Reduced Dynamics Need Not Be Completely Positive

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The reduced dynamics of a quantum system in contact with a reservoir is generally thought to be "completely positive"; this is certainly true if product initial conditions are used to define the dynamics. We show that with correlated initial conditions it need not be so. In this case the dynamics can properly be defined only on a subset of initial system states; extension, by linearity, to all possible initial states is trivially possible, but the extension may not be physically realizable and may not even be positive, let alone completely positive.

What can happen, with time, in a quantum dynamical system? If the system is closed, not much: a unitary transformation of its density operator, $\rho \rightarrow U\rho U^*$. If the system is open, the possible transformations are thought [1,2] to be the "completely positive" transformations $\rho \rightarrow \Lambda\rho = \sum_n W_n \rho W_n^*$. Here $\{W_n\}$ is a sequence, not necessarily finite, of linear operators on the system Hilbert space, restricted only by the condition $\sum_n W_n^* W_n = I$, which guarantees that $\mathrm{tr}\rho$ does not change.

Much is still forbidden under completely positive transformations. A two-state system relaxes to equilibrium; suppose that, in the basis of eigenvectors of ρ^{eq},

$$\rho = \begin{pmatrix} p^{\mathrm{eq}} + \varepsilon & \delta \\ \bar{\delta} & 1 - p^{\mathrm{eq}} - \varepsilon \end{pmatrix} \xrightarrow{\Lambda}$$

$$\begin{pmatrix} p^{\mathrm{eq}} + \alpha\varepsilon & \beta\delta \\ \beta\bar{\delta} & 1 - p^{\mathrm{eq}} - \alpha\varepsilon \end{pmatrix}$$

with α and β positive and ≤ 1. Write

$$W_n = \begin{pmatrix} a_n & c_n \\ d_n & b_n \end{pmatrix}$$

and regard the sequences $\{a_n\}, \{b_n\}, \ldots$ as vectors $a, b, \ldots$. One finds that $\beta = (a, b)$, $\alpha = (a, a) + (b, b) - 1$, and therefore, by the Schwarz inequality, $\beta \leq (\alpha + 1)/2$. The diagonal elements cannot relax much faster than the off-diagonal elements; if the relaxation is exponential $[\alpha = \exp(-t/T_1), \beta = \exp(-t/T_2)]$ then $T_2 \leq 2T_1$.

Where does the notion of "complete positivity" come from? Suppose the system S is in contact with a "reservoir" R and that $S + R$ is closed. The dynamics of $S + R$ ($\rho_{SR} \rightarrow U\rho_{SR}U^*$) is "reduced" to dynamics of S by a partial trace operation tr_R: One uses a product basis $|sr\rangle$ for $S + R$ and sums over reservoir states r; then

$$\rho_S = \mathrm{tr}_R \rho_{SR} \rightarrow \Lambda\rho_S = \mathrm{tr}_R(U\rho_{SR}U^*).$$

Of course many different ρ_{SR} reduce to a given ρ_S. To define Λ without ambiguity one assigns to each ρ_S a single ρ_{SR}; this is the "initial condition." The assignment of initial conditions $\rho_S \rightarrow \rho_{SR}$ is required to be linear, in the sense of preserving mixtures—i.e., $f\rho_{S1} + (1 - f)\rho_{S2} \rightarrow f\rho_{SR1} + (1 - f)\rho_{SR2}, 0 \leq f \leq 1$—and is

usually taken to be of product form, $\rho_S \rightarrow \rho_S \otimes \rho_R$ where $\rho_R = \exp(-\beta H_R)/Z$ is a fixed equilibrium state of R by itself. With this assignment one can show explicitly that Λ is completely positive [2].

The definition of dynamics for S is internally consistent if $\rho_{SR}(t)$ stays for all time within the set generated by the assignment $\rho_S \rightarrow \rho_{SR}$. Consistency is never enforced. With product initial conditions, consistency would mean zero system-reservoir interaction. Instead, one hopes that $\rho_{SR}(t)$, for a long time, stays "close" to the set generated by the assignment $\rho_S \rightarrow \rho_{SR}$. Product initial conditions are therefore appropriate to weak coupling. If S/R coupling is strong, different initial conditions should be used.

Still the motion of S is thought to be completely positive. The general argument [1] uses the Heisenberg picture and the map Λ^*, conjugate to Λ, that moves observables of S: $\mathrm{tr}\{(\Lambda\rho_S)A\} = \mathrm{tr}\{\rho_S(\Lambda^* A)\}$. One introduces an N-state "witness" system W, apart from $S + R$. The witness is in fact blind—no interaction with $S + R$—and dead—$H_W = 0$. On the observables of $S + W$ the Heisenberg dynamics must then be the product of Λ^* for S and the identity for W, $\Lambda_{SW}^* = \Lambda^* \otimes I_W$. Λ_{SW}^* should be positive—i.e., map positive operators to positive operators—no matter what the size N of W, and it turns out that can be true only if Λ itself is completely positive.

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 $T_2 \leq 2T_1$ for exponential two-state relaxation. One's doubts are strengthened by calculations of Skinner and co-workers [3] on strong coupling models for two-state relaxation; in some cases the relaxation looks almost exponential, but with $T_2 > 2T_1$.

Here we show that complete positivity is an artifact of product initial conditions. In general, reduced dynamics need not be completely positive.

Our first result is a bit of bad news. If the assignment of initial conditions $\rho_S \rightarrow \rho_{SR}$ is defined for all ρ_S and is

linear, in the sense of preserving mixtures, then ρ_{SR} *must* be of product form, $\rho_S \otimes \rho_R$, where ρ_R is a *fixed* density operator on reservoir space.

We outline the proof for the case that S is two state.

First, if ρ_S is pure state (i.e., $\rho_S = |s\rangle\langle s|$) then the ρ_{SR} assigned to it *must* be a product, $\rho_{SR} = \rho_S \otimes \rho_R(s)$, where ρ_R may depend on the state s; for if $|s'\rangle$ is any state in H_S orthogonal to $|s\rangle$, we have $\langle s'r\,|\rho_{SR}|\,s'r\rangle \le \langle s'\,|\rho_S|\,s'\rangle = 0$, which implies that $\rho_{SR}|s'r\rangle = 0$. ρ_{SR} is nonzero only on states $|sr\rangle$, and ρ_R is defined by $\langle r'\,|\rho_R|\,r\rangle = \langle sr'\,|\rho_{SR}|\,sr\rangle$.

The idea now is to take some pure state ρ_S's, not all independent, and deduce a contradiction unless the ρ_R's assigned to them are all the same. A two-state ρ can be represented as a point in the sphere $x^2 + y^2 + z^2 \le \frac{1}{4}$ by the identification $\rho_{11} = 1/2 + z$, $\rho_{12} = x + iy$. Take four coplanar points on the surface of the sphere, where the pure state ρ's lie, say, at (1) $z = \frac{1}{2}$, (2) $z = -\frac{1}{2}$, (3) $x = \frac{1}{2}$, and (4) $x = -\frac{1}{2}$. Then

$$\frac{\rho_{S1} + \rho_{S2}}{2} = \frac{\rho_{S3} + \rho_{S4}}{2} \Rightarrow$$

$$\frac{\rho_{S1} \otimes \rho_{R1} + \rho_{S2} \otimes \rho_{R2}}{2} = \frac{\rho_{S3} \otimes \rho_{R3} + \rho_{S4} \otimes \rho_{R4}}{2}.$$

Average the latter equation over each of three states of S, the states onto which ρ_{S1}, ρ_{S2}, and ρ_{S3} project; conclude that $\rho_{R1} = \rho_{R2} = \rho_{R3} = \rho_{R4}$. Now replace ρ_{S3} and ρ_{S4} by (3') $y = \frac{1}{2}$ and (4') $y = -\frac{1}{2}$ and do the same trick. All six pure-state ρ_S's are assigned the same ρ_R, and since the six are not all coplanar this implies, by linearity, that $\rho_S \to \rho_S \otimes \rho_R$ obtains for all ρ_S.

In other words, the only linear assignment of initial conditions that works for every ρ_S is the product assignment. In general, when product initial conditions are not appropriate, not every ρ_S can play the "reduced dynamics" game. This is consistent with recent work by Suárez, Silbey, and Oppenheim [4], who find that some "slippage" of initial conditions must occur before the reduced dynamics looks Markovian—that is, before reduced dynamics describes the evolution of ρ_S sufficiently well.

As an illustration of this result, imagine trying to assign initial conditions in the case that S/R coupling is strong but R relaxes to equilibrium much faster than S; i.e., initial conditions for constrained equilibrium of R in contact with nonequilibrium S. In classical mechanics, the solution to this problem is easily seen to be

$$\rho_S(\Gamma_s) \to \rho_{SR}(\Gamma_S, \Gamma_R) = \rho_S(\Gamma_S)\rho_{SR}^{eq}(\Gamma_S, \Gamma_R)/\rho_S^{eq}(\Gamma_S),$$

and *any* ρ_S will do (with the minor caveat that it must not put density on phase points Γ_S that are not populated at equilibrium). Many quantum versions of this assignment are possible, differing in the ordering of operators; one that has been used in the recent literature [5] is

$$\rho_S \to (\rho_S\rho_S^{eq-1}\rho_{SR}^{eq} + \rho_{SR}^{eq}\rho_S^{eq-1}\rho_S)/2. \qquad (1)$$

This assignment has many nice features, but in general it cannot be positive for all ρ_S: for pure state ρ_S's it is not of the required form ($\rho_S \otimes \rho_R$) unless $\rho_{SR}^{eq} = \rho_S^{eq} \otimes \rho_R$.

Now for our main result: Once one allows correlated initial conditions, *anything* becomes possible in reduced dynamics. Specifically, for a two-state S the following is true: Given four initial states $\{\rho_{Si}\}$, independent [in the sense of noncoplanar in the (x, y, z) representation] but otherwise arbitrary, and four final states $\{\tilde{\rho}_{Si}\}$, completely arbitrary, there is a reservoir R, a linear map $\rho_S \to \rho_{SR}$ — defined at least on the set of mixtures of $\{\rho_{Si}\}$—and a unitary operator U on $S + R$ Hilbert space such that

$$\tilde{\rho}_{Si} = \mathrm{tr}_R(U\rho_{Si}U^*).$$

Proof: Let R also be two state; use a product basis $|sr\rangle$, $s = 1$ or 2, $r = 1$ or 2; define four operators in "reservoir space" by $\langle j\,|\rho_{Ri}|\,k\rangle = \langle j\,|\tilde{\rho}_{Si}|\,k\rangle$ (that is, the matrix of ρ_{Ri} in reservoir states equals the matrix of $\tilde{\rho}_{Si}$ in system states). Set $\rho_{SRi} = \rho_{Si} \otimes \rho_{Ri}$ and define $U|sr\rangle = U^*|sr\rangle = |rs\rangle$. Then

$$\langle j\,|tr_R(U\rho_{SRi}U^*)|\,k\rangle = \sum_l \langle jl\,|U\rho_{Si} \otimes \rho_{Ri}U^*|\,kl\rangle$$

$$= \sum_l \langle lj\,|\rho_{Si} \otimes \rho_{Ri}|\,lk\rangle$$

$$= \left(\sum_l \langle l\,|\rho_{Si}|\,l\rangle\right)\langle j\,|\rho_{Ri}|\,k\rangle$$

$$= \langle j\,|\rho_{Ri}|\,k\rangle = \langle j\,|\tilde{\rho}_{Si}|\,k\rangle.$$

To repeat: In general, reduced dynamics $\rho_S \to \Lambda\rho_S$ need not be completely positive. The operator Λ is defined, via reduction from unitary $S + R$ dynamics, only on a subset of all possible ρ_S's. Λ may be extended—trivially, by linearity—to the set of *all* ρ_S, but the motions $\rho_S \to \Lambda\rho_S$ so defined may not be physically realizable. The extension may even turn density operators into operators that are not. Forget complete positivity; Λ, extended to all ρ_S, may not even be positive.

Here is an illustration of this point, using the assignment $\rho_S \to \rho_{SR}$ of Eq. (1). Again, two-state S, two-state R; suppose the Hamiltonian is diagonal in reservoir states, $H = H_1 \otimes P_1 + H_2 \otimes P_2$; then, in units of time and energy such that $\hbar = \beta = 1$, we have

$$\Lambda_t\rho_S = [e^{-iH_1 t}\rho_S(e^{-H_1} + e^{-H_2})^{-1}e^{iH_1 t}e^{-H_1}$$

$$+ e^{-iH_2 t}\rho_S(e^{-H_1} + e^{-H_2})^{-1}e^{iH_2 t}e^{-H_2} + *]/2,$$

where an asterisk denotes the adjoint of the two terms written out. The extension of Λ_t from its proper domain to all ρ_S is got just by plugging *any* ρ_S into this formula. Take $H_1 = \sigma_z$, $H_2 = 2\sigma_x$, $t = \pi/2$; one calculates easily that

$$\Lambda_t\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & a \\ a & 0 \end{pmatrix},$$

where the value of a [which happens to be $-e\sinh 2/2(1 + \cosh 1 \cosh 2)$] is irrelevant; what

matters is that it is not zero, so Λ_t has taken a proper density matrix and produced one that is not.

Finally, one may ask where the general argument for complete positivity fails. Recall that the argument introduces a system W, isolated from $S + R$ and with trivial dynamics. We know the dynamics of S by itself, Λ^* in Heisenberg representation. We know the dynamics of W by itself, the identity I_W in Heisenberg representation. S and W do not interact. The mistake is to assert that we then know the dynamics of $S + W$, that it must be the product $\Lambda^* \otimes I_W$.

Select an initial state of $W + S$, ρ_{WS}. What happens to it in time? To answer the question—since S is part of $S + R$—we need the initial state of $W + S + R$, ρ_{WSR}. Traced over R, this must give ρ_{WS}; ρ_{WS}, traced over W, specifies ρ_S, the initial state of S by itself; to this ρ_S is assigned a particular initial state ρ_{SR} of $S + R$; and traced over W, ρ_{WSR} must yield ρ_{SR}. In general, there is no state ρ_{WSR} which meets all these demands. For example, if ρ_{WS} is pure state, ρ_{WSR} must be of the form $\rho_{WS} \otimes \rho_R$ and therefore ρ_{SR} of the form $\rho_S \otimes \rho_R$; but since ρ_S may not be pure state and we may not be using product initial conditions, it may not be so.

In general, we know the dynamics of $W + S$ only for product initial states $\rho_W \otimes \rho_S$; then the initial state of the entire system is $\rho_W \otimes \rho_{SR}$. From this initial state, of course, W and S evolve on their own, and the presence of W—as should be the case—has no consequence at all for S.

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