since they are defined on a contractible domain (if restricted to a Weyl chamber) there are no periodic solutions. This relies on the fact that the state space is two dimensional, see for instance [82, Thm. 6.8.2]. Moreover, given a left (right) extremal solution, another solution can only cross it from left to right (right to left); this can be shown as in the proof of [80, Thm. 5.6].

Before we can prove this section's main result we need the following topological result about reachable sets:

Lemma 6. *Let any $x \in \Delta^2$ be given. Then $\overline{\mathfrak{reach}_B(x)}$ is contractible.*

Proof. Consider the map $F : \overline{\mathfrak{reach}_B(x)} \times [0,1] \to \overline{\mathfrak{reach}_B(x)}$ defined by

$$F(y,t) = \begin{cases} e^{-\hat{B}f(t)}y & \text{if } t < 1 \\ \frac{1}{3}\mathbb{e} & \text{else,} \end{cases}$$

where $\hat{B}$ is defined as in the proof of Lem. 4 and $f : [0,1) \to [0,\infty)$ is any homeomorphism. It follows from the same lemma that F is continuous, and hence a (strong) deformation retraction. □

Lemma 7. *Invoke Assumption* ***A*** *and further assume that $d \in \Delta^2_\downarrow$ where $\Delta^2_\downarrow$ denotes the ordered Weyl chamber of the simplex. The left extremal solution starting from d lies in the complement of the interior of the stabilisable region and terminates in the boundary of the Weyl chamber in finite time, without leaving the (classical) majorisation polytope of d. The analogous result holds for the right extremal solution.*

Proof. From Cor. 5 we know that the left extremal solution remains in the majorisation polytope of d. Let us sketch why this solution cannot enter the set of stabilisable points in $\Delta^2_\downarrow$. Consider the connected region containing d and $\tau_{23}d$ which is bounded by the majorisation polytope and the set of stabilisable points, and is shaped like a "D" lying on its belly, so let's call it D, see right panel of Fig. 6.

First note that since there are no fixed points in D, every solution reaches the boundary of D in finite time, and by the above it reaches the curved part of the boundary of D. Now consider the straight part of the boundary, between d and $\tau_{23}d$. The solutions starting from points close to $\tau_{23}d$ will reach the curved boundary of D on the right side. Hence by continuity all points on the straight part of the boundary have solutions ending up on a connected part of the curved boundary. However, as we have seen before, on the boundary of the set of stabilisable points, the cone generated by the achievable derivatives is a half plane, and hence the left and right extremal vector fields point in opposite directions. Therefore in general only one kind of solution can terminate in each point. By symmetry and the above connectedness, all left extremal solutions must terminate on the right side of D, and analogously for the right extremal solution. As noted above, no solution can leave the region delimited by the extremal solutions. □

Theorem 8. *The left and right extremal solutions starting at d separate the Weyl chamber into two parts, and the inner part containing $\frac{1}{3}\mathbb{e}$ equals the intersection of $\overline{\mathfrak{reach}_B(d)} = [d]$ with $\Delta^2_\downarrow$.*

Proof. Taking the extremal solutions in the ordered Weyl chamber and all of the permuted copies yields a closed curve surrounding and contained in $\overline{\mathfrak{reach}_B(d)}$, i.e. they form the "outer boundary" of the reachable set. By Lem. 6 $\overline{\mathfrak{reach}_B(d)}$ is contractible, hence it is equal to the region enclosed by this curve. □

Corollary 6. *For every $x \in \mathfrak{stab}_B$ it holds that $x \sim d$.*

Proof. By Lem. 4 it holds that $d \twoheadleftarrow x$. Thm. 8 shows that $\overline{\mathfrak{reach}_B(d)}$ is the set enclosed by the left and right extremal solutions (and their permuted copies) starting at d and ending in the boundary of the Weyl chamber. Moreover Lem. 7 shows that this set contains $\mathfrak{stab}_B$ and hence $x \twoheadleftarrow d$. □

For starting points other than d, a similar result holds.

Corollary 7. *For any point x outside of $[d]$, we can compute the boundary of $\overline{\mathfrak{reach}_B(x)}$ in $\Delta^2_\downarrow$ by following the left and right extremal solutions until we hit either the boundary of the Weyl chamber or $[d]$. Moreover, the left extremal solution can only terminate in the right boundary of the Weyl chamber or in the left boundary of $[d]$ and vice-versa.*

Proof. Since $d > 0$ no solution tends to the boundary of the simplex. Hence the left and right extremal solutions must terminate in the boundary of the Weyl chamber or of $[d]$. The fact that the left extremal solution can only terminate in the right boundary of the Weyl chamber or in the left boundary of $[d]$ follows from the fact that integral curves do not intersect and the fact that on the symmetry lines of the simplex, the cone of achievable derivatives opens towards $\frac{1}{3}\mathbb{e}$. □

The more general case[4m] of B *not* satisfying Assumption **A** can be treated with similar methods. Note, however, that many of our arguments rely on the fact that the state space is two dimensional, and hence it is not clear how to analytically determine stabilisable and reachable sets in higher dimensions.

[4m] cp. also Rem. 5

5. Conclusions

We have analysed quantum control systems with thermal resources, where one combines coherent unitary controls with a switchable coupling to a thermal bath as additional control. To this end, we have characterised (the closure of) thermal operations ($\overline{\mathsf{TO}}$), enhanced thermal operations (EnTO), as well as Gibbs-preserving maps (Gibbs) within the framework of Lie-semigroup theory. Thereby we could determine (up to Conj. 1) the structure of the respective semigroups, their Lie wedges as well as their edges. It is important to note that the Lie wedges in turn *define* the corresponding *Markovian* counterparts as the corresponding *Lie semigroups*, to wit MTO, MEnTO, MGibbs. A worked qubit example illustrates how Markovian thermal operations sit inside all thermal operations by means of an explicit parametrisation. In case of single qubits the Markovian thermal operations MTO even exhaust the entire set of thermal operations $\overline{\mathsf{TO}}$ in the zero-temperature limit. On a general scale, Thm. 2 provides an explicit construction for (possibly all) generators of Markovian thermal operations via temperature-weighted projections out of a total Hamiltonian (preserving energy of system and bath) in the Stinespring dilation.

In view of studying reachable sets, the semigroup techniques naturally match with general concepts of majorisation (d-majorisation). For the evolution of diagonal states under such controlled Markovian dynamics, we have upper bounded the reachable sets by inclusions within the standard simplex Δ^{n-1}: they can readily be given in terms of the convex hull of extreme points of the d-majorisation polytope. — Finally, for the qutrit case, we have explicitly determined and illustrated the geometry of both, the reachable set and the stabilisable set by techniques of differential inclusion.

6. Outlook

There are several ways to generalise the toy model with all permutations as controls plus a specific generator of a one-parameter semigroup of thermal operations:

First one may define again a reduced control system still on the simplex, but now encapsulating the entire unitary control. While our results for $T = 0$ (Thms. 4 & 5) immediately carry over into this generalisation[6a], it is not obvious how to adapt our upper bounds (Thm. 7) and if analytic solutions in the three-dimensional case (Sec. 4.2.) are still obtainable. Studying the interplay between Markovian operations and general unitary dynamics will be the subject of future work [65].

[6a] see also [84, Cor. 5.1.12]

Next one could allow for arbitrary Markovian thermal operations together with all unitary maps—the generated semigroup of which we denote by $\mathsf{MTO_U}(H_0,T)$ ($\mathsf{MTO_U}$ in abuse of notation)—and ask for best approximations to the corresponding reachable sets given by the semigroup orbit $\mathsf{MTO_U}(\rho_0)$, or analogously $\mathsf{MEnTO_U}(\rho_0)$ or $\mathsf{MGibbs_U}(\rho_0)$ on a general scale. For non-zero temperatures, this question boils down to feasible state transfers under $\mathsf{MTO}(H_0,T)$ beyond the simple bath dynamics of Cor. 4. Such a setting would generalise [64] which itself characterised the reachable set $\mathsf{MEnTO}(\rho_0)$ [6b] for ρ_0 quasi-classical and led to a "Markovian" generalisation of d-majorisation.

Finally lifting considerations to the operator level, the single-qubit observation in this work that in the zero-temperature limit *Markovian* thermal operations converge to general thermal operations $\mathsf{MTO}(H_0,T) \to \overline{\mathsf{TO}(H_0,T)}$ begs the question what happens in the general case with $\mathsf{MTO}(H_0,T)$ as $T \to 0^+$. — Beyond Markovianity, in analogy to above take $\overline{\mathsf{TO}}_\mathsf{U}(H_0,T)$ (again $\overline{\mathsf{TO}}_\mathsf{U}$ for short) as the smallest semigroup now embracing all unitary operations as well as all thermal operations $\overline{\mathsf{TO}(H_0,T)}$. While the reachable sets $\overline{\mathsf{TO}}_\mathsf{U}(\rho_0)$ are known[6c] (also see the first teaser of the introduction), $\overline{\mathsf{TO}}_\mathsf{U}$ is not yet explored on the level of quantum maps either.

All these generalisations would help to understand how Markovianity interrelates with quantum thermodynamics at large.

[6b]Note that this would be $\mathsf{MEnTO_U}(\rho_0)$ if one allowed for *all* unitary maps instead of just those with H_0 as fixed point.

[6c]$\overline{\mathsf{TO}}_\mathsf{U}$ acts (approximately) transitively (i) on the set of all density operators for all $T \in [0,\infty)$ [87, Prop. 4.12] and (ii) on the set of all states majorised by the initial state if $T = \infty$ [84, Prop. 5.2.1].

Appendix A: A Simple Proof of Proposition 2 (iv)

While $\subseteq$ in Eq. (7) is obvious, for $\supseteq$ choose $\gamma \in C^1$ as in the r.h.s. of (7) with $\dot\gamma(0) =: A$. Then given any $t \geq 0$ sufficiently small we compute

$$n \log\big(\gamma(\tfrac{t}{n})\big) = n \log\big(\mathrm{id} + \tfrac{t}{n}A + \mathcal{O}(\tfrac{t}{n})\big) = n\big(\tfrac{t}{n}A + \mathcal{O}(\tfrac{t}{n})\big) \to tA$$

as $n \to \infty$. Be aware that we are allowed to apply the logarithm to $\gamma(\frac{t}{n})$ and, more importantly, $(\gamma(\frac{t}{n}))^n$ because

$$\begin{aligned}
\|\,\mathrm{id} - (\gamma(\tfrac{t}{n}))^n\| &= \|\,\mathrm{id} - (\mathrm{id} + \tfrac{t}{n}A + \mathcal{O}(\tfrac{t}{n}))^n\| \\
&= \|\,\mathrm{id} - \mathrm{id} - n\big(\tfrac{t}{n}A + \mathcal{O}(\tfrac{t}{n})\big) - \binom{n}{2}\big(\tfrac{t}{n}A + \mathcal{O}(\tfrac{t}{n})\big)^2 - \dots\| \\
&\leq \|At + n\mathcal{O}(\tfrac{t}{n})\| \cdot \|\,\mathrm{id} + n^{-1}\binom{n}{2}\big(\tfrac{t}{n}A + \mathcal{O}(\tfrac{t}{n})\big) - \dots\| \leq Ct(\|A\| + \varepsilon)
\end{aligned}$$

for all n sufficiently large as t was chosen to be suitably small. Here C can be obtained by a brute force estimate of the remaining terms of the binomial formula. Now because S is a closed semigroup we are able to conclude that

$$\lim_{n\to\infty} \gamma\big(\tfrac{t}{n}\big)^n = \lim_{n\to\infty} e^{\log\big((\gamma(\frac{t}{n}))^n\big)} = \lim_{n\to\infty} e^{n\log(\gamma(\frac{t}{n}))} = e^{tA}$$

is in S. Thus $(e^{tA})_{t\geq 0} \subseteq S$, again due to the semigroup property of S.

Appendix B: Proof of Theorem 1

(a): The result can be found in [40, Thm. V.1.13] (again under a much more general setting). Here the straightforward proof under our assumptions: let $S \subseteq \mathcal{B}(\mathcal{Z})$ be a closed subgroup and $\mathsf{L}(S)$ its Lie wedge. Then S_0 is obviously a closed subsemigroup contained in S and thus $\mathsf{L}(S_0) = \mathsf{L}(S)$. This implies $S_0 = \overline{\langle \exp\big(\mathsf{L}(S)\big)\rangle}_{\mathrm{SG}} = \overline{\langle \exp\big(\mathsf{L}(S_0)\big)\rangle}_{\mathrm{SG}}$, i.e. S_0 is a Lie subsemigroup. Moreover, let S' be any other Lie subsemigroup contained in S. Then one has $\mathsf{L}(S') \subseteq \mathsf{L}(S)$ and thus $S' = \overline{\langle \exp(\mathsf{L}(S'))\rangle}_{\mathrm{SG}} \subseteq \overline{\langle \exp(\mathsf{L}(S))\rangle}_{\mathrm{SG}} = S_0$. Hence S_0 is the largest Lie subsemigroup of S. (i): Moreover, let S' be any other Lie subsemigroup contained in S. Then one has $\mathsf{L}(S') \subseteq \mathsf{L}(S)$ and thus $S' = \overline{\langle \exp(\mathsf{L}(S'))\rangle}_{\mathrm{SG}} \subseteq \overline{\langle \exp(\mathsf{L}(S))\rangle}_{\mathrm{SG}} = S_0$. Hence S_0 is the largest Lie subsemigroup of S. (ii): For piecewise constant controls, the reachable set of the identity obviously coincides with the semigroup generated by $\exp\big(\mathsf{L}(S)\big)$. Moreover, as any locally integrable functions can be (L^1-norm) approximated on bounded intervals by piecewise constant functions, we conclude that the closure of the reachable set $\overline{\mathfrak{reach}(\mathrm{id})}$ equals $\overline{\langle \exp\big(\mathsf{L}(S)\big)\rangle}_{\mathrm{SG}} = S_0$.

(b): The case $S \subseteq \mathsf{GL}(\mathcal{Z})$ is treated in [40, Cor. VI.5.2]; the case $S \subseteq \mathcal{B}(\mathcal{Z})$ follows readily from the fact that for every Lie subsemigroup the set of its invertible elements (i.e. $S \cap \mathsf{GL}(\mathcal{Z})$) is dense in S.

Appendix C: Proof Idea of Equation (14)

A simple way of verifying (14) is to expand the exponentials:

$$\begin{aligned}
\operatorname{tr}_{\mathbb{C}^m}\left(e^{-itH}((\cdot)\otimes\omega)e^{itH}\right) &= \sum_{j,k=0}^{\infty} \operatorname{tr}_{\mathbb{C}^m}\left(\frac{(-itH)^j}{j!}((\cdot)\otimes\omega)\frac{(itH)^k}{k!}\right)\\
&= \sum_{j,k=0}^{\infty} \frac{(-1)^j(it)^{j+k}}{j!k!}\operatorname{tr}_{\mathbb{C}^m}\left(H^j((\cdot)\otimes\omega)H^k\right)\\
&= \sum_{\ell=0}^{\infty}(it)^\ell\sum_{j=0}^{\ell}\frac{(-1)^j}{j!(\ell-j)!}\operatorname{tr}_{\mathbb{C}^m}\left(H^j((\cdot)\otimes\omega)H^{\ell-j}\right)
\end{aligned}$$

Therefore the first-order term is $-it(\operatorname{tr}_{\mathbb{C}^m}(H((\cdot)\otimes\omega))-\operatorname{tr}_{\mathbb{C}^m}((\cdot)\otimes\omega)H))$ which by [86, Eqs. (14) & (15)] equals $-it(\operatorname{tr}_\omega(H)(\cdot)-(\cdot)\operatorname{tr}_\omega(H)) = -it\operatorname{ad}_{\operatorname{tr}_\omega(H)}$. Similarly, the second-order term comes out to be

$$t^2\Big(\operatorname{tr}_{\mathbb{C}^m}\left(H((\cdot)\otimes\omega)H\right) - \frac{1}{2}\operatorname{tr}_\omega(H)(\cdot) - \frac{1}{2}(\cdot)\operatorname{tr}_\omega(H)\Big)\,. \tag{27}$$

Defining $\Phi_H := \operatorname{tr}_{\mathbb{C}^m}(H((\cdot)\otimes\omega)H)$—which is completely positive—the second factor from Eq. (27) can be re-written as $\Phi_H - \frac{\Phi_H^*(\mathbb{1})}{2}(\cdot) - (\cdot)\frac{\Phi_H^*(\mathbb{1})}{2}$. This is known to be the generator of a quantum-dynamical semigroup, and one recovers Eq. (2) by choosing the V_j as Kraus operators of Φ_H, see [23, Ch. 9, Thm. 4.2 & Eq. (4.16)]. A straight-forward computation shows that a set of Kraus operators of Φ_H is given by $(\sqrt{r_k}\operatorname{tr}_{|g_k\rangle\langle g_j|}(H))_{j,k=1}^m$. Altogether this yields (14).

Appendix D: Periodic Solutions in the Qutrit System

We show that in the qutrit case, periodic solutions enclose a stabilisable point which—as we will see below—implies that $[d] = [\frac{1}{3}\mathbb{e}]$ is the only non-trivial equivalence class. We work in the setting of Sec. 4.2. using Assumption **A**, in particular we think of the control system being given in the form of the differential inclusion (25).

Lemma 8. *Let $x : S^1 \to \Delta^2$ be a smooth, periodic, injective solution of the differential inclusion with non-vanishing derivative. Then the region enclosed by x contains a stabilisable point.*

Proof. This is a direct generalisation of [5, Ch. 5.2, Thm. 1] which states that if an upper semicontinuous differential inclusion with non-empty, closed, convex values is defined on a compact convex set and satisfies a viability condition, then it has a stabilisable point. By the Schoenfliess Theorem, see [68, Ch. 9, Thm. 6], the interior region of $x(S^1)$ is homeomorphic to an open disk, and hence by the Riemann mapping theorem, there is even a biholomorphism. Now note that since x is an injective immersion and S^1 is compact, it is an embedding, and hence the image is a smooth curve. Thus, by [6, Thm. 3.1], the Riemann mapping extends to a diffeomorphism of the closure of the interior region to the closed disk. Finally we can pull back the differential inclusion to the disk and apply the aforementioned theorem to find a stabilisable point. □

The idea of the result we want to prove is that if two points are equivalent but distinct, then they must be equivalent to some stabilisable point. To prove this in general we need the following approximation result.

Lemma 9. *Let $x \neq y$ and $y \twoheadleftarrow x$, and assume that y is not stabilisable. Let a solution $\tilde{y}$ starting at y be given. Then for every $\varepsilon > 0$ small enough we can modify the differential inclusion in the region $B_\varepsilon(y)$ without creating new stabilisable points and such that there is a smooth solution $\tilde{x}$ starting at x and ending at y such that the concatenation of $\tilde{x}$ and $\tilde{y}$ is smooth.*

Sketch of proof. Using translations and rotations we may assume that $y = (0,0)$ and the cone generated by $\mathfrak{Derv}(y)$ is contained in the upper halfplane and symmetric about the vertical axis. By continuity and assuming that δ is small enough, there are inner and outer approximations of this cone in $B_\delta(y)$ which are both pointed. We may assume (e.g., by extending x backwards) that $x'(0)$ lies in the inner approximating cone. We will only modify the differential inclusion within the lower half of this disk. Now assume that for some small enough $0 < \varepsilon \ll 1$ we have a smooth solution $\tilde{x}$ starting at x that ends ε-close to y. Then by slightly enlarging the outer cone we may assume that $\tilde{x}$ enters the unit disk within the negative of the outer cone. One can see that it is possible to modify the differential inclusion inside $B_R \setminus B_r$ for some $0 < r < R < 1$ such that there is a smooth solution entering B_r inside of the inner approximating cone, while making sure that the cone always lies in the upper halfplane, so that no stabilisable points are created. □

Proposition 5. *If $x \neq y$ and $x \sim y$, then $x \sim \frac{1}{3}\mathbb{e}$.*

Proof. If x or y is stabilisable, then by Cor. 6 it is equivalent to d and we are done. Hence we assume that neither x nor y is stabilisable. Let $\varepsilon > 0$ small enough be given. Since $x \sim y$, we may apply Lem. 9 twice to obtain a smooth, periodic solution passing through x and y for a slightly modified differential inclusion, which does not introduce new stabilisable points. Without loss of generality we may assume that this solution is injective and has non-vanishing derivative. By Lem. 8 it encloses a stabilisable point. However, if we work in a Weyl chamber, the non-stabilisable set is simply-connected, and so the periodic solution intersects the stabilisable region in some point s. Hence there is a point ε-close to x which is reachable from s (and by Cor. 6 also from $\frac{1}{3}\mathbb{e}$). Letting ε go to 0 this shows that $x \twoheadleftarrow \frac{1}{3}\mathbb{e}$. □

Appendix E: Markovian Thermal Single-Qubit Operations with Different Temperatures

We compute the product of two Markovian thermal operations in the single-qubit case and show that the result is again Markovian and thermal. Recall that every thermal qubit operation in $\mathsf{MTO}(H_0, T)$ is represented by three parameters[6d]: $\mu, \varepsilon \in \mathbb{R}$, $c \in \mathbb{C}$. A matrix representation is given by

$$G(\mu, \varepsilon, c) = \begin{pmatrix} 1-\varepsilon\mu & \mu & 0 \\ \varepsilon\mu & 1-\mu & 0 \\ 0 & 0 & c \end{pmatrix}. \tag{28}$$

Considering the product $G(\mu_3, \varepsilon_3, c_3) = G(\mu_1, \varepsilon_1, c_1)\, G(\mu_2, \varepsilon_2, c_2)$ we find that

$$\begin{aligned} \mu_3 &= \mu_1 + \mu_2 - \mu_1\mu_2(1+\varepsilon_1) \\ \varepsilon_3\mu_3 &= \varepsilon_1\mu_1 + \varepsilon_2\mu_2 - \mu_1\mu_2(1+\varepsilon_1)\varepsilon_2 \end{aligned}$$

as well as $c_3 = c_1 c_2$. Note that this product in general is not commutative.

Actually, in order for (28) to describe a thermal operation recall that $\mu, \varepsilon \in [0,1]$ and $|c|^2 \le (1-\varepsilon\mu)(1-\mu)$, and for the operation to be Markovian the latter condition is replaced by $|c|^2 \le 1 - \mu(1+\varepsilon)$.

Lemma 10. *Let parameters $\mu_1, \varepsilon_1, \mu_2, \varepsilon_2 \in [0,1]$, $c_1, c_2 \in \mathbb{C}$ be given and set $(\mu_3, \varepsilon_3, c_3) := (\mu_1, \varepsilon_1, c_1) \cdot (\mu_2, \varepsilon_2, c_2)$. Then the latter is thermal, and if the initial parameters are Markovian, then so is $(\mu_3, \varepsilon_3, c_3)$.*

Proof. Because the above composition rule on $\mathbb{R}^2 \times \mathbb{C}$ is defined via (28), i.e. $\mu_3 = \mu_1(1-\mu_2) + (1-\varepsilon_1\mu_1)\mu_2$ and $\varepsilon_3\mu_3 = \varepsilon_2\mu_2(1-\mu_1) + \varepsilon_1\mu_1(1-\varepsilon_2\mu_2)$, the assumption $\mu_1, \varepsilon_1, \mu_2, \varepsilon_2 \in [0,1]$ directly implies $\mu_3, \varepsilon_3 \ge 0$. Next, using $1-\mu_3 = (1-\mu_1)(1-\mu_2) + \mu_1\mu_2\varepsilon_1$ and $1-\varepsilon_3\mu_3 = (1-\varepsilon_1\mu_1)(1-\varepsilon_2\mu_2) + \varepsilon_1\mu_1\mu_2$ we find $1-\mu_3 \ge 0$, $\mu_3 - \mu_3\varepsilon_3 \ge 0$, and $|c_3|^2 \le (1-\varepsilon_3\mu_3)(1-\mu_3)$. Together this shows that $(\mu_3, \varepsilon_3, c_3)$ is thermal. Finally, the statement about Markovianity follows from $1 - \mu_3 - \varepsilon_3\mu_3 = (1-\mu_1-\varepsilon_1\mu_1)(1-\mu_2-\varepsilon_2\mu_2)$. □

[6d] Strictly speaking, one has to replace ε by $\mu\varepsilon$ since the former leads to an ill-defined composition rule if $\mu = 0$. However, this special case can easily be dealt with, so for the sake of simplicity and clarity we will treat ε as independent.

Hence the union of $\mathsf{MTO}(H_0, T)$ over all T yields a semigroup which we denote by $\mathsf{MTO}(H_0)$. One readily verifies that $\mathsf{MTO}(H_0)$ is weakly exponential, and it turns out that it is even locally exponential: to see this we need to find a neighbourhood basis of the identity which is exponential. Since $\mathsf{MTO}(H_0)$ decomposes into a stochastic part and a complex part (as shown above), it suffices to argue for each separately. Indeed the neighbourhood basis $\mathcal{U}_k = \{(\mu, \varepsilon, c) \in \mathsf{MTO}(H_0) : \mu, \varepsilon\mu, |\ln(c)| < 1/k\}$ is exponential, since the one parameter semigroups in the stochastic part are straight lines and the image of c under ln forms a halfdisk.

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