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PHYSICS LETTERS A
Physics Letters A 341 (2005) 48–54
www.elsevier.com/locate/pla

Who's afraid of not completely positive maps?

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Received 13 February 2005; received in revised form 15 March 2005; accepted 14 April 2005

Available online 22 April 2005

Communicated by P.R. Holland

Abstract

The arguments that are often put forward to justify the singular importance given to completely positive maps over more generic maps in describing open quantum evolution are studied. We find that these do not appear convincing on closer examination. Positive as well as not positive maps are good candidates for describing open quantum evolution.

PACS: 03.65.Yz; 03.67.Mn; 03.65.Ta

Keywords: Open quantum systems; Reduced dynamics; Entanglement; Not completely positive maps

1. Introduction

The most general evolution of a quantum mechanical system is by linear transformations that map density matrices to density matrices. It follows from the properties of density matrices that the mappings must preserve Hermiticity, trace and positivity [1]. When certain approximations hold [2,3] and the linear maps form a semi-group, a Markovian master equation called the Kossakowski–Lindblad equation [4–6] can also be used to describe open quantum dynamics. The maps on density matrices and quantum master equations along with other approaches like the influence functional method [7] are significant pieces in the effort to understand and characterize the dynamics of open quantum systems and their evolution [8].

There has been a substantial amount of interest in studying a sub-class of linear maps on density matrices called completely positive maps (see, for example, [9–14]). Such maps do not exhaust all possible dynamical behavior an open quantum system may exhibit. In spite of this, the more general possibilities allowed in open quantum dynamics have received only limited attention [15–17] compared to completely positive maps. The aim of this Letter is to examine closely the arguments that have been put forward to favor completely positive maps over more general maps as pos-

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0375-9601/$ – see front matter
doi:10.1016/j.physleta.2005.04.029

sible descriptions of the evolution of quantum systems subject to external influences.

2. Choi's theorem, complete positivity and the witness

Choi, in his seminal work on completely positive maps [18], describes the distinction between positive and completely positive maps on C^*-algebras. Choi's definition of a completely positive map may be paraphrased as follows: Consider a linear map $\Phi : \mathfrak{A} \to \mathfrak{B}$ between two C^*-algebras $\mathfrak{A}$ and $\mathfrak{B}$. The map Φ is *positive* if $\Phi(A) \geqslant 0$ for all positive $A \in \mathfrak{A}$. Let $\mathcal{M}_n$ be the collection of all $n \times n$ complex matrices and $\mathcal{M}_n(\mathfrak{A}) = \mathfrak{A} \otimes \mathcal{M}_n$ be the C^*-algebra of $n \times n$ matrices over $\mathfrak{A}$; meaning all $n \times n$ (block) matrices with the elements of the matrices being elements of $\mathfrak{A}$. Now define $\Phi \otimes \mathbf{1}_n : \mathcal{M}_n(\mathfrak{A}) \to \mathcal{M}_n(\mathfrak{B})$ by $\Phi \otimes \mathbf{1}_n((A_{jk})_{1 \leqslant j,k \leqslant n}) = (\Phi(A_{jk}))_{1 \leqslant j,k \leqslant n}$. Here $(A_{jk})_{jk}$ denotes a block matrix with $A_{jk} \in \mathfrak{A}$ occupying the jk-th block. We say that Φ is n-positive if $\Phi \otimes \mathbf{1}_n$ is positive. The set of all n-positive linear maps on $\mathfrak{A}$ is denoted by $\mathbb{P}_n[\mathfrak{A}, \mathfrak{B}]$.

Φ is said to be *completely positive* if $\Phi \in \mathbb{P}_\infty[\mathfrak{A}, \mathfrak{B}]$.

Choi goes on to prove several theorems on positivity and complete positivity including the useful result that if a map $\Phi : \mathfrak{A} \to \mathcal{M}_n$ is n-positive then it is completely positive, where n is the dimensionality of the Hilbert space on which the C^*-algebra $\mathfrak{A}$ is defined.

2.1. The witness

Let us leave Choi's definition of complete positivity aside for a moment and look at the "physical arguments" given for accepting only completely positive maps as describing the evolution of open quantum systems. The following passage is representative of similar arguments seen widely in the literature.[1]

> A completely positive map is not only a reasonable map from density operators to density operators for S, but it is extensible in a trivial way to a reasonable map from density operators to density operators on any larger system $S + W$. Since we cannot exclude a priori that our system S is in fact initially entangled with some distant isolated system W, any acceptable Φ had better satisfy this condition.

The reduced dynamics of the system S described by the map Φ is induced by the coupled unitary evolution of S and a suitable environment R. At this point there is no restriction of complete positivity on the map. The trick by which complete positivity is imposed on Φ is to introduce an auxiliary system called the *witness* W that is separate from R. The witness is assumed to be 'blind' in the sense that it does not interact with S and 'dead' in that it has no free evolution of its own. Pechukas, in [15], was one of the first to question the implications of introducing the witness that is statistically coupled to S but otherwise inert. In Pechukas' own words:

> One may reasonably doubt this argument. It is very powerful magic: W sits apart from $S + R$ and does absolutely nothing; by doing so, it forces the motion of S to be completely positive with dramatic physical consequences such as $T_2 \leqslant 2T_1$ for exponential two-state relaxation.

The motivation for introducing the witness is clear. From Choi's result it appears that to keep the action of $\Phi \otimes \mathbf{1}_W$ positive on the states of $S + W$, Φ must be completely positive. Expecting $\Phi \otimes \mathbf{1}_W$ to be positive is perfectly reasonable because just the mere presence of W cannot suddenly make the dynamics of $S + W$ unphysical.

2.2. The significance of S and W being entangled

The first step in analyzing the effect of introducing the witness on Φ is to understand the role of the entanglement between S and W in imposing complete positivity. We do this by working out explicitly a couple of simple examples. We assume that the system S is as simple as it gets and is a *qubit* with density matrix ρ. Since the map Φ acts on a two-dimensional Hilbert space, it is sufficient to show that Φ is 2-positive in order to show that it is completely positive. With this in mind we choose the witness to be a qubit also with

[1] We have taken the liberty of making the mathematical notation uniform in the passages quoted in this Letter.

density matrix ρ_W. Let us keep the initial states of the system and witness completely general and choose

$$\rho = \frac{1}{2}(1 + a_j\sigma_j) = \frac{1}{2}\begin{pmatrix} 1+a_3 & a_1 - ia_2 \\ a_1 + ia_2 & 1 - a_3 \end{pmatrix},$$
$$\rho_W = \frac{1}{2}(1 + w_k\tau_k) = \frac{1}{2}\begin{pmatrix} 1+w_3 & w_1 - iw_2 \\ w_1 + iw_2 & 1 - w_3 \end{pmatrix}, \tag{1}$$

where σ_j and τ_k, $j, k = 1, 2, 3$, are two sets of Pauli matrices. Let

$$\alpha = \sqrt{a_1^2 + a_2^2 + a_3^2} \quad \text{and} \quad \omega = \sqrt{w_1^2 + w_2^2 + w_3^2}.$$

For ρ and ρ_W to be states, we require $-1 \leqslant a, w \leqslant 1$. If we assume that there is no entanglement between S and W then from the way the witness is defined, we know that the initial state of $S + W$ is a simple product state

$$\mathcal{R}_{\text{sep}} = \frac{1}{4}(1 + a_j\sigma_j) \otimes (1 + w_k\tau_k).$$

The eigenvalues of $\mathcal{R}_{\text{sep}}$ are

$$\lambda_1 = \frac{1}{4}(1-\alpha)(1-\omega), \qquad \lambda_2 = \frac{1}{4}(1-\alpha)(1+\omega),$$
$$\lambda_3 = \frac{1}{4}(1+\alpha)(1-\omega), \qquad \lambda_4 = \frac{1}{4}(1+\alpha)(1+\omega), \tag{2}$$

which are all positive semi-definite. Starting from this valid two qubit state, let us apply a map on ρ which we know to be positive but not completely positive. An easy choice is the transposition map $\mathbf{T}$. The action of $\mathbf{T}$ on ρ is to change a_2 to $-a_2$ and leave a_1 and a_3 unchanged. This transformation does not change α and hence does not change λ_i. In other words, we find that $\mathcal{R}'_{\text{sep}} = (\mathbf{T} \otimes \mathbf{1}_W)\mathcal{R}_{\text{sep}}$ is also a positive matrix.

Another example is a map that Choi introduces in [18] as one that is $(n-1)$ positive but not n positive:

$$\Phi^C(A) = \{(n-1)(\operatorname{tr} A)\}\mathbf{1}_n - A.$$

The action of Φ^C (with $n = 2$) on ρ is

$$\rho' = \Phi^C(\rho) = \frac{1}{2}\begin{pmatrix} 1-a_3 & -a_1 + ia_2 \\ -a_1 - ia_2 & 1 + a_3 \end{pmatrix}. \tag{3}$$

In other words, $a_j \to -a_j$, $j = 1, 2, 3$. Again, this transformation does not change α and therefore $\mathcal{R}^C_{\text{sep}} = (\Phi^C \otimes \mathbf{1}_W)\mathcal{R}_{\text{sep}}$ is a positive matrix for all possible choices of ρ and ρ_W.

We see that two not completely positive maps $\mathbf{T}$ and Φ^C pass the "witness test" and appear to be valid descriptions of the evolution of S if we assume that there is no entanglement between S and W. For the transpose map in the two qubit case this, of course, makes a lot of sense because $\mathbf{T} \otimes \mathbf{1}_W$ is just the Peres' partial transpose criterion [19] for detecting entanglement. The partial transpose is indeed positive preserving on all separable states and ceases to be so only on entangled $\mathcal{R}$. Similarly Choi shows that Φ^C is 1-positive and not 2-positive by considering its action on the matrix $(E_{jk})_{1 \leqslant j,k,n}$ which, up to a normalization factor, is the fully entangled two qubit state. It also is a (block) matrix $M \in \mathcal{M}_2$ with each of its elements in turn being 2×2 matrices belonging to the C^*-algebra of single qubit operators. Specifically $M_{11} \sim 1 + \sigma_3$, $M_{12} \sim \sigma_1 + i\sigma_2$, $M_{21} \sim \sigma_1 - i\sigma_2$ and $M_{22} \sim 1 - \sigma_3$.

We see that the device of introducing the witness W that does not interact with S is inadequate to restrict the dynamics of S to completely positive transformations if there is no entanglement between S and W. This fact is not always emphasized when the witness is introduced even if it is pretty well known. The action of a given map Φ, when extended to $\Phi \otimes \mathbf{1}_n$ can fail to be positive on generic elements of $\mathcal{M}_n(\mathfrak{A})$ while at the same time being positive on all $\rho \otimes \rho_W$.

3. Effect of initial entanglement on the reduced dynamics

The problem at hand might well be the evolution of an open quantum system. Still, one has to assume that system along with its environment can be considered in isolation with no residual interaction or entanglement with anything outside. If S and W are entangled—a fact that seems crucial for the witness test to work—then there must have been some sort of direct or indirect interaction between the two at some point and hence W should really be part of the definition of the environment of S. The pertinent question therefore seems to be the nature of map induced on S by the coupled evolution of the system and an environment that may possibly be entangled to S and whether the reduced dynamics allows a consistent physical interpretation.

Before considering the case where S and W are entangled let us briefly review an alternate approach taken by Alicki in his reply to Pechukas to try and show that open quantum dynamics must be completely positive [20]. This approach introduces the notion of an "assignment map" that will be useful to us in the discussion that follows.

The origin of a dynamical map Φ acting on the state ρ of S can always be traced back the coupled unitary evolution of S and a reservoir (environment) R [1], i.e.,

$$\rho \to \Phi\rho = \mathrm{tr}_R\big[U\mathcal{R}U^\dagger\big], \tag{4}$$

where tr_R represents the partial trace over the reservoir, U a unitary transformation on $S+R$ and $\mathcal{R}$ being a generic initial state of $S+R$. The map Φ may now be treated as the composition of three operations, namely, the partial trace, the unitary map and an *assignment map* $\Lambda : \rho \to \mathcal{R}$ that assigns to each state ρ of S a state $\mathcal{R}$ of $S+R$. Since the partial trace and the unitary map are positive, the character of Φ depends on the nature of the assignment map.

Alicki assumes the following three reasonable properties for the assignment map:

(1) Λ is linear so that it preserves mixtures:

$$\Lambda \sum_i p_i\rho_i = \sum_i p_i \Lambda\rho_i \quad \text{with} \sum_i p_i = 1.$$

(2) The assignment map is consistent in the sense that $\mathrm{tr}_R[\Lambda\rho] = \rho$.

(3) Λ maps every ρ to *density matrices*:

$$\Lambda\rho = \mathcal{R} \geqslant 0; \qquad \mathrm{Tr}[\mathcal{R}] = 1; \qquad \mathcal{R} = \mathcal{R}^\dagger.$$

With all three conditions it is possible to show that the only allowed assignment map is $\Lambda : \rho \to \rho \otimes \rho_R^* \equiv \mathcal{R}$ that assigns to every ρ a state $\mathcal{R}$ by taking the tensor product of ρ with the *same* state ρ_R^* of the reservoir. There are several ways to now show that any map $\Phi\rho = \mathrm{tr}_R[U\rho \otimes \rho_R^* U^\dagger]$ constructed as the contraction of the unitary evolution of a *simply separable initial state* of $S+R$ is always completely positive. One way is to start from a tensor product state of the system and the environment and show that the evolution of the system is given by a transformation of the form

$$\rho \to \sum_\alpha C(\alpha)\rho C(\alpha)^\dagger \tag{5}$$

which is characteristic of completely positive maps [1,9,21].

The system and the environment being in a separable tensor product state initially is not an unreasonable assumption in a wide variety of realistic situations. For instance, for quantum information processors one can safely assume that there is sufficient control over the system to be able to initialize its state to one that is decoupled from its environment. The point here is that it is perfectly reasonable to assume that in many situations there might be initial correlations between the system and its environment. In such situations one cannot rely on completely positive maps to model the open system and a better understanding of not completely positive maps are called for.

The easiest way of understanding the subtleties in the arguments using the assignment map and addressing them is to consider the question of what happens when S and R are initially in an entangled state. This question was considered in detail in [16,17] and here we reproduce the essential aspects of an example worked out in [17].

We take both S and R to be qubits and couple them through a Hamiltonian of the form $H_{SR} = \frac{1}{2}\omega\sigma_3\tau_3$. The initial state of $S+R$ is taken to be one that is generically entangled:

$$\mathcal{R} = \frac{1}{4}(1 + a_j\sigma_j + b_k\tau_k + c_{jk}\sigma_j\tau_k). \tag{6}$$

The state of S is completely determined by a_j. The unitary evolution of $\mathcal{R}$ by $U = e^{-iHt}$ for a time t induces the following transformations on a_j

$$\begin{aligned} a_1 &\to a_1\cos\omega t - c_{13}\sin\omega t, \\ a_2 &\to a_2\cos\omega t + c_{23}\sin\omega t, \\ a_3 &\to a_3. \end{aligned} \tag{7}$$

We note here that certain *initial correlations* in $\mathcal{R}$ (c_{13} and c_{23}) appear in Eq. (7) as parameters defining the transformation on S. The choice of H determines which correlations appear. Now imagine that the assignment map Λ is such that it assigns to every ρ an $\mathcal{R}$ with specific *fixed* values for the correlations that appear as parameters in the reduced dynamics of S. This assignment map along with the unitary evolution and the partial trace operation induces the dynamics given by Eq. (7) on S. The dynamics of S treated as a map, far from being completely positive, is not even positive. To see this, consider the transformation induced on an initial state $\rho = 1/2(1 + a_1\sigma_1)$ of S. This state gets transformed to

$$\rho' = \frac{1}{2}\begin{pmatrix} 1 & a_1\cos\omega t - c_{13}\sin\omega t \\ a_1\cos\omega t - c_{13}\sin\omega t & 1 \end{pmatrix}$$

with eigenvalues

$$\nu_1 = 1 + a_1\cos\omega t - c_{13}\sin\omega t$$

and

$$\nu_2 = 1 - a_1\cos\omega t + c_{13}\sin\omega t.$$

The new state ρ' is not positive for all possible choices of a_1 and c_{13}. For instance, if $a_1 = -1$ and $c_{13} = 1$ then $\nu_1 = 1 - \sqrt{2} \leqslant 0$ for $\omega t = \pi/4$.

To make sense of the fact that unitary evolution of the initially entangled state of the system and the reservoir induces not positive reduced dynamics on S, one has to look more carefully at the assignment map $\Lambda : \rho \to \mathcal{R}$. The point is that if $\mathcal{R}$ is entangled then not all states of S are allowed. For example, $\mathrm{tr}_R[\mathcal{R}]$ cannot be a *pure* state of S. The assignment map applied blindly to all states of S with the restriction that certain correlations in $\mathcal{R}$ are to be kept fixed will map some of the states of S to negative matrices. This, in turn, makes the dynamical map induced on S *not positive*. In the discussion that follows we refer to such maps only as *not completely positive* to include both positive (but not completely positive) as well as not positive ones.

The question is whether we should treat such not completely positive evolution of S as being unphysical? The evolution in Eq. (7) is positive on a subset of states of S. In [17] we have shown explicitly that this subset is precisely the set of states which are *compatible* with two qubit states $\mathcal{R}$ containing certain fixed correlations. In other words, if the observed dynamics of a system is not positive on some of its states then that must be treated as a sign of entanglement between the system and its environment. Physical consistency is restored by noting that the states on which the action of the map is not positive are precisely those states that cannot be partial traces of the state of extended system when certain specific correlations are present in it. The set of states of the system that can appear as partial traces of physical entangled states $\mathcal{R}$ is called the *compatibility domain* of the system. For the example we have considered the compatibility domain can be worked out explicitly following the calculations in [17] and is given by the inequality

$$a_+^2 + a_-^2 + a_3^2 + c_{+3}^2 - \frac{a_+^2 c_{+3}^2}{1 - a_3^2} \leqslant 1 \tag{8}$$

with

$$a_+ = \frac{c_{13}a_1 + c_{23}a_2}{\sqrt{c_{13}^2 + c_{23}^2}}, \qquad a_- = \frac{c_{23}a_1 - c_{13}a_2}{\sqrt{c_{13}^2 + c_{23}^2}}, \tag{9}$$

and

$$c_{+3} = \sqrt{c_{13}^2 + c_{23}^2}. \tag{10}$$

The action of the map in Eq. (7) can be verified to be positive on all states in the compatibility domain and not so outside. A caricature of the compatibility domain with the choice $c_{13} = c_{23} = 1/2$ is drawn in Fig. 1.

The third condition on the assignment map is not necessary. The interpretation of the assignment of unphysical states of the extended system to some of the states of S is clear if we let S and R be entangled when the assignment is made. The meaningful thing to do is to confine the domain of action of the map to the compatibility domain. We see from the example that

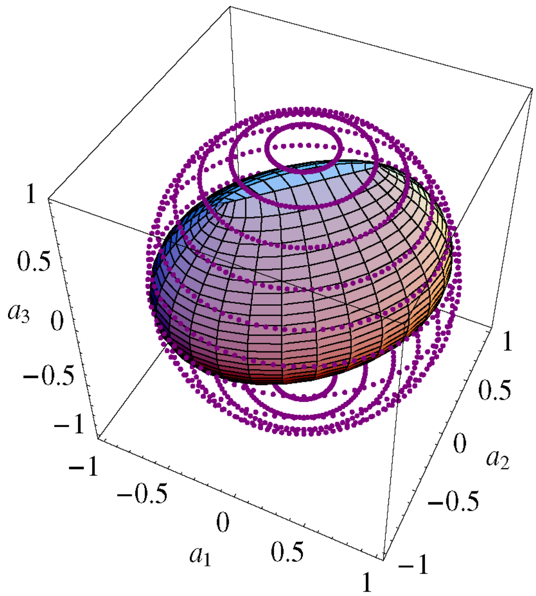

Fig. 1. The compatibility domain for the case where c_{23} and c_{13} are both $\frac{1}{2}$. The unit sphere (the Bloch sphere) that represents all possible states of the system is shown with dotted lines.

the specification of the nature of the entanglement between the system and the reservoir, that is built into the definition of the assignment map, is sufficient to delineate the domain of action of the map. We note here that the assignment map and the issues of positivity and complete positivity that come with it can be circumvented altogether if we consider Eq. (4) as a map from the overall state $\mathcal{R}$ to the state ρ of the system rather than using it to find a map from ρ to ρ. This map is just a combination of a unitary transformation and the partial trace operation; both of which are completely positive.

If we now bring back the witness which is entangled to S but not interacting with it (without changing the entanglement between S and R), all that happens is that the domain of allowed states of S is further restricted. How precisely the compatibility domain is restricted depends now of the nature of the tripartite entanglement between S, R and W. In this context we remark that even though finding the compatibility domain of large-dimensional systems entangled in specific ways to similar environments and witnesses is a well posed problem, it is technically and computationally very demanding. But what we do know about the new compatibility domain in the presence of the witness is that it must be a *subset of the compatibility domain without the witness*. So $\Phi \otimes \mathbf{1}_W$ on all the states $\mathcal{R}_{SRW}$ such that $\rho = \mathrm{tr}_{RW}[\mathcal{R}_{SRW}]$ is positive even for not positive Φ. In short, the presence of the witness does not create any new issues with respect to the physical interpretation of not positive reduced dynamics of S. So it appears that there is no reason to restrict the reduced dynamics of an open system to being exclusively completely positive in nature. *Not completely positive maps are just as good*.

4. Conclusions

We find that the arguments that are put forward to often justify considering only completely positive maps as possible descriptions of open quantum evolution do not stand up to closer inspection. The trick of introducing the witness W that is entangled to the system S to impose complete positivity on the reduced dynamics of S really does not preclude S from undergoing not completely positive evolution with a consistent physical interpretation. An alternate approach that is sometimes utilized to force complete positivity on the reduced dynamics is to re-define the system and the environment in a suitable manner so that new "dressed" system and environment are weakly coupled. In such cases complete positivity for the dynamics of the new 'system' becomes a good approximation. On the other hand, the direct approach of using not completely positive maps to describe the open quantum evolution of the original system may provide a clearer understanding of its dynamics at least in systems with small-dimensional Hilbert spaces. We have shown that there is no reason to shy away from such a direct approach based on claims that not completely positive evolution has no consistent physical interpretation and meaning.

It must be emphasized here that once the requirement of complete positivity is relaxed then the positivity of the reduced dynamics has no special significance. Initial correlations with the environment can lead to open quantum dynamics that can be not positive also. The mathematical literature on maps of C^*-algebras that are not necessarily completely positive is extensive and rich (see, for example, [22,23] and references therein). Translating these results into the context of quantum systems interacting with and entangled to external systems can lead to further insights into the nature of decoherence, dephasing and entanglement itself.

Acknowledgements

The authors acknowledge the support of US Navy—Office of Naval research through grant Nos. N00014-04-1-0336 and N00014-03-1-0639.

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