

Conditions for strictly purity-decreasing quantum Markovian dynamics

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Abstract

The purity, $\text{Tr}(\rho^2)$, measures how pure or mixed a quantum state ρ is. It is well known that quantum dynamical semigroups that preserve the identity operator (which we refer to as unital) are strictly purity-decreasing transformations. Here, we provide an almost complete characterization of the class of strictly purity-decreasing quantum dynamical semigroups. We show that in the case of finite-dimensional Hilbert spaces, a dynamical semigroup is strictly purity-decreasing if and only if it is unital, while in the infinite dimensional case, unitality is only sufficient.

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1. Introduction

Quantum dynamical semigroups have been studied intensely in the mathematical and chemical physics literature since the pioneering work of Gorini et al. [1] and Lindblad [2]. They have a vast array of applications, spanning, e.g., quantum optics, molecular dynamics, condensed matter, and most recently quantum information [3–6].

In this work, we are interested in general conditions for dissipativity [2], namely the question of which class of quantum dynamical semigroups is guaranteed to reduce the purity of an arbitrary d -dimensional state ρ , where the purity p is defined as

$$p = \text{Tr}\rho^2. \quad (1)$$

The purity, which is closely related the Renyi entropy of order 2, $-\log \text{Tr}\rho^2$ [7], satisfies $1/d^2 \leq p \leq 1$, with the two extremes $p = 1/d^2, 1$ corresponding, respectively, to a fully mixed state and a pure state. The question we pose and answer in this work is

“What are the necessary and sufficient conditions on quantum dynamical semigroups for the purity to be monotonically decreasing ($\dot{p} \leq 0$)?”

To answer this question, we first revisit a general expression for \dot{p} using the Lindblad equation, in Section 2. We then give a derivation of a sufficient condition for purity-decreasing quantum dynamical semigroups in Section 3. This condition is valid for a large class of, even unbounded, Lindblad operators. We establish a necessary condition in Section 4, which is valid in finite-dimensional Hilbert spaces. Some examples are also discussed in this section. Concluding remarks are presented in Section 5.

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2. Purity and Markovian dynamics

The action of a quantum dynamical semigroup can always be represented as a master equation of the following form (we set $\hbar = 1$):

$$\frac{\partial \rho}{\partial t} = -i[H, \rho] + \mathcal{L}(\rho), \quad (2)$$

where H is the effective system Hamiltonian, and the Lindblad generator \mathcal{L} is

$$\mathcal{L}(\rho) = \frac{1}{2} \sum_{\alpha, \beta} a_{\alpha\beta} \left([G_{\alpha}, \rho G_{\beta}^{\dagger}] + [G_{\alpha}\rho, G_{\beta}^{\dagger}] \right). \quad (3)$$

The matrix $A = (a_{\alpha\beta})$ is positive semidefinite [ensuring complete positivity of the mapping $\exp(t\mathcal{L})$] and the Lindblad operators $\{G_{\alpha}\}$ are the coupling operators of the system to the bath [3]. One can always diagonalize A using a unitary transformation $W = (w_{\alpha\beta})$ and define new Lindblad operators $F_{\alpha} = \sqrt{\gamma_{\alpha}} \sum_{\beta} w_{\alpha\beta} G_{\beta}$ such that

$$\mathcal{L}(\rho) = \frac{1}{2} \sum_{\alpha} \left([F_{\alpha}, \rho F_{\alpha}^{\dagger}] + [F_{\alpha}\rho, F_{\alpha}^{\dagger}] \right), \quad (4)$$

where $\gamma_{\alpha} \geq 0$ are the eigenvalues of A . Note that, formally, for any A

$$\text{Tr}[\mathcal{L}(A)] = 0. \quad (5)$$

For the bounded semigroup-operators case (hence in particular in finite-dimensional Hilbert spaces) (3) provides the most general form of the completely positive trace preserving semigroup. However, the formal expression (2) makes sense with unbounded H and F_{α} provided certain technical conditions are satisfied [11]. In particular, $D = -iH - \sum F_{\alpha}^{\dagger} F_{\alpha}$ should generate a contracting semigroup of the Hilbert space and F_{α} should be well-defined on the domain of D . Under those technical conditions, one can construct the so-called *minimal solution* of (2) which may not be trace-preserving [11]. One should notice that in the unbounded case the solution $\rho(t)$ of (2) need not be differentiable unless $\rho(0)$ is in the domain of $-i[H, \cdot] + \mathcal{L}$.

In the following, when dealing with unbounded generators we tacitly assume that all these technical conditions are satisfied and then the formal mathematical expressions can be precisely defined. In particular, for unbounded A , the positivity condition $A \geq 0$ means that $\langle \phi | A | \phi \rangle \geq 0$ for all ϕ from a proper dense domain. The time-evolution of the purity can thus be expressed as

$$\begin{aligned} \dot{p} &= \text{Tr} \left(\rho \frac{\partial \rho}{\partial t} \right) + \text{Tr} \left(\frac{\partial \rho}{\partial t} \rho \right) \\ &= -i \text{Tr}(\rho[H, \rho]) - i \text{Tr}([H, \rho]\rho) + \text{Tr}(\rho \mathcal{L}(\rho)) \\ &\quad + \text{Tr}(\mathcal{L}(\rho)\rho). \end{aligned} \quad (6)$$

Recall that if A is bounded and B is trace-class then AB and BA are also trace-class, and $\text{Tr}(AB) = \text{Tr}(BA)$ [12]. Assuming bounded $\{F_{\alpha}\}$ we thus have

$$\begin{aligned} \dot{p} &= -2i \underbrace{\text{Tr}(\rho[H, \rho])}_{=0} + 2 \text{Tr}(\rho \mathcal{L}(\rho)) \\ &= \sum_{\alpha} \text{Tr}[\rho F_{\alpha} \rho F_{\alpha}^{\dagger}] - \text{Tr}[\rho^2 F_{\alpha}^{\dagger} F_{\alpha}], \end{aligned} \quad (7)$$

Thus, Hamiltonian control alone cannot change the first derivative of the purity, and hence cannot keep it at its initial value (the “no-cooling principle” [8]); the situation is different when one exploits the interplay between control and dissipation [9], or with feedback [10].

It is well-known that a sufficient condition for the purity to be a monotonically decreasing function under the Markovian dynamics, is that the Lindblad generator is *unital*, namely $\mathcal{L}(I) = 0$, where I is the identity operator [13]. But can this condition be sharpened? Indeed, we will show that unital Lindblad generators are in fact a special case of a more general class of quantum dynamical semigroups for which purity is strictly decreasing. In Section 3, we prove the following theorem:

Theorem 1. *A sufficient condition for $\dot{p} \leq 0$ under Markovian dynamics, Eqs. (2) and (4) is*

$$\mathcal{L}(I) = \sum_{\alpha} [F_{\alpha}, F_{\alpha}^{\dagger}] \leq 0 \quad (8)$$

whenever the generally unbounded formal operator (8) can be defined as a form on a suitable dense domain.

Note that Theorem 1 places no restriction on Hilbert-space dimensionality. Moreover, for particular cases condition (8) is meaningful for unbounded generators provided certain technical conditions concerning domain problems are satisfied (e.g., the amplitude raising channel, discussed below). Theorem 1 can be sharpened under an additional assumption:

Theorem 2. *In the case of finite-dimensional Hilbert spaces the purity is monotonically decreasing if and only if the Lindblad generator is unital,*

$$\mathcal{L}(I) = \sum_{\alpha} [F_{\alpha}, F_{\alpha}^{\dagger}] = 0. \quad (9)$$

This is proved in Section 4. Note that in the case of a finite-dimensional Hilbert space the Lindblad operators are automatically bounded.

3. Sufficiency

In this section we present three different proofs of sufficiency. The first is the most general, in that it is valid also for unbounded operators, under appropriate restrictions. The second and third are valid only for bounded operators and are presented for their pedagogical value.

3.1. General proof of sufficiency

We present a proof of Theorem 1 which is valid even for unbounded F_α , under the following technical conditions, which are satisfied for important examples of Lindblad generators [14]:

- There exists a dense subset $\mathcal{D} \subset \{\text{joint dense domain of all of } \{H, F_\alpha, F_\alpha^\dagger, \sum_\alpha F_\alpha^\dagger F_\alpha, \sum_\alpha F_\alpha F_\alpha^\dagger\}\}$;
- All finite range operators $\sum |\psi_k\rangle\langle\phi_k|$, where $|\psi_k\rangle, |\phi_k\rangle \in \mathcal{D}$, form a core $\mathcal{C}(\mathcal{L}')$ for the generator $\mathcal{L}' \equiv -i[H, \cdot] + \mathcal{L}$, i.e., for any ρ in the domain of \mathcal{L}' there exists a sequence $\rho_n \in \mathcal{C}(\mathcal{L}')$ such that $\rho_n \rightarrow \rho$, and $\mathcal{L}'(\rho_n) \rightarrow \mathcal{L}'(\rho)$;

It follows from condition (a) that the possibly infinite sums $\sum F_\alpha F_\alpha^\dagger \rho^2$ and $\sum F_\alpha^\dagger \rho F_\alpha \rho$ converge for all $\rho \in \mathcal{C}(\mathcal{L}')$. Therefore, the expression on the RHS of (7) is meaningful for all $\rho = \rho^\dagger \in \mathcal{C}(\mathcal{L}')$ and can be transformed into the form

$$-\frac{1}{2} \sum_\alpha \text{Tr} \left[(\rho F_\alpha - F_\alpha \rho)^\dagger (\rho F_\alpha - F_\alpha \rho) \right] + \text{Tr}(\rho^2 [F_\alpha, F_\alpha^\dagger]). \quad (10)$$

The first term is evidently negative. Then, due to Eq. (8), this leads to $\dot{p} \leq 0$ first for all $\rho \in \mathcal{C}(\mathcal{L}')$, and then by condition (b) for all ρ in the domain of \mathcal{L}' [15].

One should notice that in the finite-dimensional case condition (8) is equivalent to $\sum [F_\alpha^\dagger, F_\alpha] = 0$.

3.2. Proof using the dissipativity relation

Lindblad used properties of C*-algebras to prove (Eq. (3.2) in [2]) the general “dissipativity relation”

$$\mathcal{L}(A^\dagger A) + A^\dagger \mathcal{L}(I)A - \mathcal{L}(A^\dagger)A - A^\dagger \mathcal{L}(A) \geq 0. \quad (11)$$

This relation is valid for bounded generators \mathcal{L} (though it may be possible to extend it to the unbounded case). Taking the trace and using $\text{Tr}[\mathcal{L}(A^\dagger A)] = 0$, $A = \rho = \rho^\dagger$ then yields

$$\dot{p} = \text{Tr}[\rho(\mathcal{L}\rho)] + \text{Tr}[(\mathcal{L}\rho)\rho] \leq \text{Tr}[\rho^2 \mathcal{L}(I)]. \quad (12)$$

To guarantee $\dot{p} \leq 0$, it is thus sufficient to require $\text{Tr}[\rho^2 \mathcal{L}(I)] \leq 0$ for all states ρ . Using Eq. (4) yields $\mathcal{L}(I) = \sum_\alpha [F_\alpha, F_\alpha^\dagger]$, so that

$$\dot{p} \leq \text{Tr} \left\{ \rho^2 \sum_\alpha [F_\alpha, F_\alpha^\dagger] \right\} \leq 0. \quad (13)$$

Since $\rho^2 > 0$, it follows that it suffices for $\mathcal{F} \equiv \sum_\alpha [F_\alpha, F_\alpha^\dagger]$ to be a negative operator in order for the inequality to be satisfied [15]. We have thus proved that $\mathcal{L}(I) = \sum_\alpha [F_\alpha, F_\alpha^\dagger] \leq 0$, is sufficient.

3.3. Proof using the Schwarz inequality

We now give an alternative and more direct proof of sufficiency, which, again, is valid only in the case of bounded Lindblad operators. Let $X_\alpha = \rho F_\alpha$ and $Y_\alpha = \rho F_\alpha^\dagger$, and use this, along with $\sum_\alpha F_\alpha^\dagger F_\alpha = \sum_\alpha F_\alpha F_\alpha^\dagger - A$, where $A \leq 0$ and bounded, to rewrite Eq. (7) as

$$\begin{aligned} \dot{p} &= 2\text{Tr}(\rho \mathcal{L}(\rho)) = \text{Tr} \left(\rho \sum_\alpha ([F_\alpha, \rho F_\alpha^\dagger] + [F_\alpha \rho, F_\alpha^\dagger]) \right) \\ &= \sum_\alpha 2\text{Tr}[\rho F_\alpha \rho F_\alpha^\dagger] - \sum_\alpha \text{Tr}[\rho F_\alpha^\dagger F_\alpha \rho] \\ &\quad - \text{Tr} \left[\sum_\alpha \rho \left(\sum_\alpha F_\alpha F_\alpha^\dagger - A \right) \rho \right] \\ &= \sum_\alpha 2\text{Tr}[X_\alpha Y_\alpha] - \text{Tr}[Y_\alpha Y_\alpha^\dagger] - \text{Tr}[X_\alpha X_\alpha^\dagger] + \text{Tr}[\rho^2 A]. \end{aligned} \quad (14)$$

We can now apply the the Schwarz inequality for operators

$$\begin{aligned} |\text{Tr}(X^\dagger Y)| &\leq [\text{Tr}(X^\dagger X)]^{1/2} [\text{Tr}(Y^\dagger Y)]^{1/2} \\ &\leq \frac{1}{2} [\text{Tr}(X^\dagger X) + \text{Tr}(Y^\dagger Y)], \end{aligned} \quad (15)$$

and use the fact that $\text{Tr}[X_\alpha Y_\alpha] \geq 0$ [16] to yield

$$2\text{Tr}[X_\alpha Y_\alpha] - \text{Tr}[Y_\alpha Y_\alpha^\dagger] - \text{Tr}[X_\alpha X_\alpha^\dagger] \leq 0. \quad (16)$$

Additionally, $\text{Tr}[\rho^2 A] \leq 0$ (since $\rho^2 > 0$ and $A \leq 0$ by assumption), which completes the proof that $\dot{p} \leq 0$.

4. Necessity: a condition for finite-dimensional Hilbert spaces

We would now like to derive a necessary condition on the Lindblad operators F_α so that $\dot{p} \leq 0$ holds for all ρ . Our starting point is again Eq. (7), which is valid only for bounded F_α :

$$\dot{p} = \sum_\alpha \text{Tr}[\rho F_\alpha \rho F_\alpha^\dagger] - \text{Tr}[\rho^2 F_\alpha^\dagger F_\alpha] \leq 0. \quad (17)$$

We now restrict ourselves to the case of finite-dimensional Hilbert spaces. The inequality (17) must hold in particular for states ρ which are close to the fully mixed state, i.e., $\rho = (I \pm \varepsilon A)/\text{Tr}[I \pm \varepsilon A]$, where $0 < \varepsilon \ll 1$ and $A = A^\dagger$, $\|A\| \leq 1$, otherwise arbitrary. Let us find the constraint that must be obeyed by the F_α so that (17) is true for such states. This will be a necessary condition on the F_α .

Inserting this ρ into the inequality (17) yields

$$\begin{aligned}
0 &\geq \sum_{\alpha} \text{Tr}[(I \pm \varepsilon A)F_{\alpha}(I \pm \varepsilon A)F_{\alpha}^{\dagger}] \\
&\quad - \text{Tr}[(I \pm \varepsilon A)^2 F_{\alpha}^{\dagger} F_{\alpha}] \\
&= \sum_{\alpha} \text{Tr}[F_{\alpha} F_{\alpha}^{\dagger} \pm \varepsilon A F_{\alpha} F_{\alpha}^{\dagger} \pm \varepsilon F_{\alpha} A F_{\alpha}^{\dagger}] \\
&\quad - \text{Tr}[F_{\alpha}^{\dagger} F_{\alpha} \pm 2\varepsilon A F_{\alpha}^{\dagger} F_{\alpha}] + \text{O}(\varepsilon^2) \\
&= \sum_{\alpha} \text{Tr}[F_{\alpha}, F_{\alpha}^{\dagger}] \\
&\quad \pm \varepsilon \text{Tr}[A F_{\alpha} F_{\alpha}^{\dagger} + F_{\alpha} A F_{\alpha}^{\dagger} - 2A F_{\alpha}^{\dagger} F_{\alpha}] + \text{O}(\varepsilon^2). \quad (18)
\end{aligned}$$

The term $\text{Tr}[F_{\alpha}, F_{\alpha}^{\dagger}]$ vanishes and the second term in the last line becomes $\text{Tr}(A \sum_{\alpha} [F_{\alpha}, F_{\alpha}^{\dagger}])$. We may then divide by ε and take the limit $\varepsilon \rightarrow 0$, which yields

$$\pm \text{Tr} \left(A \sum_{\alpha} [F_{\alpha}, F_{\alpha}^{\dagger}] \right) \leq 0. \quad (19)$$

Since A is arbitrary this result can only be true for all A , if $\sum_{\alpha} [F_{\alpha}, F_{\alpha}^{\dagger}] = 0$. This is exactly the unitality condition. We have thus proved Theorem 2.

However, in the infinite-dimensional case the above argument fails since then in general $\text{Tr} F_{\alpha} F_{\alpha}^{\dagger} \neq \text{Tr} F_{\alpha}^{\dagger} F_{\alpha}$, or the trace may not even be defined. Indeed, take a (non-invertible) isometry V satisfying $V^{\dagger} V = I$ and $V V^{\dagger} = P$ (a projector). A physical example is given by the bosonic amplitude-raising semigroup (single Lindblad operator): $F = a^{\dagger} =$ the bosonic creation operator. Then $\mathcal{L}(I) = [F, F^{\dagger}] = [a^{\dagger}, a] = -I$, so the semigroup is non-unital. Yet, $\mathcal{L}(I) < 0$, so that by Theorem 1 (sufficiency) we know that this is a purity-decreasing semigroup. Another example, where $\mathcal{L}(I) \neq cI$ (c a constant), yet $\mathcal{L}(I) \leq 0$, is the case $F = a^{\dagger} a a^{\dagger}$ (this example is not even trace-preserving). We thus have:

Corollary 1. *In the infinite-dimensional case, the purity may be strictly decreasing without the Lindblad generator being unital.*

An example of a semigroup that does not satisfy $\mathcal{L}(I) \leq 0$ is the bosonic amplitude-damping semigroup, $F_{\alpha} = a$. For this semigroup $\mathcal{L}(I) = [F_{\alpha}, F_{\alpha}^{\dagger}] = [a, a^{\dagger}] = +I$. Thus, this semigroup is not in general purity-decreasing. Indeed, amplitude damping will in general purify a state ρ by taking it to the ground state $|0\rangle\langle 0|$, which is pure.

5. Conclusion

In this work we have provided necessary and sufficient conditions for Markovian open-system dynamics to be strictly purity-decreasing. These conditions are summarized in Theorems 1 and 2. It turns out that the well-known result that unital semigroups are purity-decreasing is a complete characterization (i.e., the condition is both necessary and sufficient) for finite-

dimensional Hilbert spaces. However, in the infinite-dimensional case it is possible for a semigroup to be strictly purity-decreasing without being unital. A simple example thereof is the bosonic amplitude-raising semigroup. We leave as an open question the problem of finding a necessary condition in the case of unbounded generators.

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- [13] For example R.F. Streater, Statistical Dynamics, Imperial College Press, 1995, Theorem 9.12 states that in finite dimensions any bistochastic map (which we refer to here as unital), not even completely positive, is a contraction in the Hilbert-Schmidt norm. This immediately implies that such a map is purity-decreasing. We note that in the Mathematical Physics community what we refer to as a unital map is usually referred to as bistochastic (or double stochastic). The difference is the Heisenberg versus the Schrödinger picture. Here, we adopt the terminology that is common in the Quantum Information community.
- [14] In order for Eq. (2) to be meaningful even in the case of unbounded operators we must define the domain of $\mathcal{L}' \equiv -i[H, \cdot] + \mathcal{L}$. This is assured by the stated conditions: (a) and (b). In particular, one starts with a “predomain” for which one can explicitly define $\mathcal{L}'\rho$. Such a “predomain” is given in (b), while (a) is necessary to define the action of \mathcal{L}' on an appropriate joint domain for all operators involved.
- [15] Here is a proof: $\rho^2 = \sum_j \lambda_j^2 |j\rangle\langle j|$ in the basis in which ρ is diagonal. As $\sum_{\alpha} [F_{\alpha}, F_{\alpha}^{\dagger}] < 0$ means that for all vectors $|f\rangle$, the inner product $\langle f, \sum_{\alpha} [F_{\alpha}, F_{\alpha}^{\dagger}] f \rangle < 0$, obviously

$$\text{Tr} \left(\rho^2 \sum_{\alpha} [F_{\alpha}, F_{\alpha}^{\dagger}] \right) = \sum_j \lambda_j^2 \left\langle j, \sum_{\alpha} [F_{\alpha}, F_{\alpha}^{\dagger}] j \right\rangle < 0.$$

This calculation makes sense even for unbounded $\sum_{\alpha}[F_{\alpha}, F_{\alpha}^{\dagger}]$ defined as a quadratic form, provided the vectors $|j\rangle$ belong to the domain of the quadratic form.

[16] Here is a proof:

$$\mathrm{Tr}[X_{\alpha}Y_{\alpha}] = \mathrm{Tr}[\rho F_{\alpha}\rho F_{\alpha}^{\dagger}] = \mathrm{Tr}[\rho_D F'_{\alpha}\rho_D F'^{\dagger}_{\alpha}],$$

where U is the unitary matrix that diagonalizes ρ , $\rho_D = U^{\dagger}\rho U$ is diagonal with eigenvalues $\lambda_i \geq 0$, and $F'_{\alpha} = U^{\dagger}F_{\alpha}U$. Explicitly evaluating the trace yields:

$$\mathrm{Tr}[\rho_D F'_{\alpha}\rho_D F'^{\dagger}_{\alpha}] = \sum_{ijkl} \lambda_i \delta_{ij} (F'_{\alpha})_{jk} \lambda_k \delta_{kl} (F'^{\dagger}_{\alpha})_{li} = \sum_{ik} \lambda_i \lambda_k |(F'_{\alpha})_{ik}|^2 \geq 0.$$