

General form of quantum evolution

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We propose a complete treatment of a local in time dynamics of open quantum systems. In this approach Markovian evolution turns out to be a special case of a general non-Markovian one. We provide a general representation of the local generator which generalizes well known Lindblad representation for the Markovian dynamics. It shows that the structure of non-Markovian generators is highly intricate and the problem of their classification is still open. Simple examples illustrate our approach.

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Any realistic quantum system inevitably interacts with its environment, therefore, the theory of open quantum systems and their dynamical features is of particular importance [1, 2]. Actually, this problem attracts nowadays increasing attention due to the growing interest in controlling quantum systems and applications in modern quantum technologies such as quantum communication, cryptography and computation [3].

For several decades the popular Markovian approximation which does not take into account memory effects was successfully studied and applied in a variety of problems [1, 2]. However, recent investigations in quantum information and recent technological progress calls for truly non-Markovian approach. In the last few years many analytical methods and numerical techniques have been developed to treat non-Markovian processes in quantum optics, solid state physics and quantum information [4–17]. Moreover, several measures of non-Markovianity were proposed and intensively studied [18–22].

The most general form of local in time Master Equation reads as follows

$$\frac{d\rho(t)}{dt} = \mathcal{L}(t, t_0) \rho(t), \quad \rho(t_0) = \rho_0, \quad (1)$$

where $\mathcal{L}(t, t_0)$ is a local generator which depends not only upon the current time ‘ t ’ but in principle it might depend upon the initial point ‘ t_0 ’. It is clear that dependence on ‘ t_0 ’ introduces an effective memory. The system does remember when the evolution begun. We call the evolution governed by (1) Markovian if and only if $\mathcal{L}(t, t_0)$ does not depend on ‘ t_0 ’. Otherwise the evolution is non-Markovian. It is clear that $\mathcal{L}(t, t_0)$ is defined for $t \geq t_0$ only. Note however, that in the Markovian case $\mathcal{L}_M(t)$ is defined in principle for all $t \in (-\infty, \infty)$. Any solution to (1) gives rise to the dynamical map $\Lambda(t, t_0)$ defined by $\rho(t) = \Lambda(t, t_0)\rho_0$. Clearly $\Lambda(t, t_0)$ itself satisfies the following equation

$$\frac{d}{dt} \Lambda(t, t_0) = \mathcal{L}(t, t_0) \Lambda(t, t_0), \quad \Lambda(t_0, t_0) = \mathbb{1}, \quad (2)$$

where $\mathbb{1}$ denotes an identity map. A particular class of $\mathcal{L}(t, t_0)$ is provided by the homogeneous generators, i.e. when \mathcal{L} depends on ‘ $t - t_0$ ’ only. Hence, the evolution

is governed by the 1-parameter family $\mathcal{L}(\tau)$ defined for $\tau \geq 0$. It is clear that in this case the evolution is homogeneous as well, that is $\Lambda(t + T, t_0 + T) = \Lambda(t, t_0)$ for arbitrary T , and hence one may define a 1-parameter family of dynamical maps $\Lambda(t) := \Lambda(t, 0)$. Actually, one usually fixes $t_0 = 0$ from the very beginning and considers

$$\frac{d}{dt} \Lambda(t) = \mathcal{L}(t) \Lambda(t), \quad \Lambda(0) = \mathbb{1}. \quad (3)$$

We stress that it could be done only in the homogeneous case and usually it is referred as a time convolutionless (TCL) approach [23–25].

A solution $\Lambda(t, t_0)$ to (2) is defined by the following formula

$$\Lambda(t, t_0) = \mathbb{T} \exp \left(\int_{t_0}^t \mathcal{L}(\tau, t_0) d\tau \right), \quad (4)$$

where \mathbb{T} stands for the chronological operator. In the homogeneous case it simplifies to

$$\Lambda(t, t_0) = \mathbb{T} \exp \left(\int_0^{t-t_0} \mathcal{L}(\tau) d\tau \right), \quad (5)$$

which clearly shows that $\Lambda(t, t_0)$ depends on ‘ $t - t_0$ ’. We stress that the formula (4) has only a formal character since in general the evaluation of \mathbb{T} -product is not feasible. Recall, that this formula simplifies if $\mathcal{L}(t, t_0)$ defines mutually commuting family, i.e. $[\mathcal{L}(t, t_0), \mathcal{L}(u, t_0)] = 0$ for all $t, u \geq t_0$. In this case \mathbb{T} -product drops out from (4).

A solution $\Lambda(t, t_0)$ defines a legitimate quantum dynamics if and only if $\Lambda(t, t_0)$ is completely positive and trace preserving (CPT) for all $t \geq t_0$. Now comes the natural question: how to characterize the properties of $\mathcal{L}(t, t_0)$ which guarantee that $\Lambda(t, t_0)$ corresponds to the legitimate quantum dynamics. These conditions are well known in the Markovian case: a solution to

$$\frac{d}{dt} \Lambda(t, t_0) = \mathcal{L}_M(t) \Lambda(t, t_0), \quad \Lambda(t_0, t_0) = \mathbb{1}, \quad (6)$$

is CPT if and only if the time dependent generator has the following Lindblad representation [26–28]

$$\mathcal{L}_M \rho = -i[H, \rho] + \sum_{\alpha} \gamma_{\alpha} \left(V_{\alpha} \rho V_{\alpha}^{\dagger} - \frac{1}{2} \{V_{\alpha}^{\dagger} V_{\alpha}, \rho\} \right), \quad (7)$$

where $H = H(t)$ stands for the effective time-dependent Hamiltonian and $V_\alpha = V_\alpha(t)$ are time-dependent Lindblad (or noise) operators. The time dependent coefficients γ_α satisfy $\gamma_\alpha(t) \geq 0$ and encode the information about dissipation and/or decoherence of the system.

Let us observe that a family $\Lambda(t, t_0)$ of CPT maps may be represented by

$$\Lambda(t, t_0) = e^{Z(t, t_0)} , \quad (8)$$

where $Z(t, t_0)$ has a Lindblad representation for all $t \geq t_0$. The price we pay for this simple representation is that $Z(t, t_0)$ might be highly singular. It is clear that formally $Z(t, t_0)$ is defined as a logarithm of $\Lambda(t, t_0)$ and hence it is not uniquely defined (log has an infinite number of branches). Moreover, one always meets problems when $\Lambda(t, t_0)$ possesses eigenvalues belonging to the cut of log, cf. discussion in [18]. For example a CPT map $\Lambda\rho = \sigma_z\rho\sigma_z$ cannot be represented by $\Lambda = e^Z$. Note, however, that Λ may be considered as a limit of $\Lambda(t) = e^{Z(t)}$, with $Z(t) = -\log(\cos t)L_0$, and $L_0\rho = \sigma_z\rho\sigma_z - \rho$ is a legitimate Lindblad generator for $t \in [0, \pi/2)$. One has $\Lambda = \lim_{t \rightarrow \pi/2} \Lambda(t)$ (see discussion in [17]).

Note, that condition $\Lambda(t_0, t_0) = \mathbb{1}$ is equivalent to $Z(t_0, t_0) = 0$ which is guaranteed by

$$Z(t, t_0) = \int_{t_0}^t X(u, t_0) du , \quad (9)$$

and hence the solution has the following form

$$\Lambda(t, t_0) = \exp\left(\int_{t_0}^t X(\tau, t_0) d\tau\right) . \quad (10)$$

Note, that contrary to (4) the above formula does not contain chronological T-product. The corresponding generator $\mathcal{L}(t, t_0)$ is defined by [17]

$$\mathcal{L}(t, t_0) = \frac{d}{dt}\Lambda(t, t_0) \cdot \Lambda(t, t_0)^{-1} , \quad (11)$$

where $\Lambda(t, t_0)^{-1} = e^{-Z(t, t_0)}$ denotes the inverse of $\Lambda(t, t_0)$. Note, that $\Lambda(t, t_0)^{-1}$ is not completely positive, hence can not describe quantum evolution backwards in time, unless $\Lambda(t, t_0)$ is unitary or anti-unitary. Now, to compute $d\Lambda(t, t_0)/dt$ one uses well known formula [29]

$$\frac{d}{dt}e^{A(t)} = \int_0^1 e^{sA(t)} \dot{A}(t) e^{(1-s)A(t)} ds , \quad (12)$$

where $A(t)$ is an arbitrary (differentiable) family of operators, and $\dot{A} = dA/dt$. Hence

$$\frac{d}{dt}e^{Z(t, t_0)} = \mathcal{L}(t, t_0)e^{Z(t, t_0)} , \quad (13)$$

where

$$\mathcal{L}(t, t_0) = \int_0^1 e^{sZ(t, t_0)} X(t, t_0) e^{-sZ(t, t_0)} ds . \quad (14)$$

This is the main result of our Letter. It proves that each legitimate generator $\mathcal{L}(t, t_0)$ of quantum evolution governed by the Master Equation (1) has the form defined by (14), where $Z(t, t_0)$ has a Lindblad representation for each $t \geq t_0$, and $X(t, t_0)$ is defined in (9). Hence the construction of a legitimate generator is pretty simple: each family of Lindblad operators $Z(t, t_0)$, with $Z(t_0, t_0) = 0$, gives rise via (14) to the corresponding prescription for $\mathcal{L}(t, t_0)$. Nevertheless, the formula (14) is highly nontrivial and the computation of $\mathcal{L}(t, t_0)$ out of $Z(t, t_0)$ might be highly complicated. This is the price we pay for the simple representation of evolution (10). Hence, we have a kind of complementarity: either one uses T-product formula (4) with relatively simple generator or one avoids T-product in (10) but uses highly nontrivial generator (14). The advantage of our approach is that one knows how to construct generator (in practice it might be complicated) giving rise to the legitimate quantum dynamics.

Let us observe that in the special case when $X(t, t_0)$ mutually commute, i.e. $[X(t, t_0), X(u, t_0)] = 0$ for all $t, u \geq t_0$, the formula (14) reduces to $\mathcal{L}(t, t_0) = X(t, t_0)$. Hence, a commuting family $\mathcal{L}(t, t_0)$ defines a legitimate generator if and only if $Z(t, t_0) = \int_{t_0}^t \mathcal{L}(u, t_0) du$ has a Lindblad representation for all $t \geq t_0$. In the noncommutative case this simple criterion is no longer true.

The characteristic feature of the Markovian evolution governed by (6) is that $\Lambda(t, t_0)$ satisfies local composition law

$$\Lambda(t, s) \cdot \Lambda(s, t_0) = \Lambda(t, t_0) , \quad (15)$$

for $t \geq s \geq t_0$. Actually, this property is guaranteed by the intricate action of T-product in the formula (4). Now, changing the representation from (4) into (10) the validity of composition law is no longer visible. The formula (15) implies

$$e^{Z(t, u)} \cdot e^{Z(u, t_0)} = e^{Z(t, t_0)} , \quad (16)$$

for $t \geq s \geq t_0$. Clearly, in the commutative one has simply

$$Z(t, u) + Z(u, t_0) = Z(t, t_0) . \quad (17)$$

Note however that when $Z(t, t_0)$ do not commute, the Baker-Campbell-Hausdorff formula $e^A e^B = e^C$, with

$$C = A + B + \frac{1}{2}[A, B] + \frac{1}{12}\left([A, [A, B]] - [B, [A, B]]\right) + \dots ,$$

provides highly nontrivial condition upon $Z(t, t_0)$. It shows that knowing legitimate $Z(t, t_0)$ one does not know immediately whether the corresponding dynamics is Markovian or not. Only applying (14) one can check whether $\mathcal{L}(t, t_0)$ does, or does not, depend on 't₀' and hence infer about Markovianity. This problem simplifies in the homogeneous case: now the evolution is never Markovian unless $Z(t, t_0) = (t - t_0)L_0$, i.e. $\mathcal{L}(t, t_0) = L_0$, where L_0 denotes the time independent Markovian generator.

It is clear that for a general family of Lindblad generators $Z(t, t_0)$ computation of $\mathcal{L}(t, t_0)$ via (14) is rather untractable. However, as usual, there is a class of $Z(t, t_0)$ for which the general problem simplifies considerably. Consider a special class of $Z(t, t_0)$ defined via (9) by the following family

$$X(t, t_0) = a_1(t, t_0)\mathcal{L}_1 + \dots + a_N(t, t_0)\mathcal{L}_N, \quad (18)$$

where $\mathcal{L}_1, \dots, \mathcal{L}_N$ are time independent Lindblad generators. One has

$$Z(t, t_0) = A_1(t, t_0)\mathcal{L}_1 + \dots + A_N(t, t_0)\mathcal{L}_N, \quad (19)$$

where $A_k(t, t_0) = \int_{t_0}^t a_k(u, t_0)du$. Now, $Z(t, t_0)$ has a Lindblad representation iff $A_k(t, t_0) \geq 0$. Let us observe that if $\mathcal{L}_1, \dots, \mathcal{L}_N$ close a Lie algebra, i.e. $[\mathcal{L}_j, \mathcal{L}_j] = \sum_{k=1}^N c_{ij}^k \mathcal{L}_k$, then using well known Lie algebraic methods one can easily compute $\mathcal{L}(t, t_0)$ out of (14) and gets

$$\mathcal{L}(t, t_0) = b_1(t, t_0)\mathcal{L}_1 + \dots + b_N(t, t_0)\mathcal{L}_N, \quad (20)$$

where the functions $b_k(t, t_0)$ are uniquely defined by $a_k(t, t_0)$ and the structure constants c_{ij}^k . Actually, any set $\{\mathcal{L}_1, \dots, \mathcal{L}_N\}$ of Lindblad generators may be always completed to close a Lie algebra. It follows from the fact that a set of Lindblad generators belong to the Lie algebra corresponding to the Lie group of linear maps preserving hermiticity. Note, that if $[\mathcal{L}_i, \mathcal{L}_j] = 0$, i.e. the corresponding Lie algebra is commutative, then $b_k(t, t_0) = a_k(t, t_0)$, that is, $\mathcal{L}(t, t_0) = X(t, t_0)$.

Example 1 (Commutative case) Consider the following pure decoherence model defined by the following time dependent Hamiltonian $H(t) = H_R(t) + H_S(t) + H_{SR}(t)$, where $H_R(t)$ is the reservoir Hamiltonian, $H_S(t) = \sum_n \epsilon_n(t)P_n$ ($P_n = |n\rangle\langle n|$) the system Hamiltonian and

$$H_{SR}(t) = \sum_n P_n \otimes B_n(t) \quad (21)$$

the interaction part, $B_n = B_n^\dagger$ being reservoirs operators. The initial product state $\rho \otimes \omega$ evolves according to the unitary evolution $U(t, t_0)(\rho \otimes \omega)U(t, t_0)^\dagger$ and by partial tracing with respect to the reservoir degrees of freedom one finds for the evolved system density matrix

$$\rho(t) = \Lambda(t, t_0)\rho = \sum_{n,m} c_{mn}(t, t_0)P_m \rho P_n, \quad (22)$$

where $c_{mn}(t, t_0) = \text{Tr}[U_m(t, t_0)\omega U_n(t, t_0)^\dagger]$, with $U_n(t, t_0) = \text{T exp}[-i \int_{t_0}^t Y_n(\tau)d\tau]$, and $Y_n(\tau) = \epsilon_n(\tau)\mathbb{I}_R + H_R(\tau) + B_n(\tau)$ being time dependent reservoir operators. Note that the matrix $c_{mn}(t, t_0)$ is semi-positive definite and hence (22) defines the Kraus representation of the completely positive map $\Lambda(t, t_0)$. Note that $\Lambda(t, t_0)$ defines a commutative family of maps and hence one easily finds for the corresponding generator

$$\mathcal{L}(t, t_0)\rho = \sum_{n,m} \alpha_{mn}(t, t_0)P_m \rho P_n, \quad (23)$$

where the functions $\alpha_{mn}(t, t_0)$ are defined by $\alpha_{mn}(t, t_0) = \dot{c}_{mn}(t, t_0)/c_{mn}(t, t_0)$. Note that if $\dim \mathcal{H}_S = 2$, then $c_{11} = c_{22} = 1$, and $c_{12} = \gamma$ with $|\gamma| \leq 1$. One easily finds for the local generator

$$\mathcal{L}(t, t_0)\rho = ib_1(t, t_0)[\sigma_z, \rho] - b_2(t, t_0)[\sigma_z \rho \sigma_z - \rho], \quad (24)$$

with $b_1 = \text{Im}(\dot{\gamma}/2\gamma)$ and $b_2 = \text{Re}(\dot{\gamma}/2\gamma)$. Note that this dynamics is homogeneous if and only if the Hamiltonian of $S + R$ is time independent.

Example 2 (Noncommutative case) Let us consider a simple example of exactly solvable dynamics of 2-level system defined by the following homogenous family of operators $X(t) := X(t, 0)$

$$X(t) = a_1(t)\mathcal{L}_1 + a_2(t)\mathcal{L}_2, \quad t \geq 0, \quad (25)$$

where the Markovian generators $\mathcal{L}_1, \mathcal{L}_2$ are defined by

$$\begin{aligned} \mathcal{L}_1 \rho &= \sigma^+ \rho \sigma^- - \frac{1}{2} \{ \sigma^- \sigma^+, \rho \}, \\ \mathcal{L}_2 \rho &= \sigma^- \rho \sigma^+ - \frac{1}{2} \{ \sigma^+ \sigma^-, \rho \}, \end{aligned}$$

and $\sigma^+ = |1\rangle\langle 2|$, $\sigma^- = |2\rangle\langle 1|$ are the standard raising and lowering qubit operators ($\{|1\rangle, |2\rangle\}$ denotes an orthonormal basis in the qubit Hilbert space). Since \mathcal{L}_1 and \mathcal{L}_2 do not commute $X(t)$ defines a noncommutative family. Clearly, one may add to $X(t)$ a commutative part (24) which does commute with $X(t)$ and hence do not change qualitative features of dynamic. For simplicity we consider only simplified version which is essential for non-commutativity.

The time dependent parameters $a_1(t)$ and $a_2(t)$ are arbitrary but real. Following our construction one has

$$Z(t) = A_1(t)\mathcal{L}_1 + A_2(t)\mathcal{L}_2, \quad (26)$$

where $A_k(t) = \int_0^t a_k(u)du$. Hence, the formula $\Lambda(t) = e^{Z(t)}$ defines CPT map for all $t \geq 0$ if and only if

$$A_1(t) \geq 0, \quad A_2(t) \geq 0. \quad (27)$$

Now, let us apply our basic formula (14) to find the corresponding generator $\mathcal{L}(t)$. Observing that \mathcal{L}_1 and \mathcal{L}_2 close a Lie algebra $[\mathcal{L}_1, \mathcal{L}_2] = \mathcal{L}_1 - \mathcal{L}_2$, one easily finds

$$\mathcal{L}(t) = b_1(t)\mathcal{L}_1 + b_2(t)\mathcal{L}_2, \quad (28)$$

where

$$b_1(t) = a_1(t) + f(t), \quad b_2(t) = a_2(t) - f(t), \quad (29)$$

and the time dependent function $f(t)$ reads as follows

$$f(t) = \frac{W(t)}{A(t)} \left(1 + \frac{e^{-A(t)} - 1}{A(t)} \right), \quad (30)$$

where the Wronskian $W(t) = A_1(t)a_2(t) - A_2(t)a_1(t)$, and $A(t) = A_1(t) + A_2(t)$. Note, that $f(t) = 0$ (for all

$t \geq 0$) if and only if $W(t) = 0$, i.e. functions $a_1(t)$ and $a_2(t)$ are linearly dependent. If this is the case one has $a_2(t) = \lambda a_1(t)$, and $X(t) = a_1(t)(\mathcal{L}_1 + \lambda \mathcal{L}_2)$ defines a commutative family. In this case one has $b_k(t) = a_k(t)$ and hence $\mathcal{L}(t) = X(t)$. In the general noncommutative case one has for the integral

$$\int_0^t \mathcal{L}(\tau) d\tau = B_1(t)\mathcal{L}_1 + B_2(t)\mathcal{L}_2, \quad (31)$$

with $B_1(t) = A_1(t) + F(t)$, $B_2(t) = A_2(t) - F(t)$, and $F(t) = \int_0^t f(u)du$. Note, that $B_1(t) + B_2(t) = A(t) \geq 0$. However, contrary to the commutative case, there is no need that both $B_1(t)$ and $B_2(t)$ are positive. It shows that integral $\int_0^t \mathcal{L}(\tau) d\tau$ needs not have a Lindblad representation. Note, that

$$\mathcal{L}(t) = X(t) + f(t)[\mathcal{L}_1 - \mathcal{L}_2], \quad (32)$$

which clearly shows that the last term ' $f(t)[\mathcal{L}_1 - \mathcal{L}_2]$ ' destroys the Lindblad structure of $\int_0^t \mathcal{L}(\tau) d\tau$. It proves the intricate action of T-product:

$$\text{T exp} \left(\int_0^t \left\{ X(\tau) + f(\tau)[\mathcal{L}_1 - \mathcal{L}_2] \right\} d\tau \right) = e^{Z(t)}, \quad (33)$$

that is, chronological product simply washes out the unwanted term ' $f(t)[\mathcal{L}_1 - \mathcal{L}_2]$ '. Eventually, one easily shows (using standard algebraic methods, e.g. [30]) that

$$e^{Z(t)} = e^{\ln \nu_1(t) \mathcal{L}_1} \cdot e^{\ln \nu_2(t) \mathcal{L}_2}, \quad (34)$$

where (skipping time dependence)

$$\nu_1 = \frac{A}{A_1 e^{-A} + A_2}, \quad \nu_2 = \frac{A_1 + A_2 e^A}{A}. \quad (35)$$

Note that $\nu_1 \nu_2 = e^A$. One has $\nu_k(t) \geq 1$, and hence (34) gives another representation of dynamical map as a composition of two completely positive maps generated by \mathcal{L}_1 and \mathcal{L}_2 .

In conclusion, we proposed a complete treatment of a local in time dynamics of open quantum systems based on the Master Equation (1). We provided a general representation of the local generator – formula (14) – which generalizes well known Lindblad representation for the Markovian dynamics. We stress that any local generator $\mathcal{L}(t, t_0)$ may be constructed via (14) by a suitable choice of the Lindblad family $Z(t, t_0)$. However, the problem of necessary and sufficient condition for $\mathcal{L}(t, t_0)$ which guarantee that $\Lambda(t, t_0)$ is CPT is still open. Only, if $\mathcal{L}(t, t_0)$ defines a commutative family, these conditions reduce to a simple requirement that $\int_{t_0}^t \mathcal{L}(u, t_0) du$ has a Lindblad form for $t \geq t_0$.

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