Journal of Mathematical Chemistry 6(1991)165–191

FACTORIZATION OF CERTAIN EVOLUTION OPERATORS USING LIE ALGEBRA: FORMULATION OF THE METHOD*

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Received 1 September 1989
(Revised 11 September 1990)

Abstract

In this work, a new method to factorize certain evolution operators into an infinite product of simple evolution operators is presented. The method uses Lie operator algebra and the evolution operators are restricted to exponential form. The argument of these forms is a first-order linear partial differential operator. The method has broad applications, including the areas of sensitivity analysis, the solution of ordinary differential equations, and the solution of Liouville's equation. A sequence of ξ-approximants is generated to represent the Lie operators. Under certain conditions, the convergence rate of the ξ-approximant sequences is remarkably high. This work presents the general formulation of the scheme and some simple illustrative examples. Investigation of convergence properties is given in a companion paper.

1. Introduction

Exponential operators play important roles in many branches of science and engineering. Depending on the structure of the operator argument of the exponential, various expansion techniques have been used to obtain exact or approximate expressions for the exponential. Among these methods are the Feynman ordering-operator calculus [1], use of the commutator as a super operator, Lie algebraic techniques, functional analytic methods and certain other special analytical methods [2]. A differential equation method has also been extensively used to establish certain identities involving exponential operators.

Almost all of the exponential operators of interest include a parameter which corresponds to a physical quantity, and most of the available methods necessitate differentiation with respect to this parameter as an intermediate step [3,4]. The Baker–Campbell–Hausdorff (BCH) formula [5–7] allows for the expression of the product of two exponential operators as a single exponential operator with a quite complicated operator argument. A similar formula, which contains increasing powers of

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a parameter in consecutive factors of an infinite product of exponential operators, was developed by Zassenhaus [8] to express a single exponential operator whose argument is a sum of the two linear operators.

Considerable work has been devoted to connecting quantum mechanics and classical mechanics via operator techniques [3–14]. Among these, Lie algebraic tools have been used to develop various relations for exponential operators whose arguments obey Lie algebraic rules [15–22]. The solution of first-order linear operator-differential equations via Lie algebraic methods or via commutator algebra involving exponentials has been studied [8,23–25]. Normal ordering of operators to solve these kinds of equations can be found in a number of works [22,26–31]. Many problems in statistical mechanics also make use of exponential operators [32–45] once again after using Lie groups and Lie algebraic theories [46–50]. Lie algebraic techniques are also used to calculate the classical mechanical trajectories of some systems [51–61]. Since Lie algebra and Lie groups are frequently used in mathematical physics, an abundant literature can be found in this area [62–70] including computer programs to calculate certain entities [71,72]. The concept of a vector field [73] may be used to investigate the solution of appropriate first-order differential equation systems [74]. To this end, approximate exponential operators can be constructed to characterize the solutions [75,76], and the approach often gives quite accurate results for the short-term behavior of the evolution. However, the method is subject to error accumulation, especially at long-term evolution.

This brief summary serves to show the need to evaluate exponential operators in a global and rapidly convergent manner. Although various methods are available for treating the exponential of operators, there is considerable room for new and hopefully better methods. Hence, this work is devoted to the presentation of a new factorization scheme for exponential operators, and in a companion paper we deal with the convergence properties of the scheme.

In this paper, a system with n degrees of freedom will be characterized by n complex variables $x_1, \ldots, x_n$ which are considered as the components of a vector or the coordinates of a point in an n-dimensional complex vector space. Only real variables are required in most of the cases encountered; however, convergence proofs necessitate dealing with complex variables in order to take care of possible singularities outside the real axis. If any two points in the space are related by a unique transformation Q, whose functional structure does not depend on the location of the points, then one can define an evolution operator for the system, since any two points of an n-dimensional space may be connected by a continuous curve, and it is possible to use a tracing parameter which defines the position of the system on this curve during its evolution from its initial state $\boldsymbol{x}_i$ to its final state $\boldsymbol{x}_f$. This circumstance often arises where time is the evolutionary parameter and we will accordingly denote this parameter as t. Therefore, the initial and final states of the system can be characterized by the scalar instants of time t_i and t_f. Hence, the global evolution operator $Q(t_f, t_i)$, which solely depends on the initial (t_i) and the final (t_f) instances, can be defined with the relation

$$x_f = Q(t_f, t_i) \cdot x_i. \tag{1.1}$$

In many applications, one can find practical expressions for the operator Q if t_i and t_f are sufficiently close to each other. Hence, the global evolution operator $Q(t_f, t_i)$ may be factorized into a simple sequence of evolutionary steps:

$$Q(t_f, t_i) = Q(t_f, t_m)Q(t_m, t_{m-1}) \ldots Q(t_1, t_i), \tag{1.2}$$

and by choosing a sufficiently large number of intervals in time, this factorization can characterize the global evolution of the system. If the simple short time interval solutions were exactly calculable, then the presence of a large number of such evolutions m is not important. However, in reality, even simple evolutions over the short time intervals can often be only approximately determined. In such a case, the number of increments m is significant since errors can accumulate to possibly create numerical instabilities and inaccuracies. In addition, the factorization requires operators at times other than the initial and final specified values. Therefore, a more global factorization of the evolution operator only dependent on t_i and t_f, such as suggested in this paper, would be more attractive.

The present work considers the factorization of the evolution operator into a sequence of simple *global* evolution operators. The scheme presented will maintain its validity only on a special subclass of evolution operators. First, we restrict the system under consideration to being autonomous such that the evolution operator has the following simple structure

$$Q(t_f, t_i) = Q(t_f - t_m). \tag{1.3}$$

We also restrict ourselves to autonomous evolution operators having an exponential form

$$Q(t_f, t_i) = e^{(t_f - t_i)S}, \tag{1.4}$$

where S denotes a time-independent operator. An important class of evolution operators is included in the following definition:

$$S = \sum_{j=1}^{N} f_j(x_1, \ldots, x_N) \frac{\partial}{\partial x_j}, \tag{1.5}$$

where the dimension or number of degrees of freedom of the system may be finite or infinite. The finite-dimensional case may be directly related to the corresponding initial value problem produced by the set of ordinary differential equations [73], $\dot{x}_j = f_j(x_1, \ldots, x_N)$. Since almost every partial differential equation with initial conditions can be cast into an infinite set of ordinary differential equations through an appropriately chosen basis set expansion, we may consider the Lie operator in eq. (1.5) as being capable of treating a wide class of problems. Some caution is still required since the coefficients in eq. (1.5) are scalars, while some formal reductions of partial differential equations to ordinary differential equations can produce matrix coefficients. In summary, we restrict ourselves to operators having the structure of eq. (1.5) where the f_j's are infinitely differentiable in a proper subregion of x-space, zero at the origin, and depend on a finite number of variables.

Lie operators also arise in other areas in addition to that mentioned above. For example, the investigation of analytic sympletic maps [66] and the description of the behavior of trajectories *near* a reference trajectory for a general Hamiltonian system [67] are also other applications. This latter work is distinct from the present paper where we seek a global approximation to the evolution operation that is valid within a region of space without regard to a reference trajectory. In addition, our approximation of factorizing the exponential operator into a product sequence of global operators is different from that developed before. Recent additional works [68,69,74] have considered the use of Lie transformations to perform parameter space mapping of the solution of ordinary differential equations. Other applications may also be found.

The remainder of this paper is organized in the following fashion. Section 2 gives the general formulation of the global factorization for one-dimensional systems, followed by a generalization to multidimensional systems in section 3. Some illustrative examples are treated in section 4, and concluding remarks are given in section 5.

2. Factorization procedure in the one-dimensional case

Lie exponential evolution operators defined by eqs. (1.4) and (1.5) frequently arise in many applications. One application that was mentioned above arises in the treatment of ordinary differential equations. In particular, if we can evaluate the effect of the Lie transformation

$$Q = e^{t\mathcal{L}}; \qquad \mathcal{L} = \boldsymbol{f}(\boldsymbol{x}) \cdot \nabla \tag{2.1}$$

on the position vector $\boldsymbol{x}$ around a point $\boldsymbol{a}$ in the phase space of a system defined by

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}), \tag{2.2}$$

then the solution to these equations may be written as

$$\boldsymbol{x}(\boldsymbol{a}, t) = \{e^{t\mathcal{L}}\boldsymbol{x}\}_{\boldsymbol{x}=\boldsymbol{a}}, \tag{2.3}$$

where $\boldsymbol{x}$, $\boldsymbol{a}$ and ∇ are defined in the following manner:

$$\boldsymbol{x}^{\mathrm{T}} = [x_1, x_2, \ldots, x_N], \tag{2.4}$$

$$\boldsymbol{a}^{\mathrm{T}} = [a_1, a_2, \ldots, a_N], \tag{2.5}$$

$$\nabla^{\mathrm{T}} = \left[\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots, \frac{\partial}{\partial x_N} \right]. \tag{2.6}$$

This relation between the solution of ordinary differential equations and Lie transformations may conversely be used to determine the action of the operator Q on the position vector by solving the following ordinary differential equation:

$$\dot{\xi}(\boldsymbol{x}, t) = f(\xi); \quad \xi(\boldsymbol{x}, 0) = \boldsymbol{x}. \tag{2.7}$$

This approach to determining Q is generally not preferable since eq. (2.7) is often only soluble by elaborate numerical techniques which hide the important structure of the desired transformation. Although the approach pursued here is also approximate, it will still leave the structure of the evolution operator rather apparent.

In order to appreciate the approach taken below, we recall some important properties of Lie transformations which are linear:

$$\mathrm{e}^{t\mathcal{L}}\{ f(\boldsymbol{x}) g(\boldsymbol{x})\} = \{\mathrm{e}^{t\mathcal{L}} f(\boldsymbol{x})\} \{\mathrm{e}^{t\mathcal{L}} g(\boldsymbol{x})\}, \tag{2.8}$$

$$\mathrm{e}^{t\mathcal{L}} f(\boldsymbol{x}) = f(\mathrm{e}^{t\mathcal{L}} \boldsymbol{x}). \tag{2.9}$$

The first of these equations states that a Lie transformation on a product of two functions $f(x)$, $g(x)$ can be factorized to the product of the Lie transformation on the individual functions. This property is due to the exponential structure of the Lie transformation together with the application of the Leibnitz rule of differentiation, and the relation is valid provided that f and g are infinitely differentiable functions. The penetration property in eq. (2.9) also follows due to the particular structure of the Lie transformation and the assumed infinitely differentiable nature of the function f. Finally, one additional well-known property of Lie transformations concerns the special case of the translation operator

$$\mathrm{e}^{t\boldsymbol{a}\cdot\nabla} f(\boldsymbol{x}) = f(\boldsymbol{x} + t\boldsymbol{a}), \tag{2.10}$$

which follows from a simple Taylor expansion of the right-hand side.

We now desire to investigate the factorization of Lie transformations for one-dimensional systems. Although the one-dimensional nature of the problem makes it formally rather simple, this case also provides the best means to develop the factorization scheme presented here. After developing the method, future work will be devoted to reducing the factorization of the multivariable case to a one-dimensional factorization scheme. The true utility of this work lies in its application to multivariable systems. In the present case, the Lie transformation can be written as

$$Q = \mathrm{e}^{t f(x) \frac{\partial}{\partial x}}, \tag{2.11}$$

where $f(x)$ may have a number of zeros with one assumed to exist at the origin of the complex x-plane. This assumption about the location of a zero of $f(x)$ at the origin does not create any loss of generality since a simple translation can bring one of the zeros of $f(x)$ to the origin. The assumption about the existence of at least one zero of $f(x)$ is more restrictive. However, in problems where $f(x)$ forms the right-hand side of an ordinary differential equation, there will usually be at least one stationary point for the solution. Therefore, the assumption about the existence of a zero of the function $f(x)$ may be regarded as a minor loss of generality.

We may now make the additional assumption that the function $f(x)$ may be expanded in a Taylor series:

$$f(x) = \sum_{j=1}^{\infty} f_j x^j \qquad |x| < \rho, \tag{2.12}$$

where the expansion coefficients f_j are taken as known from the definition of the system. The above expansion implies that the system is well characterized, at least in a restrictive domain around the origin of the complex x-plane. We seek the factorization of the evolution operator Q such that every factor has an independent contribution in a fashion analogous to each term in the Taylor series of eq. (2.12). To this end, we define the flexible factorized structure

$$Q = \mathrm{e}^{tf(x)\frac{\partial}{\partial x}} = \prod_{j=1}^{\infty} \mathrm{e}^{\sigma_j(t)x^j\frac{\partial}{\partial x}}, \tag{2.13}$$

where $\sigma_j(t)$ are arbitrary at this point and yet to be determined. Equation (2.13) is the factorization formula for the one-dimensional case. Its global nature is evident through the functions $\sigma_j(t)$.

There have been several previous attempts to factorize Q, such as the Baker–Campbell–Hausdorff formula, the Zassenhaus formula, etc. One can find a good review of the matter by Wilcox [4]. However, the approaches in his paper differ from this work, since some of the formulae in his paper are not global and some of them do not easily lead to ξ-approximant sequences (to be defined later) which facilitate the factorization of the evolution operator in the case of infinite-dimensional solvable Lie algebra. On the other hand, the work of Wei and Norman [25] bears an important parallel to our work. Indeed, they deal with a finite-dimensional Lie algebra and obtain the solution of a differential equation over operators in a Banach space as a finite product of certain global exponential evolution operators. By assuming the solvability of the Lie algebra under consideration, they also show that the time-dependent factors in the arguments of the exponential operators can be determined by quadrature. In this work, we also deal with solvable Lie algebra. However, there are two essential differences: first, our Lie algebra is infinite-dimensional, and second, the determination of exponential factors is accomplished in a way such that it permits us to create ξ-approximants.

Assuming that (2.13) holds and the coefficients σ_j are known, it is a simple matter to determine the effect of the operator Q on x. For this purpose, we can investigate the individual effects of the factors in eq. (2.13):

$$Q^{(j)}x = e^{\sigma_j(t)x^j \frac{\partial}{\partial x}}x. \tag{2.14}$$

By using a simple variable transformation

$$y = x^{-(j-1)}, \tag{2.15}$$

we may write

$$Q^{(j)}x = e^{-(j-1)\sigma_j(t)\frac{\partial}{\partial y}}y^{-\frac{1}{(j-1)}}, \qquad j \geq 2;$$

$$Q^{(1)}x = e^{\sigma_1(t)}x, \tag{2.16}$$

and employ the translation operator property of eq. (2.10) on the y-coordinate:

$$Q^{(j)}x = [y - (j-1)\sigma_j(t)]^{-\frac{1}{(j-1)}}, \tag{2.17}$$

or equivalently in terms of the x-coordinate:

$$Q^{(j)}x = \frac{x}{\left[1 - (j-1)\sigma_j(t)x^{j-1}\right]^{\frac{1}{(j-1)}}}, \tag{2.18}$$

where x and t are considered to be independent variables, as we shall treat them henceforth. In this formula, the positive branch of the root has been taken. This is the fundamental formula of our factorization and it is valid provided the argument of the root appearing in eq. (2.18) remains positive. We are now able to evaluate the effects of the individual factors in eq. (2.13). In applications of eq. (2.13), an approximation to Q would consist of truncating the infinite product involved.

At this point, we need to determine the coefficient functions σ_j. To this end, we can use the following relation:

$$\frac{\partial Q}{\partial t} = \left\{ \sum_{j=1}^{\infty} f_j x^j \frac{\partial}{\partial x} \right\} Q; \qquad Q(0) = I, \tag{2.19}$$

which follows from eqs. (2.12) and (2.13). If we now write

$$Q = Q^{(1)}Q_1 = e^{\sigma_1(t)x\frac{\partial}{\partial x}}Q_1, \tag{2.20}$$

we may arrive at

$$\frac{\partial Q_1}{\partial t} = e^{-\sigma_1(t)x\frac{\partial}{\partial x}} \left\{ f(x)\frac{\partial}{\partial x} - \dot{\sigma}_1(t)x\frac{\partial}{\partial x} \right\} e^{\sigma_1(t)x\frac{\partial}{\partial x}} Q_1 , \tag{2.21}$$

using the properties in eqs. (2.8) and (2.9). This result may be re-expressed as

$$\frac{\partial Q_1}{\partial t} = \left\{ \left\{ \frac{f\left(e^{-\sigma_1 x\frac{\partial}{\partial x}}x\right)}{e^{-\sigma_1 x\frac{\partial}{\partial x}}x} - \dot{\sigma}_1 \right\} x\frac{\partial}{\partial x} \right\} Q_1 . \tag{2.22}$$

The following formula,

$$e^{-\sigma_1(t)x\frac{\partial}{\partial x}}x = e^{-\sigma_1(t)}x, \tag{2.23}$$

allows for a rewriting of eq. (2.22) utilizing the expansion in eq. (2.12):

$$\frac{\partial Q_1}{\partial t} = \left\{ (f_1 - \dot{\sigma}_1) + f_2\, e^{-\sigma_1(t)}x + \dots \right\} x\frac{\partial}{\partial x} Q_1 . \tag{2.24}$$

The operator acting on Q_1 on the right-hand side of eq. (2.24) is a power series in x. Each of the terms of this series is independent and in the vicinity of the origin, the first term will be dominant. We desire to make Q_1 as slowly varying as possible and therefore demand that the leading term in the series vanishes for this purpose:

$$\dot{\sigma}_1 = f_1 ; \qquad \sigma_1(0) = 0. \tag{2.25}$$

The initial condition has been taken as zero to make the simple evolution operator $Q^{(1)}$ unitary. Equation (2.24) now has the form:

$$\frac{\partial Q_1}{\partial t} = f^{(1)}(x,t)x^2\frac{\partial}{\partial x} Q_1 ; \qquad Q_1(0) = I, \tag{2.26}$$

where $f^{(1)}(x, t)$ can be identified from the remaining series of terms in the brackets of eq. (2.24) after the separation of a factor x, so $f^{(1)}(0, t)$ is a finite nonzero function of time. Exactly this same logic may be put forth to evaluate $\sigma_2(t)$ by successively eliminating higher-order powers of x in the differential equation. To construct a general recursion, we assume knowledge of the first n of the σ_j's and write

$$Q = \left\{ \prod_{j=1}^{n} Q^{(j)} \right\} Q_n , \tag{2.27}$$

which suggests the equation

$$\frac{\partial Q_n}{\partial t} = f^{(n)}(x,t)x^{n+1}\frac{\partial}{\partial x}Q_n; \qquad Q_n(0) = I. \tag{2.28}$$

The function $f^{(n)}(x, t)$ is regular for all time instances at the origin of the x-plane and is to be determined. We may now write

$$Q_n = Q^{(n+1)}Q_{n+1} = \mathrm{e}^{\sigma_{n+1}(t)x^{n+1}\frac{\partial}{\partial x}}Q_{n+1} \tag{2.29}$$

and obtain

$$\frac{\partial Q_{n+1}}{\partial t} = \left\{f^{(n)}\left(\mathrm{e}^{-\sigma_{n+1}(t)x^{n+1}\frac{\partial}{\partial x}}x, t\right) - \dot{\sigma}_{n+1}\right\}x^{n+1}\frac{\partial}{\partial x}Q_{n+1} \tag{2.30}$$

by again utilizing the properties in eqs. (2.18) and (2.19). Employing the action of the factorization operator in (2.18) gives

$$\frac{\partial Q_{n+1}}{\partial t} = \left\{f^{(n)}\left\{\frac{x}{(1+n\sigma_{n+1}(t)x^n)^{1/n}}, t\right\} - \dot{\sigma}_{n+1}\right\}x^{n+1}\frac{\partial}{\partial x}Q_{n+1}. \tag{2.31}$$

We now apply logic analogous to that leading to eq. (2.25) and eliminate the dominant contribution to the bracketed quantity multiplying the operator $x^{n+1}\frac{\partial}{\partial x}$, yielding

$$\dot{\sigma}_{n+1} = f^{(n)}(0,t); \qquad \sigma_{n+1}(0) = 0, \tag{2.32}$$

where the initial value is again chosen as zero to make $Q^{(n+1)}$ unitary. Therefore, we conclude

$$\frac{\partial Q_{n+1}}{\partial t} = f^{(n+1)}(x,t)x^{n+2}\frac{\partial}{\partial x}Q_{n+1}; \qquad Q_{n+1}(0) = I, \tag{2.33}$$

where

$$f^{(n+1)}(x,t) = \frac{1}{x}\left\{f^{(n)}\left\{\frac{x}{(1+n\sigma_{n+1}(t)x^n)^{1/n}}, t\right\} - f^{(n)}(0,t)\right\}. \tag{2.34}$$

This is a first-order recursion relation with the initial condition

$$f^{(1)}(x,t) = \frac{1}{x^2}\left\{f\left(\mathrm{e}^{-\sigma_1(t)}x\right)\mathrm{e}^{-\sigma_1(t)} - f_1 x\right\}. \tag{2.35}$$

All of the σ-functions can be evaluated analytically in principle; however, this is a tedious task and the use of the symbolic programming language such as MACSYMA or REDUCE is recommended. The first five of the σ-functions are given below.

$$\sigma_1(t) = f_1 t, \tag{2.36}$$

$$\sigma_2(t) = f_2 g_1(t), \tag{2.37}$$

$$\sigma_3(t) = f_3 g_2(t), \tag{2.38}$$

$$\sigma_4(t) = \left(f_4 + \frac{f_2 f_3}{f_1}\right) g_3(t) - \frac{f_2 f_3}{f_1} g_2(t), \tag{2.39}$$

$$\sigma_5(t) = \left(f_5 + \frac{f_2 f_4}{f_1} + \frac{f_2^2 f_3}{2f_1^2}\right) g_4(t) + \left\{\frac{f_2 f_4}{f_1} + \frac{f_2^2 f_3}{f_1^2}\right\} g_3(t) + \frac{f_2^2 f_3}{2f_1^2} g_2(t), \tag{2.40}$$

where

$$g_n(t) = \frac{1 - e^{-n f_1 t}}{n f_1}. \tag{2.41}$$

We are now at a point to implement the factorization scheme. The essential approximation is to truncate eq. (2.13) to a finite order, thereby producing the following approximant:

$$\bar{\xi}_n(x, t) = \left\{\prod_{j=1}^{n} Q^{(j)}\right\} x. \tag{2.42}$$

If the infinite product representation of Q given by (2.13) converges, then the following result will hold:

$$\bar{\xi}(x, t) = Qx = e^{t f(x) \frac{\partial}{\partial x}} x = \lim_{n \to \infty} \bar{\xi}_n. \tag{2.43}$$

Since the action of Q on x defines the fundamental operations of concern, we now focus our attention on the $\bar{\xi}$-approximants. A recursion relation for these approximations can be obtained by first noting that

$$\bar{\xi}_{n+1} = \left\{\prod_{j=1}^{n} Q^{j}\right\} e^{\sigma_{n+1}(t) x^{n+1} \frac{\partial}{\partial x}} x. \tag{2.44}$$

An application of eq. (2.18) yields

$$\bar{\xi}_{n+1} = \left\{ \prod_{j=1}^{n} Q^j \right\} \frac{x}{(1 - n\sigma_{n+1} x^n)^{1/n}} . \tag{2.45}$$

Since a product of Lie transformations is again a Lie transformation, we may use the property in eq. (2.19) together with eq. (2.42) to conclude that

$$\bar{\xi}_{n+1}(x,t) = \frac{\bar{\xi}_n(x,t)}{\left(1 - n\sigma_{n+1} \bar{\xi}_n^n(x,t)\right)^{1/n}} . \tag{2.46}$$

This is a rather simple first-order recursion (difference equation) whose initial member is evaluated as follows:

$$\bar{\xi}_1(x,t) = \mathrm{e}^{\sigma_1(t) x \frac{\partial}{\partial x}} x = x\,\mathrm{e}^{\sigma_1(t)} = x\,\mathrm{e}^{f_1 t} . \tag{2.47}$$

Although this is a simple recursion relation, it is not typically suitable for numerical purposes. Numerical instabilities will occur if f_1 is negative, resulting in excessively small quantities for large times t or also under the conditions that x tends to zero. In these cases, error accumulation may occur due to the truncated arithmetic on the computer. To prevent this error, we may renormalize the ξ-approximants and define a new recursion relation:

$$\xi_{n+1}(x,t) = \frac{\xi_n(x,t)}{\left(1 - \bar{\sigma}_{n+1} \xi_n^n(x,t)\right)^{1/n}} , \qquad \xi_1 = 1, \tag{2.48}$$

where

$$\bar{\sigma}_{n+1} = n\sigma_{n+1}\,\mathrm{e}^{n f_1 t} . \tag{2.49}$$

The relation between the new approximants and the previous ones is

$$\bar{\xi}_n(x,t) = \xi_n(x,t) x\,\mathrm{e}^{f_1 t} , \tag{2.50}$$

which also implies

$$\bar{\xi}(x,t) = \mathrm{e}^{t f(x) \frac{\partial}{\partial x}} x = \xi(x,t) x\,\mathrm{e}^{f_1 t} . \tag{2.51}$$

Since the term $x\mathrm{e}^{f_1 t}$ characterizes the linear response of the system, we can consider $\xi(x,t)$ as a function measuring the deviations of the system from its linear response. We will accordingly refer to ξ as a "deviation function". As can be easily seen, the $\bar{\xi}$- and ξ-approximants have branch points which move on trajectories in the x-plane. The location of these trajectories determines the convergence regions of the approximants. We shall leave the discussion of this issue and a comparison of the ξ-approximants with Padé approximants to a companion paper.

3. Generalization of the factorization scheme to the multidimensional case

The logic put forth in section 2 for a systematic factorization of one-dimensional evolution operators may now be generalized to multidimensional cases. In this situation, the evolution operator acting in a space of dimension N has the form

$$Q = e^{t f(x) \cdot \nabla}, \tag{3.1}$$

where

$$x^{T} = \left[x_1, \ldots, x_n \right], \tag{3.2}$$

$$\nabla^{T} = \left[\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_N} \right], \tag{3.3}$$

$$f^{T} = \left[f_1(x), \ldots, f_N(x) \right]. \tag{3.4}$$

The function $f(x)$ is assumed to have a zero at the origin:

$$\lim_{|x| \to 0} f(x) = 0, \tag{3.5}$$

and it is also assumed to be expandable in a multidimensional Taylor series in the variable $x_1, \ldots, x_N$. This latter expansion can be written in tensor form as

$$f_i = f_{ij}^{(1)} x_j + f_{ijk}^{(2)} x_j x_k + f_{ijkl}^{(3)} x_j x_k x_l + \ldots , \tag{3.6}$$

where the convention of the explicit summation over repeated indices is used for convenience. The word "tensor" is not used in its physical sense but just to denote the indexed nature of the coefficients. Henceforth, we shall use it again in the same sense without requiring certain properties of tensors of continuum mechanics, and the order of the tensor will imply the number of indices which independently vary on their domains.

In the one-dimensional case, the operator $e^{\sigma_1 x \frac{\partial}{\partial x}}$ played a fundamental role in the first step of establishing a recursion relation for the approximants. The same situation occurs again here, and we shall denote this first-degree operator Q_L as taking on the following form:

$$Q_L = e^{x^{\mathrm{T}}\sigma^{(1)}\nabla}, \tag{3.7}$$

where $\sigma^{(1)}$ is a square matrix or, equivalently, a second-order tensor. The effect of this operator on the position vector $\boldsymbol{x}$ is

$$Q_L \boldsymbol{x} = e^{\sigma^{(1)\mathrm{T}}} x. \tag{3.8}$$

Since $Q_L \boldsymbol{x}$ must be the system linear response, we can conclude that

$$\sigma_{jk}^{(1)} = t f_{kj}^{(1)} \qquad j, k = 1, \ldots, N. \tag{3.9}$$

Henceforth, we shall denote the linear response of the system evolution by S,

$$S = e^{t f^{(1)}}. \tag{3.10}$$

Using the definition of the scalar product of two tensors of the same order

$$A_{j_1 \ldots j_n} B_{j_1 \ldots j_n} = A \odot B, \tag{3.11}$$

we can write the evolution operator in eq. (3.1) as the infinite order factorized product

$$Q = Q_L \prod_{k=2}^{\infty} e^{\sigma^{(k)} \odot \mathcal{L}^{(k)}}, \tag{3.12}$$

where $\sigma^{(k)}$ is a kth order tensor to be determined and $\mathcal{L}^{(k)}$ is a tensor valued operator

$$\mathcal{L}_{j_1 j_2 \ldots j_k}^{(k)} = x_{j_2} x_{j_3} \ldots x_{j_k} \frac{\partial}{\partial x_{j_1}}. \tag{3.13}$$

The tensor product in the argument of each exponential term in eq. (3.12) is itself a sum of operators that would be difficult to deal with in practice. Therefore, we have further factorized each individual term in eq. (3.12) (except Q_L) to obtain

$$Q = Q_L \prod_{k=2}^{\infty} \prod_{j}^{*} e^{\sigma_{j1\,j2 \ldots jk}^{(k)} L_{j1\,j2 \ldots jk}^{(k)}}, \tag{3.14}$$

where it is understood that the coefficient functions $\sigma^{(k)}$ are now distinct from the set in eq. (3.12). The starred product in this formula means that the product operation is performed over the entire domain of the j-indices. There is no unique ordering to the factorization in eq. (3.14) for a multidimensional case. However, if we define the following operators

$$\overline{Q}^{(n)} = e^{\sigma^{(n)} \odot \mathcal{L}^{(n)}}, \tag{3.15}$$

$$Q^{(n)} = \prod_{j}^{*} e^{\sigma^{(n)}_{j1\, j2 \ldots jn} \mathcal{L}^{(n)}_{j1\, j2 \ldots jn}}, \tag{3.16}$$

one can prove that

$$\{\overline{Q}^{(n)} x\} - \{Q^{(n)} x\} = O(x^{2n-1}). \tag{3.17}$$

Therefore, within this level of approximation the expressions in eqs. (3.12) and (3.14) may be considered equivalent. The form given by eq. (3.14) is practical since each of the sequence of evolution operators acts on a particular coordinate and degree of freedom.

The procedure for determining the σ-tensor is the same as in the previous section; however, all scalars (except time) must be replaced with tensor quantities and the conventional algebra must be replaced with tensor algebra. The details of these operations will not be dealt with here, but the use of symbolic programming languages would be most helpful in practice. The second degree σ-tensor is given below as an example:

$$\sigma^{(2)}_{jkl} = \int_0^t S_{jm}(\tau) f^{(2)}_{mn_1 n_2} [S^{-1}(\tau)]_{n_1 k} [S^{-1}(\tau)]_{n_2 l} \, d\tau. \tag{3.18}$$

The evaluation of the ξ-approximants can again be accomplished by using the consecutive effects of the individual factors of the evolution operator. Symbolic programming techniques would likely be the best procedure for determining the $x_1, \ldots, x_n$ and t dependence of the ξ-approximants.

4. Illustrative applications

In this section, five problems are considered, each of which exhibits different types of behavior. For the sake of comparison with the techniques introduced in the previous sections, we have chosen analytically soluble problems, as described below. The examples are chosen as very simple for the purpose of illustrating the basic underlying behavior of the ξ-approximants.

First example

$$f(x) = 1 - e^{x}. \tag{4.1}$$

From traditional linear stability analysis arguments, this system $\dot{x} = f(x)$ is stable for $x > 0$ and unstable for $x < 0$. There is also only one steady-state point located at the origin. An analytic expression for the effect of the Lie transformation on x can be written as

$$\bar{\xi}(x, t) = e^{tf(x)\frac{\partial}{\partial x}} x = -\ln\{1 - (1 - e^{-x})e^{-t}\}. \tag{4.2}$$

A careful examination of the structure of $\bar{\xi}(x, t)$ reveals that its branch point traverses the path from $-\infty$ to $+\infty$ along the horizontal axes $\pm i\pi$ as time evolves. Figure 1(a) plots the exact deviation function $\xi(x, t)$ and its first five approximants $\xi_n(x, t)$ as defined in eqs. (2.51) and (2.50), respectively, for the case $x = 0.1$. It is apparent that the approximants uniformly converge to the true deviation function as n increases. The error between the true deviation function and the $n = 5$ approximant is shown in fig. 1(b), where it is evident that the error decreases monotonically to an asymptotic value for large times. A similar pair of plots is shown in fig. 2 for $x = 5.0$. At this larger value of x, qualitatively similar behavior occurs, but the rate of convergence of the approximants is slower and the peak in the error function may be a signal of the loss of global convergence. The situation for negative values of x is different, as shown in fig. 3. Figure 3 presents the case for $x = -1.0$. The approximants in this case seem to show oscillatory nonmonotonic behavior with respect to the true deviation function. The error of each of the approximants is qualitatively similar to that of figs. 1 and 2. At a sufficiently large negative value of x, singular behavior appears, resulting in apparent non-convergence.

Second example

$$f(x) = 1 - e^{-x}. \tag{4.3}$$

This system is unstable for positive x values due to the first Taylor coefficient being positive. It has only one steady-state point located at the origin of the x-plane. The analytic expression of the Lie transformation effect on x is

$$\bar{\xi}(x, t) = \ln\{1 + (e^x - 1)e^t\}. \tag{4.4}$$

The branch point trajectory of this system matches with the negative portion of the real axis of the x-plane. The branch point moves on this line toward the origin as time evolves and reaches it in the limit that $t \to \infty$. Figure 4 shows the deviation approximants and the error of the fifth member for $x = 0.1$. Apparent convergence failure is observed; however, during a finite time interval starting from $t = 0$ there is temporary convergence.

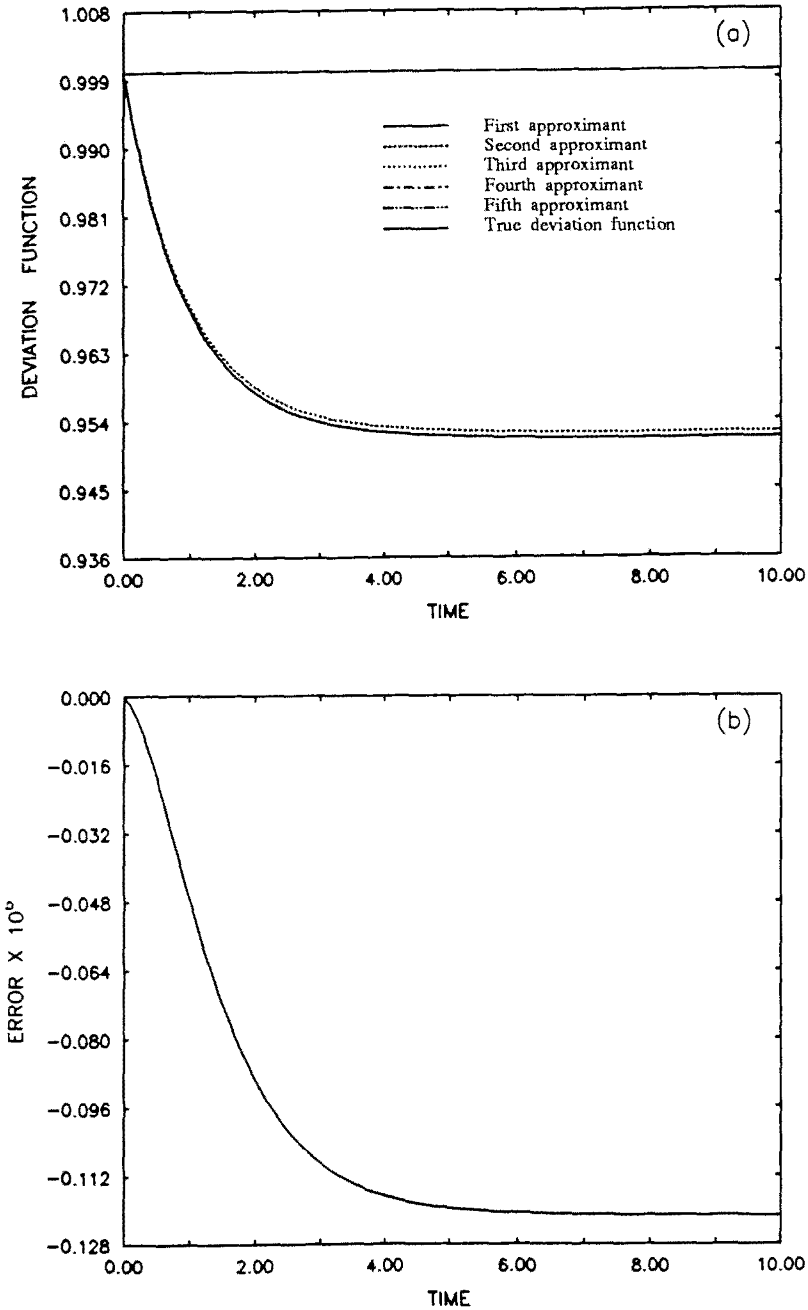

Fig. 1. Plot of the exact deviation function $\xi(x, t)$ and its first five approximants $\xi_n(x, t)$, $n = 1, \ldots, 5$ for the characteristic function in eq. (4.1) where $x = 0.1$. In (a), the last three approximants are indistinguishable from the exact result. (b) shows the error function for the approximant $n = 5$. The same line masks in (a) will be used in the remaining ξ-approximant plots.

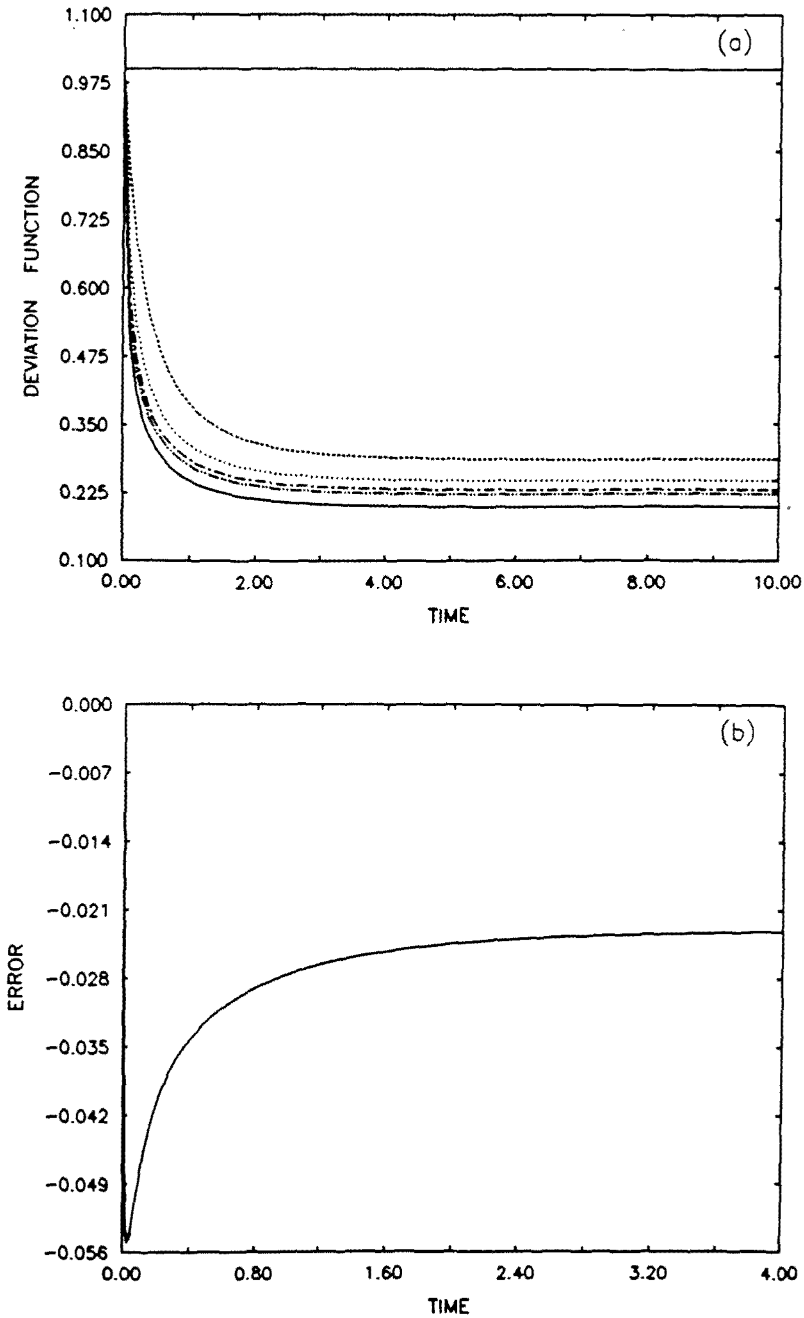

Fig. 2. The same as fig. 1 except $x = 5.0$. These results are qualitatively similar to those of fig. 1 except now the convergence rate is slower and there is a peak close to the origin in the error function.

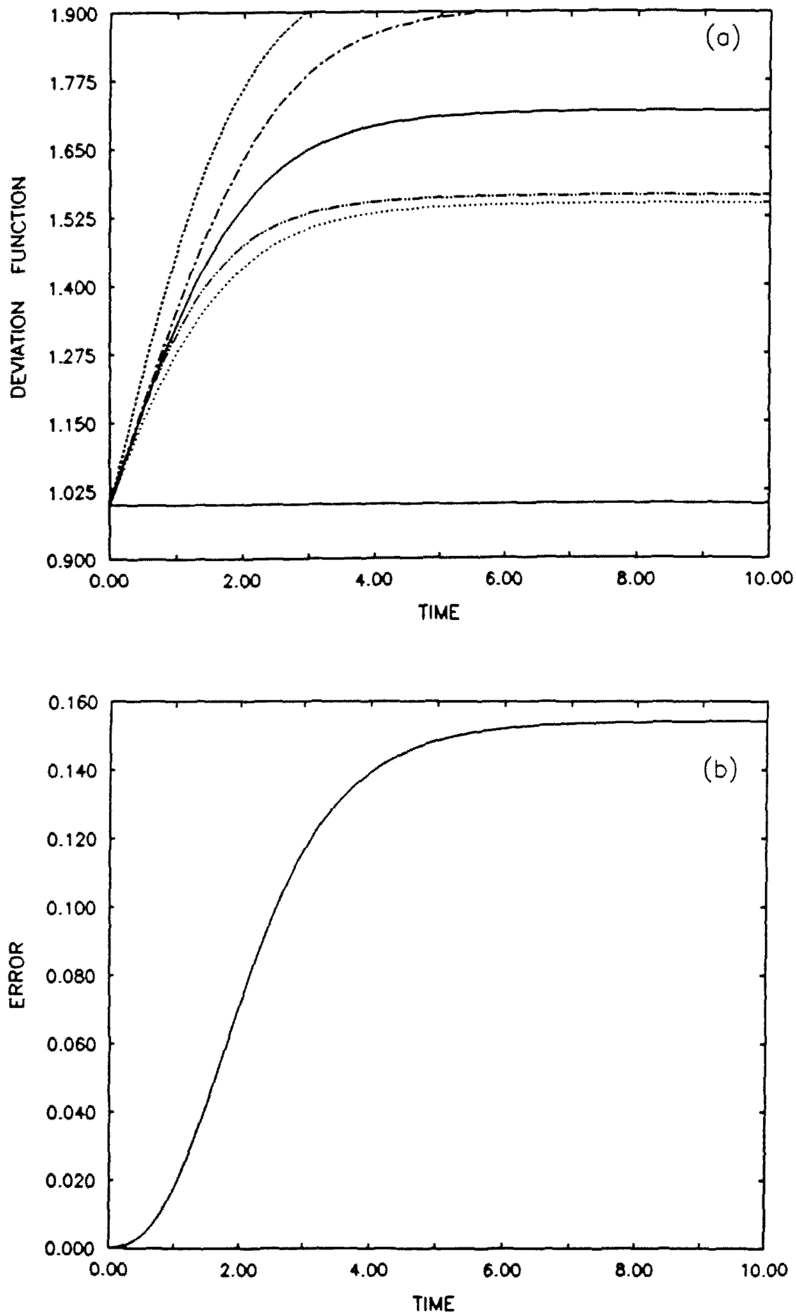

Fig. 3. The same as fig. 1 except now $x = -1.0$. Apparent oscillatory nonmonotonic behavior is exhibited with respect to the true deviation function in (a).

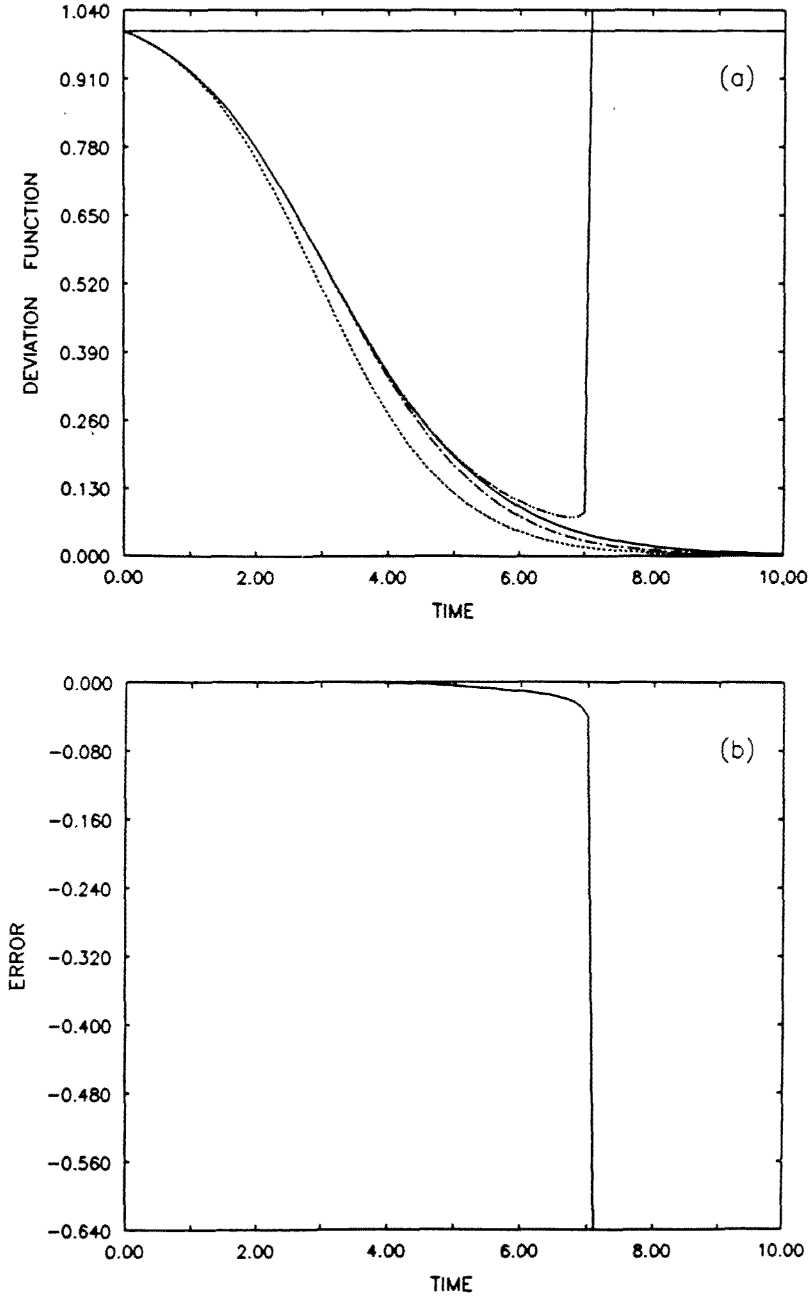

Fig. 4. (a) exhibits the exact deviation function $\xi(x, t)$ and the first five approximants $\xi_n(x, t)$, $n = 1, \ldots, 5$ corresponding to the fundamental function in eq. (4.3) at $x = 0.1$. (b) shows the error function for the $n = 5$ approximant. Apparent divergence behavior is observed at long time; however, during a finite interval around the origin there is temporary convergence. Here, only the fifth approximant goes to infinity. However, the first four approximants also have branch points close to zero but they do not make the denominator in the corresponding transformation from the previous approximant zero when $t < 10$. Some of the branch points are not even on the *positive* real axis.

Third example

$$f(x) = \sin x. \tag{4.5}$$

This system is unstable around $x = 0$ for $x > 0$; however, it has infinitely many steady-state points and they alternatively make the system either stable or unstable. Figure 5 depicts the approximant behavior for the case $x = 1.0$. There is apparent convergence behavior in the figure; however, a peak in the error function may again be a signal of the loss of global convergence. It is difficult to prove this point from only a finite number of approximants. An additional calculation is shown in fig. 6 for $x = 5.0$, which is beyond the second stationary point of $\sin(x)$. This well-behaved nature of the approximants is probably due to the fact that all the branch points of this system are purely imaginary.

Stakgold problem

This problem [75,76] is associated with the consideration of two coupled nonlinear differential equations with system coefficients given by

$$\begin{aligned} f_1(x_1,x_2) &= \lambda x_1 - x_2 - x_1\left(x_1^2 + x_2^2\right), \\ f_2(x_1,x_2) &= \lambda x_2 + x_1 - x_2\left(x_1^2 + x_2^2\right). \end{aligned} \tag{4.6}$$

The analytic expression for the effect of the Lie transformation on the position vector is

$$\begin{aligned} \overline{\xi}_1(x_1,x_2,t) &= (x_1 \cos t - x_2 \sin t)e^{-|\lambda|t}\eta(x_1,x_2,t), \\ \overline{\xi}_2(x_1,x_2,t) &= (x_1 \sin t + x_2 \cos t)e^{-|\lambda|t}\eta(x_1,x_2,t), \end{aligned} \tag{4.7}$$

where λ is assumed to be negative and η is defined as follows

$$\eta(x,t) = \left[1 + \frac{x_1^2 + x_2^2}{|\lambda|}\left(1 - e^{-2|\lambda|t}\right)\right]^{-1/2}. \tag{4.8}$$

This system is stable as long as λ remains negative. In the case of positive λ, the same condition again holds but the system does not have a steady-state solution and a limit cycle appears.

In applying the method of section 3 to eq. (4.6), we will find that the system has only the following nonzero tensor coefficients:

$$f_{11}^{(1)} = \lambda, \quad f_{12}^{(1)} = -1, \quad f_{21}^{(1)} = 1, \quad f_{22}^{(1)} = \lambda, \tag{4.9}$$

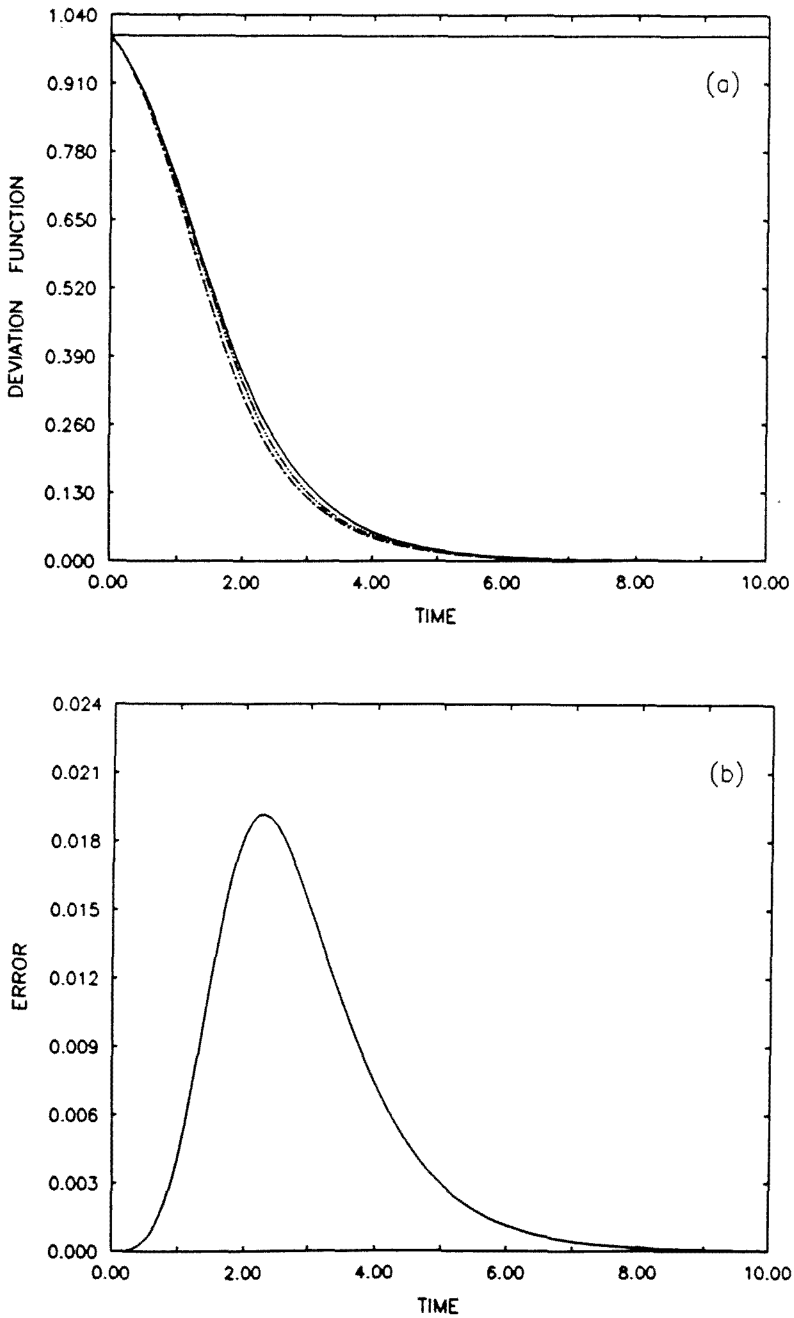

Fig. 5. The exact deviation function $\xi(x, t)$ and its first five approximants $\xi_n(x, t)$, $n = 1, \ldots, 5$ for the characteristic function in eq. (4.5) at $x = 1.0$. The first and second approximants coincide, as well as the third and fourth approximants. There is apparent convergence behavior in (a); however, a peak in the error function in (b) may signal a loss of global convergence.

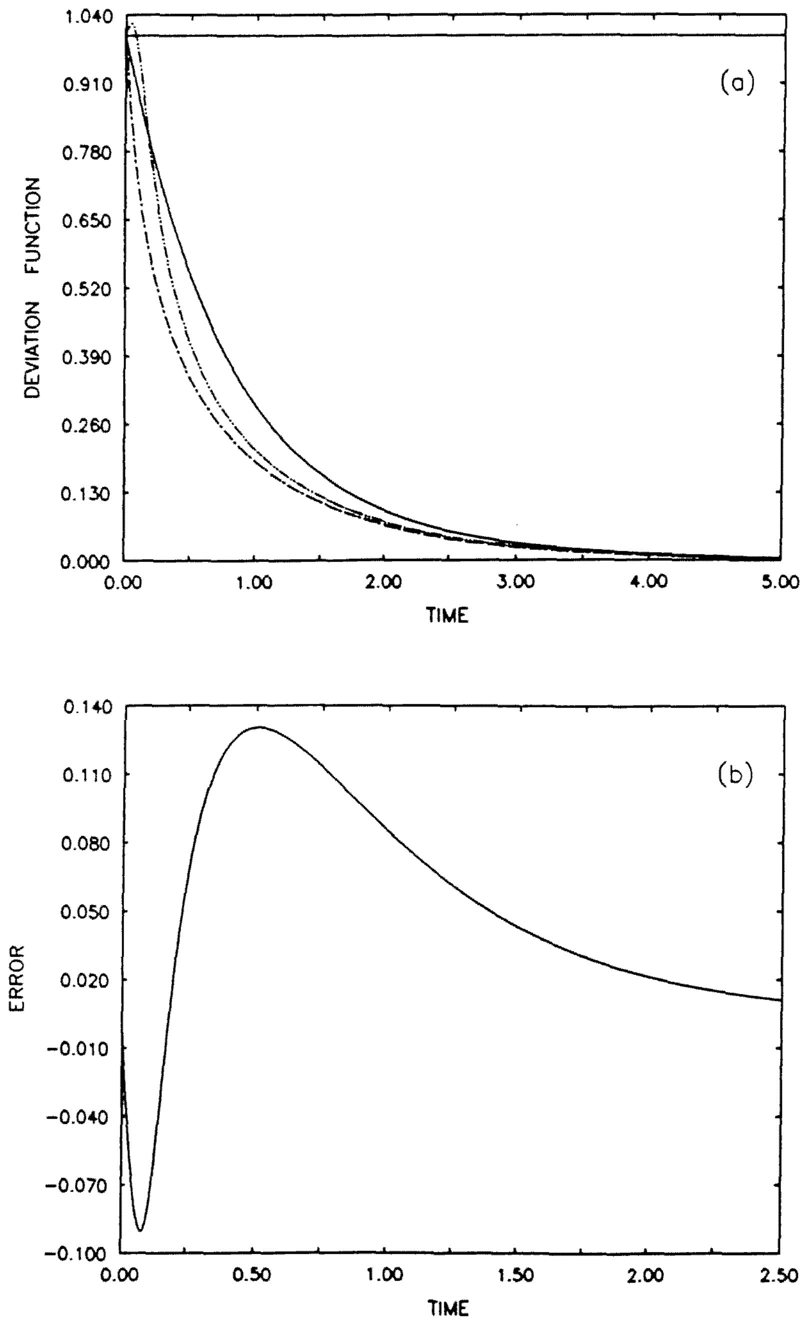

Fig. 6. The same as fig. 5 except that now $x = 5.0$.

$$f^{(3)}_{1111} = f^{(3)}_{1122} = f^{(3)}_{2211} = f^{(3)}_{2222} = -1. \tag{4.10}$$

Accordingly, the linear response term would be expressed by the tensor

$$S = e^{tf^{(1)}}, \tag{4.11}$$

and elements of this matrix and its inverse are given by the following expressions:

$$\begin{aligned} S_{11} &= e^{\lambda t}\cos t, & S_{12} &= -e^{\lambda t}\sin t, \\ S_{21} &= e^{\lambda t}\sin t, & S_{22} &= e^{\lambda t}\cos t; \end{aligned} \tag{4.12}$$

$$\begin{aligned} S^{(-1)}_{11} &= e^{-\lambda t}\cos t, & S^{(-1)}_{12} &= e^{-\lambda t}\sin t, \\ S^{(-1)}_{21} &= e^{-\lambda t}\sin t, & S^{(-1)}_{22} &= e^{-\lambda t}\cos t. \end{aligned} \tag{4.13}$$

Since the second-degree Taylor expansion coefficients are zero, it follows that

$$\sigma^{(2)} = 0. \tag{4.14}$$

The third-order terms are nonzero and $\sigma^{(3)}$ may be shown as

$$\sigma^{(3)}_{l_1 l_2 l_3 l_4} = \int_0^t S_{l_1 m_1} f^{(3)}_{m_1 m_2 m_3 m_4} S^{(-1)}_{m_3 l_2} S^{(-1)}_{m_3 l_3} S^{(-1)}_{m_4 l_4}\, d\tau, \tag{4.15}$$

where the explicit summation rule over repeated indices is employed. After some tedious algebra, one can show that all elements of the $\sigma^{(3)}$-tensor vanish except for the following four members:

$$\sigma^{(3)}_{1111}(t) = \sigma^{(3)}_{1122}(t) = \sigma^{(3)}_{2211}(t) = \sigma^{(3)}_{2222}(t) = \frac{e^{-2\lambda t} - 1}{2\lambda} \equiv \sigma_3(t). \tag{4.16}$$

This result immediately yields the tensor product

$$\sigma^{(3)} \odot \mathcal{L}^{(3)} = \sigma_3(t)\left(x_1^2 + x_2^2\right)\left(x_1 \frac{\partial}{\partial x_1} + x_2 \frac{\partial}{\partial x_2}\right). \tag{4.17}$$

As can be easily observed, the operators $\sigma^{(3)} \odot \mathcal{L}^{(3)}$ and $f^{(3)} \odot \mathcal{L}^{(3)}$ commute and therefore there will be no contribution from higher degree terms of the remainder during the elimination of the operator $\sigma^{(3)} \odot \mathcal{L}^{(3)}$ from the structure of $\mathcal{L}$. In addition, there are no higher-order terms than these already coming from the structure of $\mathcal{L}$ itself. Hence, we may conclude that the factorization exactly truncates at its second-order terms if we retain $\sigma^{(3)} \odot \mathcal{L}^{(3)}$ as a global second-degree Lie operator. Indeed, if we write

$$Qx = \mathrm{e}^{x^{\mathrm{T}} f^{\mathrm{T}(1)} \cdot \nabla} \mathrm{e}^{\sigma^{(3)} \odot \mathcal{L}^{(3)}} x = \frac{r\, \mathrm{e}^{x^{\mathrm{T}} f^{\mathrm{T}(1)} \cdot \nabla}}{\left[1 - 2\sigma_3(t) r^2\right]^{1/2}} \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \tag{4.18}$$

then it follows that

$$Qx = \frac{\mathrm{e}^{\lambda t}}{\left[1 + (\mathrm{e}^{2\lambda t} - 1)\, \frac{x_1^2 + x_2^2}{\lambda}\right]^{1/2}} \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \tag{4.19}$$

and the exact result is obtained. In this result, we have first used polar coordinates

$$r = \left(x_1^2 + x_2^2\right)^{1/2}, \quad \cos\theta = x_1 \left(x_1^2 + x_2^2\right)^{-1/2},$$

$$\sigma^{(3)} \odot \mathcal{L}^{(3)} = \sigma_3(t) r^3 \frac{\partial}{\partial r}, \tag{4.20}$$

and then returned to the Cartesian representation in eq. (4.19).

The result in eq. (4.19) is just a confirmation of the operator algebra introduced earlier in the paper. We may still go a step further and factorize the evolution operator involving $\sigma^{(3)} \odot \mathcal{L}^{(3)}$ to obtain

$$Q^{(2)} = \mathrm{e}^{\sigma_3(t) x_1^3 \frac{\partial}{\partial x_1}} \mathrm{e}^{\sigma_3(t) x_1^2 x_2 \frac{\partial}{\partial x_2}} \mathrm{e}^{\sigma_3(t) x_2^2 x_1 \frac{\partial}{\partial x_1}} \mathrm{e}^{\sigma_3(t) x_2^3 \frac{\partial}{\partial x_2}}. \tag{4.21}$$

This different factorization creates an error which is of the order of magnitude of fifth degree terms. In this case, an infinite product appears which converges about the origin.

Space extension

Consider the system defined by the function

$$f(x) = \sqrt{1 - x^2}. \tag{4.22}$$

This function has two zeros located at the points $x = +1$ and $x = -1$; however, it does not fulfill the requirements for our method. In particular, it cannot be expanded in a Taylor series around these points. Nevertheless, the problem may still be approached by extending the space to two dimensions through the introduction of a new variable in addition to x as follows:

$$y = \sqrt{1 - x^2}. \tag{4.23}$$

We can now define a new system with the descriptive functions

$$f_1(x, y) = y, \qquad f_2(x, y) = -x.$$

This new system satisfies all of the necessary conditions for factorization. Therefore, in cases such as these, the technique of space extension may make it possible to factorize Lie transformations which otherwise might not be accessible to direct treatment. This method of space extension is quite general and its full exploitation is explored in another paper [77].

5. Concluding remarks

The basic thrust of this paper is the development of a new sequence of approximants appropriate for time evolution operators with Lie generator arguments. Although we have not given convergence theorems for the ξ-approximant sequences, the results in section 4 are encouraging. Rapid and highly accurate convergence seems to be obtained at least in a sufficiently closed vicinity to the origin. The next step in this work, examined in a companion paper, is the investigation of the ξ-approximant singularities and some convergence theorems.

Actual implementation of the factorization scheme, especially for multidimensional cases, can involve a considerable amount of algebra. The use of symbolic programming on the computer would likely be a necessity in these cases, and this issue also needs further investigation for its practical implementation. A number of applications of the factorization may be envisioned, as suggested in the introduction. Evolution operators of the type studied in this paper occur in a wide variety of problems, but perhaps the most obvious and simple application would be to the solution of ordinary differential equations. The possible attraction here follows from the fact that the approximants provide a global solution in time rather than the usual sequential time stepping procedures. A number of numerical issues need to be addressed for this case as well as other applications before the optimal realm of utility of the scheme may be established.

After these tasks are realized, one can use this scheme for the solution of ordinary differential equations as well as the Liouville equation and similar equations which contain exponential evolution operators in their solutions. This factorization scheme can be employed to solve certain macroscopic level equations, such as reaction–diffusion equations, after an appropriate basis set expansion in spatial coordinates.

Perhaps one of the most important attributes of the ξ-approximant factorization is its ability to give global analytic approximations to the solution of nonlinear evolutionary differential equations.

Acknowledgement

The authors would like to thank Professor Carl Wulfman for helpful comments.

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