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Nonuniqueness of generalized quantum master equations for a single observable

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ABSTRACT
When deriving exact generalized master equations for the evolution of a reduced set of degrees of freedom, one is free to choose what quantities are relevant by specifying projection operators. However, obtaining a reduced description does not always need to be achieved through projections—one can also use conservation laws for this purpose. Such an operation should be considered as distinct from any kind of projection; that is, projection onto a single observable yields a different form of master equation compared to that resulting from a projection followed by the application of a constraint. We give a simple example to show this point and give relationships that the different memory kernels must satisfy to yield the same dynamics.

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In the study of the dynamics of large, closed quantum systems, an approach often taken is to model the dynamics of a reduced set of degrees of freedom (dofs) using the exact Nakajima–Zwanzig (NZ) equation (in units where \(\hbar = 1\)):

\[
\frac{d}{dt} \hat{\rho}(t) = -i[\hat{H}, \hat{\rho}(t)] + \hat{\theta}(t) - \int_0^t d\tau K(\tau; \rho) \hat{P}\hat{\rho}(t-\tau). \tag{1}
\]

In the above equation, \(\hat{\theta}(t) = -i[\hat{P}L e^{-iQL\hat{Q}} \hat{Q}(0)]\) is the inhomogeneous term and the memory kernel superoperator for an arbitrary projection \(\hat{P}\) is given by

\[
K(\tau; \rho) = \hat{P}L e^{-iQL\hat{Q}}L\hat{P}, \tag{2}
\]

where \(L \ldots [\hat{H}, \ldots] \) is the Liouvillian superoperator, with \(\hat{H}\) being the Hamiltonian of the entire closed quantum system. The NZ equation is derived from the quantum Liouville equation by making use of projection superoperators \(\hat{P}\) and its complement \(\hat{Q} \equiv 1 - \hat{P}\) acting on the full density matrix \(\hat{\rho}(t)\). There are no restrictions on the choice of \(\hat{P}\), so different choices will alter Eqs. (1) and (2) and give rise to different quantum master equations for the same observable, which, in principle, should yield the same dynamics for this quantity.

In this Note, we will consider a system coupled to a “bath” and derive two apparently different quantum master equations for one of the system’s populations. This example illustrates how two structurally distinct master equations, one that contains a term acting like an external drive and one that does not, can result from our choice of \(\hat{P}\) and whether we impose conservation laws on the set of reduced variables. For simplicity, we will restrict our discussion to a two-level system (TLS) coupled to some number of other dofs, which we call the bath \(B\). The general case of a D-level system coupled to other dofs is described in Sec. III of the supplementary material. Throughout this Note, we take a factorized initial condition, \(\hat{\rho}(0) = \hat{P}\hat{\rho}(0)\), so that \(Q\hat{\rho}(0) = 0\) and \(\hat{\theta}(0) = 0\).

We will now specify the two projectors used to derive two quantum master equations. For notational convenience, we define the projectors onto the \(n\)th population of the system for some arbitrary reference bath state \(\hat{\rho}_B\).
\[ \mathbb{P}^t \hat{\rho} = (|n\rangle\langle n| \otimes \hat{I}_B) \text{Tr} \left( (|n\rangle\langle n| \otimes \hat{I}_B) \hat{\rho} \right). \] (3)

In the first case, we take \( \mathbb{P} = \mathbb{P}^0 + \mathbb{P}^1 \), which results in a set of coupled master equations for the populations \( |0\rangle\langle 0| \) and \( |1\rangle\langle 1| \). From here, we can reduce the description even further since the system obeys \( \sigma_0(t) + \sigma_1(t) = 1 \) and focus solely on the \( |0\rangle\langle 0| \) component. In the second case, we consider \( \mathbb{P} = \mathbb{P}^0 \) and therefore deem the \( |0\rangle\langle 0| \) component of the reduced density matrix, \( \sigma_0(t) \equiv \rho_{00}(t) \), to be the only component of interest. We shall now show how these two procedures lead to structurally distinct generalized quantum master equations and how the associated memory kernels must relate to each other so that they produce the same dynamics for \( \sigma_0(t) \).

For the first case, we use \( \mathbb{P} = \mathbb{P}^0 + \mathbb{P}^1 \) and \( \mathbb{Q} = 1 - \mathbb{P} = \mathbb{Q}^0 - \mathbb{P}^1 \) in Eqs. (1) and (2) to obtain

\[
\frac{d\sigma_0(t)}{dt} = \int_0^t dt' K_{1,0}(t; \mathbb{P}^0 + \mathbb{P}^1) - \left[ K_{0,0}(t; \mathbb{P}^0 + \mathbb{P}^1) + K_{1,0}(t; \mathbb{P}^0 + \mathbb{P}^1) \right] \sigma_0(t-t'). \] (4)

We use the notation \( K_{m,n}(t; \mathbb{P}) \) to denote the \( (m,n) \) matrix element of the memory kernel superoperator \( \mathbb{K} \) in Eq. (2) (see the supplementary material). In obtaining Eq. (4), we have also used the relations \( \sigma_0(t) + \sigma_1(t) = 1 \) and \( K_{0,0}(t) + K_{1,0}(t) = 0 \).

For the second case, using \( \mathbb{P} = \mathbb{P}^0 \) and \( \mathbb{Q} = 1 - \mathbb{P}^0 \) in Eqs. (1) and (2), we obtain

\[
\frac{d\sigma_0(t)}{dt} = -\int_0^t dt' K_{0,0}(t; \mathbb{P}^0) \sigma_0(t-t'). \] (5)

Equation (4) superficially differs from Eq. (5) in that the former contains a term independent of the population at time \( t \) and thus plays a role like an external force in a Langevin equation. However, this force arises due to a need to satisfy a constraint, \( \sigma_0(t) + \sigma_1(t) = 1 \), which used to be enforced by the properties of the memory kernel, \( K_{0,0}(t) + K_{1,0}(t) = 0 \).

While our preceding discussion has been fully general albeit abstract, let us be more concrete by working with the simple example of a TLS with states \( |0\rangle \) and \( |1\rangle \) not coupled to any bath. The system is described by the Hamiltonian \( \hat{H} = \epsilon \hat{I}^2 + \Delta \hat{I}^z \), where \( \hat{I}^z \) (\( \alpha = x, z \)) are Pauli matrices. For the first case as outlined above, we use \( \mathbb{P} \ldots = \mathbb{P}^0 \ldots = (|n\rangle\langle n|) \text{Tr} \left( (|n\rangle\langle n|) \ldots \right) \) for \( n = 0, 1 \) and the initial condition \( \hat{\rho}(0) = |0\rangle\langle 0| \) to get explicit memory kernels (see the supplementary material),

\[ K_{0,0}(t; \mathbb{P}^0 + \mathbb{P}^1) = K_{1,1}(t; \mathbb{P}^0 + \mathbb{P}^1) = 2\Delta^2 \cos(2\tau). \] (6)

For the second case, we obtain, instead,

\[ K_{0,0}(t; \mathbb{P}^0) = 2\Delta^2 \cos(2\omega \tau), \quad \omega = \sqrt{\epsilon^2 + (1/2)\Delta^2}. \] (7)

These memory kernels are quite distinct, as shown in Fig. 1, but the population dynamics they generate are identical. It is straightforward to compute \( \hat{\rho}(t) = e^{-it\hat{H}}\hat{\rho}(0) e^{it\hat{H}} \) for the above model Hamiltonian and verify that the following function solves Eqs. (4) and (5) when \( \sigma_0(0) = 1 \):

\[ \sigma_0(t) = 1 - \frac{\Delta^2 \sin^2(\Omega t)}{\Omega^2}, \quad \Omega = \sqrt{\epsilon^2 + \Delta^2}. \] (8)

The equivalence of the dynamics between Eqs. (4) and (5) should imply relations between the memory kernels in the two equations. It is convenient to work with \( F_{m,m}(t; \mathbb{P}) \) such that its time derivative generates the memory \( K_{m,n}(t; \mathbb{P}) \),

\[ F_{m,m}(t; \mathbb{P}) = \text{Tr} \left[ (|m\rangle\langle m| \otimes \hat{I}_B) e^{-t\hat{H} - \hat{H} t} (|m\rangle\langle m| \otimes \hat{I}_B) \right], \] (9)

where \( m = 0, 1 \). The condition that the functions \( F(t) \) with respect to different projectors must generate the same \( \rho_p(t) \) is equivalent to the relation

\[ F_{m,m}(t; \mathbb{P}^0) = F_{m,m}(t; \mathbb{P}^0 + \mathbb{P}^1) - \int_0^t dt' F_{1,1}(t; \mathbb{P}^0 + \mathbb{P}^1) F_{m,m}(t - t'; \mathbb{P}^0 + \mathbb{P}^1). \] (10)

This identity is easily demonstrated by working with \( \tilde{F} \), the Laplace transform of \( F \), and applying Dyson’s identity, \( (X - Y)^{-1} = X^{-1} + X^{-1}Y(X - Y)^{-1} \). Using Eq. (10) in Laplace space, it is straightforward to show that the \( \sigma_0(t) \) solving Eq. (4),

\[ \tilde{\sigma}_0(z) = \frac{1}{z} \left[ \frac{1 + \tilde{F}_{1,1}(z; \mathbb{P}^0 + \mathbb{P}^1)}{1 + \tilde{F}_{0,0}(z; \mathbb{P}^0 + \mathbb{P}^1) + \tilde{F}_{1,1}(z; \mathbb{P}^0 + \mathbb{P}^1)} \right], \] (11)

is identical to the one solving Eq. (5); see the supplementary material. We can turn back to the TLS and note that the functions
indeed satisfy Eq. (10).

The structural difference between the master equations—arising from projections and conservation laws—is not limited to a system of two states. While our point is most striking for a TLS, differences can also appear for general $D$-level systems whenever the conservation of total population allows for the reduction of one additional dof. It is important to remember that the memory kernels associated with different projectors are not independent from each other. While time-nonlocal and complicated, relations such as Eq. (10) show that the memory kernels contain information in common about the underlying unitary dynamics. This information comes from conservation laws, the presence of which is explicitly ignored by the projection operations. Thus, our intuition is that different evolution equations can arise depending whether one imposes constraints or projects out dofs (see the supplementary material). Thus, there is no guarantee of a unique generalized quantum master equation to describe the reduced dynamics of an observable. We note that a related observation have been made about Markovian quantum master equations. 4

See the supplementary material for (1) a quick derivation of the Nakajima–Zwanzig equation with generic projection superoperators, (2) a general demonstration of how inhomogeneous terms in the Nakajima–Zwanzig equation appear if conservation laws are explicitly imposed, (3) a generalization of the time-nonlocal relation [Eq. (10)] for $D$-level systems, and (4) details on the two-level system example.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

REFERENCES

3 We put “bath” in quotations since we are using it as a shorthand for degrees of freedom we do not care about, rather than it being an infinitely large reservoir that is unchanged by coupling to a small system.