Exploring the Limits of Open Quantum Dynamics II: Gibbs-Preserving Maps from the Perspective of Majorization *

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Abstract: Motivated by reachability questions in coherently controlled open quantum systems coupled to a thermal bath, as well as recent progress in the field of thermo-/vector-majorization we generalize classical majorization from unitary quantum channels to channels with an arbitrary fixed point $D$ of full rank. Such channels preserve some Gibbs-state and thus play an important role in the resource theory of quantum thermodynamics, in particular in thermo-majorization.

Based on this we investigate $D$-majorization on matrices in terms of its topological and order properties, such as existence of unique maximal and minimal elements, etc. Moreover we characterize $D$-majorization in the qubit case via the trace norm and elaborate on why this is a challenging task when going beyond two dimensions.

Keywords: Open quantum systems, quantum control theory, reachable sets, quantum thermodynamics, majorization

1. INTRODUCTION

Studying reachable sets of control systems is necessary to ensure well-posedness of a large class of (optimal) control tasks. In Dirr et al. (2019) toy models on the standard simplex of probability vectors were studied in order to answer reachability questions of controlled $n$-level systems coupled to a bath of finite temperature such that the coupling can be switched on and off. If the closed (unitary) part of the system can be fully controlled and the bath has temperature $T = 0$ then every quantum state $\rho$ can be reached approximately from every initial state (that is, perhaps not exactly but at least with arbitrary precision). For $T = \infty$ an upper bound can be obtained by classical majorization techniques. For more details on this we refer to the first part of this talk: Exploring the Limits of Open Quantum Dynamics I: Motivation, First Results from Toy Models to Applications, as well as Section 3.3.

An obvious follow-up question is what can be said—if one can say anything at all—about the reachable set of such a system for $0 < T < \infty$? Even within the simplified diagonal toy model (cf. Part I) this is a rather difficult task and it seems that the notion necessary to handle such problems requires a more general form of majorization:

2. ON THE ROAD TO $D$-MAJORIZATION

2.1 $d$-Majorization on Vectors

Majorization relative to a strictly positive vector $d \in \mathbb{R}_{++}^n$, as introduced by Véron (1971) and in the quantum regime by Ruch et al. (1978) is defined as follows: a vector $y$ is said to $d$-majorize $x$, denoted by $x \prec_d y$, if there exists a $d$-stochastic matrix $A \in \mathbb{R}^{n \times n}$ with $x = Ay$. Recall that $A \in \mathbb{R}^{n \times n}$ is $d$-stochastic if all its entries are non-negative and $Ad = e^T A = e^T$ with $e^T := (1, \ldots, 1)^T$. A variety of characterizations of $\prec_d$ and $d$-stochastic matrices can be found in the work of Joe (1990) and vom Ende and Dirr (2019). The most useful for numerical purposes is the following: $x \prec_d y$ if and only if

$$
\sum_{j=1}^{n} x_j \leq \sum_{j=1}^{n} y_j \quad \text{and} \quad \|d, x - y, d\|_1 \leq \|d, y - y, d\|_1 \quad \text{for all} \quad i = 1, \ldots, n, \quad \text{where} \quad \|z\|_1 := \sum_{j=1}^{n} |z_j| \quad \text{is the usual vector-1-norm}.
$$

Classic majorization $\prec$, that is, $x \prec y$ for $x, y \in \mathbb{R}^n$, is originally defined via ordering $x, y$ decreasingly and then comparing partial sums: $\sum_{j=1}^{k} x_j \leq \sum_{j=1}^{k} y_j$ for all $k = 1, \ldots, n-1$ as well as $\sum_{j=1}^{n} x_j = \sum_{j=1}^{n} y_j$. For more on vector majorization we refer to Ch. 1 & 2 of Marshall et al. (2011). In particular it is well-known that setting $d = e$ in the definition of $d$-majorization recovers $\prec$—which also shows that the definition via partial sums cannot extend beyond $e^T$; as soon as two entries in $d \in \mathbb{R}_{++}^n$ differ one loses permutation invariance and reordering the vectors $x, y$ makes a conceptual difference.

The above 1-norm characterization allows to rewrite the $d$-majorization polytope $M_d(y) := \{ x \in \mathbb{R}^n \mid x \prec_d y \}$ for any

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1 A quantum state is a positive semi-definite matrix of unit trace.
trace is the Gibbs state of

by

thermodynamic equilibrium state) of the system is given

of some temperature

. Due to this result d-majorization is suited to analyse reachable sets in the toy model (cf. Part I of this talk)—yet as soon as one considers n-level quantum systems one needs a similar concept on (density) matrices.

2.2 Generalizing d-Majorization to Matrices

Classical majorization on the level of hermitian matrices uses their “eigenvalue vector” \( \lambda(\cdot) \) arranged in any order with multiplicities counted. For \( A, B \in \mathbb{C}^{n \times n} \) hermitian, \( A \) is said to be majorized by \( B \) if \( \lambda(A) < \lambda(B) \), cf. Ando (1989).

The most naive approach to define D-majorization on matrices (with \( D = \text{diag}(d) \) for some \( d \in \mathbb{R}^n_{++} \)) would be to replace \( \prec \) by \( \prec_D \) and leave the rest as it is. However such a definition is unfeasible because it depends on the arrangement of the eigenvalues in \( \lambda \), due to the lack of permutation invariance of \( d \) (unless \( d = e^T \)).

The most natural way out of this dilemma is to remember that classical majorization on matrices can be equivalently characterized via linear maps which are completely positive and trace-preserving (\( \text{cptp} \)) and which have the identity matrix \( \text{id} = \text{diag}(1, \ldots, 1) \) as a fixed point. Therefore it seems utmost reasonable to generalize d-majorization on square matrices as follows:

Definition 1. Given \( n \in \mathbb{N} \) and \( A, B \in \mathbb{C}^{n \times n} \) as well as a positive definite matrix \( D \in \mathbb{C}^{n \times n} \) we say that \( A \) is D-majorized by \( B \) (denoted by \( A \prec_D B \)) if there exists a \( \text{cptp} \) map \( T \) such that \( T(D) = A \) and \( T(D) = D \).

Such a definition is also justified by the following: given real vectors \( x, y \) and a positive vector \( d \in \mathbb{R}^n_{++} \) one can show that \( \text{diag}(x) \prec_{\text{diag}(d)} \text{diag}(y) \) if and only if \( x \prec_D y \). In other words the diagonal case reduces to d-majorization on vectors as expected.

Be aware that one could define matrix D-majorization via positive (instead of completely positive) trace-preserving maps, and that this would make a conceptual difference – unless \( D \neq \text{id} \) (Ando, 1989, Thm. 7.1), more on this at the end of Section 3.1. However, we defined D-majorization via \( \text{cptp} \) maps because this class has a richer theory behind it and because it is the more natural choice if one comes from quantum information and control.

3. PROPERTIES OF D-MAJORIZATION

Using \( \text{cptp} \) maps in Definition 1 also allows for a physical interpretation of D-majorization: Given some n-level system (with Hamiltonian \( H_0 \in \mathbb{C}^{n \times n} \) coupled to a bath of some temperature \( T > 0 \), the Gibbs state (that is, the thermodynamic equilibrium state) of the system is given by

\[
\rho_{\text{Gibbs}}^{H_0, T} := \frac{\exp(-H_0/T)}{\text{tr} (\exp(-H_0/T))} > 0.
\]

Because every positive definite \( n \times n \) matrix of unit trace is the Gibbs state of some n-level system this links \( \prec_D \) to Gibbs-preserving \( \text{cptp} \) maps. Moreover in the high-temperature limit the above definition reduces to \( \lim_{T \to \infty} \rho_{\text{Gibbs}}^{H_0, T} = \frac{1}{d} \text{diag}(1, \ldots, 1) \), which connects classical majorization to baths of infinite temperature.

3.1 Characterizations of D-Majorization

An important observation is that for any \( A, B \in \mathbb{C}^{n \times n} \) and \( D > 0 \) one has \( A \prec_D B \) if and only if \( \text{U} A \text{U}^* \prec_{\text{U} \text{D} \text{U}^*} \text{U} B \text{U}^* \) for all unitary matrices \( U \in \mathbb{C}^{n \times n} \). Thus we can w.l.o.g. assume that \( D \) is diagonal in the standard basis.

Now if one deals with qubits, i.e. two-dimensional systems, then D-majorization can be characterized as follows.

Proposition 2. Let \( d \in \mathbb{R}^2_{++}, D = \text{diag}(d) \) and \( A, B \in \mathbb{C}^{2 \times 2} \) hermitian be given. The following are equivalent.

(i) \( A \prec_D B \)

(ii) There exists a positive trace-preserving map \( T \) with \( T(D) = D \) and \( T(B) = A \).

(iii) \( \| A - tD \|_1 \leq \| B - tD \|_1 \) for all \( t \in \mathbb{R} \) with \( \| \cdot \|_1 \) being the trace norm.

(iv) \( \text{tr}(A) = \text{tr}(B) \) and \( \| A - b_1 D \|_1 \leq \| B - b_2 D \|_1 \) for \( i = 1, 2 \) as well as for the generalized fidelity

\[
\sqrt{\| A - b_1 D \sqrt{b_2 D - A} \|_1} \geq \| B - b_1 D \sqrt{b_2 D - B} \|_1.
\]

Here \( \sigma(D^{-1/2}B^{-1/2}) = \{ b_1, b_2 \} \) \( b_1 \leq b_2 \) with \( \sigma(\cdot) \) being the spectrum.

Of course property (iv) is the closest to the 1-norm characterization of \( \prec_d \) from Sec. 2.1 and, moreover, the key to easily check (e.g., on a computer) if some hermitian matrix \( D \)-majorizes another. Unfortunately none of these characterizations generalize to dimensions larger than 2 because the counterexample to the Alberti-Uhlmann theorem in higher dimensions, given by Heinosaari et al. (2012), pertains to our problem: Consider the hermitian matrices

\[
A = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & -i \\ 0 & i & 2 \end{pmatrix}, \quad B = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & i \\ 0 & -i & 2 \end{pmatrix}, \quad D = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}.
\]

Then \( \sigma(D) = \{ 2, 2 + \sqrt{2}, 2 - \sqrt{2} \} \) so \( D > 0 \). Obviously, \( B^T = A \) and \( D^T = D \) so because the transposition map is well-known to be linear, positivity- and trace-preserving one has \( \| A - tD \|_1 = \| (B - tD)^T \|_1 = \| B - tD \|_1 \) for all \( t \in \mathbb{R} \). But there exists no \( \text{cptp} \) map, i.e. no \( T \in \mathcal{Q}(n) \) such that \( T(B) = A \) and \( T(D) = D \) as shown in (Heinosaari et al., 2012, Proposition 6). For now finding simple-to-verify conditions for \( \prec_D \) beyond two dimensions remains an open problem.

3.2 Order Properties of D-Majorization

As is readily verified \( \prec_d \) is a preorder but it is not a partial order—the same holds for \( \prec_D \) and the counterexample which shows that \( \prec_d \) is not a partial order transfers to the matrix case. Moreover, now, one can characterize minimal and maximal elements in this preorder.

Theorem 3. Let \( d \in \mathbb{R}^n_{++} \) be given and let

\[
b_d := \{ X \in \mathbb{C}^{n \times n} \mid X \text{ hermitian and } \text{tr}(X) = e^T d \}
\]

\[
b_d := \{ X \in \mathbb{C}^{n \times n} \mid X \geq 0 \text{ and } \text{tr}(X) = e^T d \}
\]
be the trace hyperplane induced by $d$ within the hermitian and the positive semi-definite matrices, respectively. The following statements hold.

(i) $D = \text{diag}(d)$ is the unique minimal element in $h_d$ with respect to $\prec_D$.

(ii) $(e^{\tau d}x_k)e^T_k$ is maximal in $h_d^+$ with respect to $\prec_D$ where $k$ is chosen such that $d_k$ is minimal in $d$. It is the unique maximal element in $h_d^+$ with respect to $\prec_D$ if and only if $d_k$ is the unique minimal element of $d$.

From a physical point of view this is precisely what one expects: from the state with the largest energy one can generate every other state (in an equilibrium-preserving manner) and there is no other state with this property.

### 3.3 Reachable Sets & $D$-Majorization

Let us finally connect our notion of $D$-majorization to the reachability questions we touched upon in the introduction. Markovian quantum control systems are generally modelled via a controlled GKSL-equation [Gorini et al. (1976); Lindblad (1976)];

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

(2)

with initial state $\rho(0) = \rho_0 \in \mathbb{C}^{n \times n}$, control Hamiltonians $H_1, \ldots, H_m$, and control amplitudes $u_1, \ldots, u_m, \gamma$. Here $\Gamma(\rho) := \sum_{j \in I} (V_j^\dagger V_j \rho + \rho V_j^\dagger V_j) - V_j \rho V_j^\dagger$ describes the dissipative effect on the system by means of the matrices $(V_j)_{j \in I} \subset \mathbb{C}^{n \times n}$ which in principle can be arbitrary.

Now given any $n$-level system described by a hermitian matrix $H_S \in \mathbb{C}^{n \times n}$ with spectral decomposition $\sum_{j=1}^n E_j |j\rangle \langle j|$, $E_1 \leq \ldots \leq E_n$ and a bath of some temperature $T > 0$ the coupling of the system to said bath can be modelled by (2) if the generators of the dissipation $(V_j)_{j \in I}$ are chosen to be the modified ladder operators

$$\sigma^+_k := \sum_{j=1}^{n-1} \frac{j(n-j) e^{-E_j/T}}{e^{-E_j/T} + e^{-E_{j+1}/T}} |g_j\rangle \langle g_{j+1}|$$

$$\sigma^-_k := \sum_{j=1}^{n-1} \frac{j(n-j) e^{-E_{j+1}/T}}{e^{-E_j/T} + e^{-E_{j+1}/T}} |g_{j+1}\rangle \langle g_j|.$$ 

In order to analyze the reachable set of (2) with $H_0 = H_S$ and dissipation generators $\sigma^+_k, \sigma^-_k$ we (as in Section 2.1) define the set of all matrices which are $D$-majorized by some state $\rho$ or a collection of states $S \subseteq \mathbb{C}^{n \times n}$

$$M_D : \mathcal{P}(\mathbb{C}^{n \times n}) \to \mathcal{P}(\mathbb{C}^{n \times n})$$

$$S \mapsto \bigcup_{\rho \in S} \{X \in \mathbb{C}^{n \times n} | X \prec_D \rho\}$$

with $P$ being the power set and $M_D(X) := M_D(\{X\})$ for all $X \in \mathbb{C}^{n \times n}$. This operator is used to upper bound the reachable set of the “toy model” $\Lambda_d$ (cf. Part I) and is expected to do so in the matrix case, as well. Important properties of $M_D$ are:

(i) $M_D(X)$ is convex for all $X \in \mathbb{C}^{n \times n}$.

(ii) If $P \subset \mathbb{C}^{n \times n}$ is compact, then $M_D(P)$ is compact.

(iii) If $P$ is a collection of quantum states then $M_D(P)$ is star-shaped with respect to the Gibbs state $\frac{1}{D}(\rho)$.

(iv) When restricting $M_D$ to the compact subsets of $\mathbb{C}^{n \times n}$ then $M_D$ is non-expansive (so in particular continuous) with respect to the Hausdorff metric.

The last property formulates that for a system in the state $\rho$ which is coupled to a bath of temperature $T \geq 0$, “small” changes in $\rho$ cannot change the set of $D$-majorized states “too much”.

Coming back to footnote 3, the crucial step in the proof is to identify an extreme point of $M_D(x_0)$ which is maximal w.r.t. classical majorization. While an extreme point analysis of the set of matrices $M_D(\rho)$ is way more difficult—as the convex polytope techniques from the vector case break down—the idea of a maximal extreme point might be equally useful in analyzing general open quantum control problems in the future.

### 4. CONNECTION TO THERMO-MAJORIZATION

Over the last few years, sparked by Brandão et al. (2015); Horodecki and Oppenheim (2013) and others [Gour et al. (2015); Lostaglio et al. (2018); Sagawa et al. (2021)] thermo-majorization has been a widely discussed and studied topic in quantum physics and in particular quantum thermodynamics. In the abelian case thermo-majorization, on a mathematical level, is described by vector $d$-majorization which begs the question of how to define thermo-majorization for general quantum states.

Indeed Faist et al. (2015) have shown that it makes a conceptual difference whether one defines thermo-majorization on non-diagonal states via Gibbs-preserving maps (i.e. ctp maps having the Gibbs state $\rho = \rho_0$ as a fixed point, cf. Definition 1) or if one restricts to the smaller class of thermal operations. The latter, given some Hamiltonian of the system $H_S$ and a fixed bath temperature $T > 0$, are defined as follows, cf. also Lostaglio (2019):

**Definition 4.** A linear map $\Phi : \mathbb{C}^{n \times n} \to \mathbb{C}^{n \times n}$ is a thermal operation w.r.t. $H_S$ if there exist $m \in \mathbb{N}$, $H_R \in \mathbb{C}^{mn \times mn}$ hermitian, and $U \in \mathbb{C}^{mn \times mn}$ unitary such that

$$[U, H_S \otimes \text{id}_R + \text{id}_S \otimes H_R] = 0$$

and

$$\Phi(\rho) = \text{tr}_R(U(\rho \otimes \rho_{\text{Gibbs}}^{H_R,T})U^*)$$

for all $\rho \in \mathbb{C}^{n \times n}$ (or equivalently for all quantum states $\rho$). We denote the collection of all thermal operations by $\text{TO}(H_S, T)$.

Thermal operations are the free operations of the resource theory of quantum thermodynamics as those encompass the dynamics which preserve the Gibbs-state and which satisfy (4) (conserve the global energy, that is, the energy of the larger system $H_{SR} = H_S \otimes \text{id}_R + \text{id}_S \otimes H_R$). One readily verifies that $\text{TO}(H_S, T)$ forms a path-connected semigroup with identity and – although $\text{TO}(H_S, T)$ in general is not closed – its closure even is convex and compact.

In the vector case the state transitions possible with thermal operations are the same as with general Gibbs-preserving maps described by $d$-stochastic matrices. However in the operator case there is a discrepancy between the
two coming from the fact that there exist Gibbs-preserving maps which generate coherent superpositions of energy levels, whereas no thermal operation is capable of doing such a thing. In fact for all $H_S \in \mathbb{C}^{n \times n}$, $T \geq 0$ one finds the inclusions

$$\text{TO}(H_S, T) \subseteq \text{EnTO}(H_S, T) \subseteq Q_{e^{-H_S/T}}(n)$$

where $Q_{e^{-H_S/T}}(n)$ is the collection of all cPTP maps which have $e^{-H_S/T}$ and thus $H_S$ as a fixed point, and

$$\text{EnTO}(H_S, T) := \{ \Phi \in Q_{e^{-H_S/T}}(n) : [\Phi, \text{ad}_{H_S}] = 0 \}$$

are the enhanced thermal operations (also called “covariant Gibbs-preserving maps”). This is an important observation as the covariance property $[\Phi, \text{ad}_{H_S}] = 0$ forces that the diagonal and the off-diagonal action of any channel are strictly separated, assuming $H_S$ has non-degenerate spectrum. Note that this insight is of importance to us because the solution to the uncontrolled master equation $H_T = 0$ ($\gamma \equiv 1$) with dissipation generators $\sigma_1^d, \sigma_2^d$ from (3) lives in $\text{EnTO}$ at all times.

Be aware that in (5), if the thermal operations are replaced by their closure then the first set inclusion is an equality if $n = 2$ and becomes a strict inclusion for $n \geq 3$ as shown by Ding et al. (2021). Even worse this discrepancy between $\text{TO}$ and $\text{EnTO}$ remains when looking at the action of the respective sets on certain states; more precisely, there exist quantum states $\rho, \omega \in \mathbb{C}^{n \times n}$ and an enhanced thermal operation $\Phi$ such that $\Phi(\rho) = \omega$ but no element in $\text{TO}$ or its closure can map $\rho$ to $\omega$.

This observation is particularly important for the field of quantum control as there one usually wonders which state transitions can be realized under a given control scenario. Thus beyond qubits it makes a conceptional difference which of the sets in (5) one uses to model a quantum state transitions under Markovian thermal processes (i.e. maps from $\text{EnTO}$ which are solutions of a time-dependent GKSL-equation) in the classical realm, and they even gave algorithms to check for a Markovian path from a given initial to a given final state. While incredibly important, their work of course is but a first step in this direction and the ultimate goal will be to extend their results and concepts to general thermodynamic quantum control systems.

REFERENCES

Ando, T. (1989). Majorization, Doubly Stochastic Matrices, and Comparison of Eigenvalues. *Lin. Alg. Appl.*, 118, 163–248.

Brandão, F., Horodecki, M., Ng, N., Oppenheim, J., and Wehner, S. (2015). The Second Laws of Quantum Thermodynamics. *Proc. Natl. Acad. Sci. U.S.A.*, 112, 3275–3279.

Ding, Y., Ding, F., and Hu, X. (2021). Exploring the Gap Between Thermal Operations and Enhanced Thermal Operations. *Phys. Rev. A*, 103, 052214.

Dirr, G., vom Ende, F., and Schulte-Herbrüggen, T. (2019). Reachable Sets from Toy Models to Controlled Markovian Quantum Systems. *Proc. IEEE Conf. Decision Control (IEEE-CDC)*, 58, 2322.

Faist, P., Oppenheim, J., and Renner, R. (2015). Gibbs-Preserving Maps Outperform Thermal Operations in the Quantum Regime. *New J. Phys.*, 17, 1–4.

Gorini, V., Kossakowski, A., and Sudarshan, E. (1976). Completely Positive Dynamical Semigroups of N-Level Systems. *J. Math. Phys.*, 17, 821–825.

Gour, G., Müller, M., Narasimhachar, V., Spekkens, R., and Halpern, N. (2015). The Resource Theory of Informational Nonequilibrium in Thermodynamics. *Phys. Rep.*, 583, 1–58.

Heinosaari, T., Jivulescu, M., Reeb, D., and Wolf, M. (2012). Extending Quantum Operations. *J. Math. Phys.*, 53, 102208.

Horodecki, M. and Oppenheim, J. (2013). Fundamental Limitations for Quantum and Nanoscale Thermodynamics. *Nat. Commun.*, 4, 2059.

Joe, H. (1990). Majorization and Divergence. *J. Math. Anal. Appl.*, 148, 287–305.

Lindblad, G. (1976). On the Generators of Quantum Dynamical Semigroups. *Commun. Math. Phys.*, 48, 119–130.

Lostaglio, M. (2019). An Introductory Review of the Resource Theory Approach to Thermodynamics. *Rep. Prog. Phys.*, 82, 114001.

Lostaglio, M., Alhambra, À., and Perry, C. (2018). Elementary Thermal Operations. *Quantum*, 2, 1–52.

Lostaglio, M. and Korzekwa, K. (2021). Continuous Thermomajorization and a Complete Set of Laws for Markovian Thermal Processes.

Marshall, A., Olkin, I., and Arnold, B. (2011). *Inequalities: Theory of Majorization and Its Applications*. Springer, New York, 2 edition.

Ruch, E., Schranner, R., and Seligman, T. (1978). The Mixing Distance. *J. Chem. Phys.*, 69, 386–392.

Sagawa, T., Faist, P., Kato, K., Matsumoto, K., Nagaoka, H., and Brandão, F. (2021). Asymptotic Reversibility of Thermal Operations for Interacting Quantum Spin Systems via Generalized Quantum Stein’s Lemma. *J. Phys. A*, 54, 495303.

Veinott, A. (1971). Least $d$-Majorized Network Flows with Inventory and Statistical Applications. *Manag. Sci.*, 17, 547–567.

vom Ende, F. and Dirr, G. (2019). The $d$-Majorization Polytope.