

Quantum Semi-Markov Processes

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We construct a large class of non-Markovian master equations that describe the dynamics of open quantum systems featuring strong memory effects, which relies on a quantum generalization of the concept of classical semi-Markov processes. General conditions for the complete positivity of the corresponding quantum dynamical maps are formulated. The resulting non-Markovian quantum processes allow the treatment of a variety of physical systems, as is illustrated by means of various examples and applications, including quantum optical systems and models of quantum transport.

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The analysis of the time evolution of open systems plays a central role in many applications of modern quantum theory, including quantum information science, quantum transport theory, quantum thermodynamics, and quantum process tomography and control (see, e.g., [1]). The state of an open quantum system that is coupled to the degrees of freedom of its surroundings is represented by a time-dependent density matrix $\rho(t)$. In the Markovian regime the dynamics is governed by a master equation of the relatively simple form

$$\frac{d}{dt}\rho(t) = \mathcal{L}\rho(t), \quad (1)$$

where \mathcal{L} is a time-independent generator with the famous Gorini-Kossakowski-Sudarshan-Lindblad structure [2]

$$\mathcal{L}\rho = -i[H, \rho] + \sum_{\alpha} \left[A_{\alpha} \rho A_{\alpha}^{\dagger} - \frac{1}{2} \{A_{\alpha}^{\dagger} A_{\alpha}, \rho\} \right]. \quad (2)$$

The Hamiltonian H describes the coherent part of the time evolution and the A_{α} are certain operators representing the various decay modes. The solution of Eq. (1) can be written in terms of a linear map $V(t) = \exp(\mathcal{L}t)$ that transforms the initial state $\rho(0)$ into the state $\rho(t) = V(t)\rho(0)$ at time t . The physical interpretation of this map $V(t)$ requires that it preserves the trace and the positivity of the density matrix $\rho(t)$. According to general physical principles $V(t)$ must be a completely positive (CP) map [3,4]. Hence, $V(t)$ represents a CP dynamical semigroup known as quantum Markov process, whose generator has been proven [2] to be of the form (2).

The quantum dynamics given by Eq. (2) has a clear-cut connection to a classical Markov process for the case in which one has a closed system of equations for the populations $P_n(t) = \langle n | \rho(t) | n \rangle$ in a fixed orthonormal basis $\{|n\rangle\}$ of the open system's Hilbert space, typically the energy eigenbasis. In fact, in this case one recovers the Pauli master equation,

$$\frac{d}{dt}P_n(t) = \sum_m [\Gamma_{nm}P_m(t) - \Gamma_{mn}P_n(t)], \quad (3)$$

which describes a classical Markovian jump process with transition rates Γ_{mn} , justifying the notion of a quantum Markov process.

The most important physical assumption which underlies the master equation (1) is the validity of the Markov approximation of short environmental correlation times. If this approximation is violated non-Markovian dynamics emerges which is characterized by pronounced memory effects, finite revival times, and nonexponential relaxation and decoherence. These effects can result from long-range correlation functions, from correlations and entanglement in the initial state, as well as from the neglect of extra degrees of freedom affecting the dynamics [5,6]. As a consequence the theoretical treatment of non-Markovian quantum dynamics is generally extremely demanding. A widely used non-Markovian generalization of Eq. (1) is given by the integrodifferential equation

$$\frac{d}{dt}\rho(t) = \int_0^t d\tau \mathcal{K}(\tau)\rho(t-\tau). \quad (4)$$

In this equation one takes into account quantum memory effects through the introduction of the memory kernel $\mathcal{K}(\tau)$ which means that the rate of change of the state $\rho(t)$ at time t depends on the states $\rho(t-\tau)$ at previous times $t-\tau$. Equations of the form (4) arise, for instance, by employing the standard Nakajima-Zwanzig projection operator technique [7]. Obviously, the Markovian master equation (1) is obtained if the memory kernel is taken to be proportional to a δ function, $\mathcal{K}(\tau) = 2\delta(\tau)\mathcal{L}$.

In order to be physically acceptable the superoperator $\mathcal{K}(\tau)$ appearing in Eq. (4) must grant the CP of the resulting quantum dynamical map $V(t)$. This is a very stringent requirement and, in fact, the general structural characterization of physically admissible memory kernels is an unsolved problem of central importance in the field of

non-Markovian quantum dynamics [5,8]. It has been realized recently that even the most simple and natural choices for the memory kernel can lead to unphysical results [5,9]. To improve this situation we will construct a class of non-Markovian quantum master equations that arises naturally as a quantum mechanical generalization of classical semi-Markov processes [10]. The approach proposed here leads to important physical insights guiding the phenomenological determination of the memory kernel, and, at the same time, enables a compact formulation of sufficient conditions that guarantee the existence and the CP of the quantum dynamical map. Moreover, for a specific class of processes one can formulate CP conditions which are not only sufficient but also necessary.

We consider memory kernels with the general structure

$$\begin{aligned} \mathcal{K}(\tau)\rho = & -i[H(\tau), \rho] - \frac{1}{2} \sum_{\alpha} \{A_{\alpha}^{\dagger}(\tau)A_{\alpha}(\tau), \rho\} \\ & + \sum_{\alpha} A_{\alpha}(\tau)\rho A_{\alpha}^{\dagger}(\tau), \end{aligned} \quad (5)$$

that is to say of the form given by Eq. (2) apart from the time dependence of the considered operators. As previously done in the Markovian case let us consider the situation in which the populations obey a closed system of equations of motion, which then takes the form

$$\frac{d}{dt}P_n(t) = \int_0^t d\tau \sum_m [W_{nm}(\tau)P_m(t-\tau) - W_{mn}(\tau)P_n(t-\tau)], \quad (6)$$

where $W_{nm}(\tau) = \sum_{\alpha} |\langle n|A_{\alpha}(\tau)|m\rangle|^2$. This is the master equation for a general type of classical non-Markovian processes known as semi-Markov processes [10]. Thus, whenever the populations obey closed equations, Eq. (2) yields the classical Markovian master equation (3), while Eq. (4) with the kernel (5) leads under the same conditions to the generalized master equation (6) for a classical semi-Markov process. This justifies on the same footing as before the name quantum semi-Markov process.

To clarify the physical content of Eq. (6) let us consider as an example the situation in which the kernel functions $W_{nm}(t)$ factorize as $W_{nm}(t) = \pi_{nm}k_m(t)$, where $\pi_{nm} \geq 0$ and $\sum_n \pi_{nm} = 1$. The corresponding process can then be interpreted as describing a particle moving on a lattice with sites labeled by n , where the π_{nm} are the probabilities for jumps from site m to site n . Jumps out of a given site n take place after a certain waiting time t that follows the waiting time distribution $f_n(t)$. The characteristic feature of semi-Markov processes is the fact that, by contrast to the Markovian case, $f_n(t)$ need not be an exponential function, but can be any probability distribution, thus giving rise to memory effects. These waiting time distributions are uniquely determined by the functions $k_n(t)$ according to the relation [11]

$$f_n(t) = \int_0^t d\tau k_n(\tau)g_n(t-\tau) \equiv (k_n * g_n)(t), \quad (7)$$

where the function

$$g_n(t) = 1 - \int_0^t d\tau f_n(\tau) \quad (8)$$

denotes the probability not to have left site n by time t , the so-called survival probability, and $*$ is the usual convolution product. The generalized master equation (6) therefore provides a physically acceptable time evolution for the populations $P_n(t)$, granting, in particular, their positivity, provided the functions $k_n(t)$ allow an interpretation in terms of waiting time distributions [11,12].

However, these classical conditions are clearly not enough to ensure the existence of a well-defined dynamics in the quantum case, and a general characterization at the quantum level can hardly be achieved. Therefore our next goal is the formulation of sufficient conditions that guarantee the CP of the dynamical map $V(t)$ corresponding to the non-Markovian master equation defined by Eqs. (4) and (5), no longer assuming that closed equations for the populations exist. This map is defined by

$$\frac{d}{dt}V(t) = \int_0^t d\tau \mathcal{K}(\tau)V(t-\tau), \quad (9)$$

together with the initial condition $V(0) = I$, with I the identity map. We now employ ideas recently formulated in Ref. [13], decomposing the memory kernel as $\mathcal{K}(\tau) = B(\tau) + C(\tau)$, where $B(\tau)$ is the CP map defined by

$$B(\tau)\rho = \sum_{\alpha} A_{\alpha}(\tau)\rho A_{\alpha}^{\dagger}(\tau), \quad (10)$$

and $C(\tau)$ is given by the first line of (5). We further introduce the map $V_0(t)$ as the solution of the equation

$$\frac{d}{dt}V_0(t) = \int_0^t d\tau C(\tau)V_0(t-\tau), \quad (11)$$

with the initial condition $V_0(0) = I$. Considering the Laplace transforms of Eqs. (9) and (11) one obtains a resolventlike identity for the dynamical map leading in the time domain to the equation

$$V(t) = V_0(t) + (V_0 * B * V)(t). \quad (12)$$

Regarding formally the superoperator $B(\tau)$ as a perturbation and iterating Eq. (12) one finds that the full dynamical map $V(t)$ can be represented as a series,

$$\begin{aligned} V(t) = & V_0(t) + (V_0 * B * V_0)(t) \\ & + (V_0 * B * V_0 * B * V_0)(t) + \dots \end{aligned} \quad (13)$$

Because of the fact that the set of CP maps is closed under addition and convolution, we can conclude from Eq. (13) that $V(t)$ is CP if $V_0(t)$ is CP. To bring this condition into an explicit form let us assume that the Hermitian operators $H(\tau)$ and $\sum_{\alpha} A_{\alpha}^{\dagger}(\tau)A_{\alpha}(\tau)$ are diagonal in the time-

independent orthonormal basis $\{|n\rangle\}$, that is $H(\tau) = \sum_n \varepsilon_n(\tau) |n\rangle\langle n|$ and

$$\sum_{\alpha} A_{\alpha}^{\dagger}(\tau) A_{\alpha}(\tau) = \sum_n k_n(\tau) |n\rangle\langle n|. \quad (14)$$

Then we can solve Eq. (11) to obtain

$$V_0(t)\rho(0) = \sum_{nm} g_{nm}(t) |n\rangle\langle n| \rho(0) |m\rangle\langle m|, \quad (15)$$

where the functions $g_{nm}(t)$ are the solutions of

$$\dot{g}_{nm}(t) = - \int_0^t d\tau [z_n(\tau) + z_m^*(\tau)] g_{nm}(t - \tau), \quad (16)$$

corresponding to the initial conditions $g_{nm}(0) = 1$, and $z_n(\tau) = \frac{1}{2}k_n(\tau) + i\varepsilon_n(\tau)$. To prove Eq. (15) one first shows that $C(\tau)(|n\rangle\langle m|) = -[z_n(\tau) + z_m^*(\tau)]|n\rangle\langle m|$. Using this relation one easily demonstrates that the expression (15) indeed represents the desired solution of Eq. (11). It is important to notice that the functions $g_{nm}(t)$ do actually coincide with the survival probabilities $g_n(t)$ introduced by Eq. (8).

Employing the Kraus representation [3] we see that the map $V_0(t)$ given by Eq. (15) is CP if and only if the matrix with elements $g_{nm}(t)$ is positive,

$$G(t) = (g_{nm}(t)) \geq 0. \quad (17)$$

Hence, we arrive at a sufficient condition for CP: The quantum dynamical map $V(t)$ corresponding to the non-Markovian master equation (4) with the memory kernel (5) is CP if the condition (17) is fulfilled. A necessary condition for (17) to hold is the positivity of the diagonal elements of $G(t)$, which are given by the survival probabilities $g_n(t) = g_{nn}(t)$. This necessary condition in turn implies the positivity of the functions $f_n(t)$ according to Eq. (7), which can then be interpreted as true waiting time distributions. The positivity of the matrix $G(t)$ therefore represents a natural quantum generalization of the classical conditions.

We illustrate the result (17) with the help of several examples, which all fall into the class of quantum semi-Markov processes introduced by means of Eqs. (4) and (5). A prototypical system showing strong non-Markovian behavior is a two-level atom interacting with a damped field mode described by the memory kernel

$$\begin{aligned} \mathcal{K}(\tau)\rho = & -i\varepsilon(\tau)[\sigma_+\sigma_-, \rho] \\ & + k(\tau)\left[\sigma_-\rho\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho\}\right]. \end{aligned} \quad (18)$$

Excited and ground state are denoted by $|+\rangle$ and $|-\rangle$, respectively, and σ_{\pm} are the corresponding raising and lowering operators. The index n thus takes on the two values $n = \pm$. For a positive function $k(\tau)$ the memory kernel (18) is of the form specified above with $k_+(\tau) = k(\tau)$, $k_-(\tau) = 0$, $\varepsilon_+(\tau) = \varepsilon(\tau)$, and $\varepsilon_-(\tau) = 0$. Hence, the matrix $G(t)$ takes the form

$$G(t) = \begin{pmatrix} g_{++}(t) & g_{+-}(t) \\ g_{+-}^*(t) & 1 \end{pmatrix}, \quad (19)$$

with $g_{++}(t)$ and $g_{+-}(t)$ determined by Eq. (16). Thus we see that the condition (17) for CP is equivalent to $g_{++}(t) \geq |g_{+-}(t)|^2$. The master equation corresponding to the memory kernel (18) can be solved analytically. One then finds that for this case the condition (17) is not only sufficient but also necessary for CP.

A further very instructive example involving an infinite dimensional Hilbert space is the model of a quantum oscillator with non-Markovian damping studied in Ref. [9]. The memory kernel for this model reads

$$\mathcal{K}(\tau)\rho = k(\tau)\left[a\rho a^{\dagger} - \frac{1}{2}\{a^{\dagger}a, \rho\} \right], \quad (20)$$

where $k(\tau) = \kappa \exp(-\gamma\tau)$ and a^{\dagger} , a are the raising and lowering operators of the oscillator. This kernel is again of the form (5) with a single Lindblad operator $A(\tau) = \sqrt{k(\tau)}a$. Here, the basis states $|n\rangle$ are the number states of the oscillator, $k_n(\tau) = nk(\tau)$ and $\varepsilon_n(\tau) = 0$. Solving Eq. (16) by means of a Laplace transformation, we find

$$g_{nn}(t) = e^{-\gamma t/2} \left[\cosh(d_n t/2) + \frac{\gamma}{d_n} \sinh(d_n t/2) \right],$$

where $d_n = \sqrt{(\gamma/2)^2 - n\kappa}$. For the necessary condition $g_{nn}(t) \geq 0$ to hold d_n must be real. This shows that condition (17) is certainly violated if $4n\kappa > \gamma^2$. Because n can be arbitrary large we conclude that condition (17) is never fulfilled. The interesting aspect of this example is the fact that the non-Markovian master equation indeed violates not only CP but also positivity. This fact has been demonstrated in [9] and clearly shows again the relevance of our CP conditions.

Many further physical systems lead to a generalized master equation of the form introduced here if one applies the Nakajima-Zwanzig projection operator technique, such as the tight-binding quantum diffusion model studied in [14], and the quantum transport model introduced in [15], which leads to a memory kernel of the form

$$\mathcal{K}(\tau)\rho = k(\tau)\left[\frac{1}{2}T\rho T^{\dagger} + \frac{1}{2}T^{\dagger}\rho T - \rho \right]. \quad (21)$$

This kernel describes the motion of an excitation in a modular system consisting of weakly coupled subunits labeled by the index n , where $T = \sum_n |n+1\rangle\langle n|$ represents the corresponding translation operator. The model features strong non-Markovian behavior and a transition from diffusive to ballistic quantum transport. The memory kernel $\mathcal{K}(\tau)$ is obviously of the form introduced above. The Hamiltonian contribution vanishes, $H(\tau) = 0$, and all kernel functions are equal to each other, $k_n(\tau) = k(\tau)$, which corresponds to the special case treated in Refs. [5,13] with a loss term proportional to the identity operator. Equation (16) shows that also all matrix elements of $G(t)$ are equal, $g_{nm}(t) = g(t)$, and, hence, condition (17)

reduces to the condition $g(t) \geq 0$. Clearly this condition leads to important restrictions on the form of the kernel function $k(\tau)$ which is determined by the correlation function of the microscopic model.

As our final example we discuss memory kernels of the following general structure,

$$\begin{aligned} \mathcal{K}(\tau)\rho = & -i[H(\tau), \rho] - \frac{1}{2} \sum_n k_n(\tau) \{|n\rangle\langle n|, \rho\} \\ & + \sum_{nm} \pi_{nm} k_m(\tau) |n\rangle\langle m| \rho |m\rangle\langle n| \end{aligned} \quad (22)$$

of which (18) provides an example. For this memory kernel the coherences of the density matrix, i.e., the off-diagonal elements $\rho_{nm}(t) = \langle n|\rho(t)|m\rangle$, $n \neq m$, are simply given by $\rho_{nm}(t) = \rho_{nm}(0)g_{nm}(t)$. On the other hand, the diagonals of the density matrix, i.e., the populations $P_n(t)$ obey a closed transport equation as in (6). It is remarkable that in this case one can go one step further to derive a condition for the CP which is not only sufficient but also necessary. To this end one writes the quantum dynamical map $V(t)$ corresponding to the non-Markovian quantum master equation (4) with the memory kernel (22) in terms of the functions $g_{nm}(t)$ and of the conditional transition probabilities $T_{nm}(t)$ obeying the classical master equation (6). The quantity $T_{nm}(t)$ represents the probability that the particle is at site n at time t given that it started at site m at time $t = 0$. With the help of the resulting expression for the map $V(t)$ we then find the following result. Given a classical semi-Markov process, the quantum dynamical map $V(t)$ is CP if and only if the condition

$$\tilde{G}(t) = (\tilde{g}_{nm}(t)) \geq 0 \quad (23)$$

is satisfied. Here, the off-diagonal elements of the matrix $\tilde{G}(t)$ coincide with those of $G(t)$, while the diagonals of $\tilde{G}(t)$ are given by the conditional transition probabilities, $\tilde{g}_{nn}(t) = T_{nn}(t)$. Note that the probabilities $T_{nn}(t)$ are in fact in general greater than the corresponding survival probabilities $g_{nn}(t)$, since the system can be in state n at time t both because it has not left it and because it has come back to the initial state. Equation (23) thus provides a complete characterization of the CP of the class of quantum semi-Markov processes given by (22).

Building on an analogy with classical semi-Markov processes we have constructed a large class of non-Markovian master equations with memory kernel and formulated sufficient conditions for the CP of the resulting quantum dynamical map. The latter impose strong restrictions on the structure of physically acceptable non-Markovian quantum master equations, which are particularly useful in phenomenological approaches. For a spe-

cific class of quantum semi-Markov processes necessary and sufficient conditions for CP have also been formulated. Important further developments of the theory should include the case of temporarily negative kernel functions and effects from correlations and entanglement in the initial state.

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