Evolution of any finite open quantum system always admits a Kraus-type representation, although it is not always completely positive

D. Salgado* and J. L. Sánchez-Gómez†
Departamento de Física Teórica, Universidad Autónoma de Madrid, 28049 Cantoblanco, Madrid, Spain

M. Ferrero‡
Departamento de Física, Universidad de Oviedo, 33007 Oviedo, Spain
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We argue that a full account of the set of quantum states prevents one from applying the rigorous definition of complete positivity. However, we give three equivalent proofs that any quantum evolution of a finite system always admits a Kraus-type decomposition, i.e., a Kraus decomposition but with Kraus matrices dependent on the initial state upon which they apply.

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Initial correlations between an open quantum system and its surrounding environment have traditionally played a remarkable role to elucidate whether the reduced evolution of the open system is completely positive (CP) or not [1–3]. This property appears as an important ingredient in the study of general evolutions (both unitary and projective) of this kind of physical system [4–7].

Until recently, these initial correlations were thought to be unsurpassable for the evolution to be CP in a totally general sense [8]. However, some results have been found showing that this is not the case in particular situations, i.e., that despite the initial correlations the evolution is CP [9,10].

The physical picture where complete positivity in principle arises is surprisingly simple: consider a system and its environment with no interaction between them; then under the assumption of no evolution for the latter, the joint system must evolve from a valid state (density operator) to another valid state (density operator). And one expects that this must be so even in the presence of initial correlations between them. We will argue that despite this crystal-clear reasoning, it does not imply the complete positivity of quantum evolutions, as suggested in some places (cf., e.g., [11]).

We devote this work to elucidate further this issue and to show that the application of the mathematical notion of complete positivity should be used with care and that indeed one can find explicit examples of open systems whose evolution is not CP. However, on the contrary, we also prove that any evolution always admits a Kraus-type decomposition, i.e., an expression of the form

$$\Lambda(t)[\rho] = \sum_k M_k(t;\rho)\rho M_k^\dagger(t;\rho), \qquad (1)$$

where the Kraus matrices $M_k(t;\rho)$ depend on the initial density operator ρ upon which they apply. Only when this dependence drops out can one be sure that the evolution is truly CP.

Let us begin by recalling the mathematical definition of the set of quantum states for an arbitrary physical system [4]: the set $\mathcal{T}^{+,1}(\mathfrak{H})$ of trace-class unit-trace self-adjoint linear operators upon a complex separable Hilbert space $\mathfrak{H}$. This is a convex set,[1] but *it is not a linear space*. This is a relevant feature often not duly considered. The reader may convince himself very easily: $\mu_1\rho_1+\mu_2\rho_2$ is not a valid state for *any* μ_1,μ_2. As a consequence, one cannot claim in a rigorous mathematical sense that the evolution operator $\Lambda(t):\mathcal{T}^{+,1}\to\mathcal{T}^{+,1}$ is linear, since for an operator to be linear its domain must be a linear (sub)space [12]. At most, evolution operators preserve convexity, i.e., $\Lambda(t)[\mu_1\rho_1+\mu_2\rho_2]=\mu_1\Lambda(t)[\rho_1]+\mu_2\Lambda(t)[\rho_2]$ for all $\rho_1,\rho_2\in\mathcal{T}^{+,1}(\mathfrak{H})$ and all $\mu_1,\mu_2\in[0,1]$ such that $\mu_1+\mu_2=1$. This is how linearity is usually understood when referring to quantum evolution (cf., e.g., [13]).

As a first point, however, this distinction shows relevant consequences for the mathematical usage of complete positivity, since this is a property to be applied to *linear operators*, thus, in a rigorous sense, an evolution operator will never be CP (cf., e.g., [14,15] for the mathematical definition of complete positivity). Complete positivity should be used (and in fact it is used) in the following manner. A quantum evolution operator $\Lambda(t):\mathcal{T}^{+,1}(\mathfrak{H})\to\mathcal{T}^{+,1}(\mathfrak{H})$ is said to be CP if its extension $\tilde{\Lambda}(t):\mathcal{T}(\mathfrak{H})\to\mathcal{T}(\mathfrak{H})$ is CP, where $\mathcal{T}(\mathfrak{H})$ denotes the linear subspace of trace-class self-adjoint linear operators on $\mathfrak{H}$.

Consequently, the question of whether a given evolution operator admits more than one extension must be answered in order for it to be CP in a meaningful way. This is solved with the following result.

Proposition. Let $\Lambda: C\subset\mathfrak{A}\to C$ be a map from a convex subset C of a vector space $\mathfrak{A}$ to itself. Then (i) if C is contained in a subspace $\mathfrak{B}\subset\mathfrak{A}$, Λ admits more than one linear extension on $\mathfrak{A}$; (ii) let $\{e_i\}_{i\in\mathbb{N}}$ be elements of C, if the linear hull of $\{e_i\}_{i\in\mathbb{N}}$ is $\mathfrak{A}$, i.e., $\mathcal{V}\{e_i\}=\mathfrak{A}$, then any linear extension $\tilde{\Lambda}$ of Λ is unique.

Proof. The first part can be easily proven, since if Λ is defined only on a subset contained in a subspace $\mathfrak{B}$ of $\mathfrak{A}$, its

*Email address: david.salgado@uam.es
†Email address: jl.sanchezgomez@uam.es
‡Email address: maferrero@uniovi.es

[1]Indeed, a convex cone in the set of trace-class self-adjoint linear operators on $\mathfrak{H}$.

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action on the elements of a basis not contained in such a subspace $\mathfrak{B}$ is not defined and can, therefore, be arbitrarily defined.

For the second part, notice that, by hypothesis, one can find x_k such that $X=\Sigma_k x_k e_k$. The image of X can also be written as

$$\Lambda[X] = \sum_k y_k e_k. \tag{2}$$

Let now $\tilde{\Lambda}_1$ and $\tilde{\Lambda}_2$ be two linear extensions of Λ. Then, for all $X \in \mathfrak{A}$, we have

$$\tilde{\Lambda}_1[X] = \sum_k y_k^{(1)} e_k, \tag{3a}$$

$$\tilde{\Lambda}_2[X] = \sum_k y_k^{(2)} e_k. \tag{3b}$$

From the linearity, we can write

$$\tilde{\Lambda}_1[e_k] = \sum_p J_{kp}^{(1)} e_p, \tag{4a}$$

$$\tilde{\Lambda}_2[e_k] = \sum_p J_{kp}^{(2)} e_p, \tag{4b}$$

thus

$$y_m^{(1)} = \sum_n x_n J_{nm}^{(1)}, \tag{5a}$$

$$y_m^{(2)} = \sum_n x_n J_{nm}^{(2)}. \tag{5b}$$

Now notice that if $X \in C$, we will have $y_m^{(1)} = y_m^{(2)}$ for all m, that is, $J_{nm}^{(1)} = J_{nm}^{(2)}$ for all $X \in C$; but, since $J^{(1)}$ and $J^{(2)}$ do not depend on X, we will have $J_{nm}^{(1)} = J_{nm}^{(2)}$ for all $X \in \mathfrak{A}$, i.e., $\tilde{\Lambda}_1 = \tilde{\Lambda}_2$.

□

Since our main concern refers to finite systems, we will focus on algebras of complex matrices, i.e., the set of quantum states will be the convex subset of unit-trace positive complex matrices[2] of dimension N; the linear space $\mathfrak{A}$ will be the vector space $\mathcal{M}_N(\mathbb{C})$ of complex matrices and the extension of the evolution operators will be linear maps $\tilde{\Lambda}(t)$ such as $\tilde{\Lambda}(t): \mathcal{M}_N(\mathbb{C}) \to \mathcal{M}_N(\mathbb{C})$.

On the other hand, in order to know whether a given linear map is CP or not, one needs criteria of complete positivity, preferably of straightforward use. In this respect, we have centered on the Jamiołkowski isomorphism $\mathcal{J}: \mathcal{L}[\mathcal{M}_N(\mathbb{C})] \to \mathcal{M}_N(\mathbb{C}) \otimes \mathcal{M}_N(\mathbb{C})$, where $\mathcal{L}[\mathcal{M}_N(\mathbb{C})]$ denotes the vector space of linear maps in $\mathcal{M}_N(\mathbb{C})$, defined by

$$\mathcal{J}_E[\Lambda] \equiv \sum_{i,j=1}^{N} \Lambda[E_{ij}] \otimes E_{ij}, \tag{6}$$

where $E_{ij} \equiv |i\rangle\langle j|$ and the subscript E makes explicit reference to this choice of Weyl basis E_{ij}. This criterion then establishes that Λ is CP if and only if $\mathcal{J}_E[\Lambda]$ is positive.[3] From a physical standpoint, interest in complete positivity arises after showing that it is a necessary and sufficient condition for a linear map to admit the Kraus decomposition [17,18], i.e., the form given by

$$\Lambda[X] = \sum_k M_k X M_k^\dagger, \tag{7}$$

where the set of so-called Kraus matrices $\{M_k\}$ is not unique. This form plays a prominent role in disciplines like the Foundations of Quantum Theory [5] and Quantum Information [19]. Using the selected Weyl basis E_{ij}, the set of Kraus matrices is determined by *any* square root of[4] $\mathcal{J}_E[\Lambda]^* = QQ^\dagger$: the coordinates of M_p in the basis E_{ij} are the elements of the pth column of Q. Any other set of Kraus matrices can be obtained with the same procedure though starting with $\tilde{Q} \equiv QU$, where U is any arbitrary unitary matrix.

As a straightforward example, let us briefly discuss the well-known depolarizing channel on qubits [19] $\Lambda[\rho] = \mu\rho + [(1-\mu)/2]\mathbb{I}_2$ with $\mu \in [0,1]$. This quantum evolution admits a unique linear extension given by $\tilde{\Lambda}[X] = \mu X + [(1-\mu)/2]\mathrm{tr}[X]\mathbb{I}_2$, where $X \in \mathcal{M}_N(\mathbb{C})$, which after using the Jamiołkowski isomorphism yields the point spectrum of $\mathcal{J}_E[\Lambda]$ given by $(1-\mu)/2$ (triple) and $(1+3\mu)/2$, thus it is positive, hence Λ is CP. For the extreme case $\mu=0$, of interest for later results, a posible set of Kraus matrices is given by $M_{ij} = (1/\sqrt{2})E_{ij}$ with $i,j=1,2$, since $Q=(1/\sqrt{2})\mathbb{I}_4$. But another one can be found after using $\tilde{Q}=QU$ with

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -i \\ 0 & 0 & 1 & i \\ 1 & -1 & 0 & 0 \end{pmatrix},$$

$M_1 = \frac{1}{2}\mathbb{I}_2$, $M_2 = \frac{1}{2}\sigma_x$, $M_3 = \frac{1}{2}\sigma_y$, and $M_4 = \frac{1}{2}\sigma_z$, which straightforwardly drives one to

$$\mathbb{I}_2 = \frac{1}{2}(\rho + \sigma_x\rho\sigma_x + \sigma_y\rho\sigma_y + \sigma_z\rho\sigma_z). \tag{8}$$

With these tools, we will then show that any quantum evolution of a finite system always admits a Kraus-type decomposition, i.e., a form like

$$\Lambda(t)[\rho] = \sum_k M_k(t;\rho)\rho M_k^\dagger(t;\rho). \tag{9}$$

In general, four equivalent proofs can be given. For simplicity, let us first focus on two-level systems, that is, on qubits. Let $\Lambda(t)$ denote a general quantum evolution. Let us consider the related linear map given by $\tilde{\Lambda}_\rho(t)[X] \equiv \mathrm{tr}[X]\Lambda(t)[\rho]$, for all $X \in \mathcal{M}_2(\mathbb{C})$. This maps all initial quan-

[2]Positive Hermitian semidefinite matrices.

[3]An accesible direct simple proof of this result can be found in [16].

[4]As usual, * denotes complex conjugation. Note that *stricto sensu* Q is not the square root of $\mathcal{J}_E[\Lambda]^*$ [20]; the difference introduced for simplicity's sake is just a matter of definition.

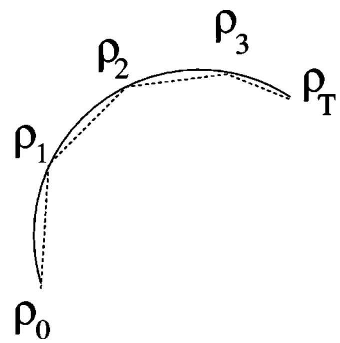

FIG. 1. Schematic construction of an approximating polygonal line.

tum states in the same state $\Lambda(t)[\rho]$ at time t. Now $\widetilde{\Lambda}_\rho$ is clearly CP, since $\mathcal{J}_E[\widetilde{\Lambda}_\rho]\geqslant 0$ and it admits a set of Kraus matrices $M_k(t;\rho)$, since $\mathcal{J}_E[\widetilde{\Lambda}_\rho(t)]^* = Q(t;\rho)Q^\dagger(t;\rho)$, thus

$$\widetilde{\Lambda}_\rho(t)[X] = \sum_k M_k(t;\rho)XM_k^\dagger(t;\rho), \tag{10}$$

which, when applied to quantum states $\sigma\in\mathcal{T}^{+,1}(\mathfrak{H})$, reduces to

$$\widetilde{\Lambda}_\rho(t)[\sigma] = \sum_k M_k(t;\rho)\sigma M_k^\dagger(t;\rho) \tag{11}$$

and in particular when $\sigma=\rho$, thus

$$\widetilde{\Lambda}_\rho(t)[\rho] = \rho(t) = \Lambda(t)[\rho] = \sum_k M_k(t;\rho)\rho M_k^\dagger(t;\rho) \tag{12}$$

for each ρ.

Equivalently, if $\rho(t)\equiv\Lambda(t)[\rho]\geqslant 0$, which is always the case, one can find a matrix $q(t;\rho)$ such that $\rho(t) = q(t;\rho)q^\dagger(t;\rho) = q(t;\rho)\mathbb{I}_2 q^\dagger(t;\rho)$ and using Eq. (8)

$$\Lambda(t)[\rho] = \frac{1}{2}q(t;\rho)(\rho + \sigma_x\rho\sigma_x + \sigma_y\rho\sigma_y + \sigma_z\rho\sigma_z)q^\dagger(t;\rho), \tag{13}$$

which clearly shows a Kraus-type form.

A third more geometrical proof can be obtained working in Bloch space [21,22], whose general structure combined with general properties of quantum dynamical maps [23] allow us to view quantum evolutions as time-continuous curves in a convex compact subset of $\mathbb{R}^{N^2-1}$, where N stands for the dimension of the quantum system. The result then follows from noticing that (i) any such time-continuous curve can be understood as the limit of a polygonal line, as in Fig. 1, and (ii) each straight segment of the approximating polygonal line is a CP map given by

$$\Lambda_k(t) = \frac{t-t_{k-1}}{t_k-t_{k-1}}\rho(t_{k-1}) + \frac{t_k-t}{t_k-t_{k-1}}\rho(t_k)$$

when $t\in[t_{k-1},t_k]$, which can be viewed as a *generalized depolarizing channel*. This channel is proven to be CP upon a direct application of the preceding criterion. It is clear that these generalized depolarizing channels which build up the whole evolution depend on the initial point of the Bloch space, i.e., a different initial state implies different generalized depolarizing channels, hence relation (1).

The fourth proof was outlined in [24], though the authors do not make explicit reference to the dependence of the Kraus matrices on the initial density operator. The generalization to any finite-dimensional quantum system is straightforward once one realizes that in the first, third, and fourth proofs, the dimension of the system was not used at all.

Note, however, that one cannot conclude from this result that any quantum evolution is CP; only when the dependence of the Kraus matrices on the initial state ρ drops out is complete positivity assured. It is clear that there are circumstances in which this dependence is spurious, as in unitary evolutions or in the preceding depolarizing channel. But one can also find examples in which the evolution cannot adopt a truly Kraus decomposition, i.e., it is not CP. Let us consider a two-level system (usually considered as representing an atom) interacting with squeezed light, whose frequency is tuned to that of the atomic transition. It can be shown that the evolution of such an atomic system is given, in Bloch decomposition language [21,22], by [25]

$$\frac{dx(t)}{dt} = -\gamma_x x(t), \tag{14a}$$

$$\frac{dy(t)}{dt} = -\gamma_y y(t), \tag{14b}$$

$$\frac{dz(t)}{dt} = -\gamma_z z(t) - \gamma, \tag{14c}$$

where $x(t)$, $y(t)$, and $z(t)$ denote the Bloch vector components of the atomic system, and γ_x, γ_y, γ_z, and γ are positive constants (cf. [25] for their origin and meaning). After a little bit of algebra, one finds that this evolution admits the following linear extension in the Weyl basis $E_{11}=\frac{1}{2}(\mathbb{I}_2+\sigma_z)$, $E_{22}=\frac{1}{2}(\mathbb{I}_2-\sigma_z)$, $E_{12}=\frac{1}{2}(\sigma_x+i\sigma_y)$, and $E_{21}=E_{12}^\dagger$:

$$\widetilde{\Lambda}(t)[E_{11}] = \left[e^{-\gamma_z t}\left(1+\frac{\gamma}{\gamma_z}\right) - \frac{\gamma}{\gamma_z}\right]E_{11}, \tag{15a}$$

$$\widetilde{\Lambda}(t)[E_{22}] = \left[e^{-\gamma_z t}\left(1-\frac{\gamma}{\gamma_z}\right) + \frac{\gamma}{\gamma_z}\right]E_{22}, \tag{15b}$$

$$\widetilde{\Lambda}(t)[E_{12}] = \frac{e^{-\gamma_x t}+e^{-\gamma_y t}}{2}E_{12} + \frac{e^{-\gamma_x t}-e^{-\gamma_y t}}{2}E_{21}, \tag{15c}$$

$$\widetilde{\Lambda}(t)[E_{21}] = \frac{e^{-\gamma_x t}-e^{-\gamma_y t}}{2}E_{12} + \frac{e^{-\gamma_x t}+e^{-\gamma_y t}}{2}E_{21}. \tag{15d}$$

After applying the Jamiołkowski isomorphism, one finds $\mathcal{J}_E[\widetilde{\Lambda}(t)]\not\geqslant 0$, since two of its eigenvalues are $\pm(e^{-\gamma_x t} - e^{-\gamma_y t})/2$, one of which is clearly negative provided $\gamma_x \neq \gamma_y$. Thus the unique linear extension of such a quantum evolution is not CP.

As a conclusion, we claim that complete positivity should only be applied to quantum evolution in the sense explained above, i.e., to the unique linear extension of the quantum evolution map. This stems from the fact that the set of quantum states is not a linear space and, thus, rigorous definitions cannot be applied. Notice that this also entails a revision of the physical justification of complete positivity alluded to in the third paragraph: the mathematical definition is not an exact translation of this physical picture. As a possible clever remark, it can be alleged that working in the Heisenberg picture, where observables do evolve, i.e., where self-adjoint operators are time-dependent, the alluded restriction of the application of complete positivity disappears. But let us remember that this representation rests on the duality between the space of all trace-class self-adjoint operators $\mathcal{T}(\mathfrak{H})$ and the space of linear operators $\mathcal{L}(\mathfrak{H})$ (cf. [4]), so the criticism still holds. One may object that this is too mathematically rigorous, but notice that from a minimal set of physical axioms for quantum theory [26] only those trace-class unit-trace self-adjoint operators are physically justified as quantum states, i.e., those belonging to $\mathcal{T}^{+,1}(\mathfrak{H})$. However, it must always be present that a Kraus-type form, which shows a physical origin [5,17], can always be ascribed to such quantum evolutions. Only in certain circumstances do these evolutions adopt a truly Kraus decomposition, thus being CP. In this sense, the question of initial correlations and complete positivity has been reformulated, and the connection between them and the dependence of Kraus matrices upon initial states appears as a new possibility to understand the role of those initial correlations.

This result also entails relevant consequences for the structure of the evolution equation of quantum states. Lindblad's theorem [11,27] establishes such a structure in the case of Markovian evolutions under the complete positivity hypothesis, namely

$$\frac{d\rho(t)}{dt} = -i[H,\rho(t)] + \Psi[\rho(t)] - \frac{1}{2}\{\Psi[\mathbb{I}],\rho(t)\}, \qquad (16)$$

where Ψ denotes a CP map. From our results and reconstructing the proof of this theorem as in [7], the complete positivity assumption may drop out and still we have a structure similar to Eq. (16) for any Markovian evolution,

$$\frac{d\rho(t)}{dt} = -i[H,\rho(t)] + \Psi(\rho(t))[\rho(t)] - \frac{1}{2}\{\Psi(\rho(t))[\mathbb{I}],\rho(t)\}, \qquad (17)$$

but now the map $\Psi(\rho)$ depends on the density operator and admits a Kraus-type form,

$$\Psi(X)[X] = \sum_k M_k(X) X M_k^{\dagger}(X). \qquad (18)$$

Note that again the study of the conditions upon which the dependence of the Kraus matrices upon the initial state appears is the key concept. The case of non-Markovian evolution still awaits equal exploration.

We conclude with Pechukas [1] (cf. also [2,3]) that quantum evolution need not be completely positive. Furthermore, *stricto sensu*, it is never CP, though the role of the initial correlations with the environment should be further elucidated in the form of the dependence of the Kraus matrices upon the initial state of the system.

Though we have dealt only with finite systems, we are convinced that the generalization to infinite-dimensional systems is just a technical matter and there should be no physical difference in the conclusions.

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