OPERATOR SPLITTING METHODS FOR NON-AUTONOMOUS DIFFERENTIAL EQUATIONS

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ABSTRACT

OPERATOR SPLITTING METHODS FOR NON-AUTONOMOUS DIFFERENTIAL EQUATIONS

In this thesis, convergency and stability analysis are studied for the non-autonomous differential equations. Not only classical operator splitting methods; Lie Trother splitting, symmetrically weighted splitting and Strang splitting but also iterative splitting method which is recent popular technique of operator splitting methods are considered. We concentrate on how to improve the operator splitting methods with the help of the Magnus expansion. In addition, we construct a new symmetric iterative splitting scheme. Then, we also study its convergence properties by using the concepts of stability, consistency and order. For this purpose, we use C_0 semigroup techniques. Finally, several numerical examples are illustrated in order to confirm our theoretical results by comparing the new symmetric iterative splitting method with frequently used operator splitting methods.

ÖZET

ZAMANA BAĞLI DENKLEMLER İÇİN OPERATÖR AYIRMA METODLARI

Bu tezde zamana bağlı denklemler için yakınsaklık ve kararlılık analizleri incelenmiştir. Sadece klasik operatör ayırma methodları; Lie Trother splitting, symmetrically weighted splitting ve Strang splitting değil aynı zamanda operatör ayırma metodlarının son zamanlarda popüler olan tekniği iterative splitting metodu da ele alınmıştır. Operatör ayırma metodlarını Magnus seri açılımı ile nasıl geliştirildiğine yoğunlaşılmıştır. Buna ek olarak, yeni bir simetrik iterative splitting şeması oluşturulmuştur. Sonra bu metodun kararlılık, tutarlılık ve mertebe konseptleri ile yakınsaklık özellikleri üzerine çalışılmıştır. Bu amaçla, C_0 yarıgrup teknikleri kullanılmıştır. Son olarak, teorik sonuçları doğrulamak için yeni simetrik iterative splitting methodu ile sık kullanılan operatör ayırma methodları karşılaştırılarak nümerik örnekler gösterilmiştir.

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CHAPTER 1

INTRODUCTION

1.1. Introduction

Operator splitting is a widely used procedure in the numerical solution of large systems of partial differential equations. It can be regarded as a time-discretization method. Thus, it can be called as time splitting method. The basic idea behind the operator splitting methods is based on splitting of complex problem into simpler sub-problems. Then, each of which are solved by an efficient method. The connections between the sub-systems are the initial conditions. Instead of the original problem, we deal with simpler sub-problem. Thus, this technique gives rise to error which is called splitting error. This error can be estimated theoretically.

The idea of sequential splitting, which is known as Lie-Trotter splitting, dates back to the 1950s. In (Bagrinovskii and Gudunov, 1957), this method was first applied to a partial differential equations. During the years 1960-1970, the first splitting methods were developed. They were in connection with finite difference methods. A renovation of the methods was done in the 1980s while using the methods for complex processes underlying partial differential methods (Crandall and Majda, 1980). The simplest kind is sequential splitting, which, in terms of the local splitting error, is the first order accurate in time. A second order and, therefore, more popular method is Strang splitting in (Marchuk, 1968), (Strang, 1968). In (Strang, 1963), Strang proposed a splitting method where a weighted sum of splitting solutions, obtained by different ordering of the sub-operators, are computed at each time step. The symmetrically weighted sequential (SWS) splitting is second order accurate, as popular as Strang splitting. Its analysis can be found by *Csomós et al.* in (Csomós et al., 2003). There is another sort of splitting method, iterative splitting, which is recently popular technique of operator splitting methods. The earliest detection of iterative method era 1995s, (Kelly, 1995), was seemingly far in advance of its time. In (Kanney et al., 2003), they focused on the convergence of iterative splitting procedure for nonlinear reactive transport problems. In (Faragó and Geiser, 2007), they suggest a new scheme which is based on the combination of splitting time interval and traditional iterative operator splitting. Then, this technique is used in (Geiser, 2008); (Geiser, 2008). In the current study, we propose a new method which is found by the combining with the

Magnus expansion and the iterative operator splitting which is suggested in (Faragó and Geiser, 2007).

Magnus integrators are an interesting class of numerical methods for Hamiltonian problems. The problem which Magnus expansion (ME) solves has a history dating back at least to the study of *Peano*, by the end of 19th century, and *Baker* at the beginning of the 20th. They combine the theory of differential equations with an algebraic formulation. In connection with these treatments from the beginning, is the study of so called Baker-Campbell-Hausdorff formula. (Magnus, 1954) have been considered as birth certificate of Magnus Expansion. The work of *Pechukas* and *Light* gave for the first time a more specific convergence analysis of the problem than the ambiguous considerations in Magnus paper. *Wei* and *Norman* did the same for existence problem. The study of *Robinson*, (Robinson, 1963), seems to be the first application of the ME to a physical problem. During the years between 1971 and 1990, ME was successfully applied to a wide spectrum of fields in Physics and Chemistry. In the last decay of 20th century ME has been adapted for specific types of equations: Floquet theory, stochastic differential equations etc. In numerical analysis, using ME as a geometric integrator along the lines of work pioneered by *Iserles and Nørsett* in (Iserles and Nørsett, 1999).

In this thesis, to discuss the analysis and applications, we concentrate on an approximate solution of non-autonomous systems of the following form

$$\begin{aligned} \frac{d}{dt}u(t) &= A(t)u(t), \ \ t \geq 0 \\ u(0) &= u_0 \in X \end{aligned}$$

on some (complex) Banach space X with the norm $\|.\|_{X \leftarrow X}$. Since the Magnus expansion (Blanes et al., 2008); (Blanes and Moan, 2006) is an attractive and widely applied method of solving explicitly time-dependent problems, in order to solve such non-autonomous system, as a numerical method, we apply operator splitting methods combining with Magnus expansion. It is often the case that $A(t) = T + V(t)$, where only the potential operator $V(t)$ is time-dependent and T is the differential operator see (Baye et al., 2003); (Baye et al., 2004); (Chin and Chen, 2002); (Aguilera-Navarro et al., 1990); (Chin and Anisimov, 2006). To analyze the convergence of the given methods, we study on two different approaches;

- For the case of T and $V(t)$ are bounded, we use Taylor series expansion.
- For the case of T is unbounded and $V(t)$ is bounded, we use C_0 semigroup ap-

proaches

The idea of using strongly continuous semigroup (C_0 semigroup) approaches for the convergency of operator splitting methods as an abstract homogeneous Cauchy problem goes back at least to *Pazy* in (Pazy, 1983). *Bjørhus* analyze the operator splitting method for the linear inhomogeneous abstract Cauchy problem in (Bjørhus, 1998). In the paper (Bátkai et al., 2011), they investigate the convergence of operator splitting methods by using evolution semigroups. You can also see (Jahnke and Lubich, 2000); (Hansen and Ostermann, 2009) for obtaining estimates on the order of convergence. By this to investigate the convergence of any method, the concepts of stability, consistency and order are used. Both (Geiser and Tanoğlu, 2011) and (Geiser, 2008) deal with the consistency of different splitting schemes has been thoroughly investigated in the terms of the local splitting error for autonomous systems. In addition, the convergence of iterative splitting method for the autonomous case in (Gücüyenen and Tanoğlu, 2011). In this thesis, we focused on the convergence of introduced splitting methods and especially the convergence of the new iterative splitting method.

1.2. Layout of the Thesis

Our aim is to develop and analyze the operator splitting methods combining with Magnus expansion. In particular, we focused on iterative splitting method. The main object of this thesis will be two fold: First, we construct a new symmetric iterative splitting scheme for non-autonomous problem. Second, its convergence properties are analyzed using the concepts of stability, consistency, and order as an abstract Cauchy problem via analytic semigroup approach. Finally, we test these schemes on several numerical examples to confirm our theoretical results.

The purpose of Chapter 2 is to present Magnus expansion for solving the time-dependent part of problem. We also give some conditions for convergence of Magnus expansion (ME). The next step in present thesis is to combine Magnus expansion with operator splitting methods. Thus, Chapter 3 introduces the operator splitting methods, which are based on Magnus expansions. In the first, we give the algorithm of traditional operator splitting methods. Then we embedded ME into operator splitting methods. We concentrate on to construct a new algorithm for the iterative splitting method which has time-symmetry property.

In Chapter 4, the consistency of the methods are discussed. Not only bounded case but also unbounded case is considered. Chapter 5 deals with in detail the stability issue for general case of the splitting methods, which are introduced in previously. We study this issue as an abstract Cauchy problem. In Chapter 6, we present the convergence results of the splitting methods which follow the line of telescoping identity and ”Lady windermere’s fan” argument.

In Chapter 7, we give some numerical examples to confirm our theoretical results and to demonstrate the effectiveness of suggested scheme. For this purpose, we use ODEs and PDEs. Since ME is an attractive and widely applied method of solving explicitly harmonic oscillator, we test our method in Matheui equation. We compare our new scheme with traditional schemes in this test problem. Since its efficiency, we apply it into Schrödinger equation. We present the results as tables and figures.

Finally, we conclude with a brief discussion of the study fulfilled in Chapter 8.

CHAPTER 2

MAGNUS EXPANSION

In the present chapter, we summarize a brief overview of Magnus expansion (ME). In order to present our point of view of ME, we may distinguish two main directions :

- We report the recurrence formulation of Magnus expansion.
- For what values of t does the series converge ? We describe this question as the convergence problem. Thus, in Section 2.2 we will sum up the convergence conditions for the ME.

2.1. Magnus Expansion

The Magnus integrator was introduced as a tool to solve non-autonomous linear differential equations for linear operators of the form

$$\frac{du}{dt} = A(t)u(t) \ , \tag{2.1}$$

with solution

$$u(t) = \exp(\Omega(t))u(0). \tag{2.2}$$

This can be expressed as:

$$u(t) = \mathcal{T}\left(\exp(\int_0^t A(s)\ ds\right) u(0) \ , \tag{2.3}$$

where the time-ordering operator $\mathcal{T}$ is given in (Dyson, 2008).

The Magnus expansion is defined as:

$$\Omega(t) = \sum_{n=1}^{\infty} \Omega_n(t) \ , \tag{2.4}$$

where the first few terms are (Blanes et al., 2008):

$$\begin{aligned}
\Omega_1(t) &= \int_0^t dt_1 A_1 \\
\Omega_2(t) &= \frac{1}{2}\int_0^t dt_1 \int_0^{t_1} dt_2 [A_1, A_2] \\
\Omega_3(t) &= \frac{1}{6}\int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([A_1, [A_2, A_3] + [A_3, [A_1, A_2]]) \\
& \cdots\cdots \qquad \text{etc.}
\end{aligned} \tag{2.5}$$

where $A_n = A(t_n)$. In practice, it is more useful to define the nth order Magnus operator

$$\Omega^{[n]}(t) = \Omega(t) + O(t^{n+1}) \tag{2.6}$$

such that

$$u(t) = \exp\left[\Omega^{[n]}(t)\right] u(0) + O(t^{n+1}). \tag{2.7}$$

Thus, the second-order Magnus operator is

$$\begin{aligned}
\Omega^{[1]}(t) &= \int_0^t dt_1 A(t_1) \\
&= e^{tA\left(\frac{1}{2}t\right)} + O(t^3)
\end{aligned} \tag{2.8}$$

or

$$\begin{aligned}
\Omega^{[1]}(t) &= \int_0^t dt_1 A(t_1) \\
&= e^{\frac{t(A(t))+(A(0))}{2}} + O(t^3).
\end{aligned} \tag{2.9}$$

and a fourth-order Magnus operator (Blanes et al., 2008); (Blanes and Moan, 2006) is

$$\Omega^{[4]}(t) = \frac{1}{2}t(A_1 + A_2) - c_3 t^2 [A_1, A_2] \tag{2.10}$$

where $A_1 = A(c_1 t)$, $A_2 = A(c_2 t)$ and

$$c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}, \qquad c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6}, \qquad c_3 = \frac{\sqrt{3}}{12}. \tag{2.11}$$

The necessity of doing time integrations and evaluating nested commutators make Magnus integrators beyond the fourth-order rather complex.

Remark 2.1 *The Magnus expansion can be generalized in different ways, e.g., commutatorless expansion, Volsamber iterative method, Floquet-Magnus expansion, etc. (Blanes et al., 2008). However, none reduces the number of needed operators at high orders.*

2.2. Convergency of Magnus Expansion

To study the convergence of the Magnus expansion, we investigate the conditions on $A(t)$. In the pioneering work Wilhelm Magnus studied its convergence in 1954. He proposed the Magnus series does not converge unless t is sufficiently small value. In literature, many bounds to the actual radius of convergence in terms of $A(t)$ have been obtained. For achieving this radius, the following statement is used.

Proposition 2.1 *If $\Omega_m(t)$ denotes the homogeneous element with $m-1$ commutators in the Magnus series, then $\Omega(t) = \sum_{m=1}^{\infty}$ is absolutely convergent for $0 \leq t < T$,*

$$T \;=\; \max\left\{ t \geq 0 : \int_0^t \|A(s)\|_2 ds < r_c \right\}. \tag{2.12}$$

Both *Pechukas and Light* (Pechukas and Light, 2008) and *Karasev and Mosolova* (Karasev and Mosolova, 1977) obtained $r_c = \ln 2 = 0.6931...$. In 1987, *Strichartz* (Strichartz, 1987) had rediscovered the explicit expression for Ω_n found by *Bialynicki-Birula et al.* (Bialynicki-Birula et al., 1969), stated in terms of Lie brackets. He used this to prove $r_c = 1$. This bound is improved independently in 1998 by *Blanes et al.* (Blanes et al., 1998) and *Moan* (Moan, 1998) as $r_c = 1.086868....$ In 2001, *Moan and Oteo* (Moan and Oteo, 2001) derived the bound $r_c = 2$ by similar techniques, except that they avoided the use of commutators as they seemed to introduce needless complications in the convergence bound. Finally, *Moan and Niesen* have been able to prove that $r_c = \pi$ if only real matrices are involved.

CHAPTER 3

OPERATOR SPLITTING METHODS BASED ON MAGNUS EXPANSION

Operator splitting is a powerful method for the numerical investigation of complex time-dependent models. In this chapter, we embedded the Magnus expansion into the operator splitting methods. In what follows, we introduce four possible splitting procedures. Finally, the new symmetric iterative splitting scheme will be given.

3.1. Lie-Trotter Splitting Based on Magnus Expansion

We consider the following problem,

$$\frac{\partial u}{\partial t} = A(t)u(t), \quad u(0) = u_0, \quad a \leq t \leq b. \tag{3.1}$$

The operator $A(t)$ of the problem (3.1) can be splitted as a sum $T + V(t)$. We, then, solve differential equation with the simplest splitting methods which is called as sequential splitting, defined by the following sequence of sub-problems:

$$\frac{\partial u^*(t)}{\partial t} = V(t)u^*(t) \qquad \text{with } t \in [t_n, t_{n+1}] \quad \text{and} \quad u^*(t_n) = u_{sp}^n, \tag{3.2}$$

$$\frac{\partial u^{**}(t)}{\partial t} = Tu^{**}(t) \quad \text{with } t \in [t_n, t_{n+1}] \quad \text{and} \quad u^{**}(t_n) = u^*(t_{n+1}) \tag{3.3}$$

for $n = 0, 1, ..., N-1$ whereby $u_{sp}^0 = u_0$ is given from (3.1). The approximated split solution at the point $t = t_{n+1}$ is defined as $u_{sp}^{n+1} = u^{**}(t_{n+1})$. Let us denote the split solution of Lie-Trotter splitting (3.2, 3.3) as $U_{sp}(t_{n+1}) = u^{**}(t_{n+1})$ on each sub-interval $[t_n, t_{n+1}]$. For simplicity denote the split solution $U_{sp}(h)$ on $(0, h]$ where h is the splitting time step. The split solution can be written in terms of the fundamental set of solutions of each sub equations (3.2, 3.3) as

$$U_{sp}(h) \quad = \quad e^{Th}\, e^{\Omega_V(h)} u_0 \tag{3.4}$$

where the exponent $\Omega_V(h)$ is an infinite sum of nested integrals and commutators belongs to the time dependent operator $V(t)$ explained in Section (2.1). To analyze the order of the Lie-Trotter splitting, we need to compare (3.4) with the exact solution of unsplit problem which we will write in the form

$$u(h) \quad = \quad e^{\Omega_A(h)} u_0 \tag{3.5}$$

where the exponent $\Omega_A(h)$ is an infinite sum of nested integrals and commutators belong to the time dependent operator $A(t)$ explained in Section (2.1). If we rearranged the equation (3.5) by substituting the $\Omega_A(h)$ then, we have

$$u(h) \quad = \quad e^{hA(h/2)} u_0. \tag{3.6}$$

3.2. Symmetrically Weighted Splitting Based on Magnus Expansion

We consider $A(t) = T + V(t)$. The weighted splitting can be obtained by using two sequential splittings as in the following algorithm:

$$\frac{\partial u^*(t)}{\partial t} = V(t)u^*(t) \qquad \text{with } t \in [t_n, t_{n+1}] \quad \text{and} \quad u^*(t_n) = u^n_{sp}, \tag{3.7}$$

$$\frac{\partial u^{**}(t)}{\partial t} = Tu^{**}(t) \quad \text{with } t \in [t_n, t_{n+1}] \quad \text{and} \quad u^{**}(t_n) = u^*(t_{n+1}) \tag{3.8}$$

and

$$\frac{\partial v^*(t)}{\partial t} = Tv^*(t) \qquad \text{with } t \in [t_n, t_{n+1}] \quad \text{and} \quad v^*(t_n) = v^n_{sp}, \tag{3.9}$$

$$\frac{\partial v^{**}(t)}{\partial t} = V(t)v^{**}(t) \quad \text{with } t \in [t_n, t_{n+1}] \quad \text{and} \quad v^{**}(t_n) = v^*(t_{n+1}) \tag{3.10}$$

for $n = 0, 1, ..., N-1$ whereby $u_{sp}^0 = u_0$ is given from (3.1). The approximated split solution at the point $t = t_{n+1}$ is defined as $u_{sp}^{n+1} = u^{**}(t_{n+1})$. Let us denote the split solution of Lie-Trotter splitting (3.2, 3.3) as $U_{sp}(t_{n+1}) = u^{**}(t_{n+1})$ on each sub-interval $[t_n, t_{n+1}]$. The split solution can be written in terms of the fundamental set of solutions of each sub equations (3.9, 3.10) as

$$U_{sp}^*(h) = e^{\Omega_V(h)} e^{Th} u_0. \tag{3.11}$$

The numerical solution is computed as a weighted average of the solutions obtained by the two sequential splitting steps. Let us denote the split solution of symmetrically weighted splitting(SWS) as $U_{sw}(t_{n+1})$ on sub-interval. Therefore, we can write the split solution as follows,

$$\begin{aligned} U_{sw}(h) &= \frac{U_{sp}(h) + U_{sp}^*(h)}{2} \\ U_{sw}(h) &= \frac{e^{Th} e^{\Omega_V(h)} + e^{\Omega_V(h)} e^{Th}}{2} u_0. \end{aligned} \tag{3.12}$$

3.3. Strang Splitting Based on Magnus Expansion

We split the $A(t)$ as in previous techniques. Then, we apply another splitting technique which is known as Strang-Marchuk splitting, where for one splitting time-step three sub-problems should be solved:

$$\frac{\partial u^*(t)}{\partial t} = Tu^*(t), \quad \text{with } t \in [t_n, t_{n+1/2}] \quad \text{and} \quad u^*(t_n) = u_{sp}^n \tag{3.13}$$

$$\frac{\partial u^{**}(t)}{\partial t} = V(t)u^*(t), \quad \text{with } t \in [t_n, t_{n+1}] \quad \text{and} \quad u^{**}(t_n) = u^*(t_{n+1/2}), \tag{3.14}$$

$$\frac{\partial \tilde{u}(t)}{\partial t} = T\tilde{u}(t), \quad \text{with } t \in [t_{n+1/2}, t_{n+1}] \quad \text{and} \quad \tilde{u}(t_{n+1/2}) = u^{**}(t_{n+1}) \tag{3.15}$$

for $n = 0, 1, ..., N-1$ whereby $u_{sp}^0 = u_0$ is given from (3.1). The approximated split solution at the point $t = t_{n+1}$ is defined as $u_{sp}^{n+1} = u^{**}(t_{n+1})$. Let us denote the split solution of Strang Marchuk splitting (3.2, 3.3) as $U_{sm}(t_{n+1}) = \tilde{u}(t_{n+1})$ on each sub-interval $[t_n, t_{n+1}]$. For simplicity denote the split solution $U_{sm}(h)$ on $(0, h]$ where h is the splitting time step. The split solution can be written in terms of the fundamental set of solutions of each sub equations (3.13, 3.15) as

$$U_{sm}(h) = e^{Th/2}\, e^{\Omega_V(h)}\, e^{Th/2} u_0. \tag{3.16}$$

Example 3.1 *By substituting the $\Omega_V(h)$ as in equation (2.8) which is given in section (2.1), we get*

$$\begin{aligned} e^{\Omega^{[2]}(h)} &= e^{h[T+V(h/2)]} \\ &= e^{\frac{1}{2}hT} e^{hV(h/2)} e^{\frac{1}{2}hT} + O(h^3). \end{aligned} \tag{3.17}$$

3.4. Iterative Splitting Method

In the present section, we will introduce traditional iterative splitting method. In this thesis our main focus is to create a new scheme for iterative splitting method. In the subsection 3.5, we develop the proposed method.

3.4.1. Algorithm for Iterative Splitting

In this section, we summarize brief overview the iterative splitting scheme. We consider the following problem,

$$\frac{\partial u}{\partial t} = (A+B)u(t), \;\; u(0) = u_0. \tag{3.18}$$

where A and B are linear operators and u_0 is initial condition.

The method is based on iteration by fixing the splitting discretization step size h on time interval $[t_n, t_{n+1}]$. The following algorithms are then solved consecutively for $i = 1, 3, \ldots, 2p+1$,

$$\frac{\partial u_i}{\partial t} = Au_i(t) + Bu_{i-1}(t) \;\text{ with }\; u_i(t_n) = u^n, \tag{3.19}$$

$$\frac{\partial u_{i+1}}{\partial t} = Au_i(t) + Bu_{i+1}(t) \;\text{ with }\; u_{i+1}(t_n) = u^n \tag{3.20}$$

where u^n is the known split approximation at time level $t = t_n$ and $u_0 \equiv 0$ is our initial guess. The split approximation at the time-level $t = t_{n+1}$ is defined as $u^{n+1} = u_{2p+2}(t_n)$, see (Geiser, 2009); (Faragó and Geiser, 2007).

The exact solutions of this system of equation then can be written by using the variation of constant formula as follows:

$$u_i(t) = \exp(At)u_0 + \int_0^t \exp((t-s)A)Bu_{i-1}(s)\, ds \quad (3.21)$$

$$u_{i+1}(t) = \exp(Bt)u_0 + \int_0^t \exp((t-s)B)Au_i(s)\, ds. \quad (3.22)$$

We summarize our algorithm in the following steps:

- Step 1: Consider the time interval $[t_0, t_{end}]$, divide it into N subintervals so that time step is $h = (t_{end} - t_0)/N$.
- Step 2: On each subinterval, $[t_n, t_n + h], n = 0, 1..N$, use the algorithm by considering the initial conditions for each step as $u(t_0) = u_0, u_i(t_n) = u_{i-1}(t_n) = u(t_n)$,

$$u_i(t_n + h) = e^{A(t_n+h)}u_0 + A^{-1}Bu_{i-1}(t_{n+1}) - A^{-1}e^{hA}Bu_{i-1}(t_n)$$

$$u_{i+1}(t_n + h) = e^{B(t_n+h)}u_0 + B^{-1}Au_i(t_{n+1}) - B^{-1}e^{hB}Au_i(t_n)$$

  where t_{n+1} denotes $t_n + h$.

- Step 3: Check the condition

$$|u_i - u_{i-1}| \leq Tol,$$

  if it is satisfied stop the iteration on this interval,

- Step 4: $u_i(t_n + h) \rightarrow u(t_n + h)$
- Step 5: Repeat this procedure for the next interval until the desired time T is achieved.

Theorem 3.1 *Let A, B $\in \mathcal{L}(X)$, where X is a Banach space, be given linear bounded operators. The Cauchy problem is in (3.18). Then the problem has a unique solution. The error bounds of the iterations (3.19), (3.20) are given by*

- *for **i** is **odd***

$$\|e_i\| \leq (K_1.\|A\|)^{\frac{i-1}{2}}.(K_2.\|B\|)^{\frac{i+1}{2}}.\|e_0\|\frac{t^i}{i!}, \tag{3.23}$$

- *for **i** is **even***

$$\|e_i\| \leq (K_1.\|A\|)^{\frac{i}{2}}.(K_2.\|B\|)^{\frac{i}{2}}.\|e_0\|\frac{t^i}{i!} \tag{3.24}$$

where $\|e_0\|$ is the difference between the exact solution and initial guess, $\|exp(At)\| \leq K_1$, $\|exp(Bt)\| \leq K_2$ for $t \geq 0$.

Proof The algorithms of the method are given by

$$u_i'(t) = Au_i(t) + Bu_{i-1}(t) \tag{3.25}$$

$$u_{i+1}'(t) = Au_i(t) + Bu_{i+1}(t) \tag{3.26}$$

with initial condition $u_i(0) = u_0$ and $u_{i+1}(0) = u_0$ where $i = 1, 3, \ldots, 2p+1$ for $[0, t]$. For the first iteration, from the variation of constant formula, we have

$$\Longrightarrow u_1(t) = e^{At}u_0 + \int_0^t e^{A(t-s)}Bu_0\,ds, \tag{3.27}$$

and we know the exact solution

$$\Longrightarrow u(t) = e^{At}u_0 + \int_0^t e^{A(t-s)}Be^{(A+B)s}u_0\,ds. \tag{3.28}$$

For the second iteration, from the variation of constant formula, we have

$$\Longrightarrow u_2(t) = e^{Bt}u_0 + \int_0^t e^{B(t-s)}Au_1\,ds \tag{3.29}$$

and we know the exact solution

$$\Longrightarrow u(t) = e^{Bt}u_0 + \int_0^t e^{B(t-s)} A e^{(A+B)s} u_0 \, ds. \tag{3.30}$$

Let's denote $e_i = u(t) - u_i(t)$. Assume that A, B are linear bounded operators and $\|exp(At)\| \leq K_1$, $\|exp(Bt)\| \leq K_2$ for $t \geq 0$.

For $i = 1$, we have the error bound

$$\|u(t) - u_1(t)\| = \| \int_0^t e^{A(t-s)} B(e^{(A+B)s}u_0 - u_0) \, ds\| \tag{3.31}$$

$$\|e_1\| = \| \int_0^t e^{A(t-s)} B e_0 \, ds\| \tag{3.32}$$

$$\|e_1\| \leq K_1.\|B\|.\|e_0\|t, \tag{3.33}$$

for $i = 2$, we get

$$\|u(t) - u_2(t)\| = \| \int_0^t e^{B(t-s)} A(e^{(A+B)s}u_0 - u_1) \, ds\| \tag{3.34}$$

$$\|e_2\| = \| \int_0^t e^{B(t-s)} A(e_1) \, ds\| \tag{3.35}$$

$$\|e_2\| \leq K_2 \int_0^t \|A\|.\|e_1\| \, ds \tag{3.36}$$

$$\|e_2\| \leq K_2.K_1.\|A\|.\|B\|.\|e_0\|\frac{t^2}{2} \tag{3.37}$$

and for $i = 3$

$$\|u(t) - u_3(t)\| = \| \int_0^t e^{A(t-s)} B(e^{(A+B)s}u_0 - u_2) \, ds\| \tag{3.38}$$

$$\|e_3\| = \| \int_0^t e^{A(t-s)} B e_2 \, ds\| \tag{3.39}$$

$$\|e_3\| \leq K_1 \int_0^t \|B\|.\|e_2\| \, ds \tag{3.40}$$

$$\|e_3\| \leq K_1.K_2.K_1.\|B\|.\|A\|.\|B\|.\|e_0\|\frac{t^3}{6} \tag{3.41}$$

then by induction we get:

For **i** is **odd**

$$\|e_i\| \leq (K_1.\|A\|)^{\frac{i-1}{2}}.(K_2.\|B\|)^{\frac{i+1}{2}}.\|e_0\|\frac{t^i}{i!} \tag{3.42}$$

For **i** is **even**

$$\|e_i\| \leq (K_1.\|A\|)^{\frac{i}{2}}.(K_2.\|B\|)^{\frac{i}{2}}.\|e_0\|\frac{t^i}{i!}. \tag{3.43}$$

Note that in (Faragó et al., 2008) they give the same error bounds implicitly. This explicit form can be found in (Gücüyenen and Tanoğlu, 2011). □

Remark 3.1 *Iterative splitting method provides the higher order accuracy in approximate solution with increasing number of iteration steps.*

3.5. New Symmetric Iterative Splitting Method

Let us consider the initial value problem (IVP) given in (3.1) on the time interval $[0, t_{end}]$ where $t_{end} \in R$. We assume for $A(t)$ a two-term splitting

$$T + V(t).$$

Let us divide the integration interval $[0, t_{end}]$ in N equal parts by the points $t_0, t_1, ..., t_n$, where the length of each interval is $h = t_{n+1} - t_n = t_{end}/N, j = 0, 1..N - 1$. The approximated solution and exact solution at time $t = t_n$ are $U(t_n)$ and $u(t_n)$, respectively.

Our technique is close to that used in (Blanes and Ponsoda, 2008). We apply second order iterative process described as below on each subinterval $[t_n, t_{n+1}]$,

$$\dot{u}_1 = Tu_1 + V(t)U(t_0) \quad u_1(t_n) = U(t_n) \tag{3.44}$$
$$\dot{u}_2 = Tu_1 + V(t)u_2 \quad u_2(t_n) = U(t_n) \tag{3.45}$$

where $u_2(t_n) = U(t_n)$ denotes the numerical approximation to the true solution $u(t_n)$ at the time $t = t_n$ and $U(t_0) = u_0$. The formal solution of the sub equations given in (3.44) and (3.45) on the time interval $[t, t+h]$ can be written by

$$u_i(t+h) \;=\; \Phi_i(t+h,t)\,u_i(t) + \int_t^{t+h} \Phi_i\,(t+h,s)F_i(s)\,ds, \qquad i = 1,2$$

where $F_1 = V(t)U(t)$ and $F_2 = Tu_1(t+h)$. Furthermore, Φ_i is given as follows

$$\begin{aligned}\Phi_1(t+h,t) &= e^{(h)T}\\ \Phi_2(t+h,t) &= e^{\frac{h}{2}[V(t+h)+V(t)]}\end{aligned}$$

which is the second order approximation of the Magnus series given in equation (2.9). Next we use the trapezoidal rule to approximate the integral

$$\int_t^{t+h} \Phi_i\,F_i\,ds \;=\; \frac{h}{2}[F_i(t+h) + \Phi_i(t+h,t)F_i(t)] + O(h^3). \tag{3.46}$$

Note that $\Phi_i(t+h,t+h) = I$. After combining approximation (3.46) with the iterative schemes (3.44), (3.45) and rearranging expressions, we get the first order approximation

$$u_1(t_n+h) \;=\; e^{Th}[u_1(t_n) + \frac{h}{2}V(t_n)u_0(t_n)] + \frac{h}{2}V(t_n+h)u_0(t_n) \tag{3.47}$$

and the second order approximation,

$$u_2(t_n+h) \;=\; e^{\frac{h}{2}[V(t_n+h)+V(t_n)]}[U(t_n) + \frac{h}{2}Tu_1(t_n)] + \frac{h}{2}Tu_1(t_n+h) \tag{3.48}$$

where $U_{n+1} = u_2(t_n+h)$. Repeat this procedure for next interval until the desired time t_{end} is reached.

Proposition 3.1 *New iterative scheme preserve the time-symmetry property.*

Proof

The time- symmetry preservation can be easily seen by interchanging t_{n+1},

$u_i(t_{n+1}),\ h$ by $t_n,\ u_i(t_n),\ -h$, respectively.

$$u_1^n \;=\; e^{-hT}[u_1^{n+1} - \frac{h}{2}V(t_{n+1})u_0^n] - \frac{h}{2}V(t_n)u_0^n. \qquad (3.49)$$

By rearranging the equation (3.49), we have

$$\begin{aligned} e^{hT}[u_1^n + \frac{h}{2}V(t_n)u_0^n] &= [u_1^{n+1} - \frac{h}{2}V(t_{n+1})u_0^n] \\ u_1^{n+1} &= e^{hT}[u_1^n + \frac{h}{2}V(t_n)u_0^n] + \frac{h}{2}V(t_{n+1})u_0^n. \end{aligned}$$

Similarly, when we consider the second order scheme to prove the time symmetry property, we use the same procedure as above.

$$u_2^n \;=\; e^{-\frac{h}{2}[V(t_n)+V(t_{n+1})]}[u_2^{n+1} - \frac{h}{2}Tu_1^{n+1}] - \frac{h}{2}Tu_1^n. \qquad (3.50)$$

When we arrange the equation (3.50) for u_2^{n+1} , they are equivalent to equations in (3.45).

□

CHAPTER 4

CONSISTENCY ANALYSIS OF OPERATOR SPLITTING METHODS

In chapter (3), we obtained modified first and second order splitting methods with the help of the Magnus expansion. This chapter is related to find the error bound for these methods. We will study on the following equation

$$\begin{aligned} \frac{d}{dt}u(t) &= A(t)u(t) = (T + V(t))u(t), \;\; 0 \leq t \leq t_{end} \qquad (4.1) \\ u(0) &= u_0 \in X. \end{aligned}$$

where X is any Banach space and $A(t) = T + V(t)$.

4.1. Consistency Analysis for Bounded Operators

The main idea of this section is to analyze the error bounds for the bounded operators, T and $V(t)$. These bounds are represented with the help of Taylor expansion in the following subsections.

4.1.1. Error Analysis of Lie Trotter Splitting

Proposition 4.1 *The Lie-Trotter splitting is at least first order for the system of equation given as (4.1) with the error bound*

$$\|u(h) - U_{sp}(h)\| \;\; \leq \;\; A_1 h^2. \qquad (4.2)$$

Here A_1 only depends on $\|[T, V(h/2)]\|$ and $\|u_0\|$.

Proof The numerical split solution (3.4) takes the following form after using the Taylor expansion for e^{Th} and the second order Magnus expansion as in (2.8) for $e^{\Omega_V(h)}$

$$U_{sp}(h) = (I + Th + \frac{1}{2}T^2h^2 + O(h^3))(I + V(\frac{h}{2})h + \frac{1}{2}V^2(\frac{h}{2})h^2 + O(h^3))u_0 \quad (4.3)$$

After collecting the terms under the powers of h, we have

$$U_{sp}(h) = (I + (T + V(\frac{h}{2}))h + (\frac{1}{2}V^2(\frac{h}{2}) + TV(\frac{h}{2}) + \frac{1}{2}T^2)h^2 + O(h^3))u_0. \quad (4.4)$$

We will approximate the exact solution (3.5) up to the second order also according to Magnus expansion which is proposed in (2.8). This yields

$$\begin{aligned} u(h) &= (I + (T + V(\frac{h}{2}))h + \frac{1}{2}(V^2(\frac{h}{2}) + TV(\frac{h}{2}) + V(\frac{h}{2})T + T^2)h^2 \\ &+ O(h^3))u_0 \end{aligned} \quad (4.5)$$

where $A(t) = T + V(t)$. In order to find the error bound, we compare (4.4) with the exact solution (4.5). Subtracting (4.4) from (4.5) leads to

$$u(h) - U_{sp}(h) = \frac{1}{2}(TV(\frac{h}{2}) - V(\frac{h}{2})T)h^2\, u_0 + O(h^3). \quad (4.6)$$

Hence, the error bound of Lie-Trotter splitting is

$$\|u(h) - U_{sp}(h)\| \leq \frac{1}{2}\|[T, V(h/2)]\|\|u_0\|h^2. \quad (4.7)$$

□

4.1.2. Error Analysis of Strang Splitting

Proposition 4.2 *The Strang-Marchuk splitting is at least second order for the system of equation given as (4.1) with the error bound*

$$\|u(h) - U_{sm}(h)\| \quad \leq \quad A_2 h^3$$

where A_2 is a function of $\|T\|, \|u_0\| \text{ and } \|\mathrm{V(t)}\|$.

Proof The numerical split solution which is defined in equation (3.16) as Strang splitting takes the following form after using the Taylor expansion for e^{Th} and the second order Magnus expansion which is given in equation (2.8) for $e^{\Omega_V(h)}$

$$\begin{aligned} U_{sm}(h) &= (I + \frac{1}{2}Th + \frac{1}{8}T^2h^2 + \frac{1}{48}T^3h^3 + O(h^4))(I + V(\frac{h}{2})h + \frac{1}{2}V^2(\frac{h}{2})h^2 \\ &+ \frac{1}{6}V^3(\frac{h}{2})h^3 + O(h^4))(I + \frac{1}{2}Th + \frac{1}{8}T^2h^2 + \frac{1}{48}T^3h^3 + O(h^4))u_0. \end{aligned}$$

After collecting the terms under the powers of h, we have

$$\begin{aligned} U_{sm}(h) &= \Bigg[I + (T + V(\frac{h}{2}))h + (\frac{1}{2}V^2(\frac{h}{2}) + \frac{T}{2}V(\frac{h}{2}) + V(\frac{h}{2})\frac{T}{2} + \frac{1}{2}T^2)h^2 \\ &+ \Bigg(\frac{1}{6}V^3(\frac{h}{2}) + \frac{T^2V(\frac{h}{2}) + V(\frac{h}{2})T^2}{8} + \frac{TV^2(\frac{h}{2})V^2(\frac{h}{2})T}{4} \\ &+ \frac{TV(\frac{h}{2})T}{4} + \frac{1}{6}T^3\Bigg)h^3\Bigg]u_0 + O(h^4). \end{aligned} \tag{4.8}$$

We will approximate the exact solution by using Magnus expansion as in numerical solution. This yields

$$\begin{aligned} u(h) &= \Bigg[I + (T + V(\frac{h}{2}))h + \frac{1}{2}(V^2(\frac{h}{2}) + TV(\frac{h}{2}) + V(\frac{h}{2})T + T^2)h^2 \\ &+ \frac{1}{6}\Bigg(V^3(\frac{h}{2}) + T^2V(\frac{h}{2}) + TV(\frac{h}{2})T + TV^2(\frac{h}{2}) + V(\frac{h}{2})T^2 \\ &+ V(\frac{h}{2})TV(\frac{h}{2}) + V^2(\frac{h}{2})T + T^3\Bigg)h^3\Bigg]u_0 + O(h^4) \end{aligned} \tag{4.9}$$

where $A(t) = T + V(t)$.

Substraction the (4.9) and (4.8) leads to

$$\begin{aligned} u(h) - U_{sm}(h) &= [\frac{1}{24}(T^2V(\frac{h}{2}) + V(\frac{h}{2})T^2) \\ &- \frac{1}{12}(TV^2(\frac{h}{2}) + V^2(\frac{h}{2})T + TV(\frac{h}{2})T) + \frac{1}{6}V(\frac{h}{2})TV(\frac{h}{2})]h^3u_0 \\ &+ O(h^4). \end{aligned} \tag{4.10}$$

The error bound of Strang splitting is obtained as

$$\begin{aligned} \|u(h) - U_{sm}(h)\| &\leq \frac{1}{12}\|T^2V(\frac{h}{2})\| + \frac{1}{6}\|TV^2(\frac{h}{2})\| \\ &+ \frac{1}{12}\|TV(\frac{h}{2})T\| + \frac{1}{6}\|V(\frac{h}{2})TV(\frac{h}{2})\|\|u_0\|h^3. \end{aligned} \tag{4.11}$$

□

4.1.3. Error Analysis of Symmetrically Weighted Splitting

Proposition 4.3 *The Symmetrically weighted splitting is at least second order for the system of equation given as (4.1) with the error bound*

$$\|u(h) - U_{sw}(h)\| \leq A_3h^3. \tag{4.12}$$

where A_3 *depends on* $\|[T, [V(\frac{h}{2}), T]]\|$ and $\|[\mathrm{V}(\frac{\mathrm{h}}{2}), [\mathrm{V}(\frac{\mathrm{h}}{2}), \mathrm{T}]]\|$ *and* $\|u_0\|$.

Proof

The symmetrically weighted splitting solution in (3.9, 3.10) takes the form

$$\begin{aligned} U^*_{sp}(h) &= (I + V(\frac{h}{2})h + \frac{1}{2}V^2(\frac{h}{2})h^2 + \frac{1}{6}V^3(\frac{h}{2})h^3 + O(h^4))(I + Th \\ &+ \frac{1}{2}T^2h^2 + \frac{1}{6}T^3h^3 + O(h^4))u_0. \end{aligned} \tag{4.13}$$

After collecting the terms under the powers of h, we have

$$\begin{aligned} U_{sp}^*(h) &= \big[I + (T + V(\frac{h}{2}))h + (\frac{1}{2}V^2(\frac{h}{2}) + TV(\frac{h}{2}) + \frac{1}{2}T^2)h^2 \\ &+ \Big(\frac{1}{6}V^3(\frac{h}{2}) + \frac{1}{2}V^2(\frac{h}{2})T \\ &+ \frac{1}{2}V(\frac{h}{2})T^2 + \frac{1}{6}T^3\Big)h^3 + O(h^4)\big]\, u_0. \end{aligned} \tag{4.14}$$

and the symmetrically weighted solution is

$$U_{sw}(h) \;=\; \frac{U_{sp}(h) + U_{sp}^*(h)}{2}\, u_0,$$

or equal to

$$\begin{aligned} U_{sw}(h) &= \Big[I + (T + V(\frac{h}{2}))h + \frac{1}{2}(V^2(\frac{h}{2}) + TV(\frac{h}{2}) + V(\frac{h}{2})T + T^2)h^2 \\ &+ \Big(\frac{1}{6}V^3(\frac{h}{2}) + \frac{1}{4}TV^2(\frac{h}{2}) + \frac{1}{4}T^2V(\frac{h}{2}) + \frac{1}{4}V(\frac{h}{2})T^2 \\ &+ \frac{1}{4}V^2(\frac{h}{2})T + \frac{1}{6}T^3\Big)h^3\Big)\, u_0 + O(h^4). \end{aligned} \tag{4.15}$$

We know the exact solution is

$$\begin{aligned} u(h) &= \Big[I + (T + V(\frac{h}{2}))h + \frac{1}{2}(V^2(\frac{h}{2}) + TV(\frac{h}{2}) + V(\frac{h}{2})T + T^2)h^2 \\ &+ \frac{1}{6}\Big(V^3(\frac{h}{2}) + T^2V(\frac{h}{2}) + TV(\frac{h}{2})T + TV^2(\frac{h}{2}) + V(\frac{h}{2})T^2 \\ &+ V(\frac{h}{2})TV(\frac{h}{2}) + V^2(\frac{h}{2})T + T^3\Big)h^3\Big] u_0 + O(h^4) \end{aligned} \tag{4.16}$$

Subtracting (4.15) from (4.16) leads to

$$u(h) - U_{sw}(h) \;=\; \frac{1}{12}([T, [V(\frac{h}{2}), T]] + [V(\frac{h}{2}), [V(\frac{h}{2}), T]])u_0h^3 + O(h^4). \tag{4.17}$$

Therefore, symmetrically weighted splitting is bounded by

$$\|u(h) - U_{sw}(h)\| \;\leq\; \frac{1}{12}(\|[T, [V(\frac{h}{2}), T]]\| + \|[V(\frac{h}{2}), [V(\frac{h}{2}), T]]\|)\|u_0\|h^3. \tag{4.18}$$

□

4.1.4. Error Analysis of Iterative Splitting

The operator $A(t)$ of the problem (4.1) can be splitted as a sum $T + V(t)$. We, then, solve the following algorithms consecutively for $i = 1, 3, \ldots, 2p + 1$.

$$\frac{\partial u_i(t)}{\partial t} = Tu_i(t) + V(t)u_{i-1}(t) \quad t \in [t_n, t_{n+1}] \text{ and } u_i(t_n) = u_{sp}^n, \tag{4.19}$$

$$\frac{\partial u_{i+1}(t)}{\partial t} = Tu_i(t) + V(t)u_{i+1}(t) \quad t \in [t_n, t_{n+1}] \text{ and } u_{i+1}(t_n) = u_{sp}^n \tag{4.20}$$

for $n = 0, 1, ..., N - 1$ whereby $u_{sp}^0 = u_0$ is given from (4.1) and $u_0 \equiv 0$ is our initial guess. The split approximation at the time-level $t = t_{n+1}$ is defined as $U_{itsp}^{n+1} = u_{i+1}(t_n)$, see (Geiser, 2009); (Faragó and Geiser, 2007).

Proposition 4.4 *The iterative splitting is at first order if we consider one iteration for the system of equation given as (4.1) with the error bound*

$$\|u(h) - U_{itsp}(h)\| \quad \leq \quad A_4 h^2. \tag{4.21}$$

Here A_4 depends on $\|T\|$ and $\|V(t)\|$.

Proof

Each sub equation, (4.19) and (4.20) have the following solutions

$$u_1(h) \quad = \quad e^{Th}u_0 + \int_0^h e^{T(h-s)}V(s)u_0 \text{ for each } [0, h], \tag{4.22}$$

If we use the Taylor expansion for e^{Th}, then (4.22) yields

$$u_1(h) \quad = \quad (I + Th + \frac{1}{2}T^2h^2)(I + \int_0^h (I - Ts)V(s)ds)u_0.$$

Due to midpoint rule for approximating integral in (4.23), one obtains

$$
\begin{aligned}
u_1(h) &= (I + Th + \frac{1}{2}T^2h^2) \\
&\quad \big(I + h(V(\frac{h}{2}) - \frac{h}{2}TV(\frac{h}{2}))\big)u_0 + O(h^3).
\end{aligned} \tag{4.23}
$$

By rearranging the equation above, we have

$$
\begin{aligned}
u_1(h) &= (I + (V(\frac{h}{2}) + T)h + \frac{1}{2}h^2(T^2 + 2TV(\frac{h}{2}) + V^2(\frac{h}{2})))u_0 \\
&+ O(h^3)
\end{aligned} \tag{4.24}
$$

where $U_{itsp}(h) = u_1(h)$. The exact solution is

$$
\begin{aligned}
u(h) &= (I + (T + V(\frac{h}{2}))h + \frac{1}{2}(V^2(\frac{h}{2}) + TV(\frac{h}{2}) + V(\frac{h}{2})T + T^2)h^2)\, u_0 \\
&+ O(h^3).
\end{aligned} \tag{4.25}
$$

The error of the iterative splitting method is obtained by subtracting (4.24) from (4.25). One obtains

$$
\|u(h) - U_{itsp}(h)\| \leq \frac{1}{2}(\|[T, V(\frac{h}{2})]\|\|u_0\|h^2. \tag{4.26}
$$

□

Proposition 4.5 *The iterative splitting is at first order if we consider two iterations for the system of equation given as (4.1) with the error bound*

$$
\|u(h) - U_{itsp}(h)\| \leq A_5h^3 \tag{4.27}
$$

where A_5 depends on $\|T\|$ and $\|V(t)\|$.

Proof The proof follows the line of previous one. □

4.2. Consistency Analysis for Unbounded Operators

In this section, our main aim is to illustrate the error bounds for operators which are assumed T is unbounded and $V(t)$ is bounded in Eq.(4.1). To obtain these bounds, we commence with describing semigroup theory and employed assumptions. Then, we will give error bounds the given methods.

4.2.1. Semigroup Theory

In the current subsection, we will summarize semigroup theory, since it will be used to get some basic assumptions in the next subsection. This theory is developed to solve operator ODE. Consider the initial value problem,

$$\frac{\partial u(t)}{\partial t} = Au(t) \quad \text{with} \quad \mathrm{t} \in [0, \mathrm{t_{end}}],\ \mathrm{u}(0) = \mathrm{u_0}, \tag{4.28}$$

with given matrix $A \in \mathbf{R}^{n\times n}$. The solution of equation above can be written as following,

$$u(t) = e^{tA}u_0. \tag{4.29}$$

In preceding section, we represented if A is a linear bounded operator in Banach space, $U(t)$ still has this form. However, in many interesting cases, it is unbounded which don't admit this form. This to some extend shows the richness of semigroup theory.

For its application, semigroup theory uses abstract methods of operator theory to treat initial boundary value problems for linear and nonlinear equations that describe the evolution of a system.

Theorem 4.1 *(Gelfand) Denote* $\sigma(M) = \{\lambda \in \mathbf{C} | \lambda I - M \text{is not invertible}\}$ *to be the spectrum of bounded linear operator* A*. We have*

- $\sigma(A)$ *is closed bounded nonempty set in* $\mathbf{C}$
- *Let* $\mid \sigma(M) \mid = \max_{\lambda\in\sigma(M)} \mid \lambda \mid$*. We have* $\sigma(M) = \lim_{k\to\infty} \mid M^k \mid^{\frac{1}{k}}$.

Remark 4.1 *For any power series,* $f(z) = \sum a_n z^n$*, suppose the convergence circle of* f *is* $B(0, R)$*. Then if* $R > \mid \sigma(M) \mid, f(M) = \sum a_n M^n$ *is well-defined. For instance,*

$e^M = \sum \frac{M^n}{n!}$ *is well defined for any bounded operator M.*

Definition 4.1 *A one-parameter strongly continuous semigroup of operators over a real or complex Banach space X is a map such that,*

$$S : X \mapsto X$$

i *S(0)=I*

ii *for all* $t, s \geq 0$ $S(t+s) = S(t)S(s)$

iii $\forall x \in X$ *such that* $\|S(t)x - x\| \to 0 \text{ as t} \to 0.$

The first two axioms are algebraic, and state that $S(t)$ is a representation of the semigroup (X, X); the last is topological, and states that the map $S(t)$ is continuous in the strong operator topology.

Theorem 4.2 $S(t)$ *be one-parameter semigroup of operator that is strongly continuous at* $t = 0$ *then, there exist constants* b, k *such that* $S(t) \leq be^{kt}$.

Definition 4.2 *The infinitesimal generator A of* $S(t)$ *is given by:*

$$Ax \ := \ \lim_{t \downarrow 0} \frac{1}{t} \left(S(t)x - x \right)$$

whenever the limit exists and $D(A)$ *is its domain.*

Theorem 4.3 $S(t)$ *be a strongly continuous semigroup of operators. Then,*

- *It is uniquely determined by its infinitesimal generator.*
- *if* $x \in D(A)$ *then* $S(t)x \in D(A)$ *and* $AS(t)x = S(t)Ax$.
- $D(A^n)$ *is dense for any* $n \in \mathbf{N}$, *where* $D(A^n) := \{u \in D(A^{n-1}) | A^{n-1}u \in D(A)\}$.
- *A is closed operator.*

For bounded linear operator M, the resolvent set is the complement of spectrum $\sigma(M)$, denote by $\rho(M)$. So for any $\lambda \in \rho(M), \lambda I - M$ is invertible. And its resolvent is $R(\lambda) = (\lambda I - M)^{-1}$. However for unbounded operator A, we need change the definition to $\lambda I - A$ is bijective between $D(A)$ and X. The resolvent of A is still $R(\lambda) = (\lambda I - A)^{-1}$, but the map is $X \mapsto D(A)$. For any $\lambda \in \mathbf{C}$ whose real part is bigger than $k($ where $\mid S(t) \mid \leq be^{kt})$, we can define Laplace transform of $S(t)$ by $L(\lambda)x = \int_0^\infty e^{-\lambda t}S(t)xdt$. The following theorem states the properties of the resolvent of A.

Theorem 4.4 *(Hille-Yosida) The infinitesimal generator A of contractions,i.e. $\mid S(t) \mid \leq 1$ for all $t \geq 0$ has every positive, real in its resolvent and $\mid R(\lambda) \mid = \mid (\lambda I - A)^{-1} \mid \leq \frac{1}{\lambda}$.*

The detailed proof of this theorem can be found in (Pazy, 1983).

4.2.2. Assumptions

For our analysis we need the following assumptions:

Assumption 4.1 *Suppose that closed linear operator $A(t) : D \to X$ where D is dense subset of X and that $A(t)$ is uniformly sectorial for $0 \leq t \leq t_{end}$. Then, there exist constants $a \in \mathbb{R}, 0 < \varphi < \pi/2$,and $M_1 \geq 1$ such that $S_\varphi(a) = \{\lambda \in \mathbb{C} : \mid arg(a - \lambda) \mid \leq \varphi\} \cup \{a\}$,*

$$\|(\lambda I - A(t))^{-1}\|_{X \leftarrow X} \leq \frac{M_1}{\mid (a - \lambda) \mid} \quad \text{for any } \lambda \in \mathbb{C} \setminus \mathrm{S}_\varphi(\mathrm{a}). \tag{4.30}$$

Then for fixed $0 \leq s \leq t_{end}$, the analytic semigroup $e^{tA(s)}$satisfy $\| e^{tA(s)} \| \leq Me^{\omega t}$ for some constants $\omega < 0$ and $M \geq 1$. Our general references on semigroups are (Ostermann et al., 2006), (Bátkai et al., 2011).

Assumption 4.2 *Let $D(T) = D(A(t))$. We assume that T is linear closed operator and that generates a strongly continuous semigroup e^{tT} on X. By semi group property, we assume $\| e^{Tt} \| \leq 1$.*

Assumption 4.3 *We assume that $V(t)$ is bounded linear operator on X. Then we get $e^{\Omega_V(t)} \leq e^{t\|V(t)\|}$ where $\Omega_V(t) \approx \Omega_2(t)$ with the help of the equation (2.9). As the convergence of Magnus expansion is guaranteed if $\| \Omega(t) \| < \pi$. The details can be found in (Moan and Niesen, 2008).*

Lemma 4.1 *Let T be an infinitesimal generator of a $\mathcal{C}_0$ semigroup $S(t)$, $t \geq 0$. Let $t_{end} > 0$. If for any $V(t)U \in \mathcal{D}(T)$ satisfying $V(t)U, TV(t)U \in \mathbf{C}^1([0, t_{end}]; X)$ then the* *solution of problem satisfies* $u(t) \in \mathcal{D}(A^2(t))$ *for* $0 \le t \le t_{end}$ *whenever* $u_0 \in \mathcal{D}(A^2(t))$, *and we have*

$$\sup_{0 \le t \le t_{end}} \|T^i u(t)\| \le E_i(t_{end}), \quad i = 0, 1, 2 \tag{4.31}$$

where E_i *depends on the specific choice of* $t_{end}, T, V(t)U$ *and* u_0. *For the detailed proof see (Bjørhus, 1998).*

Assumption 4.4 *We assume that there are non-negative constants* $\tilde{C}, R$ *with*

$$\sup_{0 \le t \le t_{end}} \|V(t)\| \le \tilde{C}.$$

$$\|u\| \le R \quad \textit{on} \quad 0 \le t \le t_{end}.$$

4.2.3. Analysis

Under the assumptions which are given in previous subsection, we will analyze the consistency. In order to get the error bounds we use the techniques are close to that use in (Jahnke and Lubich, 2000); (Hansen et al., 2008).

4.2.3.1. Lie-Trotter Splitting

Proposition 4.6 *Let Assumption 4.2 and 4.4 be fulfilled. Then, the Lie Trotter splitting method is first order accuracy, i.e., the local error satisfies the bound*

$$\|u(h) - U(h)\| \le C_1 h^2 \tag{4.32}$$

where C_1 *is a function of* $\tilde{C}$ and R.

Proof We start from the variation of constant formula for the exact solution

$$u(h) \;=\; e^{Th}u_0 + \int_0^h e^{T(h)}V(h-s)u(h-s)ds.$$

By using midpoint rule for approximating integral, we get

$$u(h) \quad = \quad e^{Th}u_0 + he^{T(h)}V(h/2)u(h/2) + O(h^2).$$

Taylor expansion of $u(0 + h/2)$ at $t = 0$ leads to

$$u(h) \quad = \quad e^{Th}u_0 + he^{T(h)}V(h/2)u(0) + O(h^2). \tag{4.33}$$

On the one hand, the split solution is given by

$$U(h) \quad = \quad e^{Th}u_0 + he^{Th}V(h/2)u_0 + F_1. \tag{4.34}$$

where

$$F_1 = \frac{h^2}{2}e^{Th}V^2(h/2)u_0 + O(h^3).$$

Due to our assumptions F_1 is bounded by $\frac{h^2}{2}\tilde{C}^2$, i.e. $F_1 \leq \frac{h^2}{2}\tilde{C}^2$.

The proof follows the subtracting numerical solution in equation (4.34) from the exact solution given in (4.33). Henceforth, we have

$$\begin{aligned} \|u(h) - U(h)\| &\leq F_1 + O(h^2) \\ \|u(h) - U(h)\| &\leq C_1 h^2 \end{aligned} \tag{4.35}$$

where C_1 is function of $\tilde{C}$ and R. □

4.2.3.2. Strang Splitting

We, now, show that Strang splitting method is consistent for the abstract Cauchy problem in 4.1 under the assumptions which we determined in the subsection 4.2.2.

Proposition 4.7 *Let Assumption 4.2 and 4.4 be fulfilled. Then, the Strang-Marchuk splitting is second order accuracy, i.e., the local error satisfies the bound*

$$\|u(h) - U(h)\| \;\; \leq \;\; C_2 h^3$$

where C_2 is a function of $\tilde{C}^3, R$.

Proof

We start with the numerical solution. Using Taylor expansion with the help of the equation (2.8) for $e^{\Omega_V(h)}$ leads

$$\begin{aligned} U(h) &= e^{T\frac{h}{2}}(I + hV(h/2) + \frac{h^2}{2}V^2(h/2) + \frac{h^3}{6}V^3(h/2) + O(h^4))e^{T\frac{h}{2}}u_0 \\ &= e^{Th}u_0 + he^{T\frac{h}{2}}V(h/2)e^{T\frac{h}{2}}u_0 + \frac{h^2}{2}e^{T\frac{h}{2}}V^2(h/2)e^{T\frac{h}{2}}u_0 + F_2 \qquad (4.36) \end{aligned}$$

where $F_2 = \frac{h^3}{6}e^{T\frac{h}{2}}V^3(h/2)e^{T\frac{h}{2}}u_0 + O(h^4)$. The bound of F_2 follows the line of *Assumption* 4.2 and 4.4 and it is defined as

$$F_2 \leq \frac{h^3}{6}\tilde{C}^3 \,\|u_0\|.$$

On the other side, as in proof of proposition 4.6, we represent the variation of constant formula for the exact solution. Expressing the last term of integral, we substitute the $u(h)$ by the same formula, at the end of this process we have

$$\begin{aligned} u(h) &= e^{Th}u_0 + \int_0^h e^{T(h-s)}V(s)e^{Ts}u_0\,ds \\ &+ \int_0^h \int_0^s e^{T(h-s)}V(s)e^{T(s-\rho)}V(\rho)e^{T\rho}u(\rho)d\rho\,ds. \qquad (4.37) \end{aligned}$$

We define $g_1(s) = e^{T(h-s)}V(s)e^{Ts}u_0$ and $g_2(s,\rho) = e^{T(h-s)}V(s)e^{T(s-\rho)}V(\rho)e^{T\rho}u(\rho)$. With the aid of $g_1(s), g_2(s,\rho)$ the equation (4.37) can be rewritten as

$$\begin{aligned} u(h) &= e^{Th}u_0 + \int_0^h g_1(s)u_0\,ds \\ &+ \int_0^h \int_0^s g_2(s,\rho)d\rho\,ds. \end{aligned} \tag{4.38}$$

We use midpoint rule to approximate the integrals. Hence we obtain

$$\begin{aligned} u(h) &= e^{Th}u_0 + h(e^{T\frac{h}{2}}V(h/2)e^{T\frac{h}{2}} + O(h^2)) \\ &+ \frac{h^2}{2}e^{T\frac{h}{2}}V(h/2)V(h/2)e^{T\frac{h}{2}}u(h/2) + O(h^3). \end{aligned}$$

Again using Taylor expansion of $u(0+h/2)$ at $t=0$ leads to

$$\begin{aligned} u(h) &= e^{Th}u_0 + h(e^{T\frac{h}{2}}V(h/2)e^{T\frac{h}{2}}) + \frac{h^2}{2}e^{T\frac{h}{2}}V^2(h/2)e^{T\frac{h}{2}}u_0 \\ &+ O(h^3). \end{aligned} \tag{4.39}$$

By subtracting (4.36) from (4.39), one obtains

$$\begin{aligned} \|u(h) - U(h)\| &\leq \|F_1\| + O(h^3) \\ \|u(h) - U(h)\| &\leq C_2h^3 \end{aligned} \tag{4.40}$$

where C_2 depends on $e^{Th}, V(h/2)$ and R. Therefore, by means of our assumptions, C_2 is bounded by a function of $\tilde{C}^3$ and R. □

4.2.3.3. Symmetrically Weighted Splitting

Proposition 4.8 *Let Assumption 4.2 and 4.4 be fulfilled. Then, the symmetrically weighted splitting is second order accuracy, i.e., the local error satisfies the bound*

$$\|u(h) - U(h)\| \;\leq\; C_3 h^3.$$

Proof

The proof proceeds by starting numerical solution. As in proof proposition 4.7, using exponential series with the help of the equation (2.8) for $e^{\Omega_V(h)}$ leads to

$$\begin{aligned} U(h) &= \frac{e^{Th}(I + hV(h/2) + \frac{h^2}{2}V^2(h/2)) + (I + hV(h/2) + \frac{h^2}{2}V^2(h/2))e^{Th}}{2} u_0 \\ &+ O(h^3) \\ &= e^{Th}u_0 + \frac{h}{2}(e^{Th}V(h/2) + V(h/2)e^{Th})u_0 + \frac{h^2}{4}(e^{Th}V^2(h/2) + V^2(h/2)e^{Th})u_0 \\ &+ O(h^3). \end{aligned} \quad (4.41)$$

Consequently, by variation of constants formula ,we obtain the following representation of exact solution:

$$\begin{aligned} u(h) &= e^{Th}u_0 + \int_0^h e^{T(h-s)}V(s)e^{Ts}u_0\, ds \\ &+ \int_0^h \int_0^s e^{T(h-s)}V(s)e^{T(s-\rho)}V(\rho)e^{T\rho}u_0 d\rho\, ds + F_2 \end{aligned}$$

where

$$F_3 = \int_0^h e^{T(h-s)}V(s) \int_0^s e^{T(s-\rho)}V(\rho) \int_0^\rho eT(\rho - \xi)V(\xi)u(\xi)d\xi\, d\rho\, ds$$

which is bounded by $\|F_3\| \leq \frac{h^3}{6}\tilde{C}^3\, \|R\|$. We define $g(s) = e^{T(h-s)}V(s)e^{Ts}u_0$ and $\omega(s,\rho) = e^{T(h-s)}V(s)e^{T(s-\rho)}V(\rho)e^{T\rho}u_0$. By using trapezium rule to approximate the integrals, i.e. we substitute $\frac{h}{2}(g(h) + g(0))$ for the second term and substitute $\frac{h^2}{4}(\omega(0,0) + \omega(h,h))$ for the last term, one obtains

$$u(h) \;=\; e^{Th}u_0 + \frac{h}{2}(V(h)e^{Th} + e^{Th}V(0))u_0 + \frac{h^2}{4}(e^{Th}V^2(0) + V^2(h)e^{Th})u_0 + O(h^3).$$

We use Taylor expansion of $V(h/2 + h/2)$ at $h/2$ and also $V(h/2 - h/2)$ at $h/2$ leads to

$$\begin{aligned} u(h) &= e^{Th}u_0 + \frac{h}{2}(V(h/2)e^{Th} + e^{Th}V(h/2))u_0 \\ &+ \frac{h^2}{4}(e^{Th}V^2(h/2) + V^2(h/2)e^{Th})u_0 + O(h^3). \end{aligned} \tag{4.42}$$

In order to get the order of this method, we take a look at the error $e_j = \|u(t_j) - U(t_j)\|$. Subtracting 4.41 from and using the assumptions leads to

$$\|u(h) - U(h)\| \;\le\; C_3 h^3. \tag{4.43}$$

Here C_3 is a function of $\tilde{C}$ and R. □

4.2.4. Symmetric Iterative Splitting

Proposition 4.9 *The symmetric iterative splitting is first order if we consider only one iteration given in (3.44) with the error bound*

$$\|u(h) - U(h)\| \;\le\; Kh^2 \tag{4.44}$$

Here K only depends on $\tilde{C}, R, E_1(t_{end})$.

Proof

We define the local error by $e_j = U(t_j) - u(t_j)$, $j = 0, 1, 2, \ldots, n$. For simplicity, we only consider the time interval [0,h]. The exact solution of the equation (4.1) can be written as,

$$u(h) \;=\; e^{Th}u_0 + \int_0^h e^{Th}V(h-s)u(h-s)ds. \tag{4.45}$$

We derive the error bound for the equation (4.1) by using first order iterative splitting scheme.Thus, the numerical solution of (4.1),

$$U(h) \;=\; e^{Th}u_0 + \int_0^h e^{Th}V(h-s)u_0 ds. \tag{4.46}$$

By subtracting (4.46) from (4.45) leads to

$$\begin{aligned} \|u(h) - U(h)\| &= \|\int_0^h e^{Th}V(h-s)[u(h-s) - u_0]ds\| \\ &\leq h\tilde{C}\|u(h-s) - u_0\| \end{aligned} \tag{4.47}$$

where $\tilde{C} = \sup_{0 \leq t \leq t_{end}} \|V(t)\|$. To obtain the error bound for $\|u(h) - u_0\|$ we use the *Lemma 4.1* and *Assumption 4.4* ,

$$\begin{aligned} u(h) &= u_0 + \int_0^h A(s)u(s)ds \\ \|u(h) - u_0\| &= h\|A(s)u\| = h\|(T + V(s))u\| \leq h \parallel Tu \parallel + \parallel V(s)u \parallel \\ \|u(h) - u_0\| &\leq h(E_1(t_{end}) + \tilde{C}R). \end{aligned} \tag{4.48}$$

By substituting (4.48) in the equation (4.47), we have

$$\|u(h) - U(h)\| \;\leq\; h^2\tilde{C}(E_1(t_{end}) + \tilde{C}R) = Kh^2 \tag{4.49}$$

where $K = \tilde{C}(E_1(t_{end}) + \tilde{C}R)$. □

Proposition 4.10 *The symmetric iterative splitting is the second order if we consider two iterations given in (3.45) with the error bound*

$$\|u(h) - U(h)\| \;\leq\; \tilde{K}h^3 \tag{4.50}$$

Here $\tilde{K}$ *only depends on* $\tilde{C}, R, E_1(t_{end})$.

Proof

We write the equation for second order iterative splitting as follows,

$$U(h) = e^{Th}u_0 + \int_0^h e^{Th}V(h-s)u_1 ds. \tag{4.51}$$

For estimating the error bound, we subtract the (4.51) from the equation (4.45), remaining term is

$$\begin{aligned} \|u(h) - U(h)\| &= \| \int_0^h e^{Th}V(h-s)[u(h-s) - u_1]ds\| \\ &\le h\tilde{C}\|u(h-s) - u_1\|. \end{aligned} \tag{4.52}$$

Here u_1 is the solution of the equation in (3.44). The proof follows that of the bound of $\|u(t-s) - u_1\|$ in (4.49), we have

$$\|u(h) - U(h)\| \le h^3\tilde{C}^2(E_1(t_{end}) + \tilde{C}R) = h^3\tilde{K}. \tag{4.53}$$

□

CHAPTER 5

STABILITY ANALYSIS FOR OPERATOR SPLITTING METHODS

This chapter deals with the stability of any linear ordinary differential equation (ODE). We investigate this subject in two main fold. Firstly, the autonomous case is considered both bounded and unbounded operators. In the sequel, non-autonomous case is discussed.

5.1. Stability for Autonomous Linear ODE Systems

In this section, we summarize the stability issue in order not to ruin the general flow of thesis. Our main reference on stability of linear autonomous differential equations is the book *Hundsdorfer and Verwer*, see (Hundsdorfer and Verwer, 2003). To analyze the stability of autonomous differential equations, we focused on the equation in (4.28) with the exact solution (4.29).

5.1.1. Stability Analysis for Bounded Operators

In the present subsection, we take a look at properties of ODEs and particularly at influence of perturbations at such systems. Consider the (IVP) in 4.28 with exact solution . Then, take into account perturbed system,

$$\frac{\partial \tilde{U}(t)}{\partial t} = A\tilde{U}(t) + g(t) \quad \text{with} \quad \mathrm{t} \in [0, \mathrm{t_{end}}],\ \tilde{\mathrm{U}}(0) = \tilde{\mathrm{U}}_0. \tag{5.1}$$

Then by subtracting equation (4.29) from the solution of equation (5.1) which is found by using variation of constant formula, leads to

$$\delta(t) = e^{tA}\delta(0) + \int_0^t e^{(t-s)A}\delta(s)ds \tag{5.2}$$

where $\delta(t)$ denotes to $\tilde{U}(t) - U(t)$. Then, the norm estimation can be found as

$$\|\delta(t)\| \leq \|e^{tA}\|\|\delta(0)\| + \int_0^t \|e^{(t-s)A}\|ds \max_{0\leq s\leq t} \|\delta(s)\|.$$

As a result, if we have the following stability condition,

$$\|e^{tA}\| \leq Ke^{tw} \quad \text{for all t} \geq 0,$$

with constants $K > 0$ and $w \in \mathbf{R}$. Therefore, we obtain

$$\|\delta(t)\| \leq Ke^{tw}\|\delta(0)\| + \frac{K}{t}(e^{tw} - 1) \max_{0\leq s\leq t} \|\delta(s)\|, \tag{5.3}$$

with arranging $(e^{tw} - 1)/w = t$ in case $w = 0$. This inequality shows that the overall error $\|\delta(t)\|$ can be bounded in terms of error $\|\delta(0)\|$ and perturbations $\|\delta(s)\|$, $0 \leq s \leq t$. In general, the term stability will be used to indicate that small perturbations give a small overall effect. Next, we concentrate on bound for $\|e^{tA}\|$. Suppose that A is diagonalizable, that is $A = P\Lambda P^{-1}$, where $\Lambda = diag(\lambda_k)$. Hence, the norm as follows,

$$\|e^{tA}\| \leq \|P\|\|\Lambda\|\|P^{-1}\| = cond(P) \max_{1\leq k\leq t} \mid e^{t\lambda_k} \mid . \tag{5.4}$$

Consequently, if we know that $cond(P) = \|P\|\|P^{-1}\| \leq K$ and $Re(\lambda_k) \leq w$, then (5.3) follows with

$$w = \max_{1\leq\leq k\leq m\leq} \mid e^{t\lambda_k} \mid . \tag{5.5}$$

In particular, if A is a normal matrix, i.e. $A^*A = AA^*$ where A^* denotes conjugate transpose of A, then the eigenvectors of P is unitary. Since $e^{tA} = Pe^{t\Lambda}P^{-1}$, the matrix e^{tA} is also normal. Thus

$$\|e^{tA}\|_2 = \max_{1\leq k\leq m} \mid e^{t\lambda_k} \mid .$$

Suppose for A, two-term splitting in equation (4.28) as

$$A = A_1 + A_2. \tag{5.6}$$

The solution of (4.28) is given by

$$U(t_{n+1}) = e^{hA}U(t_n) \tag{5.7}$$

where $h = t_{n+1} - t_n$ on each subintervals $[t_n, t_{n+1}]$, where $n = 0, 1, ..N - 1$. Instead of full A, if we wish to use only A_1 and A_2 separately , then (5.7) can be approximated by

$$U_{n+1} = e^{hA_2}e^{hA_1}U_n \tag{5.8}$$

where U_n denotes to $U(t_n)$. With regard to stability, if we have $\|e^{tA_k}\| \leq 1,\ k = 1, 2,$ then it follows that $\|U_{n+1}\| \leq \|U_n\|$ for the equation (5.8). General stability results under the weaker condition that $\|e^{tA_k}\| \leq K$ for $0 \leq \mathrm{h} \leq \mathrm{t_{end}}$. In general, if the matrix A is not normal, an estimate $cond(U)$ in some suitable norm may be difficult to obtain. Therefore we will look a more general concept to get bounds for $\|e^{tA}\|$. A useful concept for stability results with non-normal matrices is the logarithmic norm of a matrix A in $\mathbf{R^{m\times m}}$, defined as

$$\mu(A) = \lim_{t\downarrow 0} \frac{\|I + tA\|}{t}. \tag{5.9}$$

In terms of logarithmic matrix norms, $\|e^{tA_k}\| \leq 1$ means that $\mu(A_k) \leq 0$.

5.1.2. Stability Analysis for Unbounded Operators

Consider the linear abstract Cauchy problem in a Banach space X,

$$\begin{aligned} \frac{d}{dt}u &= Au + f(t), \quad t > 0 & (5.10) \\ u(0) &= u_0. & (5.11) \end{aligned}$$

Let $\|.\|$ be the norm in X, and let $\|.\|_{Ł(X)}$ denote the corresponding induced operator norm. Let A be a densely defined closed linear operator in X for which there exist real constants $M \geq 1$ and w such that the resolvent set $\rho(A)$ satisfies $\rho(A) \supset (w, \infty)$, and we have resolvent condition

$$\|(\lambda I - A)^{-n}\|_{Ł(X)} \leq \frac{M}{(\lambda - w)^n}, \quad \text{for} \quad \lambda > \mathrm{w}, \mathrm{n} = 1, 2, ... \tag{5.12}$$

These are necessary and sufficient conditions for A to be the infinitesimal generator of C_0 semigroup of bounded linear operator, which we denote by $S(t), t \geq 0$, satisfying

$$\|S(t)\|_{Ł(X)} \leq Me^{wt} \tag{5.13}$$

(Pazy, 1983). Then, if $u_0 \in D(A)$ and $f \in C^1([0, t_{end}], X)$, our Cauchy problem has unique solution $[0, t_{end}]$ given by

$$u(t) = S(t)u_0 + \int_0^t S(t-s)f(s)ds. \tag{5.14}$$

where $S(t) = e^{At}$ is a C_0 semigroup. If we define F by

$$F(t, h) = \int_h^t S(t-s)f(s)ds \quad t \geq h \geq 0, \tag{5.15}$$

we can write (5.14) as

$$u(t) = S(t)u_0 + F(t,0). \tag{5.16}$$

Assume that,

$$A = A_1 + A_2 \quad D(A) = D(A_1) = D(A_2) \tag{5.17}$$

where A_1 and A_2 are infinitesimal generators of such C_0-semigroups $\{S_1(t)\}_{t\geq 0}$ and $\{S_2(t)\}_{t\geq 0}$,respectively. Let $f_1, f_2 \in C^1([0, t_{end}], X)$. By using the notation $u(t-) := \lim_{\varepsilon\downarrow 0} u(t-\varepsilon)$ and we choose to approximate $u(t_n)$ by $u_2(t_n)$, where u_1 and u_2 are defined piecewise on the intervals $[t_n, t_{n+1}]$ where $t_n = nh, n = 0, 1, 2, ...[t_{end}/h]$,

$$\begin{aligned} \frac{d}{dt}u_1 &= Au_1 + f_1 \quad t_n < t < t_{n+1} \\ u_2(t_n) &= u_1(t_{n+1}-) \end{aligned} \tag{5.18}$$

and

$$\begin{aligned} \frac{d}{dt}u_2 &= Au_2 + f_2 \quad t_n < t < t_{n+1} \\ u_1(t_n) &= u_2(t_n-). \end{aligned} \tag{5.19}$$

Here we note that (5.18) and (5.19)are called mild solution. We use the convention that $u_2(0-) = U_0 \in D(A_1)$ where $U_0 \approx u_0$ and if we denote the approximation $u_2(t_n-)$ by U_n, a single step of the operator splitting method can be expressed in the form

$$U_{n+1} = S_2(h)S_1(h)U_n + S_2(h)F_1(t_{n+1}, t_n) + F_2(t_{n+1}, t_n). \tag{5.20}$$

Iterating on this expression, we can formulate the method in terms of U_0 as

$$\begin{aligned} U_{n+1} &= (S_2(h)S_1(h))^{n+1}U_0 + \sum_{j=0}^{n}(S_2(h)S_1(h))^j \\ &\times \ [S_2(h)F_1(t_{n-j+1}) + F_2(t_{n-j+1}, t_{n-j})]. \end{aligned} \tag{5.21}$$

Definition 5.1 *The method is said to be* stable *on [0,T] if there are constants K_T, h' such that*

$$\|(S_{spl}(h))^j\| = \|[S_2(h)S_1(h)]^j\|_{Ł(X)} \leq K_T \tag{5.22}$$

for all $j = 0, 1, 2, ...$ and $0 < h < h'$ satisfying $jh \leq t_{end}$.

It is important to note that the verification of the stability of a particular splitting is not entirely trivial. Using the naiver estimate

$$\|[S_2(h)S_1(h)]^j\| \leq \|S_1(h)\|^j\|S_2(h)\|^j \tag{5.23}$$

and simply plugging in the growth estimates of $S_1(t)$ and $S_2(t)$, by using (5.13),

$$\|[S_2(h)S_1(h)]^j\| \leq (M_1e^{w_1h})^j(M_2e^{w_2h})^j = (M_1M_2)^je^{(w_1+w_2)hj}. \tag{5.24}$$

The right-hand side is unbounded as $j \to \infty, jh \leq t_{end}$ if and only if $M_1M_2 > 1$. Thus we get a sufficient condition for stability: *The method is stable if S_1 and S_2 satisfy the growth estimates*

$$\|S_1(t)\| \leq e^{w_1t} \quad , \quad \|S_2(t)\| \leq e^{w_2t}. \tag{5.25}$$

5.2. Stability for Non-autonomous Linear ODE Systems

In the present section, we analyze the stability behavior of the operator splitting schemes introduced in chapter (3). For deducing the stabilities of the schemes, we use both the formulation which are obtained from the algorithms in Chapter (3) and the assumptions which are given in Subsection (4.2.2) for equation (4.1).

5.2.1. Stability Analysis of Sequential Splitting

We are primarily interested in the sequential splitting. It is also known as Lie-Trotter splitting. As a first step towards to stability of this scheme, we rewrite the formulation as

$$U_{sq}(t_{n+1}) \;=\; e^{Th}\, e^{\Omega_V(h)} U_{sq}(t_n).$$

In the following proposition we analyze the stability of this procedure.

Proposition 5.1 *The sequential splitting is stable on* $[0, t_{end}]$ *with the bound*

$$\| \, U_{sq}^n \, \| \leq e^{t_{end}\tilde{C}} \|u_0\|.$$

Proof The proof is an immediate consequence of the *Assumptions* 4.2 and 4.4.

$$\begin{aligned} \|U_{sq}(h)\| &= \|e^{Th}\, e^{\Omega_V(h)} u_0\| \\ \|U_{sq}(h)\| &= \|e^{Th}\|\|e^{\Omega_V(h)}\|\|u_0\| \\ \|U_{sq}(h)\| &\leq \|e^{h\tilde{C}}\|\|u_0\|. \end{aligned}$$

By successively we get the stability of the scheme as

$$\begin{aligned} \|U_{sq}^n(h)\| &\leq e^{nh\tilde{C}}\|u_0\| \\ \|U_{sq}^n(h)\| &\leq e^{t_{end}\tilde{C}}\|u_0\|. \end{aligned} \tag{5.26}$$

□

5.2.2. Stability Analysis of Strang-Marchuk Splitting

In order to obtain a stability condition for Strang-Marchuk splitting which is given by

$$U_{sm}(t_{n+1}) \;=\; e^{Th/2}\, e^{\Omega_V(h)}\, e^{Th/2} U_{sm}(t_n) \tag{5.27}$$

where $U_{sm}(t_0) = u(t_0) = u_0$.

Proposition 5.2 *The Strang-Marchuk splitting is stable on* $[0, t_{end}]$ *with the bound*

$$\| \; U_{sm}^n \; \| \leq B_1$$

where B_1 *only depends on* t_{end}, $\tilde{C}$ and $\|\mathrm{u}_0\|$.

Proof The proof proceeds by applying the following procedure,

$$\begin{aligned} \|U_{sm}(h)\| &= \|e^{Th/2}\, e^{\Omega_V(h)}\, e^{Th/2} u_0\| \\ \|U_{sm}(h)\| &= \|e^{Th/2}\| \|e^{\Omega_V(h)}\| \|e^{Th/2}\| \|u_0\| \end{aligned}$$

by using both *Proposition* 4.2 and *Assumption* 4.4, we get

$$\|U_{sm}(h)\| \;\leq\; e^{h\tilde{C}} \|u_0\|$$

By induction one can see that

$$\begin{aligned} \|U_{sm}^n(h)\| &\leq e^{nh\tilde{C}} \|u_0\| \\ \|U_{sm}^n(h)\| &\leq e^{t_{end}\tilde{C}} \|u_0\| \end{aligned} \tag{5.28}$$

The proof is concluded. □

5.2.3. Stability Analysis of Symmetrically Weighted Splitting

Our purpose is to show that symmetrically weighted splitting method is stable for the abstract Cauchy problem in 3.1 under the assumptions which we determined previously. To prove the assertion, we rewrite the following formula

$$U_{sw}(t_{n+1}) = \frac{e^{Th}\, e^{\Omega_V(h)} + e^{\Omega_V(h)}\, e^{Th}}{2} U_{sw}(t_n) \tag{5.29}$$

where $U_{sw}(t_0) = u_0$.

Proposition 5.3 *The symmetrically weighted splitting scheme is stable on* $[0, t_{end}]$ *with the bound*

$$\| U_{sw}^n \| \leq B_2$$

where B_2 *only depends on* t_{end}, $\tilde{C}$ and $\|\mathrm{u}_0\|$.

Proof The statement of *Proposition* 5.3 remains valid under the *Assumption* 4.2 and *Assumption* 4.4

$$\begin{aligned}
\|U_{sw}(h)\| &= \| \frac{e^{Th}\, e^{\Omega_V(h)} + e^{\Omega_V(h)}\, e^{Th}}{2} u_0 \| \\
\|U_{sw}(h)\| &\leq \| \frac{e^{Th}\, e^{\Omega_V(h)}\| + \|e^{\Omega_V(h)}\, e^{Th}\|}{2} \|u_0\| \\
\|U_{sw}(h)\| &\leq \frac{\|e^{h\tilde{C}}\| + \|e^{h\tilde{C}}\|}{2} \|u_0\| \\
\|U_{sw}(h)\| &\leq \|e^{h\tilde{C}}\| \, \|u_0\|.
\end{aligned}$$

Recursively, we get the following stability condition

$$\begin{aligned}
\|U_{sw}^n(h)\| &\leq e^{nh\tilde{C}} \|u_0\| \\
\|U_{sw}^n(h)\| &\leq e^{t_{end}\tilde{C}} \|u_0\|.
\end{aligned} \tag{5.30}$$

□

5.2.4. Stability Analysis of Symmetric Iterative Splitting

Proposition 5.4 *The symmetric second order iterative splitting scheme is stable on* $[0, t_{end}]$ *with the bound*

$$\| U^n \| \leq e^{t_{end}\tilde{C}} \|u_0\| + he^{2h\tilde{C}} E_1(t_{end})(\frac{1 - e^{t_{end}\tilde{C}}}{1 - e^{h\tilde{C}}}).$$

Proof

For proving the stability bounds above, we employ the standard techniques. For this purpose, we start with the needed auxiliary stability bound of the first order iterative splitting as in following proof,

$$U^1 = U(h) \;=\; e^{Th}U^0 + F_1, \quad U^0 = u_0 \tag{5.31}$$

where

$$F_1 = \int_0^h e^{Th}V(h-s)u_0$$

which is bounded by $\|F_1\| \leq h\tilde{C}\|u_0\|$ where $\tilde{C} = \sup_{0\leq t\leq t_{end}} \|V(t)\|$. By rearranging the equation (4.28),

$$\begin{aligned} \|U^1\| &= \|e^{Th}U^0 + F_1\| \\ \|U^1\| &\leq \|e^{Th}U^0\| + \|F_1\| \\ \|U^1\| &\leq \|u_0\| + \|h\tilde{C}u_0\| = (1 + h\tilde{C})\|u_0\|. \end{aligned} \tag{5.32}$$

Recursively we get the stability polynomial for iterative scheme at first order,

$$\|U^n\| \;\leq\; (1 + h\tilde{C})^n\|u_0\| = e^{t_{end}\tilde{C}}\|u_0\|. \tag{5.33}$$

On the other hand, for finding the stability result of the second order iterative splitting we use closeness and linearity of T. It follows as,

$$U^1 \;=\; e^{\Omega_V(h)}U^0 + F_2 \tag{5.34}$$

where

$$F_2 = \int_0^h \Phi_2(t,s) T u_1$$

which is bounded by $\|F_2\| \le h e^{2h\tilde{C}} \|Tu_1\|$. Since T is closed operator and for all $i = 1, 2 ... n$, by using *Lemma 4.1*, $\|TU\| \le E_1(t_{end})$. Substituting the bound of F_2 into the (4.29) leads to

$$\begin{aligned}
\|U^1\| &\le \|e^{\Omega_V(h)} U^0\| + \|F_2\| \\
\|U^1\| &\le \|e^{h\frac{(V(h)+V(0))}{2}} U^0\| + h e^{2h\tilde{C}} E_1(t_{end}) \\
\|U^1\| &\le \|e^{h\tilde{C}} U^0\| + h e^{2h\tilde{C}} E_1(t_{end}) \\
\|U^1\| &\le \|e^{h\tilde{C}} U^0\| + h\hat{H}
\end{aligned} \tag{5.35}$$

where $\hat{H} = e^{2h\tilde{C}} E_1(t_{end})$.

By recursively,

$$\begin{aligned}
\|U^1\| &\le \|e^{h\tilde{C}} U^0\| + h\hat{H} \\
\|U^n\| &\le e^{nh\tilde{C}} \|u_0\| + h\hat{H}[1 + e^{h\tilde{C}} + \ldots + e^{h(n-1)\tilde{C}}] \\
\|U^n\| &\le e^{nh\tilde{C}} \|u_0\| + h\hat{H} \sum_{i=0}^{n-1} e^{ih\tilde{C}} \\
\|U^n\| &\le e^{t_{end}\tilde{C}} \|u_0\| + h\hat{H}\left(\frac{1 - e^{t_{end}\tilde{C}}}{1 - e^{h\tilde{C}}}\right) \\
\|U^n\| &\le e^{t_{end}\tilde{C}} \|u_0\| + h\hat{S}
\end{aligned} \tag{5.36}$$

where $\hat{S} = e^{2h\tilde{C}} E_1(t_{end}) (\frac{1 - e^{t_{end}\tilde{C}}}{1 - e^{h\tilde{C}}})$ and $\tilde{\mathrm{C}} = \sup_{0 \le \mathrm{t} \le \mathrm{t_{end}}} \|\mathrm{V(t)}\|$.

□

CHAPTER 6

CONVERGENCY ANALYSIS FOR OPERATOR SPLITTING METHODS

The aim of this chapter is to collect the results of Chapter 5 and Chapter 5. We investigate convergence issues of the given methods. In particular, we focused on our proposed method

6.1. Convergence analysis of the Traditional Methods

Objective. We are concerned with deducing an estimate for the global error $y_N - y(t_{end})$ of an exponential operator splitting method when applied to the initial value problem (3.1); to this purpose, we follow a standard approach based on a *Lady Windermere's Fan* argument as follows.

Local error and order. In the present situation, the local error equals

$$d_n = D(h_{n-1})y(t_{n-1}) = (\phi(h_{n-1}) - E(h_{n-1}))y(t_{n-1}), \quad 1 \leq n \leq N, \tag{6.1}$$

Therefore, the numerical method is consistent of order p whenever the defect operator D fulfills

$$D(h) = \mathcal{O}(h^{p+1}) \tag{6.2}$$

Theorem 6.1 ***Lady Windermere's Fan.*** *In order to relate the global and local error, we employ the telescopic identity,*

$$y_N - y(t_N) \;=\; \prod_{j=0}^{N-1} \phi(h_j)(y_0 - y(t_0)) + \sum_{n=1}^{N} \prod_{j=n}^{N-1} \phi(h_j) d_n \tag{6.3}$$

Proof The validity of relation (6.3) is verified by a short calculation as follows

$$
\begin{aligned}
& \prod_{j=0}^{N-1} \phi(h_j)(y_0 - y(t_0)) + \sum_{n=1}^{N} \prod_{j=n}^{N-1} \phi(h_j) d_n \\
= \; & \prod_{j=0}^{N-1} \phi(h_j)(y_0 - y(t_0)) + \sum_{n=1}^{N} \prod_{j=n}^{N-1} \phi(h_j)(\phi(h_{n-1}) - E(h_{n-1}))y(t_{n-1}) \\
= \; & \prod_{j=0}^{N-1} \phi(h_j) y_0 - \prod_{j=0}^{N-1} \phi(h_j) y(t_0) \\
+ \; & \sum_{n=1}^{N} \prod_{j=n-1}^{N-1} \phi(h_j) y(t_{n-1}) - \sum_{n=1}^{N} \prod_{j=n}^{N-1} \phi(h_j) y(t_n) \\
= \; & y_N - \prod_{j=0}^{N-1} \phi(h_j) y(t_0) + \sum_{n=0}^{N-1} \prod_{j=n}^{N-1} \phi(h_j) y(t_n) - \sum_{n=1}^{N} \prod_{j=n}^{N-1} \phi(h_j) y(t_n) \\
= \; & y_N - \prod_{j=0}^{N-1} \phi(h_j) y(t_0) + \prod_{j=0}^{N-1} \phi(h_j) y(t_0) - y(t_N) \\
= \; & y_N - y(t_N).
\end{aligned}
$$

□

Proposition 6.1 *The traditional splitting schemes are convergent.*

Proof The proof of this assertion follows the line of the given theorem above. In terms of theorem, if a scheme is consistent and stable then it is convergent. In chapter 4 and 5 we gave the conditions which are desired. As a result, the schemes which are known as Lie Trotter, Strang splitting and symmetrically weighted splitting are convergent with the aid of the *Lady Windermere's Fan Argument*. □

6.2. Convergency of Proposed Method

In this subsection we consider convergency for proposed scheme of iterative splitting method. With the help of telescoping identity, we will prove the following statement.

Proposition 6.2 *The global error of iterative splitting is bounded by*

$$\|U^n(h) - u^n(h)\| \;\; \leq \;\; G\, h^2$$

Here G only depends on $t_{end}, \parallel u_0 \parallel, R$ and $\tilde{\mathrm{C}}$.

Proof

We use the following insignificant modification of theorem in (Jahnke and Altıntan, 2004). We can show by induction that the error after $n > 0$ steps,

$$U^n(h) - u^n(h) = \sum_{i=0}^{n-1} U_h^i (U_h - u_h) e^{(n-1-i)\Omega(h)} u_0 \tag{6.4}$$

where U_h is iterative scheme. Since $\|U_h^i\| \leq \|e^{t_{end}\tilde{C}} u_0 + h\hat{S}\|$ and $e^{(n-1-i)\Omega(h)} u_0 = u(t_{n-1-i})$, this yields

$$\begin{aligned}\|U^n(h) - u^n(h)\| &\leq \sum_{i=0}^{n-1} \|e^{t_{end}\tilde{C}}\|u_0\| + h\hat{S}\|\|(U_h - u_h^n)u_{n-1-i}\| \\ &\leq (e^{t_{end}\tilde{C}}\|u_0\| + \|h\hat{S}\|) \sum_{i=0}^{n-1} \|U_h - u_h^n\|\|u_{n-1-i}\| \end{aligned} \tag{6.5}$$

and it follows from *Proposition 5.4* that

$$\|U^n(h) - u^n(h)\| \leq h^2 G + \mathcal{O}(h^3) \tag{6.6}$$

where $G = t_{end} R e^{t_{end}\tilde{C}} \|u_0\|$. Here R denotes to bound of $\|u(t_{n-1-i})\|$. □

CHAPTER 7

NUMERICAL EXPERIMENTS

This Chapter deals with numerical experiments. We compare our new symmetric iterative splitting method(SISM) with standard splitting methods. Throughout this section, $SISM_i$ denotes i^{th} order symmetric iterative splitting. The examples include Mathieu equation, radial Schrödinger equation and a complex Schrödinger equation. All computations are done in Mathworks MATLAB. The codes will be given in Appendix part.

7.1. Mathieu equation

We first consider the Mathieu equation,

$$q'' + (\omega^2 - \varepsilon \cos(t))q \;=\; 0. \tag{7.1}$$

Now the time dependent oscillator corresponds to

$$\begin{aligned} A(t) &= \begin{pmatrix} 0 & 1 \\ -(\omega^2 - \varepsilon \cos t) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \varepsilon \cos t & 0 \end{pmatrix} && (7.2) \\ &\equiv T + V(t). && (7.3) \end{aligned}$$

We take as initial condition $p(0) = 1.75$ and $q(0) = 0$, integrate up to $t_{end} = 10$ and measure the average error for different time steps.

h	$SISM_1$/Order	Lie Trotter/Order
0.1	0.0610	0.1015
0.01	0.0066 (0.9658)	0.0105 (0.9853)
0.001	6.6819e-004 (0.9946)	0.0011 (0.9798)

Table 7.1. Comparison of errors for several h on $[0, 10]$ interval with various methods where $\omega = 0.6$ and $\varepsilon = 0.3$. The expected order is 1.

Another table deals with the comparison of second order methods.

h	$SISM_2$/ order	Strang Splitting/ order	SWS/ order
0.1	9.8067e-004	0.0011	0.0062
0.01	8.3542e-006 (2.0696)	1.0839e-005 (2.0064)	6.3187e-005 (1.9918)
0.001	8.2197e-008 (2.0070)	1.0801e-007 (2.7672)	6.3309e-007 (1.9992)

Table 7.2. Comparison of errors for different h on $[0, 10]$ interval with several methods where $\omega = 0.6$ and $\varepsilon = 0.3$. Accepted exact solution is fourth order Magnus expansion. The expected order is 2.

The numerically observed order in the discrete L^∞ norm is approximately $1 \text{ and } 2$, which is supported by propositions in chapter 4. This number is in perfect agreement with table 7.2. We also observed in Table 7.2 that second order proposed iterative splitting scheme($SISM_2$) is more efficient than not only Strang splitting but also symmetrically weighted splitting.

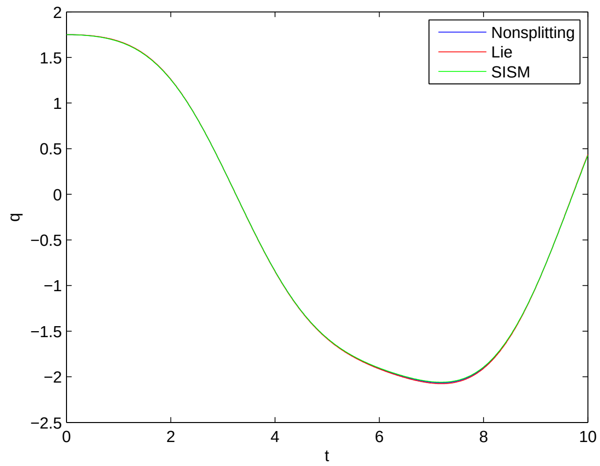

Figure 7.1. Comparison of 2nd order Magnus and first order approximation for equation (7.1) for various schemes for small time step $h = 0.01$ on $[0, 10]$.

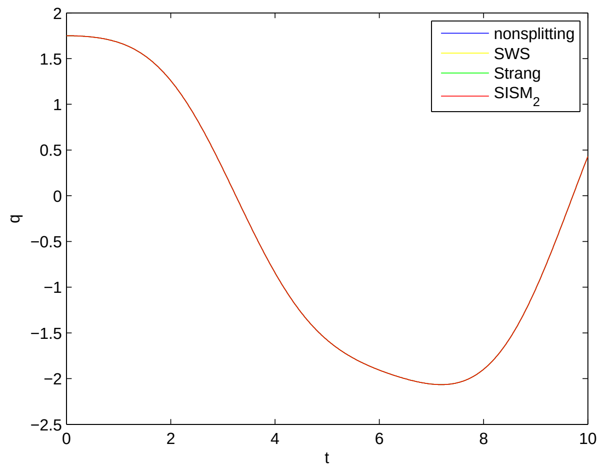

Figure 7.2. Comparison of 2nd order Magnus and first order approximation for equation (7.1) for various schemes for small time step $h = 0.01$ on $[0, 10]$.

7.2. Radial Schrödinger equation

Consider the radial Schrödinger equation, (Chin and Anisimov, 2006)

$$\frac{\partial^2 u}{\partial r^2} = f(r, e)u(r) \tag{7.4}$$

where

$$f(r, E) = 2V(r) - 2E + \frac{l(l+1)}{r^2}. \tag{7.5}$$

The Eqn. (7.4) can be transformed as a harmonic oscillator with a time dependent spring constant after relabeling $r \to t$ and $u(r) \to q(t)$ and defining

$$k(t, E) = -f(t, E). \tag{7.6}$$

By redefining the variables as $u(t) = q(t)$ and $\dot{u}(t) = p(t)$, and $Y(t) = (q(t), p(t))$, Eqn. (7.4) can be put into the system of equation as

$$\dot{Y}(t) = A(t)Y(t) \tag{7.7}$$

and Hamiltonian of the system reads as

$$H = \frac{1}{2}p^2 + \frac{1}{2}k(t, E)q^2. \tag{7.8}$$

For specific example, the ground state of hydrogen atom can be modeled as Schrodinger equation with the parameters $l = 0$, $E = -1/2$, $V(t) = -1/(t-a)$, a is arbitrary constant. Now the time dependent oscillator corresponds to

$$A(t) = \begin{pmatrix} 0 & 1 \\ f(t) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ f(t) & 0 \end{pmatrix} \equiv T + V(t), \tag{7.9}$$

with

$$f(t) = (1 - \frac{2}{t-a}). \tag{7.10}$$

The exact solution for this model with the initial conditions $q(0) = -a$, $p(0) = 1 + a$, $a = 0$ is

$$q(t) = (t-a)e^{-t}. \tag{7.11}$$

The comparison of exact solution and first order methods is illustrated in Figure 7.2. In addition, we compare exact solution with the second order methods in Figure 7.2. These computations are exhibited in for $t_{end} = 6$ and $h = 0.0001$.

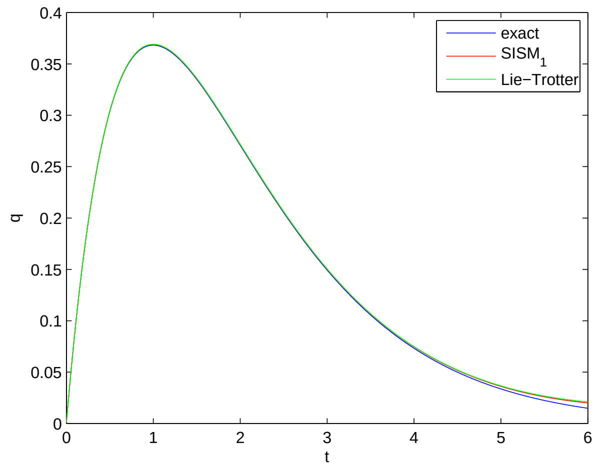

Figure 7.3. Comparison first order methods for equation (7.4) for small time step $h = 0.0001$ on $[0, 6]$.

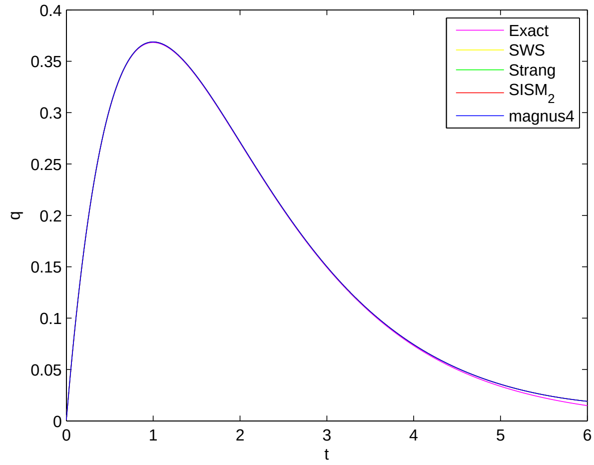

Figure 7.4. Comparison of exact and approximation solution for equation (7.4) for various schemes for small time step $h = 0.0001$ on $[0, 6]$.

The following table deals with the errors of methods for radial Schrödinger equation. The errors at the endpoint $t = 6$ are computed in a discrete L_∞ norm.

h	Iterative Splitting 2	Strang Splitting	SWS	Magnus 4	Magnus 2
0.001	4.1483e-002	4.1666e-002	4.1580e-002	4.1554e-002	4.1646e-002
0.0001	4.1677e-003	4.1699e-003	4.1689e-003	4.1686e-003	4.1697e-003

Table 7.3. Comparison of errors for several h on $[0, 6]$ interval with several methods where $a = -0.001$ with exact solution.

We notice that our scheme is more efficient than fourth order Magnus expansion. The following figure is the comparison of Magnus Expansion and SISM method.

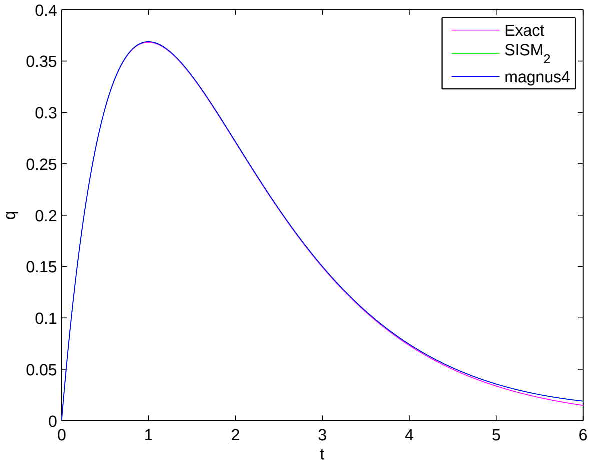

Figure 7.5. Comparison fourth order Magnus expansion and second order SISM for equation (7.4) for small time step $h = 0.0001$ on $[0, 6]$.

7.3. Schrödinger Equation

Another experiment is time dependent Schrödinger equation as following form,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{H}\psi(x,t)$$

where $\psi(x,t)$ denotes the probability amplitude for the particle to be found at position $x$at time t and $\hat{H}$ is the Hamiltonian operator for a single particle in a potential.

In our study, we choose one-dimensional harmonic oscillator in the finite time interval $t \in [0, t_{end}]$ has the form

$$\begin{aligned} i\frac{\partial\psi(x,t)}{\partial t} &= \big(-\frac{1}{2}\frac{\partial^2}{\partial x} + \frac{\omega^2(t)(x^2-1)}{2}\big)\psi(x,t) \\ \psi_0(x) &= \sqrt[4]{\frac{1}{\pi}}\exp\big(-\frac{1}{2}x^2\big) \end{aligned} \tag{7.12}$$

with $\omega^2(t) = 4 - 3e^{-t}$.

We take into account the system as following form,

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 & A(t,x) \\ -A(t,x) & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}$$

where $\psi(x,t) = u(x,t) + iv(x,t)$,then consider the splitting methods with ODE system split in the form,T corresponds to spatial derivative $\partial^2\psi(x,t)/\partial x^2$, we use the second order center difference scheme in order to approximate it, thus we get $2N \times 2N$ system.

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 & T \\ -T & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} 0 & V(t,x) \\ -V(t,x) & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}$$

For exhibited figure, we suppose that the system is defined in the interval $x \in [-10, 10]$, which

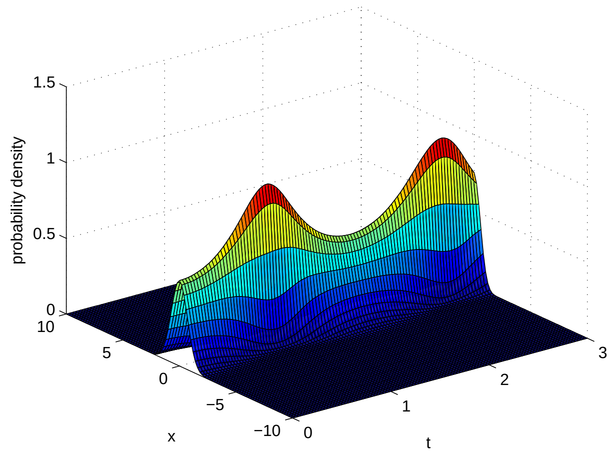

Figure 7.6. The probability of density, $|\Psi(x,t)|^2$, for the particle in (7.12) with $\omega^2(t) = 4 - 3e^{-t}$ by using the symmetric iterative splitting.

is split into $N = 100$ parts of length $\Delta x = 0.2$. We integrate the system using proposed method with the time-step size $\Delta t = 0.03$ up to final time $t = 3$.

We apply this method for the same problem with different potential. We choose potential as $\omega^2(t) = \cos^2(t)$ for equation (7.12). In the following figure, we suppose that the system is defined in the interval $x \in [-20, 20]$, which is split into $N = 100$ parts of length $\Delta x = 0.4$. We integrate the system using $SISM_2$ with the time-step size $\Delta t = 0.05$ up to final time $t = 5$.

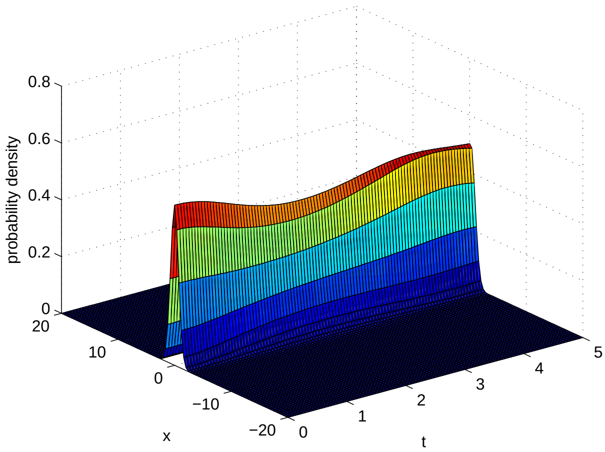

Figure 7.7. The probability of density, $|\Psi(x,t)|^2$, for the particle in (7.12) with $\omega^2(t) = \cos^2(t)$ by using $SISM_2$.

CHAPTER 8

CONCLUSION

In this thesis, we introduced the operator splitting methods; sequential splitting, Strang splitting, symmetrically weighted splitting and iterative splitting methods which are obtained by combining with Magnus expansion. We have developed the new symmetric iterative splitting method (SISM) for non-autonomous systems with the help of the Magnus expansion.

We have also discussed the consistency and stability properties for the standard splitting methods. In the linear bounded case for the operators we have studied by means of Taylor expansion and in the linear unbounded case, we use the semigroup properties. Then, we investigated the convergence issue of the introduced schemes. For that purpose, we use both *Lady Windermere's Fan Argument* and *telescoping identity*.

To confirm the theoretical results, we apply the new scheme into a test problem by comparing traditional operator splitting methods. The method also provides the higher order accuracy in approximate solution with increasing number of iteration steps.

Not only proposed method but also traditional methods of operator splitting are applied to physical problems. We found out that our new scheme is applicable for obtaining the numerical solution of the harmonic oscillators for example Schrödinger equation in quantum mechanics since it preserves the time symmetry.

Finally, numerical experiments reveal that our proposed method is efficient. It can be seen in Table 7.1 and Table 7.2. In Figures 7.3 and 7.3 illustrated the probability of density for the particle which is defined by the equation 7.12. This indicates that our scheme preserves not only time symmetry but also probability density. Thus, the new scheme is easily adapted to solve such problems numerically.

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APPENDIX A

MAT-LAB CODES

A.1. Codes for Mathieu equation

FIRST ORDER METHODS FOR MATHIEU EQUATION

```
clear all;
close all;
E=0.3;
w=0.6;
h=0.01;
tson =10;    t=0:h:tson ;
N=tson/h;
p0=1.75;
q0=0;
C0=[p0;q0];
At=zeros(N+1,1); At(1)=p0;
AAt=zeros(N+1,1);  AAt(1)=p0;
T=[0,1;-w^2,0];
%%%%%%%%%%  magnus-2  %%%%%%%%%%%%%%
yini=C0;
for k=2:N+1,
H=expm(h*(T+mat(E,t(k)+h/2)))*yini;
yini=H;
AAt(k)=yini(1,1);
end
%Lie-Trother
L(:,1)=C0;  L1(:,1)=C0;  lie(1)=p0;
for i=2:N+1
    A1=mat(E,t(i)+(h/2));
    L1(:,i)=expm(h*A1)*L1(:,i-1);
    L(:,i)=expm(T*h)*L1(:,i);
```

```
    L1=L;
    lie(i)=L1(1,i);
end

% Iterative order 1
 IT(:,1)=C0; Itr(1)=p0;  IT1(:,1)=C0;
for i=2:N+1
    IT(:,i)=expm(T*h)*(IT(:,i-1));
    IT1(:,i)=(expm((h/2)*(mat(E,t(i)+h)+
    mat(E,t(i))))*(IT1(:,i-1)
    +((h/2)*T*IT(:,i-1))))+((h/2)*T*IT(:,i));
    IT=IT1;
    Itr(i)=IT1(1,i);
end

% Errors
    for i=1:N+1
        EL(i)=abs(lie(i)-AAt(i));
        EI(i)=abs(Itr(i)-AAt(i));
    end
    nmL=max(EL)
    nmI=max(EI)

    figure(1)
    plot(t,AAt,t,lie,'r',t,Itr,'g')
    legend('magnus','Lie','SISM_1')
    xlabel('t')
    ylabel('q')
%   figure(2)
%   plot(t,EL,t,EI,'r')
%   legend('errlie','errItr')
```

SECOND ORDER METHODS FOR MATHIEU EQUATION

```
clear all;
close all;
```

```
E=0.3;
w=0.6;
h=0.1;
tson =10;    t=0:h:tson ;
N=tson/h;
p0=1.75;
q0=0;
C0=[p0;q0];
At=zeros(N+1,1); At(1)=p0;
AAt=zeros(N+1,1);  AAt(1)=p0;
T=[0,1;-w^2,0];
%%%%%%%%%  magnus-4  %%%%%%%%%%%%
c1=(1/2)-(sqrt(3)/6);
c2=(1/2)+(sqrt(3)/6);
yini2=C0;
for k=2:N+1,
   A1=T+mat(E,t(k)+c1*h);
   A2=T+mat(E,t(k)+c2*h);
F=expm(((h/2)*(A1+A2))-((sqrt(3)/12)*(h^2)*commut(A1,A2))
+((1/80)*(h^3)*commut(A1-A2,commut(A1,A2))))*yini2
; yini2=F; At(k)=yini2(1,1); end

%%%%%%%%%%%%% magnus-2 %%%%%%%%%%%%%%%
yini=C0;
for k=2:N+1,
H=expm(h*mat1(E,t(k)+h,w))*yini;
yini=H;
AAt(k)=yini(1,1);
end

 % symmetrically weighted splitting
 SW1(:,1)=C0;  SWS(:,1)=C0;
 SW2(:,1)=C0;  Swsss(1)=p0;
 for i=2:N+1
```

```
    H1=mat(E,t(i)+(h/2));
    SW1(:,i)=expm(T*h)*expm(h*H1)*SWS(:,i-1);
    SW2(:,i)=expm(h*H1)*expm(T*h)*SWS(:,i-1);
    SWS(:,i)=(SW1(:,i)+SW2(:,i))/2;
    Swsss(i)=SWS(1,i);
end
% Strang-Marchuk Splitting
ST=zeros(2,N+1);
ST(:,1)=C0;  Str(1)=p0;ST1(:,1)=C0;ST2(:,1)=C0;
for i=2:N+1
    H=mat(E,t(i)+(h/2));
    A1=expm((h)*H);
    ST(:,i)=expm(T*(h/2))*A1*expm(T*(h/2))*ST(:,i-1);
    Str(i)=ST(1,i);
end

% Iterative 2

IT2=zeros(2,N+1);ITS=zeros(2,N+1);
IT1=zeros(2,N+1); Tr2=zeros(1,N+1);
 IT2(:,1)=C0; IT1(:,1)=C0;  Tr2(1)=p0;
 ITS(:,1)=C0;
for i=2:N+1
% IT2(:,i)=(expm(T*h)*(IT2(:,i-1)+((h/2)*mat(E,t(i))*C0)))
%+((h/2)*mat(E,t(i)+h)*C0);
% ITS(:,i)=(expm((h/2)*(mat(E,t(i)+h)
%+mat(E,t(i))))*(ITS(:,i-1)+((h/2)*T*IT2(:,i-1))))
%+((h/2)*T*IT2(:,i));
% C0=ITS(:,i);
% IT2=ITS;
% Tr2(i)=ITS(1,i);
%%%%%%%%%
IT2(:,i)=(expm((h/2)*(mat(E,t(i)+h)
+mat(E,t(i))))*(IT2(:,i-1)+((h/2)*T*C0)))+((h/2)*T*C0);
```

```
ITS(:,i)=(expm(h*T)*(ITS(:,i-1)+((h/2)*mat(E,t(i))
*IT2(:,i-1))))+((h/2)*mat(E,t(i)+h)*IT2(:,i));
C0=ITS(:,i); IT2=ITS; Tr2(i)=ITS(1,i); end

for i=1:N+1
    ESt(i)=abs(At(i)-Str(i));
    ESw(i)=abs(At(i)-Swsss(i));
    EIt(i)=abs(At(i)-Tr2(i));
    EM2(i)=abs(At(i)-AAt(i));
end
%COMP=[ESt,ESw,EIt]

strang=max(ESt)
sim=max(ESw)
tr=max(EIt)
M2=max(EM2)

 plot(t,At,t,Swsss,'y',t,Str,'g',t,Tr2,'r')
legend('Magnus_2','SWS','Strang','SISM_2')
xlabel('t')
ylabel('q')
```

THE PROGRAMMES WHICH ARE USED IN FIRST AND SECOND ORDER METHODS

```
%%%%%%% mat
%time dependent part
function y=mat(ep,it)
K=zeros(2);
K(2,1)=ep*cos(it);
y=K;
%%%%%%% commut
% commutators
function y=commut(A,B)
K1=zeros(2);
K1=A*B-B*A;
y=K1;
```

A.2. Codes for Radial Schrödinger equation

FIRST ORDER METHODS

```
clear all;
close all;
h=0.0001;
a=-0.001;
tson =6;    t=0:h:tson ;
N=tson/h;
p0=-a;
q0=1+a;
C0=[p0;q0];
At=zeros(N+1,1); At(1)=p0;
AAt=zeros(N+1,1);  AAt(1)=p0;
T=[0,1;0,0];
%%%%%%%%%%% Exact Solution %%%%%%%%%%%%
PP=zeros(N+1,1);
for i=1:N+1
    PP(i)=(t(i)-a)*exp(-t(i));
end

%Lie-Trother
L(:,1)=C0;  L1(:,1)=C0;  lie(1)=p0;
for i=2:N+1
    A1=std(a,t(i)+(h/2));
    L1(:,i)=expm(T*h)*expm(h*A1)*L1(:,i-1);
    lie(i)=L1(1,i);
end

%%%%%%%%%%  magnus-2  %%%%%%%%%%
yini=C0;
for k=2:N+1,
H=expm(h*(T+std(a,t(k)+(h/2))))*yini;
yini=H;
```

```
AAt(k)=yini(1,1);
end

% Iterative order 1
 IT(:,1)=C0; Itr(1)=p0;  IT1(:,1)=C0;
for i=2:N+1
%     IT(:,i)=expm(T*h)*(IT(:,i-1));
%     IT1(:,i)=(expm((h/2)*(std(a,t(i)+h)
%+std(a,t(i))))*(IT1(:,i-1)+((h/2)*T*IT(:,i-1))))
%+((h/2)*T*IT(:,i));
%     IT=IT1;
%     Itr(i)=IT1(1,i);
    IT(:,i)=expm((h/2)
    *((std(a,t(i)+h)+std(a,t(i)))))*IT(:,i-1);
    IT1(:,i)=(expm(T*h))*(IT1(:,i-1)
    +((h/2)*std(a,t(i))*IT(:,i-1)))
    +((h/2)*(std(a,t(i)+h)*IT(:,i)));
    IT=IT1;
    Itr(i)=IT1(1,i);
end

% Errors
    for i=1:N+1
        EL(i)=abs(lie(i)-PP(i));
        EI(i)=abs(Itr(i)-PP(i));
        EM2(i)=abs(AAt(i)-PP(i));
    end
    nmL=max(EL)
    nmI=max(EI)
    nmG=max(EM2)
% plot(t,PP,t,Itr,'-.',t,lie,'+')
plot(t,PP); hold on; plot(t,Itr,'-.');
hold on; plot(t,lie,'r');
legend('exact','SISM_1','Lie-Trotter')
```

```
xlabel('t') ylabel('q')
```

SECOND ORDER METHODS

```
clear all;
close all;
h=0.0001;
a=-0.001;
tson =6; t0=0;   t=t0:h:tson ;
N=(tson-t0)/h;
p0=-a;
q0=1+a;
C0=[p0;q0];
At=zeros(N+1,1); At(1)=p0;
AAt=zeros(N+1,1);  AAt(1)=p0;
T=[0,1;0,0];
%%%%%%%%%%%% Exact Solution %%%%%%%%%%%%%%
PP=zeros(N+1,1);
for i=1:N+1
    PP(i)=(t(i)-a)*exp(-t(i));
end

%%%%%%%%%%%%%%  magnus-4  %%%%%%%%%%%%%%%%
c1=(1/2)-(sqrt(3)/6);
c2=(1/2)+(sqrt(3)/6);
yini2=C0;
for k=2:N+1,
   A1=T+std(a,t(k)+c1*h);
   A2=T+std(a,t(k)+c2*h);
F=expm(((h/2)*(A1+A2))-((sqrt(3)/12)*(h^2)*commut(A1,A2))
+((1/80)*(h^3)*commut(A1-A2,commut(A1,A2))))*yini2 ;
yini2=F;
At(k)=yini2(1,1);
end

%%%%%%%%%%%%%%%% magnus-2 %%%%%%%%%%%%%%%%
```

```
yini=C0;
for k=2:N+1,
H=expm(h*(T+std(a,t(k)+(h/2))))*yini;
yini=H;
AAt(k)=yini(1,1);
end

 % symmetrically weighted
    SWS(:,1)=C0;       Swsss(1)=p0;
 GG=expm(h*T);
 for i=2:N+1
     H1=std(a,t(i)+(h/2));
     AAa=GG*expm(h*H1)*SWS(:,i-1);
     BBb=expm(h*H1)*GG*SWS(:,i-1);
     SWS(:,i)=(AAa+BBb)/2;
     Swsss(i)=SWS(1,i);
 end
 % Strang Splitting
 ST=zeros(2,N+1);
 ST(:,1)=C0;  Str(1)=p0;ST1(:,1)=C0;ST2(:,1)=C0;
 YO=expm(T*(h/2));
 for i=2:N+1
     H=std(a,t(i)+(h/2));
     A1=expm((h)*H);
     ST(:,i)=YO*A1*YO*ST(:,i-1);
     Str(i)=ST(1,i);
 end

 % Iterative 2

IT2=zeros(2,N+1);ITS=zeros(2,N+1);
 IT1=zeros(2,N+1); Tr2=zeros(1,N+1);
 IT2(:,1)=C0; IT1(:,1)=C0;  Tr2(1)=p0;
 ITS(:,1)=C0;
```

```
for i=2:N+1
 IT1(:,i)=expm((h/2)
 *((std(a,t(i)+h)+std(a,t(i)))))*IT1(:,i-1);
 IT2(:,i)=(GG*(IT2(:,i-1)+((h/2)*std(a,t(i))*IT1(:,i-1))))
 +((h/2)*std(a,t(i)+h)*IT1(:,i));
 ITS(:,i)=(expm((h/2)*(std(a,t(i)+h)
 +std(a,t(i))))
 *(ITS(:,i-1)+((h/2)*T*IT2(:,i-1))))+((h/2)*T*IT2(:,i));
 IT2=ITS;
 IT1=ITS;
 Tr2(i)=ITS(1,i);
 %%%%%%%%%%
 % IT2(:,i)=(expm((h/2)*(std(a,t(i)+h)+std(a,t(i))))
 %*(IT2(:,i-1)+((h/2)*T*IT2(:,i-1))))+((h/2)*T*IT2(:,i-1));
 % ITS(:,i)=(GG*(ITS(:,i-1)+((h/2)*std(a,t(i))*IT2(:,i-1))))
 %+((h/2)*std(a,t(i)+h)*IT2(:,i));
 % IT2=ITS;
 % ITS=ITS;
 % Tr2(i)=ITS(1,i);
 %%%%%%%%%%%
end

% Runge-Kutta4 for testing
 %RUNG(:,1)=C0; RK2(1)=p0;
%
%for i=2:N+1
%    KUTTA=T+(std(a,t(i)));
%    KUT=T+(std(a,t(i)+h));
%    tild=RUNG(:,i-1)+(h*KUTTA*RUNG(:,i-1));
%    RUNG(:,i)=RUNG(:,i-1)
%    +((h/2)*(KUTTA*RUNG(:,i-1)+(KUT*tild)));
%    RK2(i)=RUNG(1,i);
%end
```

```
for i=1:N+1
    ESt(i)=abs(PP(i)-Str(i));
    ESw(i)=abs(PP(i)-Swsss(i));
    EIt(i)=abs(PP(i)-Tr2(i));
    EM2(i)=abs(PP(i)-AAt(i));
    EM4(i)=abs(PP(i)-At(i));
    %ERK2(i)=abs(PP(i)-RK2(i));
end
% COMP=[ESt,ESw,EIt]
format short e
strang=max(ESt)
sim=max(ESw)
tr=max(EIt)
M2=max(EM2)
M44=max(EM4)
%Runge=max(ERK2)

 plot(t,PP,'m',t,Swsss,'y',t,Str,'g',t,Tr2,t,At)
 legend('Exact','SWS','Strang','SISM_2','magnus4')
 xlabel('t')
 ylabel('q')
%  plot(t,PP,t,At,'g',t,Tr2,'r')
%  legend('Exact','Magnus-4','SISM_2')
```

THE PROGRAMME WHICH IS USED IN FIRST AND SECOND ORDER METHODS

```
 %%%%%%% std
 %time dependent part
function y=std(a,it)
K=zeros(2);
K(2,1)=1-(2/(it-a));
y=K;
```

A.3. Codes for Schrödinger Equation

FIRST ORDER METHODS

```
  clear all;
  close all;
  N=100; t0=0; tson=3; h=(tson-t0)/(N);
  x0=-10; xson=10; dx=(xson-x0)/N;
  ep=1;
  t=t0:h:tson;
  x=x0:dx:xson;
%%%%%%%%%initial condition
 coeff=0.751125544;
 C0=zeros(N+1,1);
for i=1:N+1
   C0(i)=coeff*exp((-1/2)*(((ep*x(i)))^2));
%    C0(i)=sin(x(i));
end
%%%%%%%%%%%%%% scalar matrix %%%%%%%%%%%%%%%%%%
n=N; UU=toeplitz([-2 1 0 0  zeros(1,n-3)], [-2 1 0 0 zeros(1,n-3)]);
US=(1/((dx)^2))*full(UU); BB=(-1/2)*US;

 T=[zeros(N+1) BB;-BB zeros(N+1)];

%%%%%%%%%%%%% Time-dependent matrix %%%%%%%%%%%%%%
H=zeros(N+1,N+1); R1=zeros(N+1,N+1); R2=zeros(N+1,N+1);
for i=1:N+1
   H(i,i)=shrodin(t(i)+(h/2),x(i));
end
H1=[zeros(N+1) H;-H zeros(N+1)]; % the matrix

% for iterative splitting time dependent matrix
 KT=zeros(N+1,N+1);   KT1=zeros(N+1,N+1);
for i=1:N+1
   KT(i,i)=shrodin(t(i)+(h),x(i));
```

```
   KT1(i,i)=shrodin(t(i),x(i));
end
 KTT=[zeros(N+1) KT;-KT zeros(N+1)];
 KT11=[zeros(N+1) KT1;-KT1 zeros(N+1)];

%%%%%%%%%%%% Initial Condition %%%%%%%%%%%%%
yini=[C0;zeros(N+1,1)];
yini1=yini;

%%%%%%%%%%%%%% magnus-2 %%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%% No-splitting %%%%%%%%%%%%%%%
 yini2=yini; AAt(:,1)=yini;
for k=2:N+1,
 R=expm(h*(T+H1))*yini2;
 yini2=R;
 AAt(:,k)=yini2;
end
%%%%%%%%%%%% METHODS %%%%%%%%%%%%%%%%%%%%%
%Lie-Trother
L(:,1)=yini;  L1(:,1)=yini;
for i=2:N+1
    L1(:,i)=expm(h*H1)*L1(:,i-1);
    L(:,i)=expm(T*h)*L1(:,i);
    L1=L;
end

% Iterative order 1
  IT(:,1)=yini;  IT1(:,1)=yini; Y0=zeros(size(yini));
for i=2:N+1
    IT(:,i)=expm(T*h)
    *(IT(:,i-1)+(h/2)*KT11*Y0)+((h/2)*KTT*Y0);
    IT1(:,i)=(expm((h/2)*(KTT+KT11))*(IT1(:,i-1)
    +((h/2)*T*IT(:,i-1))))+((h/2)*T*IT(:,i));
    Y0=IT1(:,i);
```

```
    IT=IT1;
%      IT(:,i)=expm((h/2)*(KTT+KT11))*(IT(:,i-1));
%      IT1(:,i)=(expm(T*h)*(IT1(:,i-1)
%+((h/2)*KT11*IT(:,i-1))))+((h/2)*KTT*IT(:,i));
%      IT=IT1;
%      IT(:,i)=expm((h/2)*((mat(E,t(i)+h)
%+mat(E,t(i)))))*(IT(:,i-1));
%      IT1(:,i)=(expm(T*h))*(IT1(:,i-1)
%+((h/2)*mat(E,t(i))*IT(:,i-1)))
%+((h/2)*(mat(E,t(i)+h)*IT(:,i)));

end

for i=1:N+1
    UL(i)=L1(i,end);
    UI(i)=IT1(i,end);
    EX2(i)=AAt(i,end);
end

for i=1:N+1
    ELie(i)=abs(UL(i)-EX2(i));
    EIt(i)=abs(UI(i)-EX2(i));
end

lie=max(ELie)
tr=max(EIt)

 plot(t,EX2,t,UL,'r',t,UI,'g')
 legend('Magnus','Lie-Trotter','Iterative')
 break
```

SECOND ORDER METHODS

```
 %%shrödinger equation with the potential is 4-3exp(-t)
 clear all;
 close all;
```

```
 N=100; t0=0; tson=3; h=(tson-t0)/(N);
 x0=-10; xson=10; dx=(xson-x0)/N;
 ep=1;
 t=t0:h:tson;
 x=x0:dx:xson;
%%%%%%%%initial condition
 coeff=0.751125544;
 C0=zeros(N+1,1);
for i=1:N+1
   C0(i)=coeff*exp((-1/2)*(((ep*x(i)))^2));
end
%%%%%%%%%%%% scalar matrix %%%%%%%%%%%%%%
 n=N;
 UU=toeplitz([-2 1 0 0    zeros(1,n-3)],
 [-2 1 0 0  zeros(1,n-3)]);
 US=(1/((dx)^2))*full(UU);
 BB=(-1/2)*US;
 T=[zeros(N+1) BB;-BB zeros(N+1)];
%%%%%%%%%  Time-dependent matrix %%%%%%%%
 H=zeros(N+1,N+1); R1=zeros(N+1,N+1); R2=zeros(N+1,N+1);
for i=1:N+1
   H(i,i)=shrodin(t(i)+(h/2),x(i));
end
 H1=[zeros(N+1) H;-H zeros(N+1)]; % the matrix
% for iterative splitting
 KT=zeros(N+1,N+1);   KT1=zeros(N+1,N+1);
for i=1:N+1
   KT(i,i)=shrodin(t(i)+(h),x(i));
   KT1(i,i)=shrodin(t(i),x(i));
end
 KTT=[zeros(N+1) KT;-KT zeros(N+1)];
 KT11=[zeros(N+1) KT1;-KT1 zeros(N+1)];
 KUT=T+KTT;
 KUTTA=T+KT11;
```

```
%%%%%%%%%%%% Initial Condition %%%%%%%%%%%
yini=[C0;zeros(N+1,1)];
yini1=yini;
%%%%%%%%%%%%%%% magnus-4  %%%%%%%%%%%%%
%Attt(:,1)=yini;
% M1=zeros(N+1,N+1); M2=zeros(N+1,N+1);
% c1=(1/2)-(sqrt(3)/6);
% c2=(1/2)+(sqrt(3)/6);
% for i=1:N+1
%     M1(i,i)=shrodin(t(i)+c1*h,x(i));
%     M2(i,i)=shrodin(t(i)+c2*h,x(i));
% end
% M11=[zeros(N+1) M1;-M1 zeros(N+1)];
% M22=[zeros(N+1) M2;-M2 zeros(N+1)];
%    A1=T+M11;
%    A2=T+M22;
% for k=2:N+1,
% F=expm(((h/2)*(A1+A2))-((sqrt(3)/12)*(h^2)*commut(A1,A2))
+((1/80)*(h^3)*commut(A1-A2,commut(A1,A2))))*yini1 ;
% yini1=F;
% Attt(:,k)=yini1;
% end
%%%%%%%%%%%% magnus-2 %%%%%%%%%%%%%%%
% %%%%%%%%%%%  No-splitting %%%%%%%%%%%%%%%%%
 yini2=yini; AAt(:,1)=yini;
 for k=2:N+1,
 R=expm(h*(T+H1))*yini2;
 yini2=R;
 AAt(:,k)=yini2;
 end
% %%%%%%%%%%%%% METHODS %%%%%%%%%%%%%%%%%%
 % symmetrically weighted
 SW1(:,:,1)=yini;    SWS(:,:,1)=yini;
 SW2(:,:,1)=yini; K1= expm(h*H1);  GG=expm(T*h);
```

```
 for i=2:N+1
     SW1(:,:,i)=GG*K1*SWS(:,:,i-1);
     SW2(:,:,i)=K1*GG*SWS(:,:,i-1);
     SWS(:,:,i)=(SW1(:,:,i)+SW2(:,:,i))/2;
 end
 % Strang Splitting
  ST(:,:,1)=yini;
 for i=2:N+1
    ST(:,:,i)=expm(T*(h/2))*K1*expm(T*(h/2))*ST(:,:,i-1);
 end

%  % Iterative 2
%  GG=expm(T*h);
%  JJ=expm((h/2)*(KT11+KTT));
% %   IT2(:,1)=yini; IT1(:,1)=yini;
% %  ITS(:,1)=yini;
%  IT2(:,:,1)=yini; IT1(:,:,1)=yini;
%  ITS(:,:,1)=yini;
 for i=2:N+1
 %%This part can be used for the probability for different
 %% potential at a certain time.
% % IT1(:,i)=JJ*(IT1(:,i-1));
% % IT2(:,i)=(GG*(IT2(:,i-1)+
% %(h/2)*KT11*IT1(:,i-1)))+((h/2)*KTT*IT1(:,i));
% % ITS(:,i)=(JJ*(ITS(:,i-1)
% %+((h/2)*(T)*IT2(:,i-1))))+((h/2)*T*IT2(:,i)) ;
% % IT1=ITS;
% % IT2=ITS;
% %%%%%%%%%%%%
 IT1(:,:,i)=JJ*(IT1(:,:,i-1));
 IT2(:,:,i)=(GG*(IT2(:,:,i-1)+(h/2)*KT11*IT1(:,:,i-1)))
 +((h/2)*KTT*IT1(:,:,i));
 ITS(:,:,i)=(JJ*(ITS(:,:,i-1)+((h/2)*(T)*IT2(:,:,i-1))))
 +((h/2)*T*IT2(:,:,i));
```

```
 IT1=ITS;
 IT2=ITS;
 end

%%%%%%%Runge-Kutta
%  RUNG(:,1)=yini;
% for i=2:N
%      tild=RUNG(:,i-1)+(h*KUTTA*RUNG(:,i-1));
%      RUNG(:,i)=RUNG(:,i-1)+((h/2)*
%(KUTTA*RUNG(:,i-1)+(KUT*tild)));
% end
%%%Probability part
for i=1:N+1
 ENEIT(i,:,:)= (ITS(i,:,:).^2 +ITS(N+1+i,:,:).^2);
 %ENESTR(i,:,:)= (ST(i,:,:).^2 +ST(N+1+i,:,:).^2);
 %ENESWS(i,:,:)= (SWS(i,:,:).^2 +SWS(N+1+i,:,:).^2);
 %%prob. for certain time
 %ENEIT(i,:)= (ITS(i,:).^2 +ITS(N+1+i,:).^2);
end

figure(1)
 [X,Y] = meshgrid(t0:h:tson, x0:dx:xson);
 Z = ENEIT;
 surf(X,Y,Z)
 xlabel('t')
 ylabel('x')
 zlabel('probability density')
%figure(2)
%
%[X,Y] = meshgrid(t0:h:tson, x0:dx:xson);
%Z = ENESWS;
%surf(X,Y,Z)
%xlabel('t')
%ylabel('x')
```

```
%zlabel('probability density of SWS')

%figure(3)
%[X,Y] = meshgrid(t0:h:tson, x0:dx:xson);
%Z = ENESTR;
%surf(X,Y,Z)
%xlabel('t')
%ylabel('x')
%zlabel('probability density of SMS')

%%%%plottin for probability for a certain time
%plot(x,ENEIT(:,end),x,ENEIT(:,1),'r')% figure
%  legend('t=t_{end}','t=t_0')
%  xlabel('x')
%  ylabel('probability')
%break
```

THE PROGRAMME WHICH IS USED IN FIRST AND SECOND ORDER METHODS

```
  %time dependent part
function y=shrodin(t,x)
ep=1;
 K=ep*((4-(3*(exp(-t))))*((x^2)-1))/2;
 %K=ep*((cos(t))^2)*((x^2)-1))/2;
 y=K;
```