
Positivity for matrix systems: a case study from quantum mechanics

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Abstract. We discuss an example from quantum physics of “positive system” in which the state (a density operator) is a square matrix constrained to be positive semidefinite (plus Hermitian and of unit trace). The positivity constraint is captured by the notion of complete positivity of the corresponding flow. The infinitesimal generators of all possible admissible ODEs can be characterized explicitly in terms of cones of matrices. Correspondingly, it is possible to determine all linear time-varying systems and bilinear control systems that preserve positivity of the state space.

1 Introduction

For a matrix system, i.e., a system of ODEs having as state space a set of square matrices, the idea of state that can assume only positive values naturally generalizes to operator positivity i.e., to positive (semi)definiteness of the square matrix representing the state variables. Such a concept is not new in applied mathematics and for example it has long been used in modeling quantum dissipative systems. Assume that the system obeys to a time-invariant linear (matrix) ODE. To preserve positivity of the state it is not sufficient to have a flow which is itself positive; it is necessary to impose the stronger concept of *complete positivity* of the flow. Infinitesimally, for positive (semi)definite state matrices that are hermitian and have trace equal to 1 i.e., densities in quantum mechanical language, the set of generators that satisfy complete positivity is well-known under the name of Lindbladian and the type of equations resulting is normally referred to as quantum Markovian master equation [8, 6]. In this note we first expose the general form of the Lindbladian for the particular case of density operators and then we reformulate the matrix system as a vector system in \mathbb{R}^n , for suitable n , using a variant of the $vec(\cdot)$ operation. At the same time, we rewrite the constraints that the complete positivity imposes on such a system on \mathbb{R}^n . Finally we show how the control inputs can enter into such a system (thus making it a bilinear control

system) while preserving positivity. In fact, the description we obtain is in terms of invariant cones of matrices and therefore all time-varying generators contained in the admissible cone for all times are compatible with the problem. Likewise, control inputs (some constrained, some unconstrained) can be added that also preserve positivity of the state matrix making the system into a bilinear control system.

Remarkably, all the Lindbladians admissible by the complete positivity assumption form the set of all possible affine dynamics that leave the unit ball invariant. In the particular case that the dynamics are linear, rather than affine, we obtain the set of semistable matrices belonging to the cone generated by choosing the identity as quadratic form in the Lyapunov equation i.e., $\{A \in \mathbb{R}^{n \times n} \text{ s.t. } A + A^T \leq 0\}$. In other words, all possible linear dynamics obtained in this way are contracting in the natural inner product of \mathbb{R}^n .

2 Completely positive linear maps

Assume that the state matrix $\rho \in \mathbb{C}^{N \times N}$ of our system is positive semidefinite (and therefore Hermitian): $\rho \geq 0$. We want to compute what kind of ODE $\dot{\rho} = \mathcal{L}(\rho)$ or control system $\dot{\rho} = \mathcal{L}(\rho, u)$ are compatible with the assumption $\rho(t) \geq 0 \forall t \geq 0$. A theorem by Choi [5] completely characterizes all linear transformations $A_t : \mathbb{C}^{N \times N} \rightarrow \mathbb{C}^{N \times N}$ such that $\rho(0) \geq 0$ implies $A_t(\rho(0)) \geq 0$. Imposing $A_t \geq 0$ is not enough, as we have the following well-known fact (see Appendix A of [6] for a practical example):

$$\textit{Remark 1. } \rho = \rho^{(1)} \otimes \rho^{(2)}, A^{(1)}(\cdot) \geq 0, A^{(2)}(\cdot) \geq 0 \not\Rightarrow (A^{(1)} \otimes A^{(2)})(\rho) \geq 0$$

The stronger requirement that must be imposed on A_t is known under the name of *complete positivity*. The symbol “ \otimes ” indicates the tensor product (for matrices it coincides with the so-called Kronecker product, see [4]).

Definition 1. *The map $A_t : M(N) \rightarrow M(N)$ is completely positive if the tensor product map $\hat{A}_t = A_t \otimes I_m$ is positive $\forall m \in \mathbb{N}$*

The general form of a completely positive map is also known as the Stinespring representation [9] and is given by $A(\rho) = \sum_{k=1}^{N^2} W_k \rho W_k^\dagger$, where the N^2 operators W_k are $N \times N$ matrices and $W^\dagger = (W^*)^T$ (conjugate transposed). To verify complete positivity it is enough to test positive semidefiniteness on the elementary matrices E_{jk} (having 1 in the (j, k) slot and 0 elsewhere):

Theorem 1. ([5], Theorem 2) *The map A_t is completely positive if and only if $(A_t(E_{jk}))_{1 \leq j, k \leq N} \geq 0$.*

If, in addition, we impose $A_t(I) = \sum_{k=1}^{N^2} W_k^\dagger W_k = I$, then A_t is also trace preserving. This is the case discussed here thereafter.

3 Quantum dynamical semigroups

The state of a quantum mechanical system in an N -dimensional complex space $\mathbb{C}^{N \times N}$ can be described in terms of a positive semidefinite Hermitian operator ρ , called the density matrix, having trace $\text{tr}(\rho) = 1$ and $\text{tr}(\rho^2) \leq 1$. Assume that the system of state ρ is governed by a time-invariant matrix ODE with flow at time t Λ_t . Λ_t is a one-parameter semigroup $\rho(t) = \Lambda_t(\rho(0))$, $t \in \mathbb{R}^+$, such that:

- $\Lambda_t(\Lambda_s(\cdot)) = \Lambda_{t+s}(\cdot)$ (semigroup property of the flows);
- for $\rho \geq 0$ $\Lambda_t(\rho) \geq 0$ (positive semidefiniteness of the state);
- $\text{tr}(\Lambda_t(\rho)) = \text{tr}(\rho) = 1$ (preservation of the trace).

Problem 1. Characterize Λ_t infinitesimally i.e., provide an explicit expression for the infinitesimal generators $\mathcal{L}(\cdot)$ such that $\dot{\rho} = \mathcal{L}(\rho)$ has $\forall t \geq 0$, $\rho(t) = \rho^\dagger(t) \geq 0$, $\text{tr}(\rho(t)) = 1$ and $\text{tr}(\rho^2) \leq 1$.

If $n = N^2 - 1$, the infinitesimal form corresponding to Λ_t is known under the name of Lindblad (or Gorini-Kossakowski-Sudarshan) form [6] $\mathcal{L}_D(\rho)$ and is given by

$$\begin{aligned} \mathcal{L}_D(\rho) &= \frac{1}{2} \sum_{j,k=1}^n a_{jk} \left([\lambda_j, \rho \lambda_k^\dagger] + [\lambda_j \rho, \lambda_k^\dagger] \right) \\ &= \frac{1}{2} \sum_{j,k=1}^n a_{jk} (2\lambda_j \rho \lambda_k - \{\lambda_k \lambda_j, \rho\}) \end{aligned} \quad (1)$$

where $A = A^\dagger = (a_{jk}) \geq 0$ i.e., $n \times n$ Hermitian positive semidefinite matrix, $[\cdot, \cdot]$ is the commutator of matrices, $[A, B] = AB - BA$, $\{\cdot, \cdot\}$ is the anticommutator, $\{A, B\} = AB + BA$, and λ_k the N -dimensional Pauli matrices λ_j , see for example [7] for their explicit expression (or Appendix A of Part II of [1] for $N = 2, 3, 4$).

Example 1. For $N = 2$

$$\lambda_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \lambda_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \lambda_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

The anticommutator for the λ_k matrices is given by $\{\lambda_j, \lambda_k\} = \frac{2\sqrt{2}}{N} \delta_{jk} \lambda_0 + \sum_{l=1}^n d_{jkl} \lambda_l$, with d_{jkl} fully symmetric two-tensor and $\lambda_0 = N^{-\frac{1}{2}} I$.

To \mathcal{L}_D (which is normally called the *relaxation* or *dissipation* part of the dynamics) one must add the Hamiltonian part given by

$$\mathcal{L}_H = -i[H, \rho] \quad (2)$$

where $-iH$ is a skew-Hermitian matrix in the special unitary Lie algebra $\mathfrak{su}(N)$ that can be expressed in terms of basis elements as $H = \sum_{m=1}^n h_m \lambda_m$ (see [2] for details). The set of admissible infinitesimal generators for our problem is then $\mathcal{L}(\rho) = \mathcal{L}_H(\rho) + \mathcal{L}_D(\rho)$ and is known under the name of quantum Markovian master equation. In fact $\mathcal{L} = \frac{d}{dt} (\Lambda_t)_{t=0}$.

4 Density operators and vectors of coherences

From (1) and (2) the ODE $\dot{\rho} = \mathcal{L}(\rho)$ does not look linear (neither affine) at first sight. However, its linearity can be emphasized by transforming the matrix system into a vector system with larger state update matrices. Operations like $vec(\cdot)$ (which stacks the columns of ρ thus obtaining a vector of dim N^2) are well-known in control theory, see e.g. [4], and can be used for this scope. For density operators, a physically motivated variant of $vec(\cdot)$ is the so-called vector of coherences formulation [1]. By dimension counting, the state matrix ρ depends on $n = N^2 - 1$ real parameters, since $\rho = \rho^\dagger$ and $\text{tr}(\rho) = 1$. Up to the imaginary unit, $N \times N$ traceless Hermitian matrices like our λ_k form the Lie algebra $\mathfrak{su}(N)$ of dimension exactly n . If to it we add the (properly normalized) unit vector λ_0 , then we obtain a complete basis for the density operator of an N -dimensional quantum mechanical system. In fact, the N -dimensional Pauli matrices λ_j and the identity matrix λ_0 , form a complete orthonormal set of basis operators for ρ (orthonormal in the sense that $\text{tr}(\lambda_j \lambda_k) = \delta_{jk}$). In particular, then, $\rho = \sum_{j=0}^n \text{tr}(\rho \lambda_j) \lambda_j = \sum_{j=0}^n \rho_j \lambda_j$, with $\rho_0 = N^{-\frac{1}{2}}$ fixed constant and the n real parameters ρ_j giving the parameterization of ρ .

Example 2. In the case of $N = 2$

$$\rho = \begin{bmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{bmatrix} = \rho_0 \lambda_0 + \rho_x \lambda_x + \rho_y \lambda_y + \rho_z \lambda_z$$

where $\rho_0 = \frac{1}{\sqrt{2}}$, $\rho_1 = \sqrt{2} \text{Re}[\rho_{01}]$, $\rho_2 = -\sqrt{2} \text{Im}[\rho_{01}]$ and $\rho_3 = \frac{1}{\sqrt{2}} (\rho_{00} - \rho_{11})$.

Call $\boldsymbol{\rho} = [\rho_1 \dots \rho_n]^T$ such *vector of coherences* of ρ . Due to the constant component along λ_0 , $\boldsymbol{\rho}$ is living on an affine space characterized by the extra fixed coordinate $\rho_0 = N^{-\frac{1}{2}}$. Such n dimensional space of affine vectors $\bar{\boldsymbol{\rho}} = [\rho_0 \rho_1 \dots \rho_n]^T = [\rho_0 \boldsymbol{\rho}^T]^T$ has Euclidean inner product given by the trace metric: $\|\bar{\boldsymbol{\rho}}\| = \sqrt{\langle \bar{\boldsymbol{\rho}}, \bar{\boldsymbol{\rho}} \rangle} = \sqrt{\text{tr}(\rho^2)}$. The condition $\text{tr}(\rho^2) \leq 1$ then translates in $\bar{\boldsymbol{\rho}}$ -space as $\bar{\boldsymbol{\rho}}$ belonging to the solid affine ball of radius 1 centered at $[\rho_0 \ 0 \ \dots \ 0]^T$, call it \mathbb{B}^n , for all positive times.

5 Admissible infinitesimal generators in the vector of coherences form

In $\bar{\boldsymbol{\rho}}$ -space, the terms $\mathcal{L}_H(\cdot)$ and $\mathcal{L}_D(\cdot)$ are linear $n \times n$ operators, also called *superoperators* in the Physics literature. Their expression is as follows:

$$\begin{aligned}\mathcal{L}_H(\rho) &= \bar{\mathcal{L}}_H \bar{\rho} = -i \left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & \text{ad}_H \end{array} \right] \bar{\rho} = -i \sum_{l=1}^n h_l \left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & \text{ad}_{\lambda_l} \end{array} \right] \bar{\rho} \\ &= - \sum_{l=1}^n h_l \left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & c_{lj}^k \end{array} \right] \bar{\rho} = \sum_{l=1}^n h_l \bar{C}_l \bar{\rho}\end{aligned}\quad (3)$$

$$\mathcal{L}_D(\rho) = \bar{\mathcal{L}}_D \bar{\rho} = \frac{1}{2} \sum_{1 \leq j, k \leq n} a_{jk} \left[\begin{array}{c|c} 0 & 0 \\ \hline \mathbf{v}_{jk} & L_{jk} \end{array} \right] \bar{\rho} = \frac{1}{2} \sum_{1 \leq j, k \leq n} a_{jk} \bar{L}_{jk} \bar{\rho} \quad (4)$$

where c_{ij}^k are the (real and fully skew-symmetric) structure constants of the Lie algebra $\mathfrak{su}(N)$ ($\text{ad}_{\lambda_l} = (\text{ad}_{\lambda_l})_{kj} = ic_{lj}^k$), the $n \times n$ matrices L_{jk} are given by:

$$L_{jk} = (L_{jk})_{lr} = \frac{1}{4} \sum_{m=1}^n ((c_{jr}^m - id_{jr}^m)c_{km}^l + (c_{kr}^m + id_{kr}^m)c_{jm}^l)$$

and the $n \times 1$ real vectors \mathbf{v}_{jk} are

$$\mathbf{v}_{jk} = \frac{i}{\sqrt{N}} [c_{jk}^1 \cdots c_{jk}^n]^T$$

These expressions were obtained in [1], Part II, eq. (II.4.18)-(II.4.19). The partition lines in the matrices above emphasize the use of homogeneous coordinates for the treatment of affine vector fields. The sum (4) contains only real linear combinations of real matrices, as it is shown in [3] Sec. IV.B by properly rearranging A and L_{jk} .

Example 3. In the case $N = 2$, from (3) one obtains the three 4×4 real skew symmetric matrices

$$\bar{M}_1 = \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{array} \right], \quad \bar{M}_2 = \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{array} \right], \quad \bar{M}_3 = \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]$$

while from (4) one gets the nine 4×4 real symmetric or “purely” affine matrices (see again [3] for the details)

$$\begin{aligned}\bar{M}_4 &= \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right], & \bar{M}_5 &= \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 \end{array} \right] \\ \bar{M}_6 &= \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{array} \right], & \bar{M}_7 &= \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]\end{aligned}$$

$$\bar{M}_8 = \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array} \right], \quad \bar{M}_9 = \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]$$

$$\bar{M}_{10} = \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{array} \right], \quad \bar{M}_{11} = \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{array} \right], \quad \bar{M}_{12} = \left[\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right]$$

As it is clear from the example of $N = 2$, the n^2 matrices \bar{L}_{jk} and the n matrices \bar{C}_l form a basis of the semidirect product of real Lie algebras $M(n, \mathbb{R}) \ltimes \mathbb{R}^n$ (of dimension $n^2 + n$).

From the Physics of the problem, the condition $\text{tr}(\rho^2) \leq 1$ can be reformulated as follows:

Proposition 1. *The dynamical system*

$$\dot{\bar{\rho}} = (\bar{\mathcal{L}}_H + \bar{\mathcal{L}}_D) \bar{\rho} \quad (5)$$

is defined and invariant on $\bar{\mathbb{B}}^n$.

6 The case of linear generators

Due to the presence of affine generators, the system (5) may have an equilibrium point which is different from the origin, which substantially complicates the intuition of the problem. For sake of simplicity, we only treat here the case of $\bar{\mathcal{L}}_D$ linear, rather than affine:

$$\bar{\mathcal{L}}_D = \left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & \mathcal{L}_D \end{array} \right]$$

Consider the inner product $\langle \cdot, \cdot \rangle$ in \mathbb{R}^{n+1} . Notice first that $\bar{\mathcal{L}}_H$ is linear and skew-symmetric and therefore $\langle \bar{\rho}, \bar{\mathcal{L}}_H \bar{\rho} \rangle = 0$. If also $\bar{\mathcal{L}}_D$ is linear, then $\langle \bar{\rho}, \bar{\mathcal{L}}_D \bar{\rho} \rangle = \rho^T \mathcal{L}_D \rho$. Furthermore, if $\mathcal{L}_D = \mathcal{L}_{D_s} + \mathcal{L}_{D_k}$ with \mathcal{L}_{D_s} symmetric and \mathcal{L}_{D_k} skew-symmetric, then $\langle \bar{\rho}, \bar{\mathcal{L}}_D \bar{\rho} \rangle = \rho^T \mathcal{L}_{D_s} \rho$. In order for $\bar{\mathbb{B}}^n$ to be invariant, it has to be $\rho^T \mathcal{L}_{D_s} \rho \leq 0$. To verify this, it is enough to consider any $\bar{\rho}_o$ such that $\|\bar{\rho}_o\| = 1$: the only (linear) infinitesimal generators admissible in this case in (5) are those determined by $\langle \bar{\rho}_o, \bar{\mathcal{L}}_D \bar{\rho}_o \rangle \leq 0$, which, again, correspond to $\text{tr}(\rho^2) \leq 1$ in the original problem formulation. Since this must hold for the entire sphere $\|\bar{\rho}\| = 1$, then it must be $\mathcal{L}_D \leq 0$.

7 Linear time-varying systems and bilinear control systems preserving positivity

The condition $A \geq 0$ on the $\bar{\mathcal{L}}_D$ part of the dynamics identifies a cone of matrices that can serve as Lindbladian for our matrix system. Each choice

of the n^2 parameters a_{jk} of A satisfying the constraint $A \geq 0$ preserve the positivity of the state space matrix ρ . Concerning the $\bar{\mathcal{L}}_H$ part, any linear combination of the \bar{L}_k is admissible.

For sake of simplicity, here we discuss only the case of \bar{L}_{jk} linear already treated in Section 6.

Proposition 2. *Consider the system*

$$\dot{\bar{\rho}} = \bar{\mathcal{L}}_H \bar{\rho} + \bar{\mathcal{L}}_D \bar{\rho} = \sum_{l=1}^n h_l \bar{C}_l \bar{\rho} + \frac{1}{2} \sum_{1 \leq j, k \leq n} a_{jk} \bar{L}_{jk} \bar{\rho} \quad (6)$$

with $\bar{C}_l = \begin{bmatrix} 0 & 0 \\ 0 & C_l \end{bmatrix}$, $\bar{L}_{jk} = \begin{bmatrix} 0 & 0 \\ 0 & L_{jk} \end{bmatrix}$ and $A = (a_{jk}) \geq 0$.

1. Any linear time-varying system $h_l = h_l(t)$ and $a_{jk} = a_{jk}(t)$ is admissible for the problem provided that $A(t) = (a_{jk})(t) \geq 0$, $\forall t \geq 0$;
2. Any of the time-varying parameters $h_l(t)$ and $a_{jk}(t)$ such that $(a_{jk})(t) \geq 0$, $\forall t \geq 0$ can be intended as a control input.

Proof. From the discussion at the end of Section 6

$$\langle \bar{\rho}, \dot{\bar{\rho}} \rangle = \rho^T \mathcal{L}_H \rho + \rho^T \mathcal{L}_D \rho = \rho^T \mathcal{L}_{D_s} \rho \leq 0$$

Thus the dynamics can at most contract toward $\rho = 0$, regardless of the values of the $h_l(t)$ and $a_{jk}(t)$ provided that $A(t) = (a_{jk})(t) \geq 0$, $\forall t \geq 0$. \square

Corollary 1. *All linear dynamics admissible by the problem are semistable and must belong to the cone generated by the identity as quadratic form in the Lyapunov equation i.e., $(\bar{\mathcal{L}}_H + \bar{\mathcal{L}}_D) + (\bar{\mathcal{L}}_H + \bar{\mathcal{L}}_D)^T \leq 0$.*

8 Conclusion

The main goal of this paper is to present the general class of linear dynamics that are preserving the positivity (and the trace) of a square Hermitian matrix. Such a model is well-studied in quantum mechanics and is of fundamental importance to avoid formal inconsistencies in the dynamical evolution of a density operator. It is arguable that such a characterization (and its intuitive interpretation given by the coherence vector) may be of interest also in other contexts where positive semidefiniteness of operators under dynamics (also controlled dynamics) is an issue.

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