Completely Positive Maps with Memory

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The prevailing description for dissipative quantum dynamics is given by the Lindblad form of a Markovian master equation, used under the assumption that memory effects are negligible. However, in certain physical situations, the master equation is essentially of a non-Markovian nature. This paper examines master equations that possess a memory kernel, leading to a replacement of white noise by colored noise. The conditions under which this leads to a completely positive, trace-preserving map are discussed for an exponential memory kernel.

We first review the canonical form of the generator that leads to the quantum Markovian master equation for the system density operator. The Gorini-Kossakowski-Sudarshan generator \( \hat{L} \) has the form

\[
L\rho = -i[H, \rho] + \frac{1}{2} \sum_{i,j=1}^{n^2-1} c_{ij} \left\{ [F_i, \rho F_j^\dagger] + [F_i^\dagger, \rho F_j] \right\}
\]

for \( \rho \in \mathcal{M}_n \) (\( \mathcal{M}_n \) denotes the set of \( n \times n \) complex matrices), where \( H = H^\dagger, \text{Tr}(H) = 0, \text{Tr}(F_i) = 0, \text{Tr}(F_i F_j^\dagger) = \delta_{ij} \), and \( \{c_{ij}\} \) is a complex positive semidefinite matrix.

The first term describes the unitary evolution while the second term defines the Lindblad superoperator \( \mathcal{L} \) describing the dissipative dynamics due to the interaction of the system with the environment. The solution \( \rho(t) = e^{L t} \rho(0) \) to Eq. (1) defines a linear operator \( \Phi_t : \rho \rightarrow \rho_t \) that maps the system density operator at some initial time to the system density operator at some time in the future. The expression in Eq. (1) has been shown to generate a completely positive dynamical semigroup that has the following properties:

\[
\begin{align*}
(i) & \quad \| \Phi_t \rho \|_1 = \| \rho \|_1 \quad \forall \rho \in V_i^+ (\mathcal{H}), \ t \geq 0, \\
(ii) & \quad \Phi_t \otimes I_n \geq 0 \quad \forall \ n \in \mathbb{Z}_+, \\
(iii) & \quad \lim_{t \downarrow 0} \Phi_t = I, \\
(iv) & \quad \Phi_t \Phi_s = \Phi_{t+s}, \ t, s \geq 0,
\end{align*}
\]

where \( \| \cdot \|_1 \) denotes the trace norm in the space of linear operators on the Hilbert space \( \mathcal{H} \) and \( V_i^+ (\mathcal{H}) \) is the cone of all positive semidefinite elements in the space \( \mathcal{S} \). The first property states that the map is trace-preserving for all density operators at all times. The second property states that the map is not only positive, but completely positive, i.e., any extension to a larger space remains a positive map \( \mathcal{S} \). The third property expresses the continuity at the origin and hence for all time. Finally, \( iv \) is the semigroup property. This property arises when the environment or reservoir is delta-function correlated in time as is the case for white noise diffusive processes.

The prevailing description for dissipative dynamics is given by \( \rho = \mathcal{L} \rho \), where \( \mathcal{L} \) is given by the second term corresponding to the dissipative dynamics due to the interaction of the system with the environment or reservoir. The overall system-environment state can be neglected. This leads to the ubiquitous quantum Markovian master equation for the system density operator, which can be used under the assumption that memory effects are negligible. However, in certain physical situations, this occurs in all branches of physics \( [6] \) it is of considerable importance to develop a general formalism that extends beyond the Markov approximation and resulting Lindblad evolution.
in Eq. (11). Instead, we consider dissipative dynamics described by
\[ \dot{\rho} = KL\rho, \] 
where $K$ is an integral operator that depends on time of the form $K\phi = \int_{0}^{t} k(t-t')\phi(t')dt'$. The kernel function $k(t-t')$ is a well-behaved, continuous function that determines the type of memory in the physical problem. The solution to the master equation can be found by taking the Laplace transform
\[ s\hat{\rho}(s) - \rho(0) = \tilde{K}(s)L\hat{\rho}(s), \] 
determining the poles, and inverting the equation in the standard way. The solution to Eq. (3) defines a linear map $\Phi_t: \rho \rightarrow \rho_t$ that describes the evolution of a system coupled to an environment provided that $\Phi_t$ satisfies properties (i), (ii), and (iii). Because the master equation is no longer of the Lindblad form, the semigroup property is lost. However, this property is not necessary to describe a physically acceptable state evolution. All that is required is that the linear map be a completely positive, trace-preserving map.

The evolution of quantum systems is described by unitary operators. Therefore, $\Phi_t$ should describe an evolution of the system that arises from an overall unitary evolution of the system and environment
\[ \Phi_t(\rho) = \text{Tr}_R\{U(\rho \otimes |\gamma_0 \rangle\langle \gamma_0|)U^\dagger\}, \] 
where $\Gamma$ denotes the environment degrees of freedom and $\gamma_0$ is some initial state of the environment. One should imagine that the state $\rho$ is prepared at some time $t = 0$ and so is initially uncorrelated with the external system. The state and the environment evolve unitarily for some time and they become correlated. One may think of the environment as extracting information from the system as it will typically map pure states into mixed states. This noise process is described by a linear map involving only operators on the system of interest so that it has a Kraus decomposition
\[ \Phi_t(\rho) = \sum_k A_k^\dagger \rho A_k, \] 
where the condition $\sum_k A_k^\dagger A_k = I$ ensures that unit trace is preserved for all time. A map has a Kraus decomposition if and only if it is completely positive. Physically, the existence of a Kraus decomposition ensures that the system evolution is compatible with a unitary evolution on the system-environment Hilbert space.

In solving Eq. (3) it is advantageous, in practice, to find a damping basis for the superoperator $L$ that diagonalizes the master equation. Solving the eigenvalue equation $L\rho = \lambda\rho$ produces a complete, orthogonal basis with which to expand the density operator at any time. This results in a set of eigenvalues $\{\lambda_i\}$ and right and left eigenoperators, $\{R_i\}, \{L_i\}$, that satisfy the duality relation $\text{Tr}\{L_iR_j\} = \delta_{ij}$. Once the initial state is known $\rho(0) = \sum_i \text{Tr}\{L_i\rho(0)\}R_i$, the state of the system at any later time can be found through $\rho(t) = \sum_i \text{Tr}\{L_i\rho(0)\}A_i(t)R_i = \sum_i \text{Tr}\{R_i\rho(0)\}A_i(t)L_i$. The $A_i(t)$ are general functions that determine the time evolution. The damping basis allows for the replacement of $L$ by the eigenvalues $\lambda_i$ so that Eq. (11) may be written as
\[ \bar{\rho}(s) = \sum_i \frac{1}{s - K(s)\lambda_i} \text{Tr}\{L_i\rho(0)\}R_i. \] 

We now present a concrete example of a system that has a master equation of the form of Eq. (3). Consider the time-dependent Hamiltonian
\[ H(t) = \hbar \sum_{i=1}^{3} \Gamma_i(t)\sigma_i, \] 
where $\Gamma_i(t)$ are independent random variables and $\sigma_i$ are the Pauli operators. Each random variable obeys the statistics of a random telegraph signal, which is defined by $\Gamma_i(t) = a_i(-1)^{n_i(t)}$. The random variable $n_i(t)$ has a Poisson distribution with a mean equal to $\tau_i/2\tau_i$, while $a_i$ is an independent coin-flip random variable. By abuse of notation, the random variable $a_i$ takes the values $\pm 1$. The random telegraph signal is a wide sense stationary stochastic process with zero mean. This model is applicable to any two-level quantum system that interacts with an environment possessing random telegraph signal noise. For example, this could describe a two-level atom subjected to a fluctuating laser field that has jump-type random phase noise. In the language of nuclear magnetic resonance, this model describes a spin-1/2 particle in the presence of three orthogonal magnetic fields. Each field has a constant magnitude $a_i$ and inverts randomly in time with a distribution given by $n_i$. The strength of the coupling of the system to the external influence is given by the parameters $\tau_i$. The flipping or fluctuation rate is inversely given by $\tau_i$.

The equation of motion for the density operator is given by the von Neumann equation $\dot{\rho} = -\frac{i}{\hbar}[H, \rho] = -i \sum_k \Gamma_k(t)[\sigma_k, \rho]$ that has the solution
\[ \rho(t) = \rho(0) - i \int_0^t \sum_k \Gamma_k(s)[\sigma_k, \rho(s)]ds. \] 
Upon substitution of Eq. (3) back into the von Neumann equation and performing a stochastic average, one obtains
\[ \bar{\rho}(t) = -i \int_0^t \sum_k e^{-i\tau_k a_k^2[\sigma_k, [\sigma_k, \rho(t')]]} dt', \] 
where the correlation functions of the random telegraph signal $\langle \Gamma_j(t)\Gamma_k(t') \rangle = a_k^2 e^{-\frac{(t-t')^2}{2\tau_k^2}} \delta_{jk}$ have been employed. Equation (10) is an incoherent combination of exact equations of motion for the mean value of the density matrix, i.e., the ensemble average over the random fluctuations for each component $k = 1, 2, 3$. After averaging
over the reservoir variables, we are left with a homogeneous Volterra equation for the system density operator that has an exponential memory kernel. The state of the system at time \( t \) depends on its past history. The power spectrum of the environment is given by a Fourier transform of the exponential correlation function, which is an unnormalized Lorentzian with a maximum of \( 2\kappa^2 \tau^2 \) and a full width at half maximum equal to \( 1/(\pi\tau) \). In the case of white noise, the delta-function correlation in time leads to a flat power spectrum for the environment with a strength given by a diffusion constant. The system is equally coupled to all frequencies of the external system. In the case of colored noise, the system prefers certain frequencies. Thus, \( a \) is the coupling strength of the system with the external system while \( \tau \) determines which frequencies the system prefers most. Increasing both \( a \) and \( 1/\tau \) corresponds to a more noisy environment. Therefore, the dimensionless product \( a\tau \) is the fundamental quantity that determines the amount of fluctuation.

Having derived a master equation of the form of Eq. (9) with an exponential kernel function, we now determine the damping basis and solve the master equation. We assume that the fluctuation rates \( \tau_i \) are equal so that they obey the same Poisson statistics. This leads to a single kernel operator acting on the Lindblad superoperator, rather than a linear superposition of such operators:

\[
\hat{\rho} = \mathcal{L}_1 \rho + \mathcal{L}_2 \rho + \mathcal{L}_3 \rho \rho.
\]

The damping basis for Eq. (10) is found to be the following set of eigenvalues and eigenoperators:

\[
\{\lambda_0, \lambda_1, \lambda_2, \lambda_3\} = \{0, -4(a_1^2 + a_2^2), -4(a_1^2 + a_3^2), -4(a_2^2 + a_3^2)\} \quad \text{and} \quad \{R_0, R_1, R_2, R_3\} = \{L_0, L_1, L_2, L_3\} = \{I, \sigma_1, \sigma_2, \sigma_3\}
\]

which are self dual. Using the damping basis, the Laplace transform of Eq. (10) becomes

\[
\tilde{\rho}(s) = \sum_{i} \frac{s + 1/\tau}{s(1 + s/\tau)} \text{Tr}\{\sigma_i \rho(0)\} \sigma_i.
\]

This can be inverted to give the solution

\[
\rho(t) = \sum_{i} \text{Tr}\{\sigma_i \rho(0)\} \Lambda_i(t) \sigma_i.
\]

In terms of the dimensionless time \( \nu = t/2\tau \), the functions \( \Lambda_i(\nu) = e^{-\nu}\left[\cos(\mu_i \nu) + \frac{\sin(\mu_i \nu)}{\mu_i}\right] \) are damped harmonic oscillators having frequencies \( \mu_i = \sqrt{(4\kappa_i \tau_i)^2 - 1} \) with \( \kappa_i^2 = a_i^2 + a_k^2 \) for \( i \neq j \neq k \). This differs from the Markovian case, where the functions are purely exponential functions in time with parameters defining the characteristic lifetimes. A power series expansion gives \( \Lambda(\nu) = 1 - \frac{\nu^2}{2!} + O(\nu^3) \), which shows that the linear term in \( \nu \) is missing. Thus, the standard white noise diffusion term vanishes. This is a general property of the memory kernel and a fundamental difference between white noise and colored noise.

The function \( \Lambda(\nu) \) has two regimes – pure damping and damped oscillations. The fluctuation parameter, given by the product \( \kappa \tau \), determines the behavior of the solution. When \( 0 \leq \kappa \tau < 1/4 \) the solution is described by damping. The frequency \( \mu \) is imaginary with magnitude less than unity. When \( \kappa \tau = 1/4 \) the function \( \Lambda(\nu) = e^{-\nu(1 - \nu)} \) is unity at the initial time and approaches zero as time approaches infinity. In addition to pure damping, damped harmonic oscillations in the interval \([-1, +1]\) exist in the regime \( \kappa \tau > 1/4 \).

The functions \( \Lambda_i(\nu) \) determine the evolution of each component of the Bloch vector. The bound \( |\Lambda(\nu)| \leq 1 \) ensures that the density operator evolves only to states on or inside the Bloch sphere so that \( \Phi \) always maps positive operators to positive operators. For Markovian master equations, the dissipation results in a contraction of each component, which is a consequence of the semigroup property. This property is absent for colored noise, so that the dissipation results in contractions with oscillations. The information exchange between the system and the environment leads to an exchange of entropy between the two. The entropy of the average system state can oscillate in time with an overall decay.

The solution to the master equation (12) defines a linear map \( \Phi_t : \rho \rightarrow \rho_t \) on \( \mathcal{M}_2 \). This has a Kraus decomposition \( \Phi_t(\rho) = \sum_{k} A_k \rho A_k^\dagger \) with Kraus operators given by \( A_1 = \sqrt{\xi_1(\nu)} \sigma_1, A_2 = \sqrt{\xi_2(\nu)} \sigma_2, A_3 = \sqrt{\xi_3(\nu)} \sigma_3 \) and \( A_4 = \sqrt{\xi_4(\nu)} I \), provided the following linear combinations are nonnegative:

\[
4\xi_1(\nu) = 1 + \Lambda_1 - \Lambda_2 - \Lambda_3 \geq 0,
4\xi_2(\nu) = 1 - \Lambda_1 + \Lambda_2 - \Lambda_3 \geq 0,
4\xi_3(\nu) = 1 - \Lambda_1 - \Lambda_2 + \Lambda_3 \geq 0,
4\xi_4(\nu) = 1 + \Lambda_1 + \Lambda_2 + \Lambda_3 \geq 0.
\]

We now show which properties (2) hold. Clearly, this mapping is trace-preserving and property 2(i) is satisfied. Property 2(iii) is satisfied because \( \lim_{t \to 0} \Lambda_i(t) = 1 \). The system evolves continuously in time and the evolution is described by the identity map at the initial time. The semigroup property 2(iv) is lost as \( \Lambda_i(t) \Lambda_i(s) \neq \Lambda_i(t+s) \).

The map is completely positive if \( \Phi_t \otimes I_{n} \geq 0 \), \( \forall n \in \mathbb{Z}_+ \). It is sufficient to show that the composite operation on a maximally entangled state is positive. For a linear map from \( \mathcal{M}_2 \) to \( \mathcal{M}_2 \), we need only show that the composite map \( \Phi_t \otimes I (|\beta_0\rangle \langle \beta_0|) \) on \( \mathcal{M}_4 \) is positive semidefinite, where \( |\beta_0\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \) is the maximally entangled Bell state. Hence the map is completely positive if and only if the eigenvalues of the composite map are nonnegative. The eigenvalues \( \{\xi_j\} \) are exactly those given by Eqs. (13). Therefore, property 2(ii) is satisfied for all \( a_i \tau \) and every \( \nu \) if and only if

\[
\inf_{(a_i \tau)} \xi_j(\nu) \geq 0, \quad j = 1, 2, 3, 4.
\]

This follows from the fact that the existence of a Kraus decomposition and the composite operation on the maximally entangled state are both necessary and sufficient to show complete positivity.

Condition (14) is not satisfied for all values of the parameters. A case where it is satisfied occurs when two
or more of the $a_i$ are zero. For example, if two of the $a_i$ are zero and one is nonzero then $\Phi_i$ defines a depolarizing channel with colored noise. Suppose $a_2 = a, a_1 = a_3 = 0$. In this case, $A_1(\nu) = A_2(\nu) = \Lambda(\nu)$ and $A_3(\nu) = 1$. This map has Kraus operators given by $A_1 = \sqrt{[1 + \Lambda(\nu)]/2} \ I$ and $A_2 = \sqrt{[1 - \Lambda(\nu)]/2} \ \sigma_3$. This map is a completely positive, trace-preserving map for all values of the fluctuation parameter $\sigma \tau$ because $|\Lambda(\nu)| \leq 1$ for all times $\nu$. The Hamiltonian $H = \hbar^2 \sigma_3$ implies that the $z$ component of the spin-1/2 particle is a constant of the motion so that the two states $|\pm\rangle$ are fixed points and do not evolve. As a physical model, a constant magnitude magnetic field is applied in the $z$-direction which inverts randomly in time. If the field is unobserved, the average trajectory for the density operator of the spin-1/2 system is dissipative. As time approaches infinity, there is maximum uncertainty in the $x$ and $y$ components of the spin system. A steady state $\Phi(t)\sigma_{ss} = \frac{1}{2}(\rho + \sigma_3 \rho \sigma_3)$ is reached; the entire Bloch sphere evolves to a line connecting the north and south poles.

An example where condition (14) fails is given by $a_1 = a_2 = a$ and $a_3 = 0$. Then each component of the Bloch vector evolves with frequencies given by $\mu_1 = \mu_2 = \sqrt{(4\alpha \tau)^2 - 1}$ and $\mu_3 = \sqrt{(3\sigma \tau)^2 - 1}$. There are no fixed points except the maximally mixed state. In this case, it is found numerically that $\alpha \tau < 0.8$ leads to a completely positive map. This means that there is a limit on the environment power spectrum. The bandwidth may be large provided the coupling is made small and vice versa.

We find that if two or more of the $a_i$ are nonzero then there are regimes for the fluctuation parameters where complete positivity is lost. Assume the frequencies $\mu_i$ are equal. Then only the last eigenvalue in (13) need be considered. Setting the time equal to $\nu = \pi/\mu$ we find that if the frequencies are less than or equal to $\pi/\ln(3)$ the map defined by Eq. (12) is completely positive for all time. Complete positivity is lost as the frequencies become large. The case of three equal frequencies sets an upper bound. We have the following sufficient condition for (14) to be satisfied: If $\mu^* = \max\{\mu_1, \mu_2, \mu_3\} \leq \pi/\ln(3)$ then the map is completely positive for all time.

We recover the Markovian master equation by letting $\tau \to 0$ and $a \to \infty$ in such a way that $2a^2\tau$ becomes a constant. The random telegraph signal reduces to a Gaussian white noise in this singular limit and Eq. (10) becomes

$$\dot{\rho}(t) = -\int_0^t \delta(t - t') \sum_k 2a_k \sigma_k \rho(t') \| \sigma_k, \rho(t') \| dt'.$$

(15)

This master equation is local in time, leading to $\Lambda_i(t) = \exp(-\gamma_i t)$ in Eq. (12) with inverse lifetimes $\gamma_i = 4a_i^2\tau$. We point out that, even in the case of white noise, there are examples of maps that are positive but not completely positive [7, 13, 14]. For Markovian dynamics, the relations (16) are satisfied if and only if $\gamma_i \leq \gamma_j + \gamma_k$ for all permutations of the indices.

By construction of our example, complete positivity holds in the white noise limit. We conclude that the loss of complete positivity, when the memory kernel is present, is a feature of the colored noise. The validity of Eq. (9) has been questioned [15]. This Letter shows conditions under which a memory kernel is valid and shows that such conditions can be achieved. We have presented an example of a completely positive, trace-preserving map that results from a system-environment coupling that is essentially non-Markovian. From this, it was shown that a memory kernel can be physically valid. The results reveal that interesting features arise from the colored noise of the environment, which are not present in the limit of white noise. White noise is an idealization of real noises and under certain conditions cannot be used. Thus, more work needs to be done in the study of more general noises that include memory effects.

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