

# SOLUTION OF FRIEDRICH'S MODEL THROUGH EXACT MARKOVIAN MASTER EQUATION

BY M. FRANKOWICZ

Department of Theoretical Chemistry, Institute of Chemistry, Jagellonian University, Cracow\*

AND C. JĘDRZEJEK

Department of Theoretical Physics, Institute of Physics, Jagellonian University, Cracow\*\*

(Received January 26, 1978)

Up to now the existence of the inverse superoperator  $N^{-1}$  appearing in the simplest convolutionless exact master equation (EME), namely Fuliński-Kramarczyk master equation, has not been proven in the general case. Recently we have constructed this superoperator for Kreuzer-Nakamura model. In present work we show the existence of superoperator  $N^{-1}$  for Friedrichs model, widely investigated by Brussels school in the resolvent formalism.

## 1. Introduction

Standard method of investigating the time evolution of classical and quantum systems is so called master equation (ME) formalism. It describes the time dependence of certain quantities (usually density matrix or some observables) split on "relevant" and "irrelevant" parts with the use of a projection superoperator. Although this method is purely formal and fully equivalent to using original Liouville-von Neumann equation, it serves as a convenient tool in making various approximations (e.g. density expansion, weak-coupling limit) and in investigating of asymptotic properties (long time approximation).

First exact ME was derived by Van Hove [1]. A great impulse into studying such equations was given by Zwanzig [2] and Nakajima [3] who introduced projection operator method. In those times there was a belief that the only possible form of the exact ME was of the convolution type which suggested nonmarkovianity of an exact ME. This type of EME was widely exploited, particularly by Prigogine and co-workers [4-6]. Next the Brussels school worked out methods of investigating the approach to equilibrium leading to the asymptotic markovian ME [7].

---

\* Address: Zakład Chemii Teoretycznej, Instytut Chemii UJ, Krupnicza 41, 30-060 Kraków, Poland.

\*\* Address: Zakład Fizyki Teoretycznej, Instytut Fizyki UJ, Reymonta 4, 30-059 Kraków, Poland.

There are two types of the exact ME: nonmarkovian and markovian, the latter first derived in works of Fuliński and Kramarczyk [8–11]. Although this kind of ME was further investigated by many authors [12–16], they are not in such common use as the nonmarkovian ones. One reason is that usually markovian forms of ME are obtained by various approximations from nonmarkovian ones, which created a view that nonmarkovianity is inherent in the exact time evolution. The other reason is that although Lugiato [17] has given a rigorous proof of the existence of certain forms of the markovian ME, such a proof of the existence of the simplest markovian ME, namely Fuliński-Kramarczyk ME [10], is lacking in the general case.

This gap was partly filled by us by constructing the superoperator  $N^{-1}$  for the Kreuzer-Nakamura model [18]. In this work we give still one more example, namely we construct this superoperator for the Friedrichs model, extensively investigated by Brussels school and other authors by means of the resolvent formalism [19] and of the theory of subdynamics [20–22]. Our hope is to show a possibility of extending the use of markovian ME on systems with more complicated interactions. We believe that this approach can also be fruitful with respect to devising various new approximation schemes.

## 2. Markovian master equations

There are two types of generalized (exact) ME obtained from the Liouville-von Neumann equation

$$i\partial_t \varrho(t) = [H, \varrho(t)] \equiv L\varrho, \quad \hbar = 1, \quad (1)$$

by means of the projection operator method. The projector  $P$  picks out from the density matrix the “relevant” or “interesting” part, called the master part. The first one, of the convolution form, was derived in a general way by Zwanzig [2] and for particular cases by many others [23–27]. It was extensively studied by many authors, especially by Prigogine and co-workers [4–7]. Recently, it was generalized to describe open systems [28–30]. The form of this ME, given by Zwanzig, is

$$\begin{aligned} \partial_t P\varrho(t) = & -iPLP\varrho(t) - iPLe^{-iQLt}Q\varrho(t_0) \\ & - \int_0^t dt_1 PLe^{-iQLt_1}QLP\varrho(t-t_1), \end{aligned} \quad (2)$$

where  $Q = 1 - P$ .

The other type of ME, without convolution, is called “markovian” ME. It was derived first by Fuliński [9]. The simplest convolutionless ME was derived by Fuliński and Kramarczyk [10]

$$\partial_t P\varrho(t) = (\partial_t N)N^{-1}(Q\varrho(t_0) + P\varrho(t)), \quad (3)$$

where

$$N = 1 + P(Z(t, t_0) - 1), \quad (4)$$

and  $Z(t, t_0)$  is the time evolution superoperator defined through the relation

$$\varrho(t) = Z(t, t_0)\varrho(t_0). \quad (5)$$

Lugiato [17] gave the rigorous proof of the existence of two similar ME

$$\partial_t P \varrho(t) = (\partial_t K_1) K_1^{-1} (\alpha \varrho(t_0) + P \varrho(t)), \quad (6)$$

$$\partial_t P \varrho(t) = (\partial_t K_2) K_2^{-1} ((\alpha - 1) \varrho(t_0) + Q \varrho(t_0) + P \varrho(t)), \quad (7)$$

where

$$K_1(t, t_0) = \alpha + PZ(t, t_0), \quad \alpha \text{ real, } |\alpha| > 1, \quad (8)$$

$$K_2(t, t_0) = \alpha + P(Z(t, t_0) - 1), \quad \alpha \text{ real, } |\alpha| > 2. \quad (9)$$

The most general form of EME, containing both above possibilities and additionally "shifted markovian" EME and EME with partial memory, was given recently by Fuliński [31]. It was shown that for suitable choices of superoperators it is formally possible to obtain EME with desired properties, e.g. Zwanzig ME, Fuliński-Kramarczyk ME, Shimizu ME [14] etc. by direct transformation. All these forms are mathematically equivalent and carry the same physical information if certain superoperators appearing in these equations exist.

### 3. The Friedrichs model

The model we will deal with belongs to a class considered first by Friedrichs [32]. This model has been used by Brussels school [20-22] which examined the ergodic properties of quantum systems and tested subdynamics and transformation theory on that model.

Middleton and Schieve [19] have found the explicit solution of the Prigogine-Resibois generalized ME in the special case of the Lorentzian interaction and of the spontaneous emission initial conditions. They also calculated the collision operator  $\psi(z)$  for this model.

Following them we choose the basis consisting of a state  $|E\rangle$  and a nondegenerate continuum of states  $\{|\omega\rangle\}$ . The orthonormality of these states is assumed:

$$\langle E|E\rangle = 1, \quad \langle \omega|\omega'\rangle = \delta(\omega - \omega'), \quad \langle E|\omega\rangle = \langle \omega|E\rangle = 0. \quad (10)$$

In this basis the complete Hamiltonian has the form

$$H = E|E\rangle \langle E| + \int d\omega \omega |\omega\rangle \langle \omega| + \int d\omega V(\omega) (|\omega\rangle \langle E| + |E\rangle \langle \omega|). \quad (11)$$

Further we assume that  $V(\omega)$  is a real function. The Liouville superoperator in the above basis has the following nonvanishing matrix elements:

$$L_{\omega\mu E\nu} = L_{E\nu\omega\mu} = V(\omega)\delta(\mu - \nu), \quad (12)$$

$$L_{\nu E\mu\omega} = L_{\mu\omega\nu E} = -V(\omega)\delta(\mu - \nu), \quad (13)$$

$$L_{\omega EEE} = L_{EEE\omega} = V(\omega), \quad (14)$$

$$L_{E\omega EE} = L_{EEE\omega} = -V(\omega), \quad (15)$$

$$L_{E\omega E\mu} = (E - \omega)\delta(\omega - \mu), \quad (16)$$

$$L_{\omega E\mu E} = -(E - \omega)\delta(\omega - \mu), \quad (17)$$

$$L_{\omega\mu\nu\xi} = (\omega - \mu)\delta(\omega - \nu)\delta(\mu - \xi). \quad (18)$$

The time evolution superoperator  $Z(t, t_0)$  can be calculated directly from the von Neumann equation

$$\partial_t Z = -iLZ, \quad (19)$$

or by means of the time evolution operator  $U(t, t_0)$

$$Z_{mm'n'} = U_{mm'} U_{n'n}. \quad (20)$$

We first calculate the operator  $U$ . This operator fulfills the equation

$$\partial_t U(t, t_0) = -iH U(t, t_0). \quad (21)$$

After performing the Laplace transformation of Eq. (21) and exploiting the fact that considered Hamiltonian is time independent we obtain

$$s\tilde{U}(s) - U(t_0) = -iH\tilde{U}(s). \quad (22)$$

From now on we put  $t_0 = 0$ . Let  $U(0) = 1$ . Then we have

$$s\tilde{U}_{EE}(s) - 1 = -iE\tilde{U}_{EE}(s) - i \int V(\omega) \tilde{U}_{\omega E}(s) d\omega, \quad (23)$$

$$s\tilde{U}_{\omega E}(s) = -iV(\omega)\tilde{U}_{EE}(s) - i\omega\tilde{U}_{\omega E}(s), \quad (24)$$

and thus

$$\tilde{U}_{\omega E}(s) = -\frac{iV(\omega)}{s+i\omega} \tilde{U}_{EE}(s). \quad (25)$$

Putting (25) into (23) we obtain

$$U_{EE}(s) = \left[ s+iE + \int \frac{[V(\omega)]^2}{s+i\omega} d\omega \right]^{-1}. \quad (26)$$

Let us assume that the interaction has the Lorentzian form

$$[V(\omega)]^2 = \lambda\gamma^2 [(\omega - E)^2 + \gamma^2]^{-1}, \quad (27)$$

where  $\gamma$  is the peak width and  $\lambda$  its height. Now, we have to calculate

$$G(s) = \int \frac{[V(\omega)]^2}{s+i\omega} d\omega. \quad (28)$$

For interaction (27) and with assumption that  $\omega$  changes from  $-\infty$  to  $+\infty$  we obtain

$$G(s) = \lambda\gamma^2 \int_{-\infty}^{+\infty} \frac{d\omega}{(s+i\omega)(\omega - E - i\gamma)(\omega - E + i\gamma)} = \frac{\pi\lambda\gamma}{i(E - i\gamma - is)}. \quad (29)$$

Then

$$U_{EE}(s) = \frac{s+a}{(s+a)^2 + b^2} + \frac{\gamma}{2} \frac{1}{(s+a)^2 + b^2}, \quad (30)$$

where

$$a = \frac{\gamma + 2iE}{2}, \quad b^2 = \gamma \left( \pi\lambda - \frac{\gamma}{4} \right). \quad (31)$$

The inverse Laplace transform of the expression (30) gives us the value of the element  $U_{EE}(t)$

$$U_{EE}(t) = e^{-at} \left( \cos bt + \frac{\gamma}{2b} \sin bt \right). \quad (32)$$

We can calculate the element  $U_{\omega E}(t)$  from Eq. (25), inverting the product of Laplace transforms. Then we get

$$U_{\omega E}(t) = \frac{-iV(\omega)e^{-i\omega t}}{(a-i\omega)^2 + b^2} \left\{ e^{-(a-i\omega)t} \left[ \left( \frac{\gamma}{2} - a + i\omega \right) \times \sin(bt) - \left( \frac{\gamma(a-i\omega)}{2b^2} - b \right) \cos(bt) \right] + \frac{\gamma(a-i\omega)}{2b^2} - b \right\}. \quad (33)$$

Since operator  $U$  is unitary and  $V(\omega)$  is real,

$$U_{E\omega}(t) = U_{\omega E}(t). \quad (34)$$

For the sake of completeness we also give the expression for  $U_{\omega\omega'}(t)$

$$U_{\omega\omega'}(t) = e^{-i\omega t} \delta(\omega - \omega') - iV(\omega) e^{-i\omega t} \int_0^t e^{i\omega' t'} U_{E\omega'}(t') dt'. \quad (35)$$

#### 4. Fuliński-Kramarczyk equation for the Friedrichs model

The Fuliński-Kramarczyk ME for the Friedrichs model has the form

$$\begin{aligned} \partial_t \rho_{EE}(t) &= F_{EEEE} \rho_{EE}(t) + \int (F_{EE\omega\omega'} \rho_{E\omega}(0) \\ &+ F_{EE\omega E} \rho_{\omega E}(0) + \int F_{EE\omega\omega'} \rho_{\omega\omega'}(0) d\omega') d\omega. \end{aligned} \quad (36)$$

We have used the projector  $P$  of the form

$$(P)_{mnp\tau} = \delta_{mE} \delta_{nE} \delta_{pE} \delta_{\tau E}, \quad (37)$$

which picks out from the density matrix the diagonal element representing the probability that the discrete state is occupied. The superoperator  $F$  is defined by the relation

$$F(t) = [\partial_t N(t)] N^{-1}(t). \quad (38)$$

For the above choice of the projector the only non-vanishing matrix elements of  $N$  are

$$N_{EEmn} = Z_{EE} \delta_{mn}, \quad (mn \neq EE), \quad (39)$$

$$N_{E\omega E\omega'} = \delta(\omega - \omega'), \quad (40)$$

$$N_{\omega\mu\nu\xi} = \delta(\omega - \nu) \delta(\nu - \xi). \quad (41)$$

The matrix elements of  $N^{-1}$  can be calculated from the definition

$$(NN^{-1})_{mnp r} = (N^{-1}N)_{mnp r} = \delta_{mp}\delta_{nr}.$$

As a result we have

$$(N^{-1})_{EEEE} = (Z_{EEEE})^{-1}, \quad (42)$$

$$(N^{-1})_{EE mn} = -Z_{EE mn}(Z_{EEEE})^{-1}, \quad (mn \neq EE) \quad (43)$$

$$(N^{-1})_{E\omega E\omega'} = (N^{-1})_{\omega E\omega' E} = \delta(\omega - \omega'), \quad (44)$$

$$(N^{-1})_{\omega\mu\nu\xi} = \delta(\omega - \nu)\delta(\mu - \xi). \quad (45)$$

Now we can write down all needed matrix elements of the superoperator  $F$ :

$$F_{EEEE} = (\partial_t Z_{EEEE})(Z_{EEEE})^{-1}, \quad (46)$$

$$F_{EEE\omega} = (Z_{EEEE})^{-1}(Z_{EEEE}\partial_t Z_{EEE\omega} - Z_{EEE\omega}\partial_t Z_{EEEE}), \quad (47)$$

$$F_{EE\omega E} = (F_{EEE\omega})^*, \quad (48)$$

$$F_{EE\omega\omega'} = \partial_t Z_{EE\omega\omega'}. \quad (49)$$

Having determined  $U(t)$  we can evaluate all needed matrix elements of  $Z$ . These are

$$Z_{EEEE} = e^{-\gamma t} \left( \cos^2(bt) \pm \frac{\gamma^2}{4|b|^2} \sin^2(bt) + \frac{\gamma}{2b} \sin(2bt) \right), \quad (50)$$

$$\begin{aligned} Z_{EE\omega E} = & -C_1(\omega)e^{-\gamma t} \left[ C_2(\omega) \cos^2(bt) \mp \frac{i\gamma}{2b^*} (E - \omega) \sin^2(bt) \right. \\ & \left. - \frac{1}{2} i \left( (E - \omega) \mp \frac{\gamma}{2b^*} C_2(\omega) \right) \sin(2bt) \right] + C_1(\omega)C_2(\omega) \\ & e^{-\left(\frac{\gamma}{2} - i(E - \omega)\right)t} \left( \cos(bt) \pm \frac{\gamma}{2b^*} \sin(bt) \right), \quad (51) \end{aligned}$$

$$\begin{aligned} Z_{EE\omega\omega'} = & C_1(\omega)C_1^*(\omega')e^{-i(\omega - \omega')t} [e^{-(\gamma - i(\omega - \omega'))t} \\ & (C_2(\omega)C_2^*(\omega') \cos^2(bt) \pm (E - \omega)(E - \omega') \sin^2(bt) \\ & - \frac{1}{2} i(C_2^*(\omega')(E - \omega) \mp C_2(\omega)(E - \omega')) \sin(2bt)) \\ & - e^{-\frac{\gamma}{2}t} (C_2(\omega)C_2^*(\omega') (e^{i(E - \omega')t} + e^{-i(E - \omega)t}) \cos(bt) \\ & - i(C_2^*(\omega')(E - \omega)e^{-i(E - \omega)t} \mp C_2(\omega)(E - \omega')e^{i(E - \omega')t}) \sin(bt) + C_2(\omega)C_2^*(\omega')], \quad (52) \end{aligned}$$

where

$$C_1(\omega) = \frac{iV(\omega)}{(a-i\omega)^2 + b^2}, \quad (53)$$

$$C_2(\omega) = \frac{2b^3 - \gamma(a-i\omega)}{2b^2}, \quad (54)$$

and upper (lower) sign relates to the case of real (imaginary)  $b$ .

Calculation of time derivatives of  $Z$  is straightforward and the results are not presented.

Now when we have obtained the superoperators appearing in Eq. (36) we have found the exact solution to the dynamics of the considered model. If we assume that for  $t = 0$   $\varrho_{EE}(0) = 1$  and all the other matrix elements vanish we find

$$\varrho_{EE}(t) = Z_{EEEE}(t), \quad (55)$$

where  $Z_{EEEE}(t)$  is given by Eq. (50). As expected, this solution agrees with the one obtained by Middleton and Schieve [19]. When  $b$  is a real number, we obtain damped oscillatory decay of the excited state, and for imaginary values of  $b$  we have monotonic exponential decay.

### 5. Final remarks

Using the Fuliński-Kramarczyk markovian ME we solved the dynamics of the Friedrichs model. The results are fully equivalent to the ones obtained via resolvent formalism. We did it showing the existence of inverse superoperator  $N^{-1}$  in Eq. (3), the existence of which has not been proven yet for the general case. Therefore, it is useful to know that it exists at least for some models. We believe that this fact can extend the application of markovian ME in studying the problem of time evolution.

We would like to extend our appreciations and thanks to Professor A. Fuliński for many helpful discussions and comments.

### REFERENCES

- [1] L. Van Hove, *Physica* **23**, 441 (1957).
- [2] R. Zwanzig, *J. Chem. Phys.* **33**, 1338 (1960).
- [3] S. Nakajima, *Prog. Theor. Phys.* **20**, 948 (1958).
- [4] I. Prigogine, *Non-Equilibrium Statistical Mechanics*, Interscience Publishers, New York 1962.
- [5] R. Balescu, *Statistical Mechanics of Charged Particles*, Interscience Publishers, London 1963.
- [6] P. Resibois, *Physics of Many-Particle Systems*, E. Meeron, Editor, Gordon and Breach, New York 1966.
- [7] M. Baus, *Bull. Cl. Sci. Acad. Roy. Belg.* **53**, 1291, 1332, 1352 (1967).
- [8] A. Fuliński, *Phys. Lett.* **24A**, 63 (1967).
- [9] A. Fuliński, *Phys. Lett.* **25A**, 13 (1967).
- [10] A. Fuliński, W. J. Kramarczyk, *Physica* **39**, 575 (1968).
- [11] W. J. Kramarczyk, Thesis, Cracow 1969.
- [12] H. Krips, *Nuovo Cimento* **3B**, 153 (1971).

- [13] A. R. Altenberger, *Physica* **62**, 379 (1972).
- [14] T. Shimizu, *J. Phys. Soc. Jap.* **28**, 1088 (1970).
- [15] V. P. Vstovsky, *J. Stat. Phys.* **15**, 105 (1976).
- [16] M. Tokuyama, H. Mori, *Prog. Theor. Phys.* **55**, 411 (1976).
- [17] L. A. Lugiato, *Physica* **49**, 615 (1970).
- [18] M. Frankowicz, C. Jędrzejek, to be published.
- [19] J. W. Middleton, W. C. Schieve, *Physica* **63**, 139 (1973).
- [20] A. Grecos, I. Prigogine, *Physica* **59**, 77 (1972).
- [21] M. De Haan, F. Henin, *Physica* **67**, 197 (1973).
- [22] M. De Haan, *Bull. Cl. Sci. Acad. Roy. Belg.* **63**, 69, 317 (1977).
- [23] E. Montroll, in *Fundamental Problems in Statistical Mechanics*, E. G. D. Cohen, Editor, North-Holland Publ.Co., Amsterdam 1962, p. 230.
- [24] L. A. Lugiato, *Physica* **44**, 337 (1969).
- [25] F. C. Andrews, *J. Math. Phys.* **2**, 91 (1961).
- [26] G. Severne, *Physica* **31**, 877 (1965).
- [27] A. Muriel, *J. Chem. Phys.* **49**, 2339 (1968).
- [28] W. Peier, *Physica* **57**, 565 (1972).
- [29] L. A. Lugiato, M. Milani, *Physica* **85A**, 1 (1976).
- [30] F. Haake, *Springer Tracts in Modern Physics* **66**, 98 (1973).
- [31] A. Fuliński, *Physica*, to appear 1978.
- [32] K. O. Friedrichs, *Commun. Pure and Applied Math.* **1**, 361 (1948).