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Reduced dynamics for entangled initial state of the full density operator

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Abstract. Starting from the Schrödinger equation for a system and a reservoir, we construct a quantum dynamical map that describes reduced dynamics. We work with an arbitrary initial state for the system and reservoir, and thus refrain from performing any factorizations. The map is found to be nonlinear, not completely positive, and not unique. To investigate the physical implications, the Bloch equations are constructed. If the freedom the new map offers us is fully exploited, then the classic inequality $\gamma_\perp \geqslant \gamma_\parallel/2$ for the damping coefficients must be replaced by a weaker condition.

1. Quantum dynamical map

Any quantum mechanical description of a dynamical process must be based on the Schrödinger equation. This fundamental statement has far-reaching consequences, if one adheres to the, let us admit, pedantic point of view that conservative processes do not exist, except for the one called nature. Then the Schrödinger equation is only valid for a composite $\mathcal{SR}$ of two systems $\mathcal{S}$ and $\mathcal{R}$, so that one is obliged to work with a direct product $\mathcal{H} = \mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{R}$ of two Hilbert spaces.

The system $\mathcal{S}$ accommodates the dynamical process at hand, and can be monitored by the experimentalist. For the sake of simplicity, we set the dimension of $\mathcal{H}_\mathcal{S}$ equal to the finite integer N. The system $\mathcal{R}$, traditionally called the reservoir, corresponds to the outside world. The evolution in time of $\mathcal{S}$ alone is governed by the following reduced density matrix:

$$\rho_\mathcal{S}(t) = \mathrm{Tr}_\mathcal{R}[\exp(-\mathrm{i}Ht)|\Psi(t=0)\rangle\langle\Psi(t=0)|\exp(\mathrm{i}Ht)]. \tag{1}$$

The Hamiltonian $\hbar H$ acts on $\mathcal{H}$, and is left unspecified in this work. The normalized initial state vector of $\mathcal{SR}$ is denoted as $|\Psi(t=0)\rangle$.

Since the vector $|\Psi(t=0)\rangle$ is not known to us, the trace in (1) should be performed such that a relation between the experimentally relevant matrices $\rho_\mathcal{S}(t)$ and $\rho_\mathcal{S}(t=0)$ is created. To that end, we utilize a well known [1] and completely general decomposition of the initial state vector. It reads

$$|\Psi(t=0)\rangle = \sum_{k=1}^{N} |\chi_k \otimes r_k\rangle. \tag{2}$$

The set $\{|\chi_k\rangle\} \subset \mathcal{H}_\mathcal{S}$ is orthonormal, and the set $\{|r_k\rangle\} \subset \mathcal{H}_\mathcal{R}$ is orthogonal. To derive (2), one should perform the decomposition with the help of the orthonormal set $\{|\chi'_k\rangle\}$; the companion set $\{|r'_k\rangle\}$ is made orthogonal by means of the unitary transformation $|\chi_k\rangle = U|\chi'_k\rangle$.

The right-hand side of (1) can be expressed in terms of the eigenvalues $\{\lambda_k = \langle r_k | r_k \rangle\}$ and eigenvectors $\{|\chi_k\rangle\}$ belonging to the reduced density matrix at $t = 0$, as well as a set of time-dependent matrices $\{W(t; m, k)\}$. These act on $\mathcal{H}_{\mathcal{S}}$, and are defined by

$$\langle \phi_1 | W(t; m, k) | \phi_2 \rangle = \langle \phi_1 \otimes \hat{r}_m | \exp(-\mathrm{i}Ht) | \phi_2 \otimes \hat{r}_k \rangle \tag{3}$$

where $|\phi_1\rangle$ and $|\phi_2\rangle$ are arbitrary elements of $\mathcal{H}_{\mathcal{S}}$. The abbreviation $|\hat{r}_k\rangle = \langle r_k | r_k \rangle^{-1/2} |r_k\rangle$ has been introduced.

An explicit evaluation of (1) yields

$$\rho_{\mathcal{S}}(t) = \sum_{k,l=1}^{N} \lambda_k^{1/2} \lambda_l^{1/2} \sum_{m=1}^{\infty} W(t; m, k) |\chi_k\rangle\langle\chi_l| W^\dagger(t; m, l). \tag{4}$$

The finite set $\{|\hat{r}_k\rangle\}_{k=1}^{N}$ has been extended to an orthonormal basis for $\mathcal{H}_{\mathcal{R}}$. The advantage of (4) over (1) is that all components on the right-hand side pertain to system $\mathcal{S}$. Hence, one can read off from (4) the explicit form of the quantum dynamical map $\Lambda(t)$, which is defined as $\rho_{\mathcal{S}}(t) = \Lambda(t)[\rho_{\mathcal{S}}(0)]$. This map turns out to be nonlinear, because (4) depends on matrix $\rho_{\mathcal{S}}(0)$ through its eigenvalues and eigenvectors. Except for the case that one eigenvalue equals unity and all others zero, $\Lambda(t)[\rho_{\mathcal{S}}(0)]$ cannot be put into the form $\sum_{j=1}^{\infty} \tilde{W}(t; j) \rho_{\mathcal{S}}(0) \tilde{W}^\dagger(t; j)$, with a free choice for the matrices $\{\tilde{W}(t; j)\}$ that act on $\mathcal{H}_{\mathcal{S}}$. In other words, the criterion for complete positivity [2, 3] is not satisfied.

In deriving (4), the reservoir $\mathcal{R}$ has been identified with the complete world surrounding system $\mathcal{S}$. In a different and more pragmatic approach, $\mathcal{R}$ loses its abstract status to become a concrete physical system. If $\mathcal{S}$ stands for a two-level atom, $\mathcal{R}$ might be the quantized electromagnetic radiation field. One assumes that from time $t = 0$ onwards, the composite $\mathcal{SR}$ constitutes a conservative quantum system. Due to past interactions with the outside world, the evolution of $\mathcal{SR}$ starts from an arbitrary mixed state

$$\rho_{\mathcal{SR}}(t = 0) = \sum_{j=1}^{\infty} \mu_j |\Psi^{(j)}(t = 0)\rangle\langle\Psi^{(j)}(t = 0)|. \tag{5}$$

The normalized state vectors $\{|\Psi^{(j)}(t = 0)\rangle\}$ belong to $\mathcal{H}$, and the positive c-numbers $\{\mu_j\}$ add up to unity.

We gain a lot from these concessions. The quantum dynamical map becomes an infinite sum of maps of type (4), in which the numbers $\{\mu_j\}$ figure as weights. A convenient representation is obtained, if use is made of the matrices $\{F_m\}_{m=0}^{N^2-1}$, which act on $\mathcal{H}_{\mathcal{S}}$. The new matrices are chosen such that the relation $\mathrm{Tr}_{\mathcal{S}}(F_m F_n^\dagger) = \delta_{m,n}$ is true for $0 \leqslant m, n \leqslant N^2 - 1$; F_0 equals $N^{-1/2}\mathbf{1}_N$ [3]. One ends up with

$$\rho_{\mathcal{S}}(t) = \sum_{j=1}^{\infty} \sum_{k,l=1}^{N} \sum_{m,n=0}^{N^2-1} \mu_j \lambda_k^{(j)1/2} \lambda_l^{(j)1/2} \Theta^{(j)}(t)_{km,ln} F_m |\chi_k^{(j)}\rangle\langle\chi_l^{(j)}| F_n^\dagger. \tag{6}$$

The time-dependent c-numbers

$$\Theta^{(j)}(t)_{km,ln} = \sum_{p=1}^{\infty} \mathrm{Tr}_{\mathcal{S}}[W^{(j)}(t; p, k) F_m^\dagger] \{\mathrm{Tr}_{\mathcal{S}}[W^{(j)}(t; p, l) F_n^\dagger]\}^* \tag{7}$$

make up an $(N^3 \times N^3)$-dimensional matrix. As a consequence of the property

$$\sum_{k,l=1}^{N} \sum_{m,n=0}^{N^2-1} \Theta^{(j)}(t)_{km,ln} c_{km} c_{ln}^* \geqslant 0 \tag{8}$$

with $\{c_{km}\}$ arbitrary complex numbers, the matrix is positive.

The orthonormality of the set $\{|\hat{r}_k^{(j)}\rangle\}_{k=1}^{\infty}$ implies that for all j

$$\Theta^{(j)}(t=0)_{km,ln} = N\delta_{k,l}\delta_{m,0}\delta_{n,0}. \tag{9}$$

Consequently, the relation between the initial reduced density matrix on the one hand, and the sets $\{\mu_j\}$, $\{\lambda_k^{(j)}\}$, and $\{|\chi_k^{(j)}\rangle\}$ on the other hand, is given by

$$\rho_{\mathcal{S}}(t=0) = \sum_{j=1}^{\infty}\sum_{k=1}^{N} \mu_j \lambda_k^{(j)} |\chi_k^{(j)}\rangle\langle\chi_k^{(j)}|. \tag{10}$$

Conservation of the trace of $\rho_{\mathcal{S}}(t)$ is guaranteed by a third property of the matrix (7), namely

$$\sum_{m,n=0}^{N^2-1} \Theta^{(j)}(t)_{km,ln} F_n^{\dagger} F_m = \mathbf{1}_N \delta_{k,l}. \tag{11}$$

To prove (11), one should employ the identity

$$\sum_{p=1}^{\infty} W^{(j)\dagger}(t;p,k) W^{(j)}(t;p,l) = \mathbf{1}_N \delta_{k,l} \tag{12}$$

and the decomposition $\rho = \sum_{m=0}^{N^2-1} \mathrm{Tr}(\rho F_m^{\dagger}) F_m$ for arbitrary ρ acting on $\mathcal{H}_{\mathcal{S}}$.

The result (6) delivers to us the quantum dynamical map describing reduced dynamics for an arbitrary initial state of the full density operator. Owing to (11) and the positivity of matrix (7), the map respects the von Neumann conditions $\mathrm{Tr}_{\mathcal{S}}\,\rho_{\mathcal{S}}(t) = 1$ and $\rho_{\mathcal{S}}(t) \geqslant 0$. Unfortunately, the map is nonlinear, not completely positive, and not uniquely defined for a given evolution of the reduced density matrix $\rho_{\mathcal{S}}(t)$.

This 'sting in the tail' needs some further explanation. Take for the initial full density operator $\rho_{\mathcal{SR}}(t=0)$ a factorized state $\rho_{\mathcal{S}}(t=0) \otimes \rho_{\mathcal{R}}(t=0)$ and prescribe for each initial condition $\rho_{\mathcal{S}}(t=0)$ how $\rho_{\mathcal{S}}(t)$ evolves. The following can now be observed: matrix (7) does not depend on the integers j, k and l; it can be evaluated on the basis of definition (6) of the quantum dynamical map; the answer is uniquely determined [4]. If we have no information at all about the initial state $\rho_{\mathcal{SR}}(t=0)$, then the situation becomes more delicate. Specification of the left-hand side of (6) for arbitrary $\rho_{\mathcal{S}}(t=0)$ no longer suffices to compute matrix (7) in a unique manner. The reason is that, in carrying out the decomposition (10), infinitely many choices for the sets $\{\mu_j\}$ and $\{\lambda_k^{(j)}\}$ can be made.

2. Bloch dynamics

We have seen that, if one wishes to avoid the customary [3, 5–8] factorization of initial states, then one is forced to abandon the concept of complete positivity. We shall demonstrate that it is indeed rewarding to do so. We integrate the Bloch equations [5]

$$\frac{\mathrm{d}}{\mathrm{d}t} p(t) = -[\gamma_{\perp} + \mathrm{i}\omega] p(t) \qquad \frac{\mathrm{d}}{\mathrm{d}t} d(t) = -\gamma_{\parallel}[d(t) - d_{\infty}] \tag{13}$$

to obtain

$$\begin{aligned} p(t) &= p(0)\exp[-(\gamma_{\perp} + \mathrm{i}\omega)t] \\ d(t) &= d_{\infty} + [d(0) - d_{\infty}]\exp(-\gamma_{\parallel} t). \end{aligned} \tag{14}$$

The coefficients $\gamma_{\perp}$, $\gamma_{\parallel}$, ω and d_{∞} are real-valued. The Bloch dynamics (14) will be constructed on the basis of map (6). It will be found that the inequality $\gamma_{\perp} \geqslant \gamma_{\parallel}/2$, one of the hallmarks of complete positivity [8], must be replaced by a weaker version. This is a relevant conclusion, because the Bloch equations (13) are known to provide an adequate description of damping phenomena in various fields, for instance, nuclear magnetic resonance [6] and quantum optics [7].

It should be emphasized that we proceed in the axiomatic fashion, which has been outlined in [8]. That is to say, we substitute (14) into the left-hand side of (6), and seek a solution for the matrix $[\Theta^{(j)}(t)_{km,ln}]$. In this setting, one no longer pays attention to relation (7). Of course, one retains the constraints (8), (9) and (11). We shall not enter into the technical implementation of the above program, because this does not teach us anything of conceptual value. We shall simply present a single realization of the Bloch dynamics that makes maximal use of the freedom map (6) offers us.

As N equals 2 now, the orthonormal set $\{|1\rangle, |2\rangle\}$ spans $\mathcal{H}_S$. Quantum expressions for the polarization and inversion must be obtained on the basis of the relations $p(t) = \langle 2|\rho_S(t)|1\rangle$ and $2d(t) = \langle 2|\rho_S(t)|2\rangle - \langle 1|\rho_S(t)|1\rangle$, respectively. Hence, for all $t \geqslant 0$ the inequality

$$|p(t)| \leqslant [\tfrac{1}{4} - d^2(t)]^{1/2} \tag{15}$$

must accompany (14), otherwise the positivity of $\rho_S(t)$ is violated.

In proposing a decomposition (10), we invoke the identity

$$\exp(\mathrm{i}\alpha) = (\sin\delta)^{-1}\sum_{j=1}^{J}\nu_j(\alpha)\exp[\mathrm{i}\delta(j-1)] \tag{16}$$

with $0 \leqslant \alpha \leqslant 2\pi$, $\delta = \pi/2^M$, $J = 2^{M+1}$, and the positive integer M arbitrary. All coefficients $\{\nu_j(\alpha)\}$ lie inside the interval [0, 1]. For $\delta(j-1) \leqslant \alpha \leqslant \delta j$, those differing from zero, read

$$\nu_j(\alpha) = \sin(\delta j - \alpha) \qquad \nu_{j+1}(\alpha) = \sin(\alpha + \delta - \delta j) \tag{17}$$

with $j = 1, 2, 3, \ldots, J-1$. For $2\pi - \delta \leqslant \alpha \leqslant 2\pi$ one has

$$\nu_1(\alpha) = \sin(\alpha + \delta) \qquad \nu_J(\alpha) = -\sin\alpha. \tag{18}$$

In addition to (16), we also employ the fact that the sum

$$\xi(M,\alpha) = (\sin\delta)^{-1}\sum_{j=1}^{J}\nu_j(\alpha) \tag{19}$$

converges to unity for $M \to \infty$. Note that ξ lies inside the interval $[1, 1/\cos(\delta/2)]$.

We are ready to present our realization of the Bloch dynamics (14). We meet (10) by means of the choices $\lambda_k^{(j)} = \delta_{k,1}$ for all j, $|\chi_2^{(1)}\rangle = |\chi_1^{(2)}\rangle = |1\rangle$, $|\chi_1^{(1)}\rangle = |\chi_2^{(2)}\rangle = |2\rangle$, $\mu_{j+2} = q\nu_j(\alpha)/\sin\delta$, and

$$\begin{aligned}
&\mu_1 = [1 - q\xi(M,\alpha)][\tfrac{1}{2} + d(0)] \qquad \mu_2 = [1 - q\xi(M,\alpha)][\tfrac{1}{2} - d(0)] \\
&|\chi_1^{(j+2)}\rangle = \exp[-\mathrm{i}\delta(j-1)][\tfrac{1}{2} - d(0)]^{1/2}|1\rangle + [\tfrac{1}{2} + d(0)]^{1/2}|2\rangle \\
&|\chi_2^{(j+2)}\rangle = [\tfrac{1}{2} + d(0)]^{1/2}|1\rangle - \exp[\mathrm{i}\delta(j-1)][\tfrac{1}{2} - d(0)]^{1/2}|2\rangle
\end{aligned} \tag{20}$$

with $j = 1, 2, 3, \ldots, J$, $q = |p(0)|[\tfrac{1}{4} - d^2(0)]^{-1/2}$, and $\alpha = \arg p(0)$. As required, the weights $\{\mu_j\}$ add up to unity, and for each j the set $\{|\chi_k^{(j)}\rangle\}_{k=1,2}$ is orthonormal. The weights μ_1 and μ_2 are non-negative for $q \leqslant \xi^{-1}$; hence, if M tends to infinity, any point of the Bloch sphere may be chosen as the initial state of the reduced density matrix, except for the points with $d(0) = \pm\frac{1}{2}$, $p(0) = 0$. However, these choices are not of interest to us, because they cause $\gamma_\perp$ to disappear from the dynamics. Finally, observe that in the limit $M \to \infty$ all weights $\{\mu_j\}$ differ from zero. Hence, by adopting the setting (20), one fully exploits the freedom of map (6). As becomes clear from (5), the second important consequence of (20) is that the full density operator starts from an entangled state.

Next, we have to come up with positive, and thus Hermitian, matrices $[\Theta^{(j)}(t)_{mn}]$ that turn map (6) into the Bloch dynamics (14). As $k = l = 1$ is valid throughout, the dependence on k and l is suppressed. We adopt the representation $|1\rangle \to (0,1)^T$, $|2\rangle \to (1,0)^T$, $\{F_k\}_{k=1}^3 \to \{\sigma_k/\sqrt{2}\}_{k=1}^3$, with $\{\sigma_k\}_{k=1}^3$ denoting the Pauli matrices. One checks that the following choice of nonzero matrix elements works out well:

$$
\begin{aligned}
&\Theta^{(1)}(t)_{00} = \Gamma_{\|,+}(t) + 2d_\infty \Gamma_{\|,-}(t)\\
&\Theta^{(1)}(t)_{11} = \Theta^{(1)}(t)_{22} = (\tfrac{1}{2} - d_\infty)\Gamma_{\|,-}(t)\\
&\Theta^{(2)}(t)_{mn} = \Theta^{(1)}(t)_{mn}[d_\infty \to -d_\infty]\\
&\Theta^{(j+2)}(t)_{00} = \Gamma_{\|,+}(t)/2 + \cos(\omega t)[\Gamma_\perp(t) - r\Gamma_{\|,-}(t)]\\
&\Theta^{(j+2)}(t)_{11} = [\tfrac{1}{2} + r\cos(\omega t - 2\delta j + 2\delta)]\Gamma_{\|,-}(t)\\
&\Theta^{(j+2)}(t)_{22} = [\tfrac{1}{2} - r\cos(\omega t - 2\delta j + 2\delta)]\Gamma_{\|,-}(t)\\
&\Theta^{(j+2)}(t)_{33} = \Gamma_{\|,+}(t)/2 - \cos(\omega t)[\Gamma_\perp(t) - r\Gamma_{\|,-}(t)]\\
&\mathrm{Im}\,\Theta^{(j+2)}(t)_{03} = \sin(\omega t)[\Gamma_\perp(t) - r\Gamma_{\|,-}(t)]\\
&\mathrm{Re}\,\Theta^{(j+2)}(t)_{12} = r\sin(\omega t - 2\delta j + 2\delta)\Gamma_{\|,-}(t)\\
&\mathrm{Re}\,\Theta^{(j+2)}(t)_{03} = -\mathrm{Im}\,\Theta^{(j+2)}(t)_{12} = d_\infty \Gamma_{\|,-}(t)
\end{aligned}
\tag{21}
$$

with $j = 1, 2, 3, \ldots, J$. The shorthand notation $\Gamma_{\|,\pm}(t) = 1 \pm \exp(-\gamma_\| t)$, $\Gamma_\perp(t) = \exp(-\gamma_\perp t)$, $r = (\frac{1}{4} - d_\infty^2)^{1/2}$ has been used. We emphasize that our construction of the Bloch dynamics holds true for any M, so the limit $M \to \infty$ poses no problems.

The choice (21) complies with the constraints (9) and (11). The requirement that for each j the matrix $[\Theta^{(j)}(t)_{mn}]$ be positive, is equivalent to the inequalities

$$
\begin{aligned}
&1 + 2\eta_1 d_\infty + (\eta_2 - 2\eta_1 d_\infty)\exp(-\gamma_\| t) \geqslant 0\\
&h(t) = \exp(\gamma_\perp t - \gamma_\| t) - \exp(-\gamma_\perp t) - 2r\exp(-\gamma_\| t) + 2r \geqslant 0
\end{aligned}
\tag{22}
$$

with $\eta_1 = \pm 1$ and $\eta_2 = \pm 1$. By taking $t \to \infty$ in the upper inequality, the condition $\gamma_\| \geqslant 0$ follows. We set $\eta_2 = -1$, divide both inequalities (22) by t, and let t decrease to zero. These steps bring us to

$$
|d_\infty| \leqslant \tfrac{1}{2} \qquad \gamma_\| \geqslant 0 \qquad \gamma_\perp \geqslant \gamma_\| [\tfrac{1}{2} - (\tfrac{1}{4} - d_\infty^2)^{1/2}]. \tag{23}
$$

The above conditions are also sufficient. For the case $\gamma_\perp \leqslant \gamma_\|/2$ one can show this by writing

$$
\frac{\mathrm{d}h(t)}{\mathrm{d}t} = \gamma_\perp t(\gamma_\| - \gamma_\perp)\exp(-\gamma_\| t)[y(\gamma_\| t - \gamma_\perp t) - y(\gamma_\perp t)] + (2r\gamma_\| - \gamma_\| + 2\gamma_\perp)\exp(-\gamma_\| t) \tag{24}
$$

and exploiting the fact that the function $y(x) = [\exp(x) - 1]/x$ does not decrease on the real axis.

In the discussion below equation (12), we have already pointed out that the choices (20) and (21) are not uniquely determined. However, constructions of the Bloch dynamics, which weaken the inequalities (23), do not exist. The reason is that one can prove the equivalence between (23) and (15), given that $\rho_S(t = 0) \geqslant 0$. Condition (15) is satisfied by all quantum dynamical maps of structure (6). The equivalence proof is set up by writing the function $|p(t)|^2 + d^2(t)$ as a parabola in $d(0)$ for the choice $q = 1$. Subsequently, one demands that the parabola be smaller than $\frac{1}{4}$ on the interval $|d(0)| \leqslant \frac{1}{2}$. The ensuing inequalities can be processed in a similar vein as explained below (23).

3. Conclusion

In previous work [9–13], it was argued that the use of a disentangled initial state for the system and reservoir does not produce the most general description of reduced dynamics. Motivated by this criticism, we have constructed the quantum dynamical map that describes reduced dynamics for an arbitrary initial state. We have found that the property of complete positivity cannot be maintained.

The new map is indeed capable of providing some new physics. The classic inequality $\gamma_\perp \geqslant \gamma_\parallel/2$ for the damping coefficients of the Bloch equations must be replaced by a weaker and more natural condition. The latter directly relates to the positivity of the reduced density matrix. One verifies that the replacement is not necessary if the initial state of the full density operator is assumed to be pure, so that the map (4) is in command of the dynamics.

Finally, we should be aware of the fact that only the axiomatic part of the job has been completed. The remaining part consists of specifying a Hamiltonian $\hbar H$ and an initial density operator $\rho_{\mathcal{SR}}(t = 0)$, which allow us to derive (23) from microscopic expressions for the Bloch parameters. What are intended are expressions that contain energy eigenvalues of the unperturbed system $\mathcal{S}$ and correlation functions of the reservoir [7]. Of course, the microscopic theory must be devised such that the positivity of the reduced density matrix is preserved. Therefore, as a mathematical tool one should not utilize a perturbative approach [14], but rather a weak-coupling [15] or singular-coupling [16] procedure that is suited for coping with entangled initial states.

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