Note on the equivalence of different approximations in the relaxation theory

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We briefly discuss relations between different variants of the second order generalized master equations (GME), in particular among different types of the Markov–Born approximation of time-convolution GME and Born approximation in time-convolutionless one. We prove that equivalence valid in the van Hove limit does not in general apply for other types of scaling. On the other hand, for other scalings one appropriate form of the interaction representation always exist that reproduces this equivalence known from the weak-coupling (van Hove) one.

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Master equations are a well known and widely used device for treatment of processes of relaxation. Their rigorous derivation was developed during the previous century, though not without difficulties. However, these difficulties and the necessity to make approximations for practical purposes resulted into development of various variants of the master equations and their approximations. The different variants of generalized master equation (GME) [1–6], and equivalence among their exact (unapproximated) formulations [7–10], were extensively discussed. Also properties of standard approximations are known (for example [11]). On the other hand, practical purposes direct scientists to use mathematically simple forms of the relaxation description, for example the simplest form — using time-independent and time-local relaxation coefficients. Although different approximations arise from different concepts, some of these approximations are equivalent according to unchanged nature of the physical problem and given mathematical structure of the model. Although this fact is not unknown, there is no (as far as we know) wider publication activity in this direction. An explicit formulation may be of some importance, because in fact some of the traditional "equivalence" may be only proved under certain conditions. We want to briefly describe the relation between the second order (Born) approximation of time-convolutionless GME (TCL-GME) and the Born–Markov approximation of time-convolution GME (TC-GME) outside the van Hove limit. This case has not been discussed so far.

Now we are at the point to specify the problem we deal with. Generalized master equations are devices for the treatment of open system evolution. We consider Hilbert space of the physical problem to be decomposed into two factorspaces. One of them we identify with "system" variables, the other one with the bath. The ge-

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nerator of dynamics — Hamiltonian — is accordingly decomposed into three parts. (This decomposition is also carried over into the Liouville space $\mathcal{L}_x = (1/\hbar)[H_x, \ldots]$ in the same way.) So

$$H = H_{\rm S} + H_{\rm B} + H_{\rm S-B}\,. \tag{1}$$

GMEs usually concern only the information about system variables and are correspondingly connected with projecting off unnecessary bath information. So, any type of bath averaging is required. In the usual formalism introduced by Zwanzig [3] it means to specify projection operators $\mathcal{P}$ in a proper way. We specify the form of bath averaging in the most popular variant [12]:

$$\mathcal{P}\ldots = \rho_B {\rm Tr}_{\rm B}\ldots, \quad \rho_{\rm B} = \frac{{\rm e}^{-\beta_T H_{\rm B}}}{{\rm Tr}_{\rm B}{\rm e}^{-\beta_T H_{\rm B}}}, \quad \mathcal{Q} = 1 - \mathcal{P}.$$

$\rho_{\rm B}$ is the canonical density matrix of the bath, which is also assumed to be its initial density matrix. We assume it uncorrelated with the initial state of the system in order to cancel inhomogeneous terms in GME. Further, we formulate some silently assumed condition of decomposition (1). (Those can be understood as mathematical definition of the decomposition (1).) In particular,

$$\mathcal{P}\mathcal{L}_{\rm S} = \mathcal{L}_{\rm S}\mathcal{P}, \quad \mathcal{P}\mathcal{L}\mathcal{P} = \mathcal{L}_{\rm S}\mathcal{P}, \quad \mathcal{P}\mathcal{L}_{\rm B} = \mathcal{L}_{\rm B}\mathcal{P} = 0, \quad \mathcal{Q}\rho(t=0) = 0. \tag{2}$$

The GME general formulae are considered according to work [3].

We are in fact unable to calculate the coefficients of GME exactly (except for trivial cases). So, we have to introduce some type of a perturbational treatment and take some finite (usually the least nontrivial, i.e. the second) order approximation.

The very popular choice is to take $H_{\rm S-B}$ as a λ-dependent perturbation (the van Hove type scaling) and to calculate relaxation coefficients up to the second order in λ (Born approximation). In this case, an equivalence between the Born–Markov TC-GME (6) and the Born TCL-GME (7) is found below. (For the correspondence see e.g. [6]) TC-GME is given by the following formula [6]:

$$\frac{{\rm d}\rho_{\rm S}(t)}{{\rm d}t} = -{\rm i}\mathcal{L}_{\rm S}\rho_{\rm S}(t) - \int_0^t {\rm d}t'{\rm Tr}_{\rm B}[\mathcal{L}_{\rm S-B}{\rm e}^{-{\rm i}(\mathcal{L}_{\rm S}+\mathcal{L}_{\rm B})t'}\mathcal{L}_{\rm S-B}\rho_{\rm B}]\rho_{\rm S}(t-t'). \tag{3}$$

In the interaction picture

$$\rho^{\rm I}(t) = {\rm e}^{{\rm i}\mathcal{L}_{\rm S}t}\rho(t), \tag{4}$$

it yields:

$$\frac{{\rm d}\rho^{\rm I}_{\rm S}(t)}{{\rm d}t} = -{\rm e}^{{\rm i}\mathcal{L}_{\rm S}t}\int_0^t {\rm Tr}_{\rm B}[\mathcal{L}_{\rm S-B}{\rm e}^{-{\rm i}(\mathcal{L}_{\rm S}+\mathcal{L}_{\rm B})t'}\mathcal{L}_{\rm S-B}\rho_{\rm B}]{\rm e}^{{\rm i}\mathcal{L}_{\rm S}t'}{\rm d}t'{\rm e}^{-i\mathcal{L}_{\rm S}t}\rho^{\rm I}_{\rm S}(t-t'). \tag{5}$$

Now the standard reasoning is to perform in (5) the Markov approximation (i.e. we consider $\rho^{\rm I}$ in the convolution term to be time independent and then we integrate the convolution kernel in the $t \to \infty$ limit) . After returning into the Schrödinger picture we obtain

$$\frac{d\rho_{\rm S}(t)}{{\rm d}t} = -{\rm i}\mathcal{L}_{\rm S}\rho_{\rm S}(t) - \int_0^\infty {\rm Tr}_{\rm B}[\mathcal{L}_{\rm S-B}{\rm e}^{-{\rm i}(\mathcal{L}_{\rm S}+\mathcal{L}_b)t'}\mathcal{L}_{\rm S-B}\rho_{\rm B}]{\rm e}^{{\rm i}\mathcal{L}_{\rm S}t'}{\rm d}t'\rho_{\rm S}(t). \tag{6}$$

With the conditions (2),(6) is clearly equivalent with the following Born approximation of TCL-GME [6](in a formal long-time limit):

$$\frac{d\rho_{\mathrm{S}}(t)}{\mathrm{d}t} = -\mathrm{i}\mathcal{L}_{\mathrm{S}}\rho_{\mathrm{S}}(t) - \int_0^\infty \mathrm{d}t' Tr_{\mathrm{B}}[\mathcal{L}_{\mathrm{S-B}}\mathrm{e}^{-\mathrm{i}(\mathcal{L}_{\mathrm{S}}+\mathcal{L}_{\mathrm{B}})t'}\mathcal{L}_{\mathrm{S-B}}\mathrm{e}^{\mathrm{i}(\mathcal{L}_{\mathrm{S}}+\mathcal{L}_{\mathrm{B}})t'}\rho_{\mathrm{B}}]\rho_{\mathrm{S}}(t). \quad (7)$$

The above two ways to the one joint final result are usually justified by taking so called van Hove limit. This amounts to performing the scaling

$$\lambda \to 0, \quad \frac{t}{\lambda^2} \to \mathrm{const.}$$

However, this scaling is well applicable from the physical point of view for treatment of open system with weak interaction between the system and the bath. In spite of its powerful usefulness one can be interested in some physically different situations when, e.g., a part of the internal system dynamics is comparable with that caused by the $H_{\mathrm{S-B}}$ interaction. The usefulness of the van Hove scaling can be then limited, and there were some other perturbational or scaling schemes suggested [13]. The goal of present work is the inspection of this case.

We point out how it is necessary to take the Markov approximation of the second order TC-GME to keep equivalence with the Born approximation TCL-GME outside the van Hove limit. We deal with the following Hamiltonian perturbational scheme:

$$H_{\mathrm{S}} = H_{\mathrm{S}}^{(0)} + H_{\mathrm{S}}^{(2)}, \qquad H_{\mathrm{S-B}} \propto \lambda, \; H_{\mathrm{S}}^{(2)} \propto \lambda^2. \quad (8)$$

Here, $H_{\mathrm{S}}^{(2)}$ may describe, e.g., the above internal system dynamics. This scaling intends to apply to the situation when the bath-assisted processes become commensurable with those of the internal system dynamics [13]. However, our result remains unchanged also for another scheme which one can derive from the Davies work [14]:

$$H_{\mathrm{S}} = H_{\mathrm{S}}^{(0)} + H_{\mathrm{S}}^{(1)}, \qquad H_{\mathrm{S-B}} \propto \lambda, H_{\mathrm{S}}^{(1)} \propto \lambda. \quad (9)$$

Born approximation TCL-GME [6], performed with (8), gives the following equation:

$$\frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} = -\mathrm{i}\mathcal{L}_{\mathrm{S}}\rho_{\mathrm{S}}(t) - \int_0^\infty \mathrm{d}t' \mathrm{Tr}_{\mathrm{B}}[\mathcal{L}_{\mathrm{S-B}}\mathrm{e}^{-\mathrm{i}(\mathcal{L}_{\mathrm{S}}^{(0)}+\mathcal{L}_{\mathrm{B}})t'}\mathcal{L}_{\mathrm{S-B}}\mathrm{e}^{\mathrm{i}(\mathcal{L}_{\mathrm{S}}^{(0)}+\mathcal{L}_{\mathrm{B}})t'}\rho_{\mathrm{B}}]\rho_{\mathrm{S}}(t). \quad (10)$$

For comparison we refer to the Born approximation TC-GME obtained as above but in connection with (8):

$$\frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} = -\mathrm{i}\mathcal{L}_{\mathrm{S}}\rho_{\mathrm{S}}(t) - \int_0^t \mathrm{d}t' \mathrm{Tr}_{\mathrm{B}}[\mathcal{L}_{\mathrm{S-B}}\mathrm{e}^{-\mathrm{i}(\mathcal{L}_{\mathrm{S}}^{(0)}+\mathcal{L}_{\mathrm{B}})t'}\mathcal{L}_{\mathrm{S-B}}\rho_{\mathrm{B}}]\rho_{\mathrm{S}}(t-t'). \quad (11)$$

In order to save the equivalence between explicitly different (10) and the Markov approximation to (11), we have to choose the interaction picture in the following way:

$$\rho^{\mathrm{I}}(t) = \mathrm{e}^{\mathrm{i}\mathcal{L}_{\mathrm{S}}^{(0)}t}\rho(t). \quad (12)$$

Further treatment is fully analogical to that by van Hove. Then and only then the Markov approximation to (11) in the interaction picture (12) coincides with (10). On the other hand if one chooses the interaction picture in the standard way according to (4), one obtains the result

$$\frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} = -\mathrm{i}\mathcal{L}_{\mathrm{S}}\rho_{\mathrm{S}}(t) - \int_0^{\infty} \mathrm{Tr}_{\mathrm{B}}[\mathcal{L}_{\mathrm{S-B}}\mathrm{e}^{-\mathrm{i}(\mathcal{L}_{\mathrm{S}}^{(0)}+\mathcal{L}_{\mathrm{B}})t'}\mathcal{L}_{\mathrm{S-B}}\mathrm{e}^{\mathrm{i}\mathcal{L}_{\mathrm{S}}t'}\rho_{\mathrm{B}}]\mathrm{d}t'\rho_{\mathrm{S}}(t). \quad (13)$$

Clearly (13) does **not** coincide with (10). So the equivalence is not preserved in the above scheme beyond van Hove limit. The equivalence remains preserved only if we keep in mind the perturbational origin of the second order treatment of TC-GME and if we take it into account in the choice of the interaction representation.

We conclude that equivalence between the Born approximation of TCL-GME and a specific form (6) of the Born–Markov approximation of TC-GME is carried over to the case of (8) scaling only in rather a specific way: it is necessary to take, in the definition of the interaction picture, only that part of the system Hamiltonian that is "unperturbed".

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References

[1] M. Tokuyama and H. Mori: Progr. Theor. Phys. **55** (1976) 411.

[2] S. Nakajima: Progr. Theor. Phys. **20** (1958) 948.

[3] R. Zwanzig: Lectures in Theoretical Physics (Boulder) **3** (1960) 106.

[4] A. Fuliński and W. J. Kramarczyk: Physica **39** (1968) 575.

[5] H. Mori: Progr. Theor. Phys. **33** (1965) 423.

[6] N. Hashitsume, F. Shibata, and M. Shingu: J. Stat. Phys. **17** (1977) 155.

[7] A. Fuliński: Phys. Lett. A **25** (1967) 13.

[8] R. Zwanzig: Physica **30** (1964) 1109.

[9] F. Shibata, Y. Takahashi, and N. Hashitsume: J. Stat. Phys. **17** (1977) 171.

[10] H. Gzyl: J. Stat. Phys. **26** (1981) 679.

[11] R. Dümcke and H. Spohn: Z. Phys. B **34** (1979) 419.

[12] P.N. Argyres and P.L. Kelley: Phys. Rev. A **134** (1964) 98.

[13] V. Čápek and I. Barvík: Physica A **294** (2001) 388.

[14] E.B. Davies: Math. Ann. **219** (1976) 147.