Acta Universitatis Carolinae. Mathematica et Physica

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Acta Universitatis Carolinae. Mathematica et Physica, Vol. 23 (1982), No. 2, 61--72

Persistent URL: http://dml.cz/dmlcz/142495

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Algebraic Representation of the Nakajima-Zwanzig's Generalized Master Equation

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Received 29 September 1982

It is shown that 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 possible wide applicability of this method. Various properties of this representation of the generalized master equation together with an illustrative example are given and discussed in detail.

В работе показано что с помощью некоторых свойств функций Бесселя возможно интегро-дифференциальное обобщенное кинетическое уравнение свести к системе линейных матричных уравнений. Простота этих уравнений позволяет широкое применение этого подхода. Детально овсуждаются разные свойства этого представления обобщенного кинетического уравнения и приводится простой пример его применения.

V práci je ukázáno, že s použitím některých vlastností Besselových funkcí lze integrodiferenciální zobecněnou kinetickou rovnici převést na systém lineárních maticových rovnic. Jednoduchost tohoto systému umožňuje širokou použitelnost navržené metody. V práci jsou uvedeny a diskutovány různé vlastnosti této reprezentace zobecněné kinetické rovnice společně s ilustrativním příkladem.

1. Introduction

Starting from the work of Pauli [1], the master equations play an important role in various fields of physics. We mention here the theory of transport phenomena and relaxation processes and the theory of lasers. Further examples and references are given e.g. in [2].

The most general form of the master equation is the so called generalized master equation (GME) [3, 4]. It is convenient for example for the unified description of the coupled coherent and incoherent motion of excitons.

The most elegant way of the derivation of GME is based on the decomposition of the density matrix ϱ into some relevant and irrelevant parts. Starting then from the Liouville equation for ϱ, the equation for the relevant part only (usually the diagonal

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of ϱ) can be derived. This non-local in time integro-differential equation is known as the generalized master equation. This equation for the relevant part of ϱ contains the kernel consisting of so called memory functions which 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), GME can be used for the evaluation of the memory functions.

In this work, we describe a new way of the solution of GME based on some properties of the Bessel functions. The simplicity of this approach leading to a system of linear matrix equations makes possible to take into account the most general form of GME with the so called non-retarded terms (section 2). The expansion of the probabilities in terms of a simple modification of the Bessel functions is discussed in section 3. Simple example illustrating the foregoing theory is given in section 4. The time scaling procedure is described in section 5. The appendix summarizes the relevant results from the theory of the Bessel functions.

2. Algebraic Representation of GME

In this work, we discuss GME in the form

$$\frac{\mathrm{d}P_m(t)}{\mathrm{d}t} = \int_0^t \sum_n K_{mn}(t-s)\, P_n(s)\, \mathrm{d}s + Q_m(t)\,, \tag{1}$$

where $P_m(t)$ are the diagonal elements of the density matrix, $K_{mn}(t)$ are the memory functions and $Q_m(t)$ are so called non-retarded terms. Although $P_m(t)$ and $Q_m(t)$ are not in general independent [4], $P_m(t)$, $K_{mn}(t)$ and $Q_m(t)$ may be from our point of view arbitrary functions satisfying (1). In many important cases the non-retarded terms vanish [2–5].

To simplify the notation, we re-write GME (1) into the matrix form. For this aim, we consider the probabilities $P_m^{(i)}(t)$ and the non-retarded terms $Q_m^{(i)}(t)$ for different initial conditions $P_m^{(i)}(0)$ and the corresponding $Q_m^{(i)}(0)$, $i = 1, 2, \ldots$ and define matrices

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

and

$$Q(t) = \begin{pmatrix} Q_1^{(1)}(t), & Q_1^{(2)}(t), & \ldots \\ Q_2^{(1)}(t), & Q_2^{(2)}(t), & \ldots \\ \vdots & \vdots & \end{pmatrix}. \tag{3}$$

GME (1) then becomes

$$\frac{dP(t)}{dt} = \int_0^t K(t-s)\,P(s)\,ds + Q(t)\,, \tag{4}$$

where $K(t-s) = \{K_{mn}(t-s)\}_{m,n=1,2,\ldots}$ is also matrix. For the problem of the order N (m runs from 1 to N) we use N independent initial conditions so that all three matrices $P(t)$, $K(t)$ and $Q(t)$ are the square matrices of the order N.

The right hand side of GME (4) contains the time convolution between $K(t-s)$ and $P(s)$. One way of its solution consists in the application of the Laplace transform to (4) which leads to a product of the corresponding transforms instead of the convolution of the originals (see e.g. [5]). Instead of using the Laplace transform, we make use of the Neumann type series (see Appendix) for the expansion of $P(t)$, $K(t)$ and $Q(t)$ as functions of time.

For this aim, we define functions

$$\bar{J}_i(t) = \frac{(i+1)\,J_{i+1}(t)}{t}\,, \quad i = 0, 1, \ldots\,, \tag{5}$$

where $J_i(t)$ are the Bessel functions of the first kind. From our point of view, these functions have the following important properties

$$\frac{d\bar{J}_0(t)}{dt} = -\tfrac{1}{2}\,\bar{J}_1(t)\,, \tag{6a}$$

$$\frac{d\bar{J}_i(t)}{dt} = \tfrac{1}{2}[\bar{J}_{i-1}(t) - \bar{J}_{i+1}(t)]\,. \quad i = 1, 2, \ldots \tag{6b}$$

and

$$\int_0^t \bar{J}_i(t-s)\,\bar{J}_j(s)\,ds = \bar{J}_{i+j+1}(t) \tag{7}$$

leading to a significant simplification of (4).

We assume now that $P(t)$, $K(t)$ and $Q(t)$ are expanded in terms of the functions $\bar{J}_i(t)$

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

$$K(t) = \sum_{i=0}^{\infty} K_i\,\bar{J}_i(t) \tag{9}$$

and

$$Q(t) = \sum_{i=0}^{\infty} Q_i\,\bar{J}_i(t)\,, \tag{10}$$

where P_i, K_i and Q_i are the matrix-type expansion coefficients. It appears that the mathematical assumptions for which the series (8)–(10) can be used are sufficiently general (see Appendix).

Substituting now (8)–(10) into GME (4) and equating the coefficients before $\bar{J}_i(t)$ on both sides of (4) we get the following infinite system of matrix equations

$$\tfrac{1}{2}P_1 = Q_0\,, \tag{11a}$$

$$\tfrac{1}{2}(P_2 - P_0) = K_0P_0 + Q_1\,, \tag{11b}$$

$$\tfrac{1}{2}(P_3 - P_1) = K_0P_1 + K_1P_0 + Q_2\,, \tag{11c}$$

$$\vdots$$

$$\tfrac{1}{2}(P_{i+1} - P_{i-1}) = \sum_{j=0}^{i-1} K_jP_{i-1-j} + Q_i\,, \quad i = 1, 2, \ldots\,. \tag{11d}$$

Thus, it appears that GME (4) is equivalent to the matrix system (11) which represent the reccurrent relations for the determination of one unknown function from $P(t)$, $K(t)$ and $Q(t)$ in terms of two remaining ones.

If the matrix coefficients K_i and Q_i are known, the matrices P_i can be evaluated in an obvious way. Assuming that the initial value $P(0)$ is given it follows from (A4) that

$$P_0 = 2P(0)\,. \tag{12}$$

Further matrices $P_1, P_2, \ldots$ can be found from (11)

$$P_1 = 2Q_0\,, \tag{13}$$

$$P_2 = 2(K_0P_0 + Q_1) + P_0\,,$$

$$P_3 = 2(K_0P_1 + K_1P_0 + Q_2) + P_1\,.$$

$$\vdots$$

If the memory functions are to be evaluated, we solve (11) in a similar way

$$K_0 = [\tfrac{1}{2}(P_2 - P_0) - Q_1]\,P_0^{-1}\,, \tag{14}$$

$$K_1 = [\tfrac{1}{2}(P_3 - P_1) - K_0P_1 - Q_2]\,P_0^{-1}\,,$$

$$K_2 = [\tfrac{1}{2}(P_4 - P_2) - K_0P_2 - K_1P_1 - Q_3]\,P_0^{-1}\,.$$

$$\vdots$$

Note that the matrix P_0 is regular for independent initial conditions so that P_0^{-1} exists. In many cases (see e.g. [5]) the initial condition has the form $P(0) = \mathbf{1}$ so that $P_0^{-1} = 0.5\,.\,\mathbf{1}$.

The evaluation of Q_i in terms of P_i and K_i is straightforward and requires no comment.

Multiplying equations (11) by $\bar{J}_0(t)$, $\bar{J}_1(t)$, ... and summing them we get the following form of GME

$$\frac{\mathrm{d}P(t)}{\mathrm{d}t} = \sum_{i=0}^{\infty}\Big(\sum_{j=0}^{i-1} K_jP_{i-1-j}\Big)\,\bar{J}_i(t) + Q(t)\,. \tag{15}$$

This equation explicitely displays the essence of our method. The "continuous" convolution in (4) is transformed to a "discrete" convolution in (15). In the discrete convolution, time t appears in the functions $\bar{J}_i(t)$ only. GME (15) is local in time, however, the value of the convolution depends on all K_i, P_i, $(i = 0, 1, \ldots$ or as it can be shown on all derivatives of $P(t)$ and $K(t)$ at $t = 0$. Truncating the series (8)–(10) i.e. assuming $P_i = K_i = Q_i = \mathbf{0}$ for $i > n$, we search for the solutions exact to the n-th power of t (see (A1)). It follows from (15) that the corresponding truncated expression for the convolution is then exact to the $(n + 1)$-th power of t so that it can also be truncated. Therefore, this form of GME is particularly suitable for finding approximate solutions exact to a given power of t.

3. Evaluation of the Matrices P_i

In this section we discuss the way by which the memory kernel $K(t)$ can be evaluated. Assuming the initial conditions for which $Q(t) = \mathbf{0}$ we find the matrix of the probabilities $P(t)$ from the solution of the corresponding Schrödinger equation Having $P(t)$, we derive the formulae from which the matrix coefficients P_i can be evaluated. The calculation of the memory kernel from (14) and (9) is then straightforward.

We consider here the problem of the motion of excitons in the coherent case (see e.g. [5]). For this aim, we assume the time independent electron hamiltonian

$$\boldsymbol{H} = \sum_{m,n} |m\rangle H_{mn} \langle n| , \tag{16}$$

where $|n\rangle$ are some localized states. We suppose here that the solutions of the Schrödinger equation

$$\boldsymbol{H}|\alpha\rangle = E_\alpha|\alpha\rangle \tag{17}$$

are known and introduce frequencies ω_α by

$$E_\alpha = \hbar\omega_\alpha . \tag{18}$$

In the representation of the states $|n\rangle$, Eq. (17) becomes

$$\sum_\alpha H_{mn}\langle n \mid \alpha\rangle = E_\alpha\langle m \mid \alpha\rangle . \tag{19}$$

Our aim, however, is to investigate solutions of the time Schrödinger equation

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \langle n \mid \psi\rangle = \boldsymbol{H}\langle n \mid \psi\rangle \tag{20}$$

which has a general solution

$$\langle n \mid \psi\rangle = \sum_\alpha c_\alpha \exp(-\mathrm{i}\omega_\alpha t) \langle n \mid \alpha\rangle . \tag{21}$$

Now, as it is usual we require the fulfilment of N independent initial conditions

$$\langle n \mid \psi(t=0)\rangle_p = \delta_{np}\,, \quad p = 1, \ldots, N\,, \tag{22}$$

i.e. we assume that the solution (21) is at $t = 0$ localized at site p, $p = 1, \ldots, N$. This requirement directly leads to

$$\langle n \mid \psi(t)\rangle_p = \sum_{\alpha} \langle n \mid \alpha\rangle \exp(-\mathrm{i}\omega_\alpha t) \langle \alpha \mid p\rangle\,. \tag{23}$$

Further let us denote the probability to find the excitation at site n by $P_n^{(p)}(t)$, where p denotes the initial localization of the excitation

$$P_n^{(p)}(0) = \delta_{np}\,. \tag{24}$$

We get from (23)

$$P_n^{(p)}(t) = |\langle n \mid \psi(t)\rangle_p|^2 = \sum_{\alpha,\beta} G_{np}^{(\alpha\beta)} \exp(-\mathrm{i}\omega_{\alpha\beta} t)\,, \tag{25}$$

where the elements of the matrix $G^{(\alpha\beta)}$ are formed by the components of the eigenvectors $\langle n \mid \alpha\rangle$

$$G_{np}^{(\alpha\beta)} = \langle n \mid \alpha\rangle \langle \alpha \mid p\rangle \langle p \mid \beta\rangle \langle \beta \mid n\rangle\,. \tag{26}$$

Therefore, the matrix of the probabilities appearing in (4) equals

$$P(t) = \sum_{\alpha,\beta} G^{(\alpha\beta)} \exp(-\mathrm{i}\omega_{\alpha\beta} t)\,. \tag{27}$$

The matrices $G^{(\alpha\beta)}$ are in general hermitian

$$G^{(\alpha\beta)} = G^{(\alpha\beta)+} \tag{28}$$

and fulfil the relation

$$G^{(\alpha\beta)} = G^{(\beta\alpha)*}\,. \tag{29}$$

For the real hamiltonian the matrix of the probabilities is symmetric

$$P(t) = \sum_{\alpha,\beta} G^{(\alpha\beta)} \cos(\omega_{\alpha\beta} t) = P(t)^{\mathrm{T}}\,. \tag{30}$$

Assuming now that $P(t)$ (27) is known we evaluate the matrices P_i in the expansion (8). Since the only time-dependent term in (27) is the exponential one it is sufficient to determine the coefficients $c_n(\omega)$ of the expansion

$$\exp(-\mathrm{i}\omega t) = \sum_{n=0}^{\infty} c_n(\omega)\, \bar{J}_n(t)\,. \tag{31}$$

First we determine $c_0(\omega)$. Putting $t = 0$ and using (A4) we get

$$1 = \sum_{n=0}^{\infty} c_n(\omega)\, \bar{J}_n(0) = \tfrac{1}{2}\, c_0(\omega) \tag{32}$$

so that

$$c_0(\omega) = 2\,. \tag{33}$$

In order to determine $c_n(\omega)$, $n = 1, 2, \ldots$ we calculate the derivative of both sides of (31) and use (A3)

$$-\mathrm{i}\omega \exp(-\mathrm{i}\omega t) = c_0(\omega)(-\tfrac{1}{2})\bar{J}_1(t) + \sum_{n=1}^{\infty} c_n(\omega)\tfrac{1}{2}(\bar{J}_{n-1}(t) - \bar{J}_{n+1}(t)) . \quad (34)$$

Substituting for $\exp(-\mathrm{i}\omega t)$ from (31) and equating the coefficients before $\bar{J}_n(t)$, $n = 0, 1, 2, \ldots$ on both sides we get the following reccurrent formulae

$$c_1(\omega) = -2\mathrm{i}\omega\, c_0(\omega) , \quad (35a)$$

$$c_{n+1}(\omega) = c_{n-1}(\omega) - 2\mathrm{i}\omega\, c_n(\omega) , \quad n = 1, 2, \ldots . \quad (35b)$$

For a given ω, these equations and Eq. (33) determine $c_n(\omega)$, $n = 0, 1, 2, \ldots$ uniquely. Because of the difference equation (35b), the coefficients $c_n(\omega)$ are closely related to the Gegenbauer and Tschebyschev polynomials [6].

The matrices P_n necessary in (11) can be now easily found. It follows from (27) or from

$$P(t) = \sum_{\alpha\beta} G^{(\alpha\beta)} \exp(-\mathrm{i}\omega_{\alpha\beta} t) = \sum_{n=0}^{\infty} P_n \bar{J}_n(t) \quad (36)$$

that

$$P_n = \sum_{\alpha\beta} G^{(\alpha\beta)} c_n(\omega_{\alpha\beta}) . \quad (37)$$

Since

$$c_n(\omega) = (-1)^n c_n(-\omega) \quad (38)$$

we get also

$$P_{2k} = 2\sum_{\alpha} G^{(\alpha\alpha)} + 2\sum_{\alpha<\beta} c_{2k}(\omega_{\alpha\beta}) \operatorname{Re} G^{(\alpha\beta)} \quad (39a)$$

and

$$P_{2k+1} = 2\mathrm{i}\sum_{\alpha<\beta} c_{2k+1}(\omega_{\alpha\beta}) \operatorname{Im} G^{(\alpha\beta)} . \quad (39b)$$

These formulae are general. If the hamiltonian is real we get

$$P_{2k+1} = 0 \quad (40)$$

and

$$P_{2k} = P_{2k}^{\mathrm{T}} . \quad (41)$$

In many cases, $P(t)$ is an even function of t so that the expansion of $\cos(\omega_{\alpha\beta} t)$ instead of $\exp(-\mathrm{i}\omega_{\alpha\beta} t)$ is necessary. The coefficients of the expansion

$$\cos \omega t = \sum_{n=0}^{\infty} b_n(\omega) \bar{J}_n(t) \quad (42)$$

can be determined analogously. First it is obvious that

$$b_n(\omega) = \operatorname{Re} c_n(\omega) \quad (43)$$

so that

$$b_{2k+1}(\omega) = 0 . \quad (44)$$

For non-zero coefficients we get the reccurrent relations

$$b_0 = 2\,, \tag{45}$$

$$b_2 = 2 - 8\omega^2\,,$$

$$b_{2k+2} = (2 - 4\omega^2)\, b_{2k} - b_{2k-2}\,.$$

It follows from (37) that the matrices P_i are determined by the energy spectrum of the hamiltonian ($\omega_{\alpha\beta} = (E_\alpha - E_\beta)/\hbar$) and the corresponding eigenvectors (matrices $G^{(\alpha\beta)}$). According to (14), the memory kernel $K(t)$ depends also on $\omega_{\alpha\beta}$ and $G^{(\alpha\beta)}$. This dependence, however, is in general complicated. For short times it is given by

$$P(t) = \sum_{i=0}^{n} P_i\, \bar{J}_i(t) \tag{46a}$$

and

$$K(t) = \sum_{i=0}^{n} K_i\, \bar{J}_i(t)\,, \tag{46b}$$

where $P_i = P_i(\omega_{\alpha\beta}, G^{(\alpha\beta)})$ and $K_i = K_i(\omega_{\alpha\beta}, G^{(\alpha\beta)})$ with the accuracy to the n-th power of t.

4. Example

In this section, a simple example illustrating the use of our approach is given. Further applications are prepared for the publication.

It is well known that the problem of the excitons in dimer with the hamiltonian

$$\boldsymbol{H} = \begin{pmatrix} 0 & \mathrm{V} \\ \mathrm{V} & 0 \end{pmatrix} \tag{47}$$

leads to the probabilities

$$P(t) = \begin{pmatrix} \cos^2 \dfrac{\mathrm{V}}{\hbar} t\,, & \sin^2 \dfrac{\mathrm{V}}{\hbar} t \\ \sin^2 \dfrac{\mathrm{V}}{\hbar} t\,, & \cos^2 \dfrac{\mathrm{V}}{\hbar} t \end{pmatrix} \tag{48}$$

and the constant memory kernel

$$K(t) = \frac{2\mathrm{V}^2}{\hbar^2} \begin{pmatrix} -1, & 1 \\ 1, & -1 \end{pmatrix}. \tag{49}$$

It can directly be verified that these $P(t)$ and $K(t)$ satisfy GME (4) with $Q(t) = \mathbf{0}$.

First we introduce a new time scale by the substitution

$$\frac{\mathrm{V}}{\hbar} t \to t\,. \tag{50}$$

Using then the method of section 3 we get as a result

$$P(t) = \begin{pmatrix} \cos^2 t, & \sin^2 t \\ \sin^2 t, & \cos^2 t \end{pmatrix} = \sum_{n=0}^{\infty} P_{2n}\, \bar{J}_{2n}(t) \tag{51}$$

and

$$K(t) = \begin{pmatrix} -2, & 2 \\ 2, & -2 \end{pmatrix} = \sum_{n=0}^{\infty} K_{2n}\, \bar{J}_{2n}(t)\,, \tag{52}$$

where

$$P_{2n} = \begin{pmatrix} 2 - 2^{4n} \sum_{s=0}^{n-1} \frac{(2n-s)!}{2^{4s} s!} \frac{(-1)^{n-s+1}}{(2n-2s)!}, & 2^{4n} \sum_{s=0}^{n-1} \frac{(2n-s)!}{2^{4s} s!} \frac{(-1)^{n-s+1}}{(2n-2s)!} \\ 2^{4n} \sum_{s=0}^{n-1} \frac{(2n-s)!}{2^{4s} s!} \frac{(-1)^{n-s+1}}{(2n-2s)!}, & 2 - 2^{4n} \sum_{s=0}^{n-1} \frac{(2n-s)!}{2^{4s} s!} \frac{(-1)^{n-s+1}}{(2n-2s)!} \end{pmatrix} \tag{53}$$

and

$$K_{2n} = \begin{pmatrix} -4, & 4 \\ 4, & -4 \end{pmatrix}. \tag{54}$$

The first few matrices P_n have the form

$$P_0 = \begin{pmatrix} 2, & 0 \\ 0, & 2 \end{pmatrix}, \quad P_2 = \begin{pmatrix} -14, & 16 \\ 16, & -14 \end{pmatrix}, \quad P_4 = \begin{pmatrix} 210, & -208 \\ -208, & 210 \end{pmatrix}, \tag{55}$$

$$P_6 = \begin{pmatrix} -2910, & 2912 \\ 2912, & -2910 \end{pmatrix}.$$

Matrices P_{2n+1} and K_{2n+1} are equal to zero.

5. Time Scaling

The method developed in this paper is based on the infinite expansions (8)–(10) of $P(t)$, $K(t)$ and $Q(t)$ in terms of the functions $\bar{J}_i(t)$. From the computational point of view, the question of the rate of the convergence of these series and the possibility of their truncation is to be analyzed. It may appear in this context that the expansion in terms of the functions $\bar{J}_i(At)$ $(A \neq 1)$ instead of $\bar{J}_i(t)$ is more convenient. This generalization leading to the change of the form of the basis functions can be taken into account in the following way.

Let us consider GME (4) and define a new time scale by

$$\tau = At\,, \quad \sigma = As\,. \tag{56}$$

Then we get from (4)

$$\frac{\mathrm{d}P'(\tau)}{\mathrm{d}\tau} = \int_0^{\tau} K'(\tau - \sigma)\, P'(\sigma)\, \mathrm{d}\sigma + Q'(\tau) \tag{57}$$

where

$$P'(\tau) = P(\tau/A), \quad Q'(\tau) = Q(\tau/A) \tag{58}$$

and

$$K'(\tau) = \frac{1}{A^2} K(\tau/A). \tag{59}$$

Solving (58) we get the original solutions from

$$P(t) = P'(At), \quad Q(t) = Q'(At) \tag{60}$$

and

$$K(t) = A^2 K'(At). \tag{61}$$

The time scaling generally leads to the change of the matrix coefficients P_i, K_i and Q_i.

For example, in case of the dimer (section 4) we put $A = 2$ so that

$$P(t) = \begin{pmatrix} \cos^2 t, & \sin^2 t \\ \sin^2 t, & \cos^2 t \end{pmatrix} = \sum_{n=0}^{\infty} P_{2n} \bar{J}_{2n}(2t) \tag{62}$$

and

$$K(t) = \begin{pmatrix} -2, & 2 \\ 2, & -2 \end{pmatrix} = 4 \sum_{n=0}^{\infty} K_{2n} \bar{J}_{2n}(2t). \tag{63}$$

The expression for P_{2n} then becomes

$$P_{2n} = \begin{pmatrix} 1 + (-1)^n (2n+1), & 1 - (-1)^n (2n+1) \\ 1 - (-1)^n (2n+1), & 1 + (-1)^n (2n+1) \end{pmatrix} \tag{64}$$

and

$$K_{2n} = \begin{pmatrix} -1, & 1 \\ 1, & -1 \end{pmatrix}. \tag{65}$$

The functions $\bar{J}_n(t)$ appearing in (8)–(10) go for $n > t$ very quickly to zero so that these series may easily be truncated. It means that to get a sufficiently exact numerical solution on the interval $(0, t)$ the number of terms of the series (8)–(10) taken into account must be roughly equal or greater than t. For example, to get $P(t)$ or $K(t)$ on the period $(0, \pi)$ with 7 digit accuracy, it is sufficient to take about 10 first terms of the series (62) or (63).

From the computational point of view, the scaling parameter A is optional and can be used for the optimalization of the convergence of the series (8)–(10).

6. Conclusions

The suggested way of the solution of GME is applicable to the most general form of GME with non-retarded terms. There is no limitation of our method as far as the spatial structure (one, two or three dimensions, perfect or distorted lattice) and the composition (different chemical components, impurities) of the investigated

systems is concerned. Because of its generality, it can be used in different fields of physics. In comparison with other methods, it leads to a simple system of algebraic equations which can be easily solved. The method is particularly suitable for searching approximate solutions exact to a given power of t.

Acknowledgements

Fruitful discussions with Prof. L. Valenta and Dr. V. Čápek are gratefully acknowledged.

Appendix

The functions

$$\bar{J}_n(t) = \frac{n+1}{2}\left(\frac{t}{2}\right)^n \sum_{m=0}^{\infty} \frac{(-1)^m \left(\frac{t}{2}\right)^{2m}}{m!\,(m+n+1)!} \tag{A1}$$

have the following properties

$$\frac{\mathrm{d}\bar{J}_0(t)}{\mathrm{d}t} = -\tfrac{1}{2}\,\bar{J}_1(t)\,, \tag{A2}$$

$$\frac{\mathrm{d}\bar{J}_i(t)}{\mathrm{d}t} = \tfrac{1}{2}[\bar{J}_{i-1}(t) - \bar{J}_{i+1}(t)]\,, \quad i = 1, 2, \ldots\,, \tag{A3}$$

$$\bar{J}_n(0) = \tfrac{1}{2}\,\delta_{n0}\,, \tag{A4}$$

$$\int_0^t \bar{J}_i(t-s)\,\bar{J}_j(s)\,\mathrm{d}s = \bar{J}_{i+j+1}(t)\,. \tag{A5}$$

The expansion of a given function in terms of the functions $\bar{J}_n(t)$ is one of the forms of the Neumann series of the first kind [7]. Any function $f(t)$ which can be expanded into the power series

$$f(t) = \sum_{l=0}^{\infty} b_l t^l \tag{A6}$$

can also be expanded into the series

$$b(t) = \sum_{n=0}^{\infty} a_n\,\bar{J}_n(t) \tag{A7}$$

with the same radius of convergence. The mutual relation between the coefficients of these series is given by

$$a_n = 2^{n+1} \sum_{s=0}^{\leqq n/2} \frac{(n-s)!}{2^{2s}s!}\,b_{n-2s} \tag{A8}$$

and

$$b_l = \frac{2^{-l-1}}{(l+1)!} \sum_{m=0}^{\leqq l/2} \frac{(-1)^m}{l-2m+1} \binom{l+1}{m} a_{l-2m} \,. \tag{A9}$$

A few examples is given below.

$$\cos t = 2 \sum_{k=0}^{\infty} (-1)^k (2k+1)\, \bar{J}_{2k}(t) \,, \tag{A10}$$

$$\sin t = 2 \sum_{k=0}^{\infty} (-1)^k 2(k+1)\, \bar{J}_{2k+1}(t) \,, \tag{A11}$$

$$1 = 2 \sum_{k=0}^{\infty} \bar{J}_{2k}(t) \,, \tag{A12}$$

$$\cos^2 t = \sum_{k=0}^{\infty} [1 + (-1)^k (2k+1)]\, \bar{J}_{2k}(2t) \,, \tag{A13}$$

$$\sin^2 t = \sum_{k=0}^{\infty} [1 - (-1)^k (2k+1)]\, \bar{J}_{2k}(2t) \,. \tag{A14}$$

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