Note on the Evaluation of the Memory-Kernel Occuring in Generalized Master Equations

P. Hänggi
Institut für Theoretische Physik, Universität Stuttgart,
Stuttgart, Federal Republic of Germany

In this communication we comment on a recent work [12] on the evaluation of the memory-kernel of the generalized master equation. We derive in a transparent and straightforward way the basic expression for the memory kernel. We demonstrate that the evaluation of this expression in [12] is carried out by use of the exact Laplace transform of the Greens function solution of the master equation.

I. Introduction

In recent years the projection operator technique and the concept of generalized master equations proved to be a very useful tool for the description of a set of macrovariables a [1–5]. Starting from the basis of microscopic first principles the projector operator method enables to contract on the minimal information necessary to describe the macroscopic dynamics. This information is collected in the relevant probability $\bar{\rho}(t)$ whose time evolution is determined by the generalized master equation

$$\dot{\bar{\rho}}(t)=\Omega\,\bar{\rho}(t)+\int_0^t K(t-\tau)\,\bar{\rho}(\tau)\,d\tau+I(t). \tag{1.1}$$

The method of master equations has seen a rapid development over the last years and recently the emphasis has shifted from the basic theoretical work to applications [3, 4, 6–9]. In spite of the flexibility of the generalized master equation there are certainly limits of its practical usefulness: The main difficulty lies in the evaluation of the rather involved formal expressions for the integral kernel $K(t)$ and the inhomogeneity $I(t)$. Recent theoretical progress has elucidated that the problem connected with the inhomogeneity is not the most serious one. By taking the preparation of the initial distribution explicitly into account one can always obtain a homogeneous generalized master equation with uniquely defined stochastic operators [10, 11]. Consequently, the major difficulty is the evaluation of the memory kernel $K(t)$. It involves the solution of a problem with the unusual propagator $\exp(1-P)\,Lt$ where L means the microscopic stochastic operator (Liouvillian) and P the appropriately chosen projector operator. An exact integral equation for the stochastic operator $K(t)$ which does not contain this unusual propagator has been derived in Ref. 10. However, it remains to be shown that a perturbation expansion based on that integral equation is more adequate than the usual procedures [3, 4].

In a very recent paper [12] on this subject, a method has been presented which allows an exact evaluation of the memory kernel $K(t)$ without using a pertubational expansion. The aim of this communication is to show that this method makes use of the exact Laplace transform of the solution of the master equation (1.1). Hence, the method is of no use if we want to determine that solution. However, it exposes some general properties of memory kernels!

II. Evaluation of the Memory Kernel

Starting from the equation of motion for the microscopic probability function $\rho(t)$

$$\dot{\rho}(t)=L\,\rho(t) \tag{2.1}$$

we obtain by use of an appropriately chosen projector operator P (i.e. this choice implies $(1-P)\,\rho(0)=0$) for the relevant part $P\rho(t)$ the generalized master equation [3, 4, 10]

$$\frac{d}{dt}P\rho = PLP\rho + \int_0^t K(t-\tau)\,P\rho(t-\tau)\,d\tau \qquad (2.2)$$

with $K(t)$ given by

$$K(t) = PL\,e^{(1-P)Lt}(1-P)\,LP. \qquad (2.3)$$

The time-evolution of the relevant part $\bar{\rho}(t) = P\rho(t)$ is described by the propagator $G(t)$ satisfying (2.2) with the initial condition $G(0) = P$; i.e.

$$\bar{\rho}(t) = G(t)\,\bar{\rho}(0) \qquad (2.4)$$

where

$$\dot{G}(t) = PLPG(t) + \int_0^t K(t-\tau)\,G(\tau)\,d\tau,$$

$$G(0) = P. \qquad (2.5)$$

Note that from (2.1) the propagator $G(t)$ is simply given by

$$G(t) = P\,e^{Lt}\,P. \qquad (2.6)$$

The method of the evaluation of the memory kernel $K(t)$ proposed by the authors of Ref. 12 has its bearing on the equation

$$\hat{K}(z) = zP - \hat{G}(z)^{-1} - PLP \qquad (2.7)$$

with

$$\hat{f}(z) = \int_0^\infty (\exp - z\,t)\,f(t)\,dt, \qquad \hat{G}(z) = P\frac{1}{z-L}P. \qquad (2.8)$$

However, Eq. (2.7) is *equivalent* to (2.5) because is just represents the usual Laplace transform of the latter relation. By use of the Laplace inversion we obtain

$$K(t) = \frac{1}{2\pi i}\int_C e^{zt}\left[zP - \left(P\frac{1}{z-L}P\right)^{-1} - PLP\right]dz \qquad (2.9)$$

where C denotes the usual path (not closed) in the complex plane [13] that passes the eigenvalues of L from the right side. Equation (2.9) is the main result of Ref. 12; it has been derived there under the implicit assumption of a bounded spectrum of L. The authors of Ref. 12 consider in this context a different path $\tilde{C}$ steming from the integral representation of the Γ-function. Under some mild mathematical restrictions this path can be deformed to a closed path such that the contributions of the analytic first and third term in (2.9) vanish and consequently can be droped for the evaluation of the memory kernel $K(t)$, $t \geqq 0$. Using the usual Laplace path C in (2.9) we obviously obtain from those two terms the singular contributions $\delta'(t)P$ and $-\delta(t)\ PLP$ respectively. However, these singular terms are compensated by the singular contributions of the second term yielding for $K(t), t \geqq 0$ a *regular* expression [11].

Also, it can be seen that a further evaluation of $K(t)$ from (2.7) or (2.9) is based on the knowledge of the propagator $G(z)$ (or up to a Laplace transformation on $G(t) = Pe^{Lt}P$) which on the other hand represents the solution of the generalized master equation (2.5). This latter fact can be seen explicitly from the examples given in [12, 14]. However, in cases where we know the propagator $G(t) = Pe^{Lt}P$ either exactly or within an approximation there is in general no need to consider the master equation (2.2). Nethertheless, equations (2.7) and (2.9) may be used for a test of approximation schemes as presented in [3, 4] in cases where the exact solution is known.

Finally, I would like to mention, that with a possible series expansion for the memory-kernel given in (2.3), generated from a small dimensionless parameter, the generalized master equation does not remain an empty concept [3, 4, 6]. Its advantage lies in the fact that the calculation of $K(t)$ is based on the projected relevant information and *not* on either an exact or perturbative solution of the microdynamics (i.e. solution for the propagator e^{Lt}).

I wish to thank the Volkswagen-Foundation for financial support of the project Synergetics. Also, I greatly appreciate clarifying discussions and the critical reading of the manuscript by Peter Talkner, Hermann Grabert and Fritz Haake.

References

1. Zwanzig, R.: J. Chem. Phys. **33**, 1338 (1960)
2. Nordholm, S., Zwanzig, R.: J. Stat. Phys. **13**, 347 (1975)
3. Haake, F.: Satistical Treatment of Open Systems by Generalized Master Equations, Springer Tracts in Modern Physics **66**, 98 (1973)
4. Hynes, J.T., Deutch, J.M.: Nonequilibrium Problems-Projector Operator Techniques, Physical Chemistry, an Advanced Treatise **XIB**, 729 Henderson, D. (ed.) New York: Academic Press 1975
5. Grabert, H.: Z. Physik B**27**, 95 (1977)
6. Agarwal, G.S.: Progress in Optics, XI Wolf, E. (ed.) Amsterdam: North Holland Publ. Co. 1973
7. Balescu, R.: Equilibrium and Nonequilibrium Statistical Mechanics. New Aork: J. Wiley 1975
8. Argyres, P.N., Kelley, P.L.: Phys. Rev. **134**A, 98 (1964)
9. Kenkre, V.M., Knox, R.S.: Phys. Rev. B**9**, 5279 (1974)
10. Grabert, H., Talkner, P., Hänggi, P.: Z. Physik B**26**, 389 (1977)
11. Grabert, H., Talkner, P., Hänggi, P., Thomas, H.: Z. Physik B**29**, 273 (1978)
12. Kühne, R., Reineker, P.: Z. Physik B**31**, 105 (1978)
13. Doetsch, G.: Handbuch der Laplace Transformation, Birkhäuser, Basel (1950)
14. Kühne, R., Reineker, P.: Phys. Stat. Sol. **89**b, 131 (1978)

Peter Hänggi
Institut für Theoretische Physik, Universität Stuttgart
Pfaffenwaldring 57/IV
D-7000 Stuttgart-80
Federal Republic of Germany