

FACTORIZATION OF CERTAIN EVOLUTION OPERATORS USING LIE ALGEBRA: CONVERGENCE THEOREMS*

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Abstract

This work concerns convergence theorems with a sequence of $\bar{\xi}$ -approximants for exponential evolution operators with Lie operator arguments. A companion paper presents the formulation of the ξ -approximants. The theorems presented in this paper give the conditions which are sufficient for convergence of the sequences. Although the main emphasis will be on convergence properties of the one-dimensional case, the generalization to multidimensional cases is quite straightforward.

1. Introduction

In a companion paper, we developed a new factorization scheme [1] for exponential evolution operators with Lie operator arguments. The factorization was based on the ordering of contributions to the evolution operator with respect to deviations from a steady-state solution. Hence, in the Lie operator of the form $f(x) \cdot \nabla$, the function $f(x)$ must vanish around the origin $x = 0$. The factorization scheme results in an infinite product of elementary evolution operators and the approximation to the desired overall evolution operators is achieved by a truncation of the infinite product to order n . This procedure produces a sequence of ξ -approximants to the desired evolution operator. The effect of the Lie transformation, or its approximate representation, on the position vector x is fundamental in the theory since many of the basic operations may be related to certain properties of Lie transformations.

ξ -approximants are rich in singularities and two consecutive elements of their sequence are related through a first-order but nonlinear recursion relation. As the limit of the sequence of the ξ -approximants is taken, infinitely many branch point trajectories may exist in the complex x -plane. The flexibility inherent in the ξ -approximants suggests that this approach may rapidly converge to accurately approximate

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the effect of the evolution operator on x . This conjecture was confirmed in a number of applications [1], although certain cases exhibited slow or non-convergent characteristics.

Such empirical evidence is helpful, but a mathematical proof of the convergent behavior is needed in order to intelligently use the method in realistic applications. It is necessary to establish not only the existence of convergence, but also to determine the criteria under which convergence is expected. The purpose of this paper is to address these latter issues.

In order to mathematically explore the convergence characteristics, section 2 will investigate the singularities of the $\bar{\xi}$ -approximants. This section will also define some useful fundamental concepts. Section 3 will present the convergence theorems for the $\bar{\xi}$ -approximant sequences. These latter developments will be carried out for the one-dimensional case, and section 4 will generalize the theorems to the multi-dimensional case. Finally, section 5 presents concluding remarks.

2. Singularities of $\bar{\xi}$ -approximants and some fundamental definitions in the one-dimensional case

The evolution operator of concern has the form $Q = e^{t f(x) \frac{\partial}{\partial x}}$, where $f(x)$ is a specified function defining the Lie operator. The action of Q on x is approximated by a sequence of $\bar{\xi}$ -approximants, $Qx \equiv \bar{\xi}_n$ such that

$$\bar{\xi}_{n+1} = \frac{\bar{\xi}_n}{[1 - n\sigma_{n+1}(t)\bar{\xi}_n^n]^{1/n}}; \quad \bar{\xi}_1(x, t) = x e^{f_1 t}, \quad (2.1)$$

where

$$Q = e^{t f(x) \frac{\partial}{\partial x}} = \prod_{j=1}^{\infty} e^{\sigma_j(t) x^j \frac{\partial}{\partial x}} \quad (2.2)$$

and

$$f(x) = \sum_{k=1}^{\infty} f_k x^k. \quad (2.3)$$

The coefficients $\sigma_j(t)$ in each of the elementary exponential operators in eq. (2.2) are global functions of time. The evaluation of these coefficients establishes the terms of the recursion relations in eq. (2.1) and the details of this operation were presented in an earlier paper [1]. The iteration in eq. (2.1) may be written in explicit form as:

$$\bar{\xi}_2(x, t) = \frac{x e^{f_1 t}}{1 - \bar{\sigma}_2 x}, \quad (2.4)$$

$$\bar{\xi}_3(x, t) = \frac{x e^{f_1 t}}{[(1 - \bar{\sigma}_2 x)^2 - \bar{\sigma}_3 x^2]^{1/2}}, \tag{2.5}$$

$$\begin{aligned} \bar{\xi}_n(x, t) &= \left[\left[\left[[1 - \bar{\sigma}_2 x]^2 - \bar{\sigma}_3 x^2 \right]^{3/2} - \bar{\sigma}_4 x^3 \right]^{4/3} \dots - \bar{\sigma}_{n-1} x^{n-2} \right]^{\frac{n-1}{n-2}} - \bar{\sigma}_n x^{n-1} \Big]^{-1/n} x e^{f_1 t}, \end{aligned} \tag{2.6}$$

where

$$\bar{\sigma}_{n+1} = n \sigma_{n+1}(t) e^{n f_1 t}. \tag{2.7}$$

The structure of $\bar{\xi}_n$ may be identified as a type of continued fraction.

The origin in the complex x -plane is not a singular point for all the $\bar{\xi}_n$'s as long as t remains finite. Since $\sigma_j(0) = \bar{\sigma}_j(0) = 0$, all singularities of the approximants are gathered at infinity at the initiation of the evolution. Each singularity moves along a trajectory in the complex x -plane as time evolves, and may or may not reach the origin when t tends to infinity. As a specific example, we will now examine the second approximant $\bar{\xi}_2(x, t)$. This approximant has a rather simple singularity, a pole, whose location is given as follows:

$$x_p = \frac{f_1}{[e^{f_1 t} - 1] f_2}, \tag{2.8}$$

where we have made use of the formula

$$\sigma_2(t) = (1 - e^{-f_1 t}) \frac{f_2}{f_1}. \tag{2.9}$$

Since the expansion coefficients f_n are assumed to be real, the pole in eq. (2.8) is evidently located on the real axis of the complex x -plane. The pole starts to move from either $+\infty$ ($f_2 > 0$) or $-\infty$ ($f_2 < 0$) to a limiting point as time t tends to infinity. If $f_2 = 0$, the pole remains at infinity. In general, two different cases occur as time evolves, assuming that $f_2 \neq 0$,

$$\lim_{t \rightarrow \infty} x_p(t) = \begin{cases} 0 & f_1 \geq 0, \\ \frac{f_1}{f_2} & f_1 < 0. \end{cases} \tag{2.10}$$

It is apparent from eq. (2.10) that if the system under consideration is unstable, $f_1 \geq 0$, then the trajectory of the singular point ends at the origin. However, if the system is stable, $f_1 < 0$, then the singular point stops at a finite location away from

the origin on the real axis. Therefore, at least for this approximant, there is a "clean" region where a singularity can never appear if $f_1 < 0$, and the origin of the complex x -plane is an interior point of this clean region. If the system under consideration is unstable, the origin may again be included in this clean region; however, in this case it becomes a point located on the border of the clean region.

In order to gain further insight into the $\bar{\xi}_n$ -approximants, we shall now examine the next approximant $\bar{\xi}_3$. This approximant has four branch points, two of which are located at infinity and the remaining ones are given below (where $\bar{\sigma}_3 \geq 0$, otherwise branch points are complex):

$$x_1 = [\bar{\sigma}_2(t) + [\bar{\sigma}_3(t)]^{1/2}]^{-1}, \quad x_2 = [\bar{\sigma}_2(t) - [\bar{\sigma}_3(t)]^{1/2}]^{-1}. \quad (2.11)$$

These singularities are algebraic branch points with two Riemann sheets. Depending on the nature of the system, $\bar{\sigma}_2^2 - \bar{\sigma}_3$ may be positive, zero or negative. If it differs from zero, then the origin becomes an interior point of the clean region for this approximant.

There is a remarkable property about the $\bar{\xi}$ -approximants, which can be stated as follows. If $\bar{\xi}_j$ has a singularity which is a branch point (except for the case $j = 2$), then every $\bar{\xi}_k$ -approximant ($k > j$) will have the same singularity. This means that when j tends to infinity there will be an abundance of branch point trajectories in the complex x -plane. Any given trajectory may or may not be in the clean regions of certain given approximants in the complex x -plane. As we shall see, the proof of the convergence of the $\bar{\xi}$ -approximant sequences completely depends on the existence of these regions and their locations.

It is now useful to make some definitions before proceeding. A given system is ultimately prescribed by the behavior of the functions $f(x)$ describing the corresponding Lie operator. If the complex x -plane of such a system has a region where any portion of the branch point trajectories of the $\bar{\xi}$ -approximants never exists, then we shall call this region a "clean region" in accord with the use of these words above. If, additionally, this region includes the origin of the complex x -plane as an interior point, then this region will be called the "main clean region" of the system. We further define a "global normal" system as follows: *iff* a system described by $f(x)$ has a main clean region with a nonzero measure, it is a global normal system, where we have used a measure in the sense that the measure of any countable infinite set vanishes. This latter measure is employed to exclude the possibility of having a clean region which only includes the origin. The interpretation of this definition of a global normal region can be made as follows: if we deal with a finite period of time, then the system will apparently have a main clean region. If we denote this region by $R(t)$, then we can write:

$$\lim_{t \rightarrow \infty} R(t) = R_\infty \supset [0], \quad m(R_\infty) > 0. \quad (2.12)$$

In other words, the main clean region will continue to have a set of uncountable points around the origin when time tends to infinity if the system is global normal. This definition may be relaxed by limiting ourselves not just to a semi-infinite time period, but to a finite one starting from $t = 0$. Therefore, we can define the "temporary normal" system as follows: a system described by $f(x)$ is temporary normal *iff* it has a main clean region with a nonzero measure (m) for a given time period $[0, T]$. Here, m is defined again in such a way that the measure of every finite or countable infinite set is zero. Finally, all remaining systems will be "abnormal". As can be observed, all global normal systems are at the same time temporary normal, and all abnormal systems can be considered as a limiting case ($T \rightarrow 0$) of temporary normal systems.

3. Convergence theorems in the one-dimensional case

From an examination of eqs. (2.1), (2.5)–(2.7), we may rewrite the approximants $\bar{\xi}_j(x, t)$ as follows:

$$\bar{\xi}_j(x, t) = \frac{x e^{f_1 t}}{\Delta_j(x, t)}. \tag{3.1}$$

The function $\Delta_j(x, t)$ in the denominator satisfies the recursion relation

$$\Delta_n(x, t) = [\Delta_{n-1}^n(x, t) - \bar{\sigma}_n x^{n-1}]^{1/(n-1)}, \quad n \geq 2; \quad \Delta_1 = 1. \tag{3.2}$$

One may conclude from this relation that the serial representation of $\Delta_n(x, t)$ in positive integer powers of x with time-dependent coefficients will converge within a finite circle of nonzero radius around the origin of the complex x -plane for some time period $[0, T]$. One can then construct a Majorant series for this function such that

$$|\Delta_n(x, t)| < D_n(x, t); \quad D_n > 1; \quad |x| < \rho_n(t); \quad n \geq 1, \tag{3.3}$$

where $\rho_n(t)$ denotes the time-dependent convergence radius of the n th Majorant series. The expression for the bound D_n may be established as follows:

$$\begin{aligned} & |\Delta_n^n(x, t)| < D_n^n(x, t) \\ \Rightarrow & |\Delta_n^n(x, t) - \bar{\sigma}_{n+1} x^n| < |\Delta_n^n(x, t)| + |\bar{\sigma}_{n+1}| |x|^n < D_n^n(x, t)(1 + |\bar{\sigma}_{n+1}| |x|^n) \\ \Rightarrow & |\Delta_{n+1}| < D_n(x, t)(1 + |\bar{\sigma}_{n+1}| |x|^n)^{1/n} \end{aligned}$$

$$\begin{aligned} &\Rightarrow \\ &|\Delta_{n+1}| < D_n(x, t)(1 + |\bar{\sigma}_{n+1}| |x|^n) \\ &\Rightarrow \\ &D_{n+1}(x, t) = D_n(x, t)(1 + |\bar{\sigma}_{n+1}| |x|^n). \end{aligned} \tag{3.4}$$

The latter result implies that

$$D_\infty(x, t) = D_N(x, t) \prod_{j=1}^\infty (1 + |\bar{\sigma}_{N+j}|^{N+j} |x|^{N+j-1}). \tag{3.5}$$

If the infinite product in eq. (3.5) is convergent, this is the region of the complex x -plane defined by $|x| < \rho(t)$ and

$$\rho(t) \geq \rho_{\min} > 0 \tag{3.6}$$

for all t values, then $D_\infty(x, t)$ will converge to a finite value. This result also implies that the function $\Delta_\infty(x, t)$ will converge for all t values in a region defined by $|x| < \rho_{\min}$. The existence of such a convergence implies that the zeros of the function $\Delta_n(x, t)$ in the complex x -plane are bounded from below in absolute value for all times. This in turn means that the system is global normal.

The condition for convergence of the infinite product in eq. (3.5) is equivalent to establishing the convergence of the following expression:

$$d_N(x, t) = \sum_{j=1}^\infty |\bar{\sigma}_{N+j}| |x|^{N+j-1}. \tag{3.7}$$

If this sum converges and remains smaller than unity for sufficiently large N values, then the infinite product in eq. (3.5) also converges. If ρ_{\min} in eq. (3.6) vanishes, then two circumstances may occur:

$$(i) \quad \rho(t) \geq \rho_{\min}(T) > 0, \quad t \in [0, T]; \tag{3.8}$$

$$(ii) \quad \rho(t) \geq \rho_{\min}(T), \quad \rho_{\min}(T) = 0 \quad (\text{except } T = 0). \tag{3.9}$$

The first of these cases corresponds to a temporary normal system, while the second implies the abnormal case. We have therefore proved the following theorem:

THEOREM 1

If the following infinite sum

$$d(x, t) = \sum_{j=1}^\infty |\bar{\sigma}_j| |x|^{j-1} \tag{3.10}$$

converges in a circle around the origin of the complex x -plane $|x| < \rho(t)$, then the following statements hold:

- (i) if $\rho(t) \geq \rho_{\min} > 0$ for $t \in [0, \infty]$, the system is global normal;
- (ii) if $\rho(t) \geq \rho_{\min}(\tau) > 0$ for $t \in [0, \tau]$ with $\tau > 0$, the system is, at least, temporary normal.

COROLLARY 1

If the first condition (i) of theorem 1 holds, then the sequence of $\bar{\xi}$ -approximants converges for all x and t values in the regions $|x| < \rho_{\min}$ and $[0, \infty]$, respectively, and they have a permanent main clean region with nonzero measure.

COROLLARY 2

If the second condition (ii) of theorem 1 holds, the sequence of $\bar{\xi}$ -approximants converges at least for all x and t values in the regions $|x| < \rho_{\min}(\tau)$ and $[0, \tau]$, $\tau > 0$, respectively, and they have at least a temporary clean region around the origin of the complex x -plane.

We now seek to more explicitly express the relation between the convergence condition of $d(x, t)$ and the nature of the system. As derived in the companion paper [1], the σ -coefficients are described as

$$\dot{\sigma}_{n+1}(t) = f^{(n)}(0, t), \tag{3.11}$$

with

$$f^{(n+1)}(x, t) = \frac{f^{(n)}(x[1 + n\sigma_{n+1}(t)x^n]^{-1/n}) - f^{(n)}(0, t)}{x} \tag{3.12}$$

and

$$f^{(1)}(x, t) = \sum_{j=0}^{\infty} f_{j+2} e^{-(j+1)\sigma_1} x^j. \tag{3.13}$$

Now, if we assume that $f(x)$ converges for $|x| \leq (\rho_f > 0)$, we can write the following inequality:

$$|f_{j+2}| \leq \frac{A_f}{\rho_f^j}. \tag{3.14}$$

This relation, however, permits us to write the following Majorant function for $f^{(1)}(x, t)$:

$$M_1(x, t) = \frac{A_f e^{-\sigma_1}}{1 - \frac{|x| e^{-\sigma_1}}{\rho_f}}, \quad |x| < \rho_f e^{\sigma_1} = \rho_f e^{f_1 t}. \tag{3.15}$$

Let us now assume that we have found a Majorant function for $f^{(n)}(x, t)$ as follows:

$$f^{(n)}(x, t) = \sum_{j=0}^{\infty} F_n^{(j)}(t)x^j; \quad |F_n^{(j)}(t)| < \frac{A_n}{\rho_n^j}; \tag{3.16}$$

$$M_n(x, t) = \frac{A_n}{1 - |x|/\rho_n}, \tag{3.17}$$

where $F_n^{(j)}$ stands for time-dependent coefficients and A_n, ρ_n denote certain time-dependent functions. The last assumption, however, makes it possible to write the following expression for M_{n+1} , the Majorant function of $f^{(n+1)}(x, t)$, as can be revealed after a careful examination of the recursion given by eq. (3.12):

$$M_{n+1}(x, t) \leq \frac{M_n(|x|[1 - n|\sigma_{n+1}||x|^n]^{-1/n}) - M_n(0, t)}{|x|}. \tag{3.18}$$

If we use the expression of M_n given by eq. (3.17), we can write

$$M_{n+1}(x, t) \leq \frac{A_n}{\rho_n} \frac{G_n(x, t)}{1 - \left[n|\sigma_{n+1}| + \frac{1}{\rho_n^n} \right]^{1/n} |x|}, \tag{3.19}$$

where

$$G_n(x, t) = \frac{g_{1,n}(x, t)}{g_{2,n}(x, t)}, \tag{3.20}$$

$$g_{1,n}(x, t) = \sum_{j=1}^{n-1} \left(1 - n|\sigma_{n+1}||x|^n \right)^{(n-j-1)/n} \rho_n^{-j} |x|^j, \tag{3.21}$$

$$g_{2,n}(x, t) = \sum_{j=1}^{n-1} \left(n|\sigma_{n+1}| + \frac{1}{\rho_n^n} \right)^{j/n} |x|^j. \tag{3.22}$$

Since $G_n(0, t) = 1$ and $G_n(x, t)$ is a monotonic decreasing function of x in a non-vanishing region of the x -complex plane around $x = 0$, we can construct the following Majorant function for the right-hand side of eq. (3.18):

$$M_{n+1}(x, t) = \frac{A_{n+1}}{1 - |x|/\rho_{n+1}}, \tag{3.23}$$

where

$$A_{n+1} = \frac{A_n}{\rho_n}; \quad A_1 = A_f e^{-f_1 t} \tag{3.24}$$

and

$$\frac{1}{\rho_{n+1}} = \left(n |\sigma_{n+1}| + \frac{1}{\rho_n^n} \right)^{1/n}; \quad \rho_1 = \rho_f e^{f_1 t}. \tag{3.25}$$

If we assume that $(n |\sigma_{n+1}|)^{1/n} e^{f_1 t}$ is bounded by v , then we can write

$$\alpha_n \leq e^{-f_1 t} \rho_n \tag{3.26}$$

$$\alpha_{n+1} = \frac{\alpha_n}{(1 + v^n \alpha_n^n)^{1/n}}, \quad \alpha_1 = \rho_f. \tag{3.27}$$

Therefore, we have made the convergence radii of the Majorant functions smaller. As can be easily shown after some intermediate steps, α_n monotonically converges to a nonzero limit, say α , as n tends to infinity. This makes it possible to write

$$B_{n+1} = \frac{B_n e^{-f_1 t}}{\alpha}; \quad B_1 = A_f, \tag{3.28}$$

$$M_n = \frac{B_n}{1 - x e^{-f_1 t} / \alpha_n}. \tag{3.29}$$

Since $\dot{\sigma}_{n+1} < M_{n+1}(0, t)$, we can obtain

$$|\sigma_{n+1}(t)| < \frac{(1 - e^{-n f_1 t}) A_f}{n f_1 \alpha^n}, \quad n \geq 1, \tag{3.30}$$

which obviously satisfies the boundedness condition of $(n |\sigma_{n+1}|)^{1/n} e^{f_1 t}$ globally for $f_1 < 0$ and temporarily for $f_1 \geq 0$. This result immediately produces the following theorem.

THEOREM 2

If the descriptive function of a given system is denoted by $f(x)$, ($f(0) = 0$), then the following statements are true:

- (i) if $f(x)$ has a finite convergence radius centered at the origin of the complex x -plane and $f_1 < 0$, then the system is global normal;
- (ii) if the same conditions of case (i) hold except that $f_1 > 0$, then the system is at least temporary normal.

Our third theorem concerns the $\bar{\xi}_n$ -approximants. Let us consider the inverse relation between $\bar{\xi}_n$ and $\bar{\xi}_{n+1}$.

$$\bar{\xi}_n = \frac{\bar{\xi}_{n+1}}{[1 + n\sigma_{n+1}\bar{\xi}_{n+1}^n]^{1/n}}. \quad (3.31)$$

If we write

$$\bar{v} = \min \left\{ \left(\left| \frac{1}{n\sigma_{n+1}} \right| \right)^{1/n} \right\}, \quad (3.32)$$

and if the following holds for a specific n

$$|\bar{\xi}_{n+1}(x, t)| \leq \bar{v}_{n+1} \leq \bar{v}, \quad (3.33)$$

then,

$$|\bar{\xi}_n| < \frac{\bar{v}_{n+1}}{[1 - n|n\sigma_{n+1}|\bar{v}_{n+1}^n]^{1/n}}. \quad (3.34)$$

Now one can choose \bar{v}_{n+1} in a way such that

$$\bar{v}_n = \frac{\bar{v}_{n+1}}{[1 - n|\sigma_{n+1}|\bar{v}_{n+1}^n]^{1/n}} \longrightarrow \bar{v}_{n+1} = \frac{\bar{v}_n}{[1 + n|\sigma_{n+1}|\bar{v}_n^n]^{1/n}} \leq \bar{v}_n, \quad (3.35)$$

where \bar{v}_n is defined as

$$|\bar{\xi}_n(x, t)| \leq \bar{v}_n < \bar{v}. \quad (3.36)$$

Therefore, we conclude

THEOREM 3

If we denote the minimum of the expression $(|1/(n\sigma_{n+1})|)^{1/n}$, $n = 1, 2, \dots$ by \bar{v} , and for a finite fixed N , the approximant $\bar{\xi}_N$ remains smaller than \bar{v} in absolute value, then all higher order approximants behave in the same way.

The interpretation of this theorem is as follows. If the system is globally normal, then the limit of the sequence of approximants $\bar{\xi}(x, t) = \lim_{N \rightarrow \infty} \bar{\xi}_N$ will remain permanently in the main clean region.

In the proofs of these theorems, we assumed that $f(x)$ has real coefficients and that x is a complex variable. We did this for the sake of simplicity. However, if $f(x)$ is assumed to be a complex quantity, nothing will change except the replacement of f_1 with $\mathcal{R}(f_1)$.

4. Generalization to the multidimensional case

In the companion paper [1] establishing the approximants, it was noted that there is a degree of flexibility in the order of the elementary factors or propagators associated with a multidimensional Lie transformation. A convenient ordering for the proof of convergence can be written as follows:

$$Q = e^{t f(x) \cdot \nabla} = e^{t x^T \cdot f^{T(1)} \cdot \nabla} \left\{ \prod_{j=0}^{\infty} e^{\mu_j^{(1)} x_1^j \frac{\partial}{\partial x_1}} \right\} \dots \left\{ \prod_{j=0}^{\infty} e^{\mu_j^{(N)} x_N^j \frac{\partial}{\partial x_N}} \right\}, \quad (4.1)$$

where $\mu_j^{(N)}$ depends on x_n 's except x_N and t . We have chosen an ordering of a product of elementary exponential operators such that the differentiation with respect to x_N is effected first. This ordering has a practical implication if we consider the effect of Q on x_1 , in which case the last $(N - 1)$ curly bracketed operators reduce to unity due to the fact that they have no effect on x_1 :

$$Q x_1 = e^{t x^T \cdot f^{T(1)} \cdot \nabla} \left\{ \prod_{j=1}^{\infty} e^{\mu_j^{(1)} x_1^j \frac{\partial}{\partial x_1}} \right\} x_1. \quad (4.2)$$

Similarly, if we deal with $Q x_j$, then we can choose the ordering or the curly bracketed operators in such a way that

$$Q x_j = e^{t x^T \cdot f^{T(1)} \cdot \nabla} \left\{ \prod_{k=1}^{\infty} e^{\mu_k^{(j)} x_j^k \frac{\partial}{\partial x_j}} \right\} x_j \quad (4.3)$$

can be written. Such changes of ordering will alter the μ_j 's, and without loss of generality, we may consider the particular ordering in eq. (4.1).

To find, for example, $\mu_0^{(1)}(x_1, \dots, x_N, t)$ we can obtain a partial differential equation which must satisfy

$$\frac{\partial \mu_0^{(1)}}{\partial t} = \bar{f}_1(-\mu_0^{(1)}, x_2, \dots, x_N) + \sum_{j=2}^N \bar{f}_j(-\mu_0^{(1)}, x_2, \dots, x_N) \frac{\partial \mu_0^{(1)}}{\partial x_j}, \quad (4.4)$$

where \bar{f}_j denotes the new descriptive vector element of the system after extraction of its linear response. This may be equivalently stated as

$$|f(\mathbf{x})|_{\mathbf{x}=\mathbf{0}} = 0, \quad \{\nabla f_j\}_{|\mathbf{x}=\mathbf{0}} = \mathbf{0}, \quad 1 \leq j \leq N. \quad (4.5)$$

The same equations are assumed to hold for $\mu_0^{(1)}$

$$\mu_0^{(1)}\{0, 0, \dots, 0, t\} = 0, \quad \{\nabla \mu_0\}_{|\mathbf{x}=\mathbf{0}} = \mathbf{0}, \quad (4.6)$$

since the first-degree terms are excluded by extraction of the linear response. Hence, eq. (4.4) may be solved by a multidimensional Taylor series with the initial condition

$$\mu_0^{(1)}(x_2, \dots, x_N, 0) = 0. \quad (4.7)$$

The convergence of such series has been thoroughly investigated in the theory of partial differential equations [2]. Therefore, $\mu_0^{(1)}$, and the other μ 's which satisfy the same kind of partial differential equations, can be assumed convergent and bounded in a closed domain around the $(n-1)$ -tuple manifold formed by the Cartesian product of the x_2, \dots, x_N complex planes. In analogy with the previous section, one may prove theorems about the convergence properties of the sequence of approximants generated by truncating the product of operators in eq. (4.2). These same type of statements follow as before except through a change of the x -plane into an n -tuple manifold constructed by the Cartesian product of the n -complex planes (x_1 -plane, \dots , x_N -plane).

5. Concluding remarks

In the first of these two papers, we presented a factorization scheme for Lie transformation evolution operators, and in the present paper we have given sufficient conditions for the convergence of the scheme. Under appropriate circumstances, these approximants form a practical tool to produce a rapidly convergent and high precision approximation to the original evolution operator. These new approximants are also richer than, for example, Padé approximants for numerical analysis. This comment follows due to the abundance of branch points, which makes it possible to characterize many types of functions having various types of singularities. These two papers are actually only the first step in the theoretical development of these new types of approximants, and much additional research needs to be done for their deeper understanding and to bring them to a truly practical level.

References

- [1] M. Demiralp and H. Rabitz, Factorization of certain evolution operators using Lie algebra: Formulation of the method, *J. Math. Chem.* 6(1991), this issue.
- [2] P.R. Garabedian, *Partial Differential Equations* (Wiley, New York, 1962).