PL ISSN 0459-6854

BULLETIN
DE LA SOCIÉTÉ DES SCIENCES ET DES LETTRES DE ŁÓDŹ
1986 Vol. XXXVI, 5

Recherches sur les déformations No. 17

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A NEW EFFICIENT METHOD OF THE SOLUTION OF THE NAKAJIMA-ZWANZIG GENERALIZED MASTER EQUATION *)

Summary

It is shown that by using some properties of the Bessel functions the integro-differential generalized master equation can be transformed into a system of linear matrix equations. The simplicity of the system makes the wide application of the method possible.

The master equations play an important role in the theory of transport phenomena and relaxation processes. The most general form of the master equation is the so-called generalized master equation (GME) ([1, 2]). It is useful, for example, for the unified description of the coupled coherent and incoherent motion of excitons.

The most elegant way of deriving GME is based on the decomposition of the density matrix ρ into some relevant and irrelevant parts. Thus, starting from the Liouville equation for ρ, the equation can be derived for the relevant part only (usually the diagonal of ρ). This non-local in time integro-differential equation is known as the generalized master equation. For the rel-

*) Trilateral Conf. Contemp. Problems of Quantum Chemistry, Łódź, Oct.25-30,1982

evant part of ρ this equation contains the kernel which consists of the so-called memory functions that are characteristic for a given system and do not depend on the dynamical process in question. For given memory functions and initial conditions, the time evolution of the relevant part of ρ is given by GME. On the other hand, if the time evolution of ρ is known (for example from the solution of the corresponding Schrödinger equation), then GME can be used for the calculation of the memory functions. For this aim only one set of independent initial conditions is necessary. Once the memory functions are known, they can be used for determining the time evolution of the relevant part of ρ for arbitrary initial conditions. In this sense the memory functions determine fully transport properties of the investigated system.

In a local representation the matrix elements of the relevant part of ρ are usually interpreted as the probabilities related to a given place. For example, they can have the meaning of finding the excitation at a given site of the molecule or crystal.

In this paper we consider the generalized master equation in the form

$$\frac{dP_m(t)}{dt} = \int_0^t \sum_n K_{mn}(t-s)\,P_n(s)\,ds + Q_m(t), \tag{1}$$

where $P_m(t)$ are the probabilities (usually of finding the excitation at a given site m), $K_{mn}(t)$ are the memory functions, and $Q_m(t)$ are inhomogenous or driving terms. Our aim is to describe here a new approach to the solution of GME (1) which leads to the solution of a simple system of matrix equations instead of (1).

First, we consider $P_m^{(i)}(t)$ and $Q_m^{(i)}(t)$ corresponding to independent initial conditions $P_m^{(i)}(0)$ and $Q_m^{(i)}(0)$, $i = 1,2,\ldots$, and define matrices

$$P(t) = \begin{pmatrix} P_1^{(1)}(t), & P_1^{(2)}(t), \ldots \\ P_2^{(1)}(t), & P_2^{(2)}(t), \ldots \\ \vdots & \end{pmatrix}, \quad Q(t) = \begin{pmatrix} Q_1^{(1)}(t), & Q_1^{(2)}(t), \ldots \\ Q_2^{(1)}(t), & Q_2^{(2)}(t), \ldots \\ \vdots & \end{pmatrix}. \tag{2}$$

Then GME (1) can be written in the matrix form

$$\frac{dP(t)}{dt} = \int_0^t K(t-s)\,P(s)\,ds + Q(t), \tag{3}$$

where $K(t-s) = \{K_{mn}(t-s)\}_{m,n=1,2,\ldots}$ is a matrix.

Further, we introduce functions

$$\bar{J}_i(t) = \frac{(i+1)\,J_{i+1}(t)}{t}, \tag{4}$$

where $J_i(t)$ are the Bessel functions of the first kind. These functions have, from our point of view, two important properties. Their derivative equals

$$\frac{d\bar{J}_i(t)}{dt} = \tfrac{1}{2}\,[\bar{J}_{i-1}(t) - \bar{J}_{i+1}(t)] \tag{5}$$

and, what is more important, the convolution between them is given analytically

$$\int_0^t \bar{J}_i(t-s)\,\bar{J}_j(s)\,ds = \bar{J}_{i+j+1}(t) \tag{6}$$

(see [3] and [4]). As it is shown below, these properties enable us to transform (3) into an algebraic form.

Expanding $P(t)$, $K(t)$, and $Q(t)$ in terms of these functions (it is the so-called Neumann expansion of the first kind ([3, 5]) we obtain

$$P(t) = \sum_{i=0}^{\infty} P_i\,\bar{J}_i(t), \tag{7}$$

$$K(t) = \sum_{i=0}^{\infty} K_i\,\bar{J}_i(t), \tag{8}$$

$$Q(t) = \sum_{i=0}^{\infty} Q_i\,\bar{J}_i(t). \tag{9}$$

Substituting into (3) and equating the coefficients before $\bar{J}_i(t)$ on both sides of (3) we get the following system of matrix equations:

$$\begin{aligned} &\tfrac{1}{2}P_1 = Q_0, \\ &\tfrac{1}{2}(P_2 - P_0) = K_0 P_0 + Q_1, \\ &\tfrac{1}{2}(P_3 - P_1) = K_0 P_1 + K_1 P_0 + Q_2, \\ &\qquad\vdots \\ &\tfrac{1}{2}(P_{i+1} - P_{i-1}) = \sum_{j=0}^{i-1} K_j P_{i-1-j} + Q_i, \quad i = 1,2,\ldots . \end{aligned} \tag{10}$$

Thus, the solution of GME (1) is equivalent to the solution of the matrix equations (10) which represent the recurrent relations for the determination of one unknown function from $P(t)$, $K(t)$ or $Q(t)$

in terms of two remaining ones.

Multiplying Eqs.(10) by $\bar{J}_0(t)$, $\bar{J}_1(t)$,..., and summing them we get another form of GME

$$(11) \qquad \frac{dP(t)}{dt} = \sum_{i=0}^{\infty} \Big(\sum_{j=0}^{i-1} K_j P_{i-1-j} \Big) \bar{J}_i(t) + Q(t),$$

which shows that although non-local in time, GME (1) can be rewritten in local-in-time form. Because of (6), the time convolution in (3) becomes the "discrete convolution" in (11). Replacing the infinite sum in (11) by the first n-terms we get the solution of (1) exact to the n-th power of t. These properties interesting from the physical point of view indicate the importance of this form of GME.

Equations (10) and (11) require the knowledge of the expansion coefficients-matrices in (7)-(9). It appears that they can be determined easily. For example, in the coherent case and for the time independent hamiltonian the elements of the matrices P_i are simple functions of the eigenvalues and eigenvectors of the hamiltonian (cf. [7, 8]).

The problem of the convergence of the series (7)-(9) is important from the computational view-point. The experience in this respect obtained till now is very good. Namely, the Bessel functions for the fixed t go very quickly to zero (see [4])

$$(12) \qquad J_n(t) \approx \frac{1}{\sqrt{n}} \frac{1}{n^n}$$

so that the series (7)-(9) can easily be truncated. For the time $0 \leq t \leq 1$ only a few first terms contribute to (7)-(9). For the longer time the number of terms which have to be taken into account increases. It appears, however, that for the fixed $t > 100$ all terms with $n > t$ give a negligible contribution and may be omitted. For a very long time the change of the time scale described in [7] may be useful. It should be mentioned that from the view-point of the convergence of (8) the coherent case is the most difficult one. In the more realistic non-coherent case where the memory functions go quickly to zero quicker convergence of (8) is generally expected.

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Presented by Leszek Wojtczak at the Session of the Mathematical-Physical Commission of the Łódź Society of Sciences and Arts on February 23, 1984

NOWA EFEKTYWNA METODA ROZWIĄZANIA OGÓLNEGO RÓWNANIA KINETYCZNEGO NAKAJIMA-ZWANZIGA

Streszczenie

W pracy zastosowano nowe podejście do rozwiązania kinetycznego równania różniczkowo-całkowego. Przy pomocy funkcji Bessela równanie to daje się zamienić na układ równań liniowych. Uproszczenie takie rozszerza skalę zastosowań równania kinetycznego.