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COMMENT

On homogeneous generalized master equations

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Abstract
It is argued that the method recently proposed by Los (Los V F 2001 *J. Phys. A: Math. Gen.* **34** 6389) turning inhomogeneous time-convolution generalized master equations (GMEs) into homogeneous ones is problematic in the quantum case. It is also shown here that the proposed method is inapplicable to time-convolutionless GMEs.

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Recently, Los [1] succeeded in transferring the initial condition term in time-convolution (i.e. non-Markovian) generalized master equations (TC-GMEs) via additional contributions to the kernel, thus turning the TC-GME of classical as well as quantum physics into a homogeneous form. In quantum physics, this result is quite important as it shows that the effects of information on initial system–bath correlations, the initial state of the bath etc contained in the so-called uninteresting part $(1-\mathcal{P})\rho(t_0)$ of the initial density matrix of the 'system + bath' complex $\rho(t)$ at the initial time t_0 and included in the inhomogeneous initial condition term can be, for purposes of evaluation of the time derivative of the interesting part $\mathcal{P}\rho(t)$ of the density matrix at any later time, turned into a change of the memory. We rewrite here the main steps of the arguments and then try to apply them to the time-convolutionless generalized master equations (TCL-GMEs), proving that this method and conclusions do not apply there.

The idea of Los [1] is based on the usual method of derivation of the Nakajima–Zwanzig identity [2–4] from the Liouville equation $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \mathcal{L}\rho(t)$ by rewriting it as

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = \mathcal{P}\mathcal{L}\mathcal{P}\rho(t) + \mathcal{P}\mathcal{L}(1-\mathcal{P})\rho(t), \tag{1}$$

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}(1-\mathcal{P})\rho(t) = (1-\mathcal{P})\mathcal{L}\mathcal{P}\rho(t) + (1-\mathcal{P})\mathcal{L}(1-\mathcal{P})\rho(t). \tag{2}$$

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Here $\mathcal{P} = \mathcal{P}^2$ is an arbitrary projector and $\mathcal{L}\ldots = \frac{1}{\hbar}[H, \ldots]$ is the Liouville superoperator. By summing up equations (1) and (2) we recover the Liouville equation while solving equation (2) yields for the uninteresting part of the density matrix $(1-\mathcal{P})\rho(t)$

$$(1-\mathcal{P})\rho(t) = \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}(1-\mathcal{P})\rho(t_0) - \mathrm{i}\int_{t_0}^{t} \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-\tau)}(1-\mathcal{P})\mathcal{L}\mathcal{P}\rho(\tau)\,\mathrm{d}\tau. \tag{3}$$

Introducing equation (3) into (1) yields the standard Nakajima–Zwanzig identity

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = {}&-\mathrm{i}\,\mathcal{P}\mathcal{L}\mathcal{P}\rho(t) - \int_{t_0}^{t} \mathcal{P}\mathcal{L}\mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-\tau)}(1-\mathcal{P})\mathcal{L}\mathcal{P}\rho(\tau)\,\mathrm{d}\tau \\ &- \mathrm{i}\mathcal{P}\mathcal{L}\mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}(1-\mathcal{P})\rho(t_0).\end{aligned} \tag{4}$$

This identity serves as a basis for all the TC-GMEs. All of them suffer, however, from one problem: this is the existence of the (generally) non-negligible inhomogeneous term, i.e. the last term on the right-hand side of equation (4). The method of Los is based on solving the linear set of equations for $(1-\mathcal{P})\rho(t)$ and $(1-\mathcal{P})\rho(t_0)$ that consists of equation (3) and

$$(1-\mathcal{P})\rho(t_0) = (1-\mathcal{P})\mathrm{e}^{\mathrm{i}\mathcal{L}(t-t_0)}(\mathcal{P}\rho(t) + (1-\mathcal{P})\rho(t)). \tag{5}$$

The result yields, upon introducing it into equation (4), the identity obtained by Los [1]

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = -\mathcal{P}\mathcal{L}\mathcal{R}(t)\left(\mathrm{i}\,\mathcal{P}\rho(t) + \int_{t_0}^{t} \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-\tau)}(1-\mathcal{P})\mathcal{L}\mathcal{P}\rho(\tau)\,\mathrm{d}\tau\right), \\ &\mathcal{R}(t) = \{1 - \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}(1-\mathcal{P})\mathrm{e}^{\mathrm{i}\mathcal{L}(t-t_0)}\}^{-1}.\end{aligned} \tag{6}$$

This is a homogeneous identity including the effect of initial system–bath correlations etc which might have broad applications (see [1] for one classical example). The reader should, however, be warned that practical applications of equation (6) to study, for example, the effect of initial system–bath correlations is hindered by the fact that $\mathcal{R}(t)$ is singular at $t = t_0$. This follows from the fact that $\mathcal{R}^{-1}(t) \to_{t\to t_0+} = \mathcal{P}$ and $\mathcal{P}$ is generally not invertible as argued below. The limit of the product of $\mathcal{R}(t)$ with the term in round brackets in equation (6) upon deducing $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t)$ at times t approaching t_0 has to be treated with care. The value of this limit is codetermined by the formally removed information contained in $(1-\mathcal{P})\rho(t_0)$. Once, however, $\mathcal{P}\rho(\tau)$ is determined in any (and even arbitrarily short) finite interval (t_0, t_1), equation (6) can in principle be used to deduce $\mathcal{P}\rho(t)$ for all $t > t_1$.

The idea appears, however, of whether one cannot use the method of Los for TCL-GMEs where neither time integration nor any memory kernel appears. We shall now repeat all the reasoning analogously, using the formalism of Shibata *et al* [5, 6]. We use here the fact that the older form of the TCL-GME by Fuliński and Kramarczyk [7, 8] is fully equivalent to that by [5, 6]—see [9]. So, following [5, 6], we turn equation (3) (using $\rho(\tau) = \mathrm{e}^{\mathrm{i}\mathcal{L}(t-\tau)}(\mathcal{P}\rho(t) + (1-\mathcal{P})\rho(t))$ into the form

$$\begin{aligned}(1-\mathcal{P})\rho(t) = {}&\left[1 + \mathrm{i}\int_0^{t-t_0} \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}\tau}(1-\mathcal{P})\mathcal{L}\mathcal{P}\mathrm{e}^{\mathrm{i}\mathcal{L}\tau}\,\mathrm{d}\tau\right]^{-1} \\ &\times\left[-\mathrm{i}\int_0^{t-t_0} \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}\tau}(1-\mathcal{P})\mathcal{L}\mathcal{P}\mathrm{e}^{\mathrm{i}\mathcal{L}\tau}\,\mathrm{d}\tau\,\mathcal{P}\rho(t)\right. \\ &\left. + \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}(1-\mathcal{P})\rho(t_0)\right].\end{aligned} \tag{7}$$

Introducing (5) into (1) yields the Shibata–Hashitsume–Takahashi–Shingu identity

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t) = -\mathrm{i}\mathcal{P}\mathcal{L}\left[1 + \mathrm{i}\int_0^{t-t_0} \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}\tau}(1-\mathcal{P})\mathcal{L}\mathcal{P}\mathrm{e}^{\mathrm{i}\mathcal{L}\tau}\,\mathrm{d}\tau\right]^{-1} \times [\mathcal{P}\rho(t) + \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}(1-\mathcal{P})\rho(t_0)]. \tag{8}$$

The idea is now to get rid, in a way analogous to that of Los [1], of the inhomogeneous initial-condition term $\propto (1-\mathcal{P})\rho(t_0)$, given by the uninteresting part of the initial density matrix of the 'system + bath' complex . Combining equation (7) (as a counterpart to equation (3)) with equation (5) we obtain for $(1-\mathcal{P})\rho(t_0)$ by excluding $(1-\mathcal{P})\rho(t)$

$$\{1-(1-\mathcal{P})[\mathrm{e}^{\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}\mathcal{P}\mathrm{e}^{-\mathrm{i}\mathcal{L}(t-t_0)} + 1 - \mathcal{P}]^{-1}\}(1-\mathcal{P})\rho(t_0) = (1-\mathcal{P})[\mathrm{e}^{\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}\mathcal{P}\mathrm{e}^{-\mathrm{i}\mathcal{L}(t-t_0)} + 1 - \mathcal{P}]^{-1}\mathrm{e}^{\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}\mathcal{P}\rho(t). \tag{9}$$

Here, we have used the fact that

$$\mathrm{i}\int_0^x \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}\tau}(1-\mathcal{P})\mathcal{L}\mathcal{P}\mathrm{e}^{\mathrm{i}\mathcal{L}\tau}\mathrm{d}\tau = \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}x}(1-\mathcal{P})\mathrm{e}^{\mathrm{i}\mathcal{L}x} - 1 + \mathcal{P}. \tag{10}$$

If we were able to express now, from this equation, $(1-\mathcal{P})\rho(t_0)$ and replace by the result this quantity in equation (8), we would have the required result: a time-local homogeneous identity for the interesting part of the density matrix $\mathcal{P}\rho(t)$ (i.e. the interesting information therein). What we shall now prove, however, is that this programme is not performable.

The reason is simple. The point is that, in contrast to a similar procedure by Los, the superoperator (i.e. its matrix representation) $\mathcal{X} \equiv \{1-(1-\mathcal{P})[\mathrm{e}^{\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}\mathcal{P}\mathrm{e}^{-\mathrm{i}\mathcal{L}(t-t_0)} + 1 - \mathcal{P}]^{-1}\}$ is not invertible. We prove this by the method of contradiction. Assume that the opposite is true. Then using some algebra, we obtain that

$$\mathcal{X} = \mathrm{e}^{\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}\mathcal{P}[\mathcal{P} + \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}(1-\mathcal{P})\mathrm{e}^{\mathrm{i}\mathcal{L}(t-t_0)}]^{-1}\mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}. \tag{11}$$

Here all the superoperators exist—compare, for example, that superoperator $[\mathcal{P}+\mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}(1-\mathcal{P})\mathrm{e}^{\mathrm{i}\mathcal{L}(t-t_0)}]^{-1}$ is, because of identity equation (10), the one that also enters equation (8). In [5,6], its existence is proven. So, $\mathcal{P} = \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}\mathcal{X}\mathrm{e}^{\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}[\mathcal{P} + \mathrm{e}^{-\mathrm{i}(1-\mathcal{P})\mathcal{L}(t-t_0)}(1-\mathcal{P})\mathrm{e}^{\mathrm{i}\mathcal{L}(t-t_0)}]$ must be invertible, too. This is, however, true only exceptionally, for just $\mathcal{P} = 1$ when no information is projected off. In the case of the Argyres–Kelley projector [10] , for example,

$$\mathcal{P}\cdots = \rho_0^B \otimes \mathrm{Tr}_B(\cdots), \qquad \mathrm{Tr}_B(\rho_0^B) = 1, \tag{12}$$

projecting off the bath and leading to generalized master equations for the density matrix of the system only, $\mathcal{P}(\rho_B \otimes \rho_S) = \rho_0^B \otimes \rho_S$, which is independent of ρ_B for arbitrary density matrix ρ_B of the bath fulfilling $\mathrm{Tr}_B\,\rho_B = 1$. Except, therefore, for the case where $\mathcal{P} = 1$, the inverse of $\mathcal{P}$ does not exist, which is the contradiction. Hence, $\mathcal{X}$ is not invertible either. $(1-\mathcal{P})\rho(t_0)$ cannot therefore be expressed from (9) and used in (8). Therefore, the method of Los [1] of deriving a homogeneous generalized master equation cannot be applied to the TCL-GME.

In summary, the influence of the uninteresting part of the initial density matrix of the 'system + bath' complex $(1-\mathcal{P})\rho(t_0)$ on the time dependence (derivative) of the interesting part of the density matrix $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{P}\rho(t)$ can be deduced from the time development of $\mathcal{P}\rho(\tau)$ in the interval $\tau \in (t_0, t)$. The latter determines the limit of $\mathcal{R}(t)$ multiplied by the round bracket in equation (6). Hence, though the derivation of the homogeneous time-nonlocal (convolution or non-Markovian) generalized master equations for the density matrix $\rho_S(t)$ of the system is formally possible by the method of Los, one is forced to deal with the hidden information contained in the formally omitted $(1-\mathcal{P})\rho(t_0)$ in another fashion. Certainly, however, one cannot derive in an analogous way homogeneous time-local (convolutionless or Markovian) generalized master equations for, for example, $\rho_S(t)$, taking initial entanglement (correlations etc) of the bath and system into account.

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