Computational methods for highly oscillatory partial differential equations

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OŚWIADCZENIA

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data *podpis*

Wyrażam zgodę na udostępnienie osobom zainteresowanym mojej pracy dyplomowej dla celów naukowo-badawczych. Zgoda na udostępnienie pracy dyplomowej nie oznacza wyrażenia zgody na kopiowanie pracy dyplomowej w całości lub w części.

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Abstract

In this dissertation, we are concerned with finding an approximate solution to the linear partial differential equations with a highly oscillatory potential function and a strongly elliptic differential operator. We consider evolution equations involving first- or second-time derivatives, such as the heat equation or the wave equation. Such equations present significant challenges in numerical treatment and standard methods are mostly ineffective for them.

In the first part of the thesis, we analytically derive the Modulated Fourier expansion for a linear partial differential equation with a multifrequency highly oscillatory potential. The Modulated Fourier expansion (MFE) is an important technique in computational mathematics used, *inter alia*, to study the long–time behavior of Hamiltonian systems with highly oscillatory solutions. Moreover, MFE can be utilized in numerical-asymptotic approach as an ansatz for finding approximate solution to linear or nonlinear highly oscillatory differential equations. To derive the Modulated Fourier Expansion for the considered problem, we show that the solution of the equation is expressed as a convergent Neumann series in the appropriate Sobolev space. Then, by using integration by parts and the theory of semigroups, we expand asymptotically each of integrals from the Neumann series into a sum of known coefficients. By organizing terms appropriately we obtain formulas for the coefficients of the Modulated Fourier expansion. The proposed approach enables, firstly, to determine the coefficients for this expansion and secondly, to derive a general formula for the error associated with the approximation of the solution by MFE.

In the second part of the thesis we propose, using the results of the first part, a third-order numerical integrator based on the Neumann series and the Filon quadrature, designed mainly for highly oscillatory partial differential equations. The method can be applied to equations that exhibit small or moderate oscillations; however, counter-intuitively, large oscillations increase the accuracy of the scheme. The proposed approach enables the easy improvement of the method's accuracy and the straightforward estimation of its error.

The proposed computational methods are illustrated with many examples. For each equation in the numerical examples of this dissertation, we know the analytical solution. Thus, we do not need to compute reference solutions using a supercomputer. Using the proposed methods, we can accurately compare the numerical approximation with the function satisfying the equation.

Streszczenie

W niniejszej rozprawie zajmujemy się problemem aproksymacji rozwiązania wysoko oscylującego równania różniczkowego cząstkowego z silnie eliptycznym operatorem różniczkowym. Rozważamy równania ewolucyjne z pierwszą lub drugą pochodną względem zmiennej czasowej. Oscylacje są wywoływane przez funkcję potencjału równania. Takie równania są trudne w aproksymacji numerycznej, ponieważ standardowe i dobrze znane metody są dla nich zazwyczaj nieskuteczne.

W pierwszej części rozprawy wyprowadzamy analitycznie zmodyfikowane rozwinięcie Fouriera dla liniowego równania różniczkowego cząstkowego z wysoko oscylującą funkcją potencjału z wieloma częstotliwościami. Zmodyfikowane rozwinięcie Fouriera (w skrócie piszemy MFE) jest ważnym narzędziem w matematyce obliczeniowej, które jest wykorzystywane między innymi do badania zachownania rozwiązania wysoko oscylującego równania Hamiltona na długim przedziale czasowym. Ponadto MFE może być również wykorzystywane w numeryczno-asymptotycznym podejściu jako ansatz w celu znale–zienia przybliżonego rozwiązania liniowego lub nieliniowego wysoko oscylującego równania różniczko–wego. Aby analitycznie wyprowadzić zmodyfikowane rozwinięcie Fouriera dla rozważanego problemu na początku pokazujemy, że rozwiązanie równania może być przedstawione jako suma zbieżnego szeregu Neumanna w odpowiedniej przestrzeni Sobolewa. Następnie, korzystając z całkowania przez części i teorii półgrup, rozwijamy asymptotycznie wyrazy szeregu Neumanna w sumy o znanych współczynnikach. Grupując odpowiednio wyrazy otrzymujemy poszukiwane rozwinięcie asymptotyczne równania. Proponowane podejście umożliwia po pierwsze wyznaczenie współczynników MFE, a po drugie oszacowanie błędu wynikającego z aproksymacji rozwiązania przez zmodyfikowane rozwinięcie Fouriera.

W drugiej części rozprawy wykorzystujemy wyniki z pierwszej części pracy i przedstawiamy metodę numeryczną tworzoną w oparciu o szereg Neumanna i kwadraturę Filona. Metoda może być stosowana do równań które nie oscylują, jednakże wbrew intuicji duże oscylacje zwiększają dokładność schematu numerycznego. Proponowane podejście pozwala na łatwe szacowanie błędu metody i umożliwia poprawę rzędu zbieżności w prosty sposób.

Metody obliczeniowe które prezentujemy w rozprawie, są ilustrowane wieloma przykładami. Dla każdego równania w przykładach numerycznych znamy rozwiązanie analityczne. Nie musimy więc obliczać rozwiązań referencyjnych za pomocą superkomputera. Możemy dokładnie porównać aproksymację numeryczną przy użyciu proponowanych metod z funkcją spełniającą równanie.

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Contents

Notations

Ω	open and bounded subset of $\mathbb{R}^m$ with smooth boundary
$L^2(\Omega)$	standard L^2 space with norm $\|u\|_2 = \left(\int_\Omega \|u(x)\|^2 \mathrm{d}x\right)^{1/2}$
$H^{2p}(\Omega)$	standard Sobolev space with norm $\|u\|_{H^{2p}(\Omega)} = \left(\sum_{\|\boldsymbol{p}\| \le 2p} \|D^{\boldsymbol{p}} u\|_2^2\right)^{1/2}$
$\boldsymbol{p} = (p_1, \ldots, p_m)$	multi-index notation, $\|\boldsymbol{p}\| = p_1 + \cdots + p_m$
$C_c^\infty(\Omega)$	set of smooth functions with compact support
$H_0^p(\Omega)$	the closure of $C_c^\infty(\Omega)$ in $H^p(\Omega)$
$\|T\|_{X \leftarrow X}$	operator norm, $\|T\|_{X \leftarrow X} = \sup_{\|v\|_X \le 1} \|Tv\|_X$, where $\| \ \|_X$ is a norm in space X
$C([0, t^\star], X)$	space of all continuous functions $u: \ [0, t^\star] \to X$ such that $\max_{t \in [0, t^\star]} \|u(t)\|_X < \infty$, where $\| \ \|_X$ is a norm in space X
$C^k([0, t^\star], X)$	space of all functions $u : [0, t^\star] \to X$ whose derivatives in $[0, t^\star]$ up to order k are in $C([0, t^\star], X)$
$\mathcal{L}$	linear differential operator
$\sigma_d(t)$	d-dimensional simplex with vertices $(0, \ldots, 0), (0, \ldots, 0, t), \ldots, (t, \ldots, t)$
$\mathcal{O}(\cdot)$	big-O notation

Chapter 1

Introduction

This thesis is concerned with presenting computational methods for highly oscillatory partial differential equations. To be precise, the subject of our consideration is the following problem

$$\begin{aligned}&\partial_t u(x,t) = \mathcal{L}u(x,t) + f(x,t)u(x,t), \qquad t \in [0,t^\star], \quad x \in \Omega \subset \mathbb{R}^m,\\&u(x,0) = u_0(x), \quad x \in \Omega,\end{aligned} \tag{1.1}$$

with zero boundary conditions, where domain Ω is an open and bounded subset of $\mathbb{R}^m$, $t^\star > 0$ and $\mathcal{L}$ is a linear differential operator. Complex valued function $f(x,t)$ from the equation (1.1) is a highly oscillatory of type

$$f(x,t) = \sum_{\substack{n=-N\\n\neq 0}}^{N} \alpha_n(x,t)e^{in\omega t}, \quad \omega \gg 1, \quad N \in \mathbb{N}, \tag{1.2}$$

where frequency parameter ω is assumed to be large. Such equations appear in many 'real-life' problems and play a significant role in electronic engineering, electromagnetics, quantum mechanics, and computing scattering frequencies. Apart from the many applications, highly oscillatory phenomena are fascinating objects to study from the mathematical point of view as they are common in many mathematical problems and are difficult in numerical approximation. For this reason, they are the subject of active study by many mathematicians.

Highly oscillatory differential equations may be split into equations with intrinsic and extortionist high oscillation. The former are generated by the inner nature of the equation. The important examples include the Airy equation

$$u''(t) + k^2 t u(t) = 0,$$

the semiclassical Schrödinger equation

$$\mathrm{i}\epsilon\partial_t u(x,t) = -\frac{\epsilon^2}{2}\Delta u(x,t) - V(x)u(x,t),$$

for $(x,t) \in \mathbb{R}^d \times \mathbb{R}$, where $\epsilon \ll 1$ is a small parameter, and the following system of differential equations

$$\ddot{x} = \Omega^2 x + g(x), \qquad \Omega = \begin{pmatrix} 0 & 0 \\ 0 & \omega I \end{pmatrix}, \tag{1.3}$$

where $\omega \gg 1$, $x = x(t)$, $\ddot{x} = x''(t)$, and g is a non-linear function. The equation (1.3) is important in computational mathematics as it is strongly connected with a Fermi–Pasta–Ulam Problem, [17].

In this thesis, we focus on finding an approximate solution for the second type of highly oscillatory differential equation, in which the highly oscillatory nature of the equation is imposed by the external source of type (1.2). An example of such an equation is (1.1), which we will work on.

1.1 Why not the standard numerical schemes?

In traditional numerical methods applied to highly oscillatory problems, it is usually required that the time step h satisfies the condition $h\omega < 1$. This causes the method to become extremely expensive when ω is large. This occurs because conventional schemes are constructed using Taylor expansions, where error formulas involve expressions with high derivatives of a highly oscillatory function. To provide a more detailed understanding of the challenges associated with the numerical approximation of highly oscillatory differential equations, let us apply Duhamel's formula to equation (1.1) and write it in the following integral form

$$u(t+h) \quad = \quad \mathrm{e}^{h\mathcal{L}} u(t) + \int_0^h \mathrm{e}^{(h-\tau)\mathcal{L}} f(t+\tau) u(t+\tau) \mathrm{d}\tau, \tag{1.4}$$

where u_0 and $f(s)$, $u(s)$ for fixed s are elements of appropriate Banach spaces and $\{\mathrm{e}^{t\mathcal{L}}\}_{t\geq 0}$ is a semigroup operator. Let us note that $f^{(k)}(t) = \mathcal{O}(\omega^k)$, and therefore the magnitudes of subsequent time-derivatives of functions u and f grow drastically. This implies that approximating the integral from equation (1.4) using standard quadrature rules, as in basic numerical schemes, leads to a significant error.

Example 1. *Consider a simple ODE*

$$\begin{aligned} &u'(t) = tu(t) + \cos(\omega t) u(t), \qquad t \in [0,1], \\ &u(0) = 1, \end{aligned} \tag{1.5}$$

with parameter $\omega \gg 1$. *The analytical solution of (1.5) is equal to*

$$u(t) = \mathrm{e}^{\sin(\omega t)/\omega + t^2/2}.$$

To find an approximate solution of equation (1.5), we employ the well-known fourth-order Runge–Kutta scheme

$$\begin{aligned} k_1 &= f(u_n, t_n), \\ k_2 &= f(u_n + \frac{k_1 h}{2}, t_n + \frac{h}{2}), \end{aligned}$$

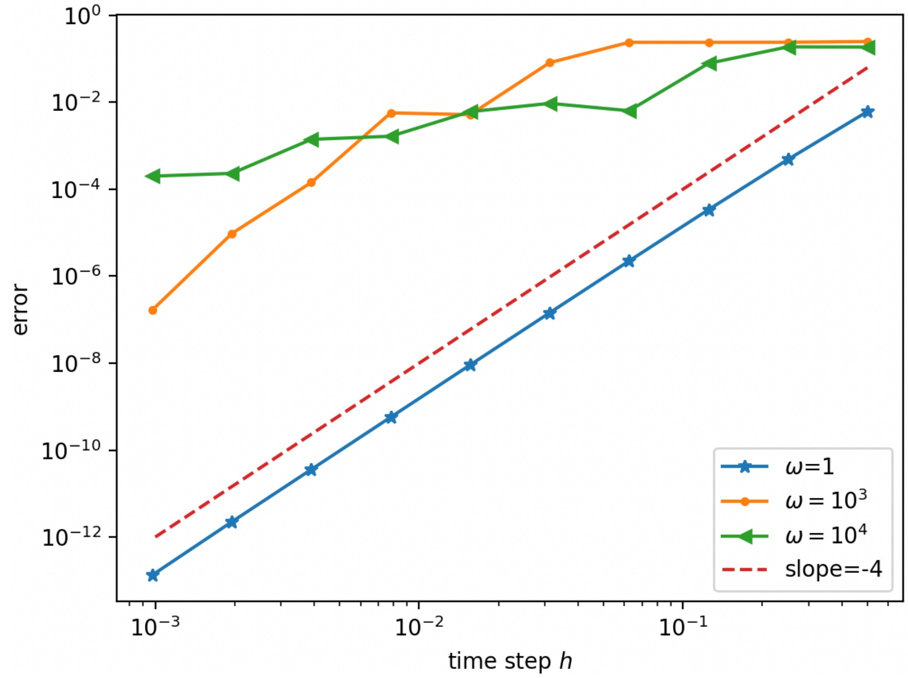


Figure 1.1: Error of approximation in the L^2-norm of the solution to equation (1.5) by the fourth-order Runge–Kutta scheme, for different values of parameter ω.

$$\begin{aligned} k_3 &= f(u_n + \frac{k_2 h}{2}, t_n + \frac{h}{2}), \\ k_4 &= f(u_n + hk_3, t_n + h), \\ u_{n+1} &= u_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4), \end{aligned}$$

where h is a sufficiently small time step, function f is given by $f(u,t) = tu + \cos(\omega t)u$ and $u_0 = u(0) = 1$. In the above scheme $u_N \approx u(1)$, $N = 1/h$. Figure (1.1) presents the error of approximation the solution to equation (1.5) by the Runge–Kutta fourth-order method, for a few values of parameter ω. While for $\omega = 1$ the numerical scheme provides the expected fourth-order accuracy, larger oscillatory parameters such as $\omega = 10^3$ or $\omega = 10^4$ spoil the convergence rate and significantly increase the error constant. The reason for this is the dependence of the method's error on higher-order time derivatives of the solution. This is unfavourable in highly oscillatory problems because the magnitude of the error is directly proportional to the magnitude of ω^m for certain $m > 1$. For that reason, there is a need to look for alternative, more efficient methods for highly oscillatory problems. As we will see, counter-intuitively, high oscillations facilitate finding approximate solutions of differential equations, as long as we consider the problem more carefully and use appropriate methods dedicated to highly oscillatory phenomena.

It should also be mentioned that modern computational mathematics focuses not only on providing fast and accurate numerical method but also that the method should preserve some relevant invariants and geometric properties of the equations. The examples of the typical invariants important in differential equations derived from physics are the conservation of energy and the preservation of unitarity. A branch of computational mathematics that focuses on the study of qualitative features of differential equations is Geometric Numerical Integration [5, 17]. This approach provides that numerical methods can be effective over a long time interval.

This dissertation is written based on two papers [28] and [29], in which we propose two methods to approximate the solution to equation (1.1). The paper [28] is a generalisation of the results first obtained in the article [23]. The research presented in articles [23, 28] was motivated by the paper [12].

1.2 Asymptotic expansion of a highly oscillatory solution

Suppose that $u(x,t)$ is the solution of the equation (1.1). In paper [28], we aim to present the solution $u(x,t)$ as the following partial sum of the asymptotic expansion

$$u(x,t) = \underbrace{p_{0,0}(x,t) + \sum_{r=1}^{R} \frac{1}{\omega^r} \sum_{s=-S}^{S} p_{r,s}(x,t) e^{is\omega t}}_{=:U_{as}^{[R]}(t)} + \frac{1}{\omega^{R+1}} E_{R,S}(x,t), \quad \omega \gg 1, \tag{1.6}$$

for any time variable $t > 0$, where coefficients $p_{r,s}(x,t)$ and magnitude of error constant $E_{R,S}(x,t)$ are independent of ω. The asymptotic expansion $U_{as}^{[R]}(t)$ of type 1.6 is also known as a Modulated Fourier expansion (MFE) or frequency expansion. Approximating the highly oscillatory solution by the sum $U_{as}^{[R]}(t)$ has several advantages. If parameter ω is large, then it seems that only the first few terms of sum (1.6) are necessary to provide a good approximation, and the remaining terms become less relevant. Furthermore, increasing the parameter ω should improve the accuracy of approximating $u(x,t)$ by sum (1.6). On the other hand, as we have already seen, the larger value of ω, the more inefficient the Runge-Kutta scheme becomes, see Figure 1.1.

The Modulated Fourier expansion (1.6) is an important technique in computational mathematics used, *inter alia*, for analysing highly oscillatory ODEs or PDEs over long times [7, 15, 16, 24, 31, 34]. A detailed description of the Modulated Fourier expansion can be found in [17]. Furthermore, MFE can be utilized in numerical-asymptotic approaches as an ansatz for solving numerically linear or nonlinear highly oscillatory differential equations [9, 10, 12]. In short, this ansatz is inserted into the equation, and subsequently, the coefficients $p_{r,s}$ in the sum (3.4) are determined either recursively or numerically by solving non-oscillatory differential equations. This approach allows us to approximate highly oscillatory equations with great accuracy.

In our approach, we do not assume that the ansatz (1.6) solves equation (1.1). Instead, we demonstrate that the solution of equation (1.1) can be expressed as a sum of type (1.6), and we derive the coefficients of expansions (1.6) purely analytically. In addition, so far it is known that the sum $U_{as}^{[R]}(t)$ approximates the solution with an error of form $C\omega^{-R-1}$, but the constant C is unknown. Our approach enables us to derive a formula for this constant. This may be important in practise, as this constant can be large, especially when the number R in sum $U_{as}^{[R]}(t)$ is big.

To express the solution of equation (1.1) as a partial sum of the asymptotic expansion of type (1.6), we show that the Neumann series converges to the solution in $H^{2p}(\Omega)$ Sobolev norm for any time variable $t > 0$, where $2p$ is the order of a differential operator $\mathcal{L}$. Any term of the Neumann series is expressed by a sum of multivariate integrals. By using integration by parts and the theory of semigroups, we expand asymptotically each of highly oscillatory integrals from the Neumann series into a sum of known coefficients. By organizing terms appropriately with respect to magnitudes ω^{-r} and frequencies $e^{is\omega t}$, we obtain sum (1.6). We also consider the occurrence of the resonance points in highly oscillatory integrals from the Neumann series. This issue will be discussed more precisely in Chapter 3. The paper [28] describes this result and will be discussed in Chapter 3.

1.3 Numerical integrator for highly oscillatory equation based on the Neumann series

The method based on the asymptotic expansion of the solution briefly described in Section 1.2, is low-cost, effective, and provides a small error for highly oscillatory equations. However, although the sum $U_{as}^{[R]}(t)$ yields an excellent numerical approximation, for fixed parameter ω in general it does not converge to the solution of the equation (1.1) as $R \to \infty$. To overcome this limitation, using the results presented in [28], in paper [29], instead of approximating the integrals which appearing in the Neumann series by the partial sum of the asymptotic expansion, we approximate them by the Filon method. The Filon method is a quadrature rule designed for highly oscillatory integrals. Using this approach, we obtain a third-order numerical scheme that converges to the solution as the step size $h \to 0$ and/or as $\omega \to \infty$. The local error of the proposed method is bounded by $C \min\left\{h^4, h^2\omega^{-2}, \omega^{-3}\right\}$, where the constant C is independent of both h and ω. Therefore, the numerical integrator can also be applied to equations with small or moderate oscillation; however, large oscillations significantly enhance the accuracy of the scheme. The proposed approach based on the Neumann series enables improvement of the method's accuracy and straightforward estimation of its error. Moreover, by representing the solution as the Neumann series, the time derivatives of the solution, which can be large for highly oscillating equations, do not appear in the error formula of the numerical scheme. The paper [29] describes this numerical method and will be presented in Chapter 4.

Due to the generality of equation (1.1), both methods can also be applied to differential equations with a second-time derivative, such as the wave equation or the Klein-Gordon equation.

The proposed numerical methods are illustrated by numerous examples. We know the analytical solution for each equation in the numerical examples of this dissertation. This facilitates an accurate and precise comparison of the solution with the numerical approximation using the proposed methods.

Let us also note that long and technical proofs of the theorems in this dissertation are provided in the Appendix.

Chapter 2

Basic tools

In this chapter, we introduce important concepts, definitions, and present some theory that will be used in Chapter 3 and Chapter 4. For more details about the applications of the semigroup theory to partial differential equations, we refer to [14, 27]. Quadrature methods for highly oscillatory integrals are presented in [13], while details about the spectral and the splitting methods can be found in [32, 33], [25].

2.1 Application of the semigroup theory to PDEs

The theory of semigroup is widely utilized in computational mathematics as a useful and practical tool for investigating partial differential equations. This chapter discusses the basic properties of the semigroup operator and application of semigroup theory to PDEs.

For certain type of differential operator $\mathcal{L}$, and suitable initial-boundary conditions, the abstract Cauchy problem

$$\begin{cases} \partial_t u(x,t) = \mathcal{L}u(x,t), \quad x \in \Omega, \quad t > 0, \\ u(x,0) = u_0(x), \end{cases} \tag{2.1}$$

has a solution that can be written as $u(x,t) = [\boldsymbol{u}(t)](x) = S(t)u_0$, for some bounded linear operator $S(t) = \mathrm{e}^{t\mathcal{L}} : H \to H$, where H is an appropriate Hilbert space. This leads to the following definitions. Let X be a Banach space.

Definition 1. *A family $\{S(t)\}_{t\geq 0}$ of bounded linear operators $S(t) : X \to X$ is called a C_0-semigroup, or strongly continuous semigroup, if*

1. $S(0)u = u, \quad \forall\, u \in X,$
2. $S(t+s)u = S(t)S(s)u, \quad \forall\, t, s \geq 0,\ \forall\, u \in X,$
3. *$\forall\, u \in X$ the mapping $[0,\infty) \ni t \mapsto S(t)u$ is continuous.*

Definition 2. *Let $D(\mathcal{L})$ be a set defined by*

$$D(\mathcal{L}) = \{u \in X : \lim_{t\to 0^+} \frac{S(t)u - u}{t} \text{ exist in } X\}. \tag{2.2}$$

Then operator $\mathcal{L} : D(\mathcal{L}) \to X$ *such that*

$$\mathcal{L}u := \lim_{t\to 0^+} \frac{S(t)u - u}{t} \quad \textit{for} \quad u \in D(\mathcal{L}), \tag{2.3}$$

is called the infinitesimal generator of the semigroup $\{S(t)\}_{t\geq 0}$.

To refer to the semigroup operator $\{S(t)\}_{t\geq 0}$ we will also write $\mathrm{e}^{t\mathcal{L}} := S(t)$ for all $t \geq 0$.

Theorem 1. *Let* $u \in D(\mathcal{L})$. *Then, for the strongly continuous semigroup operator* $\{S(t)\}_{t\geq 0}$ *the following properties hold*

1. $S(t)u \in D(\mathcal{L})$ *for each* $t \geq 0$,
2. $\frac{d}{dt}S(t)u = \mathcal{L}S(t)u = S(t)\mathcal{L}u$ *for each* $t > 0$.

Proposition 1. *For strongly continuous semigroup operator* $\{S(t)\}_{t\geq 0}$, *there exist constants* $\omega \in \mathbb{R}$ *and* $M \geq 1$ *such that*

$$\|S(t)\|_{X\leftarrow X} \leq M\mathrm{e}^{\omega t},$$

for all $t \geq 0$.

Definition 3. *A linear operator* $\mathcal{L} : D(\mathcal{L}) \to X$ *is called closed if for any sequence* $u_k \in D(\mathcal{L})$, *such that* $u_k \to u$ *and* $\mathcal{L}u_k \to v$ *as* $k \to \infty$, *then* $u \in D(\mathcal{L})$ *and* $v = \mathcal{L}u$.

Theorem 2. *If* $\mathcal{L}$ *is the infinitesimal generator of strongly continuous semigroup* $\{S(t)\}_{t\geq 0}$, *then* $D(\mathcal{L})$ *is dense in* X *and* $\mathcal{L}$ *is a closed operator.*

Theorem 3. *Suppose that* $\mathcal{L}$ *is a closed linear operator,* $\{S(t)\}_{t\geq 0}$ *is a semigroup generated by* $\mathcal{L}$ *and function* $f \in C([0,t^\star], D(\mathcal{L}))$. *Then*

$$\mathcal{L}\int_0^t S(t-\tau)f(\tau)\mathrm{d}\tau = \int_0^t S(t-\tau)\mathcal{L}f(\tau)\mathrm{d}\tau, \tag{2.4}$$

for any $t \leq t^\star$.

Proofs of the above theorems can be found in almost every book dedicated to semigroup theory (for example, in [14, 27, 30]).

We are mainly interested in the application of the semigroup theory to partial differential equations. Let Ω be an open and bounded in $\mathbb{R}^m$ set with smooth boundary $\partial\Omega$. We assume that $\mathcal{L}$ is a differential operator of order $2p$

$$\mathcal{L} = \sum_{|\boldsymbol{p}|\leq 2p} a_{\boldsymbol{p}}(x)D^{\boldsymbol{p}}, \qquad D^{\boldsymbol{p}} = \frac{\partial^{p_1}}{\partial x_1^{p_1}}\frac{\partial^{p_2}}{\partial x_2^{p_2}}\cdots\frac{\partial^{p_m}}{\partial x_m^{p_m}}, \quad x \in \Omega \subset \mathbb{R}^m, \tag{2.5}$$

where multi-index $\boldsymbol{p} = (p_1, \ldots, p_m)$ is an m-tuple of non-negative integers and $a_{\boldsymbol{p}}$ are smooth, complex-valued functions on $\bar{\Omega}$. Domain of $\mathcal{L}$ is the set $D(\mathcal{L}) = H^{2p}(\Omega) \cap H_0^p(\Omega)$, where $H^{2p}(\Omega)$ is the standard Sobolev space. The space $H_0^p(\Omega)$ is the closure of $C_c^\infty(\Omega)$ in $H^p(\Omega)$, where $C_c^\infty(\Omega)$ consists of smooth functions with compact support. The space $D(\mathcal{L}) = H^{2p}(\Omega) \cap H_0^p(\Omega)$ is also Banach space with norm $\| \ \|_{D(\mathcal{L})} = \| \ \|_{H^{2p}(\Omega)}$.

Theorem 4. *Let $u, v \in H^p(\Omega)$ and let Ω be a domain in $\mathbb{R}^m$ with smooth boundary $\partial\Omega$. If $2p > m$, then product $uv \in H^p(\Omega)$. Moreover, there exist a constant $C > 0$ depending on p, m and Ω such that*

$$\|uv\|_{H^p(\Omega)} \leq C\|u\|_{H^p(\Omega)}\|v\|_{H^p(\Omega)}. \tag{2.6}$$

Proof of the above theorem can be found in [1].

Theorem 5. *Let $\Omega \subset \mathbb{R}^m$, $4p > m$ and let functions $u \in D(\mathcal{L}) = H^{2p}(\Omega) \cap H_0^p(\Omega)$, $f \in H^{2p}(\Omega)$. Then $uf \in D(\mathcal{L})$.*

Definition 4. *Let A be the differential operator of form (2.5). We say that the operator A is strongly elliptic if there exist a constant $\theta > 0$ such that*

$$Re(-1)^p \sum_{|\boldsymbol{p}|=2p} a_{\boldsymbol{p}}(x)\xi^{\boldsymbol{p}} \geq \theta|\xi|^{2p} \tag{2.7}$$

for all $x \in \bar{\Omega}$ and $\xi \in \mathbb{R}^m$, where $\xi^{\boldsymbol{p}} = \xi_1^{p_1}\xi_2^{p_2}\dots\xi_m^{p_m}$, $|\xi| = \sum_{j=1}^m \xi_j$.

We state two important theorems that are central to the considerations presented in Chapters 3 and 4 (for more details we refer to [27]).

Theorem 6. *Let $-\mathcal{L}$ be a strongly elliptic operator of order $2p$ on a bounded domain $\Omega \subset \mathbb{R}^m$ with smooth boundary $\partial\Omega$. Then $\mathcal{L}$ is the infinitesimal generator of a strongly continuous semigroup on $L^2(\Omega)$.*

Theorem 7. *Let $\Omega \subset \mathbb{R}^m$ be a bounded domain with smooth boundary $\partial\Omega$. Assume that $-\mathcal{L}$ is a strongly elliptic operator in Ω of order $2p$ with smooth coefficients $a_{\boldsymbol{p}}(x)$ of $\bar{\Omega}$. If $u \in H^{2p}(\Omega) \cap H_0^p(\Omega)$ then the following a-priori estimate holds*

$$\|u\|_{H^{2p}(\Omega)} \leq C\left(\|\mathcal{L}u\|_{L^2(\Omega)} + \|u\|_{L^2(\Omega)}\right), \tag{2.8}$$

where constant C is independent of u.

Note that we do not need to restrict ourselves to the differential operator $\mathcal{L}$ of even degree or defined on a bounded domain Ω. It is sufficient for $\mathcal{L}$ to be an infinitesimal generator of a strongly continuous semigroup on an appropriate Banach space. The following question arises: what type of differential operators are generators of a strongly continuous semigroup? Well-known theorems, such as the Hille-Yosida theorem, the Lumer-Phillips theorem and Stone's theorem, characterize the generators of strongly continuous semigroups of linear differential operators on Banach space.

2.2 Computational methods for the Cauchy problem

A natural question arises how to effectively approximate expressions of the form $\mathrm{e}^{t\mathcal{L}}$, where $\mathcal{L}$ is a differential operator (2.5). Recall that $\mathrm{e}^{t\mathcal{L}}u_0$ is the solution of the Cauchy problem

$$\begin{cases} \partial_t u(x,t) = \mathcal{L}u(x,t), \quad x \in \Omega, \quad t > 0, \\ u(x,0) = u_0(x), \\ u(x,t) = 0, \quad x \in \partial\Omega. \end{cases} \tag{2.9}$$

With luck, we can find an analytical solution, but usually it is difficult, or even impossible to find a formula that satisfies the above problem. To compute $\mathrm{e}^{t\mathcal{L}}u_0$, we will take advantage of spectral and splitting methods, important tools in numerical analysis.

2.2.1 Spectral methods

This section describes basic facts concerning spectral methods. Suppose that $N \in \mathbb{N}$ is an even number. A periodic function can be expanded into a Fourier series, provided it is sufficiently regular. Therefore, one can approximate the 2π-periodic function v in $[0, 2\pi]$ by a trigonometrical polynomial, which results from the truncation of the Fourier series

$$v(x) \approx \sum_{k=-N/2+1}^{N/2} c_k \mathrm{e}^{\mathrm{i}kx},$$

where

$$c_k = \frac{1}{2\pi}\int_0^{2\pi} v(s)\mathrm{e}^{-\mathrm{i}ks}\mathrm{d}s.$$

If function $v(x)$ is smooth and periodic, coefficient c_k can be approximated by the trapezoidal rule with excellent accuracy

$$c_k = \frac{1}{2\pi}\int_0^{2\pi} v(s)\mathrm{e}^{-\mathrm{i}ks}\mathrm{d}s \approx \frac{1}{N}\sum_{j=1}^{N} v\left(\frac{2\pi j}{N}\right)\mathrm{e}^{-\mathrm{i}k2\pi j/N} =: \hat{v}_k.$$

Let now introduce the N-equispaced grids $\{x_1, \ldots, x_N\}$ on the interval $[0, 2\pi]$

$$x_j = jh = j\frac{2\pi}{N}, \quad 1 \le j \le N, \quad h = \frac{2\pi}{N}, \tag{2.10}$$

and the set of the corresponding values $\{v_1, \ldots, v_N\}$, where $v_j = v(x_j), \quad j = 1, \ldots, N$. A discrete Fourier transform is a sequence $\{\hat{v}_k\}_{k=-\frac{N}{2}+1}^{\frac{N}{2}}$, such that

$$\hat{v}_k = \frac{1}{N}\sum_{j=1}^{N} \mathrm{e}^{-ikx_j}v_j, \quad k = -\frac{N}{2}+1, \ldots, \frac{N}{2}. \tag{2.11}$$

The inverse discrete Fourier transform is given by

$$v_j = \sum_{k=-N/2+1}^{N/2} \mathrm{e}^{\mathrm{i}kx_j} \hat{v}_k, \quad j = 1, \ldots, N. \tag{2.12}$$

Based on (2.12) we define interpolating function p (interpolating polynomial) such that

$$p(x) = \sum_{k=-N/2+1}^{N/2} \mathrm{e}^{\mathrm{i}kx} \hat{v}_k,$$

with $\hat{v}_k$ given by (2.11). Since $\{\hat{v}_k\}$ is N-periodic, for even N we have $\hat{v}_{-N/2} = \hat{v}_{N/2}$. Straightforward calculations show that function $p(x)$ is equal to [32]

$$p(x) = \sum_{j=1}^{N} v(x_j) h_j(x), \tag{2.13}$$

where

$$h_j(x) = \frac{1}{N} \sin\left(N \frac{x - x_j}{2}\right) \cot\left(\frac{x - x_j}{2}\right).$$

In addition, one can show that function p satisfies

$$p(x_j) = v(x_j), \quad j = 1, \ldots, N,$$

therefore trigonometric polynomial p is the interpolant of function v. By w_j we denote the approximation of the derivative of the function v at the point x_j

$$w_j \approx v'(x_j).$$

Having the interpolating polynomial p we set

$$w_k = p'(x_k) = \sum_{j=1}^{N} v(x_j) h_j'(x_k) \tag{2.14}$$

The formula (2.14) can be written in a matrix form

$$\boldsymbol{w} = \mathcal{K}_1 \boldsymbol{v},$$

where

$$\begin{aligned} \boldsymbol{w} &= (w_1, w_2, \ldots, w_N)^T, \\ \boldsymbol{v} &= (v(x_1), v(x_2), \ldots, v(x_N))^T, \end{aligned}$$

and $\mathcal{K}_1 \in M_{N\times N}(\mathbb{R})$ is the first order differentiation matrix. The entries $(\mathcal{K}_1)_{k,j},\ k,j=1,\dots,N$ of matrix $\mathcal{K}_1$ can be derived explicitly by computing the derivative of function p at point $x_k,\ k=1,\dots,N$

$$(\mathcal{K}_1)_{k,j} = \begin{cases} 0 & \text{if } j=k, \\ \frac{(-1)^{k+j}}{2}\cot\frac{(k-j)h}{2} & \text{if } j\neq k. \end{cases}$$

Similarly, one can compute the entries $(\mathcal{K}_2)_{k,j},\ k,j=1,\dots,N$ of the second order differentiation matrix $\mathcal{K}_2 \in M_{N\times N}(\mathbb{R})$

$$(\mathcal{K}_2)_{k,j} = \begin{cases} -\frac{\pi^2}{3h^2}-\frac{1}{6} & \text{if } j=k, \\ \\ -\frac{(-1)^{k+j}}{2}\sin^{-2}\left(\frac{(k-j)h}{2}\right) & \text{if } j\neq k. \end{cases}$$

Both matrices $\mathcal{K}_1$ and $\mathcal{K}_2$ are circulant and symmetric, for example $\mathcal{K}_2$ is of the following form

$$\mathcal{K}_2 = \begin{pmatrix} & \ddots & \vdots & & \\ & \ddots & -\frac{1}{2}\csc^2(\frac{2h}{2}) & & \\ & \ddots & \frac{1}{2}\csc^2(\frac{h}{2}) & & \\ & & -\frac{\pi^2}{3h^2}-\frac{1}{6} & & \\ & & \frac{1}{2}\csc^2(\frac{h}{2}) & \ddots & \\ & & -\frac{1}{2}\csc^2(\frac{2h}{2}) & \ddots & \\ & & \vdots & \ddots & \end{pmatrix}$$

(where function $\csc(x)=\frac{1}{\sin(x)}$). Circulant matrix can be diagonalized using the fast Fourier transform to compute the exponential matrix $\exp(t\mathcal{K}_2)$ with a low computational cost.

Example 2. *Let v_1 and v_2 be functions such that*

$$v_1(x) = \mathrm{e}^{\cos^2(x)}, \quad x\in[0,2\pi],$$

and

$$v_2(x) = \begin{cases} \mathrm{e}^{-\frac{1}{1-x^2}} & \text{if } x\in(-1,1), \\ 0 & \text{otherwise.} \end{cases}$$

Function v_2 may be regarded as periodic. By using spectral methods, we approximate second derivative of function v_j, $\partial^2_{xx}v_j \approx \mathcal{K}_2\boldsymbol{v}_j$, $\boldsymbol{v}_j=(v_j(x_1),\dots,v_j(x_N))^T$, $j=1,2$. Figure 2.1 presents the error of such the approximation for different value of N. It is vivid that Fourier spectral methods are particularly effective for smooth and periodic functions [33].

Non-periodic functions can be approximated on a bounded interval by the Chebyshev spectral methods. Suppose we wish to approximate function f on interval $[-1,1]$ (functions defined on a different bounded domain can be rescaled to $[-1,1]$). For such functions, equispaced grids cause a big error of approximation, therefore to minimise the error, we use Chebyshev points (roots of Chebyshev

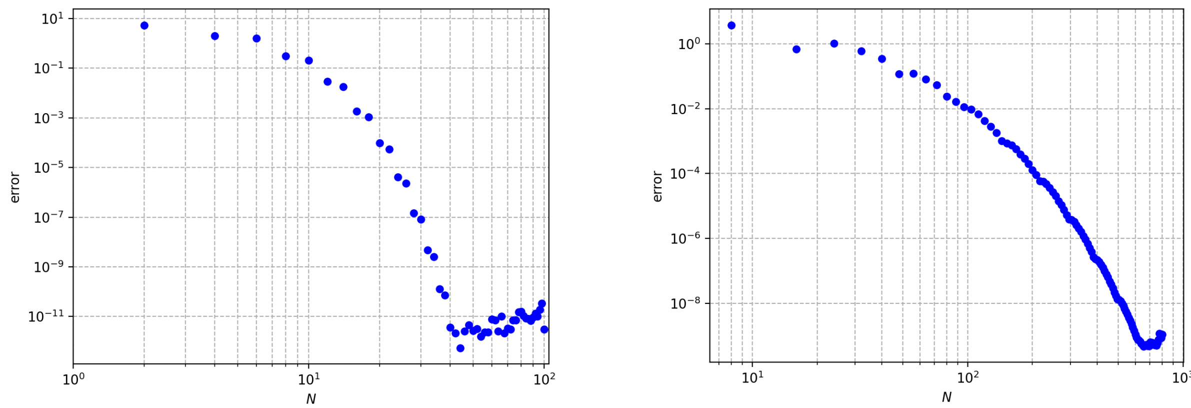


Figure 2.1: Spectral approximation of the second derivative of functions $v_1(x) = \mathrm{e}^{\cos^2(x)}$ (left graph) and $v_2(x) = \mathrm{e}^{-1/(1-x^2)}$ if $x \in (-1,1)$, $v_2(x) = 0$ otherwise (right graph). The error is evaluated in maximum norm $\| \ \|_\infty$.

polynomial) instead

$$x_j = \cos(j\pi/N), \qquad j = 0,1,\ldots,N, \qquad 1 = x_0 < x_1 < \cdots < x_N = -1, \qquad N \in \mathbb{N}. \tag{2.15}$$

For values $f(x_j) = f_j,\ j = 0,1,\ldots,N$ there exist unique polynomial of degree $\leq N$ such that $p(x_j) = f_j,\ 0 \leq j \leq N$. As in the case for periodic functions we denote $w_j \approx f'(x_j)$ and set $w_j = p'(x_j)$. To find vector $\boldsymbol{w} = (w_0, w_1, \ldots, w_N)$ that approximates the derivative of function f on interval $[-1,1]$ it is sufficient to multiply vector $\boldsymbol{f} = (f_0, f_1, \ldots, f_N)^T$ by the Chebyshev differentiation matrix $D_N \in M_{(N+1)\times(N+1)}(\mathbb{R})$

$$\boldsymbol{w} = D_N \boldsymbol{f},$$

where

$$(D_N)_{kj} = \begin{cases} \frac{2N^2+1}{6}, & \text{if} \ \ k = j = 0, \\ -\frac{2N^2+1}{6}, & \text{if} \ \ k = j = N, \\ \frac{-x_j}{2(1-x_j^2)}, & \text{if} \ \ k = j = 1,\ldots,N-1, \\ \frac{c_i}{c_j}\frac{(-1)^{i+j}}{(x_i - x_j)}, & \text{if} \ \ k \neq j, \quad i,j = 1\ldots,N-1, \end{cases}$$

and coefficients $c_0 = c_N = 2$, $c_j = 1$ for $1 \leq j \leq N-1$.

In the multivariate case $\Omega \subset \mathbb{R}^m$, $m > 1$, differential operator $\mathcal{L}$ (e.g., when $\mathcal{L} = \Delta$) can also be approximated by the spectral methods, see [33].

Spectral methods in an unbounded domain are currently an intensive object of research.

2.2.2 Splitting methods

Splitting methods are widely used in computational mathematics to solve differential equations numerically. An interesting application of such methods is presented in the article [19], in which the authors use splitting methods to numerically approximate the Korteweg-de Vries equation.

Suppose that the differential operator $\mathcal{L}$ for the Cauchy problem (2.9) is of the form $\mathcal{L} = \Delta + h$, where $h(x)$ is a space dependent function. Let $\bar{h} = (h_1, \dots, h_N) \in \mathbb{R}^N$ be a vector such that $h_j = h(x_j)$, $j = 1, \dots, N$, $\{x_j\}$ is the space grid and let $I_N \in M_{N\times N}(\mathbb{R})$ be the identity matrix. In general, we cannot diagonalize matrix $\mathcal{K}_2 + I_N\bar{h}$ similarly as before to compute effectively $\exp(t(\mathcal{K}_2 + I_N\bar{h}))$. Certainly one can find the value of $\exp(t(\mathcal{K}_2 + I_N\bar{h}))$ by computer program *expm*, but the computational cost will be large – especially in a higher space dimension. Therefore, to approximate expression $\exp(t(\mathcal{K}_2 + I_N\bar{h}))$, we may use the splitting methods. The simplest splitting is the Lie-Trotter method

$$\mathrm{e}^{h(A+B)}u_0 = \mathrm{e}^{hA}\mathrm{e}^{hB}u_0 + \mathcal{O}(h^2), \tag{2.16}$$

where A and B are some matrices that do not need to commute and $h = T/n$ is a small time step. On the whole time interval $[0, T]$ we have

$$\mathrm{e}^{T(A+B)}u_0 = \left(\mathrm{e}^{hA}\mathrm{e}^{hB}\right)^n u_0 + \mathcal{O}(h).$$

In other words, instead of considering the equation

$$u'(t) = (A + B)u(t), \quad u(0) = u_0, \tag{2.17}$$

which may be difficult in numerical approximation, we are dealing with the simpler equations ()

$$u'(t) = Au(t), \quad u(0) = u_1 \qquad \text{and} \qquad u'(t) = Bu(t), \quad u(0) = u_2. \tag{2.18}$$

Then the combination of the solutions (2.18) is the approximation of the solution (2.17). More accurate scheme is the Strang splitting

$$\mathrm{e}^{h(A+B)}u_0 \approx \mathrm{e}^{Ah/2}\mathrm{e}^{Bh}\mathrm{e}^{Ah/2}u_0 + \mathcal{O}(h^3). \tag{2.19}$$

It is possible to construct schemes which converge faster than the Lie-Trotter and Strang splitting, but it involves larger error constant and higher computational costs.

Example 3. *Consider the equation*

$$\begin{cases} u_t(x,t) = \partial^2_{xx}u(x,t) - x^2u(x,t), & x \in (-10, 10), \quad t \in [0,1], \\ u(x,0) = u_0(x) = \mathrm{e}^{-\frac{x^2}{2}}. \end{cases} \tag{2.20}$$

Function u satisfying problem (2.20) is $u(x,t) = \mathrm{e}^{-\frac{x^2}{2}}\mathrm{e}^{-t}$. Initial condition $u_0(x) = \mathrm{e}^{-\frac{x^2}{2}}$ is not periodic, but it is close to zero on the boundary, so it may be regarded as periodic in practical computations. Figure 2.2 presents the error of the Strang splitting method

$$\mathrm{e}^{h(\mathcal{K}_2 - I_N x^2)} \approx \mathrm{e}^{-hI_N x^2/2}\mathrm{e}^{h\mathcal{K}_2}\mathrm{e}^{-hI_N x^2/2}u_0$$

evaluated in supremum norm, for $N = 256$ grid points.

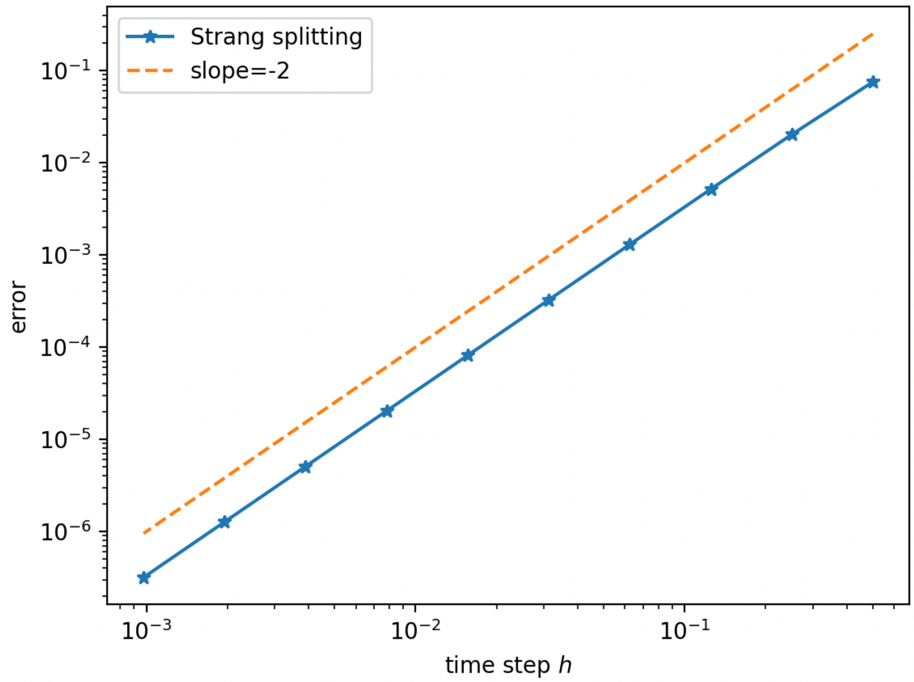


Figure 2.2: Numerical approximation of the Strang splitting method applied to the equation (2.20). The error is evaluated in supremum norm $\| \ \|_\infty$.

2.3 The Neumann series

Let us consider the following ordinary differential equation

$$Y'(t) = A(t)Y(t), \qquad Y(0) = Y_0, \tag{2.21}$$

where $Y : \mathbb{R} \to \mathbb{C}^n$ and $A(t)$ is an $n \times n$ time-dependent matrix. Equation (2.21) can be written in the following form

$$Y(t) = Y_0 + \int_0^t A(\tau)Y(\tau)\mathrm{d}\tau. \tag{2.22}$$

By iterating equation (2.22), one can show that the solution of the problem (2.22) is given by the series

$$Y(t) = \sum_{d=0}^{\infty} T^d Y_0, \tag{2.23}$$

where

$$T^d Y_0 = \int_0^t A(\tau_1) \int_0^{\tau_1} A(\tau_2) \cdots \int_0^{\tau_{d-1}} A(\tau_d) Y_0 \mathrm{d}\tau_d \ldots \mathrm{d}\tau_1.$$

The series (2.23) is known as the Neumann series and the Dyson series [20], and it converges to the solution of equation (2.22) for all values of t provided that the matrix $A(t)$ is bounded [6].

2.4 Quadrature methods for highly oscillatory integrals

As mentioned, the solution u of equation (1.1) can be expressed as a convergent Neumann series. For function f of the form (1.2), the Neumann series is an infinite sum of multivariate highly oscillatory integrals. Hence, to approximate the solution of (1.1), we need to be able to approximate such integrals.

In general, oscillatory integrals is of the following form

$$I[h,\sigma] = \int_\sigma h(\boldsymbol{s})\mathrm{e}^{\mathrm{i}\omega g(\boldsymbol{s})}\mathrm{d}\boldsymbol{s}, \tag{2.24}$$

where $\sigma \subset \mathbb{R}^d$ is a domain of the integral and $h, g : \mathbb{R}^d \to \mathbb{R}$. We assume that functions h and g are sufficiently smooth and $\omega \gg 1$. For such integrals, standard quadrature rules based on Taylor expansion are inadequate in numerical approximation due to the large error constant. There are some quadrature rules dedicated to integrals of the form (2.24), such as: the asymptotic expansion, the Filon-type method and the Levin collocation method. In this dissertation, we consider integral (2.24) with oscillator $g(\boldsymbol{s}) = \boldsymbol{n}^T\boldsymbol{s}$, where $\boldsymbol{n}, \boldsymbol{s} \in \mathbb{R}^d$, and $\sigma = \sigma(t)$ being a d-dimensional simplex with vertices $(0,\dots,0,0), (0,\dots,0,t), (0,\dots,0,t,t), \dots, (t,\dots,t,t)$. In this chapter, we briefly describe the asymptotic method, which will be used in Chapter 3, and the Filon method, which will be utilized in Chapter 4.

Asymptotic expansion

Applying integration by parts repeatedly, we obtain the following formula

$$\begin{aligned}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau}h(\tau)\mathrm{d}\tau = &\underbrace{\sum_{m=0}^{r-1}\frac{(-1)^m}{(\mathrm{i}\omega)^{m+1}}\left[\mathrm{e}^{\mathrm{i}\omega t}\partial_\tau^m h(\tau)\Big|_{\tau=t} - \partial_\tau^m h(\tau)\Big|_{\tau=0}\right]}_{=:\mathcal{S}_r(t)} \\ &+ \underbrace{\frac{(-1)^r}{(\mathrm{i}\omega)^r}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau}\partial_\tau^r h(\tau)\mathrm{d}\tau}_{=:E_r(t)}.\end{aligned} \tag{2.25}$$

Sum $\mathcal{S}_r(t)$ approximates the integral with error $|E_r(t)| \le C\omega^{-r}$, where constant C is independent of ω, but depends on t, function h and its successive derivatives. We say that $\mathcal{S}_r(t)$ is the r-partial sum of the asymptotic expansion of integral $I[h,(0,t)]$. In general, for $\omega \gg 1$ the sum $\mathcal{S}_r(t)$ provides a significant approximation of a highly oscillatory integral. However, the series $\mathcal{S}_\infty(t)$ it is not always convergent. Instead, we write

$$\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau}h(\tau)\mathrm{d}\tau \sim \mathcal{S}_\infty(t) = \sum_{m=0}^{\infty}\frac{(-1)^m}{(\mathrm{i}\omega)^{m+1}}\left[\mathrm{e}^{\mathrm{i}\omega t}\partial_\tau^m h(\tau)\Big|_{\tau=t} - \partial_\tau^m h(\tau)\Big|_{\tau=0}\right], \quad \omega \to \infty, \tag{2.26}$$

where the expression on the right hand side is a formal series. Symbol $\sim$ means that for each $N = 1, 2, \dots$ we have

$$\left|\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau}h(\tau)\mathrm{d}\tau - \sum_{m=0}^{N-1}\frac{(-1)^m}{(\mathrm{i}\omega)^{m+1}}\left[\mathrm{e}^{\mathrm{i}\omega t}\partial_\tau^m h(\tau)\Big|_{\tau=t} - \partial_\tau^m h(\tau)\Big|_{\tau=0}\right]\right| = \mathcal{O}(\omega^{-N-1}).$$

In other words, series $\mathcal{S}_\infty(t)$ may diverge, but partial sum $\mathcal{S}_r(t)$ provides excellent approximation of integral $I[h,(0,t)]$ for large parameter ω.

Throughout the dissertation, we will use the standard notation deriving from the asymptotic analysis. By $g \sim \mathcal{O}(\omega^{-d})$ we understand that function g has the asymptotic expansion whose first term decays like $\mathcal{O}(\omega^{-d})$. In (2.25) we have $\mathcal{S}_r(t) \sim \mathcal{O}(\omega^{-1})$ and $E_r(t) = \mathcal{O}(\omega^{-r-1})$.

To analyze multivariate integrals 2.24 over a domain $\sigma \subset \mathbb{R}^d$ we need the following

Definition 5. *Point $\boldsymbol{s} \in \partial\sigma$ is called a resonance point if gradient $\nabla g(\boldsymbol{s})$ of oscillator g is orthogonal to the boundary of σ. We say that the nonresonance condition is satisfied if for every $\boldsymbol{s} \in \partial\sigma$ gradient $\nabla g(\boldsymbol{s})$ is not orthogonal to the boundary of σ.*

If oscillator $g(\boldsymbol{s}) = \boldsymbol{n}^T\boldsymbol{s}$ and $\sigma(t)$ is a d-dimensional simplex, then the *nonresonance condition* means that vector $\boldsymbol{n}$ is not orthogonal to the faces of simplex $\sigma(t)$.

Theorem 8. *Suppose that $\sigma(t) \subset \mathbb{R}^d$ is a d-dimensional simplex and that the nonresonance condition is satisfied. Let h be a real valued function. Then [22]*

$$I[h,\sigma(t)] = \int_{\sigma(t)} h(\boldsymbol{s})\mathrm{e}^{\mathrm{i}\omega \boldsymbol{n}^T\boldsymbol{s}}\mathrm{d}\boldsymbol{s} \sim \mathcal{O}(\omega^{-d}).$$

Filon method

The Filon method is a quadrature rule designed for highly oscillating integrals. We restrict ourselves to describing only the simplest version of the Filon method. Suppose that Hermite interpolation polynomial p approximate function h, $p(s) \approx h(s)$. Let p satisfies the following conditions

$$p^{(k)}(0) = h^{(k)}(0), \quad p^{(k)}(t) = h^{(k)}(t), \quad k = 0,1,\ldots N.$$

Then the Filon method reads

$$\int_0^t h(s)\mathrm{e}^{\mathrm{i}\omega s}\mathrm{d}s \approx \int_0^t p(s)\mathrm{e}^{\mathrm{i}\omega s}\mathrm{d}s,$$

and the integral $\int_0^t p(s)\mathrm{e}^{\mathrm{i}\omega s}\mathrm{d}s$ is computed explicitly. One can show that the error of the above approximation satisfies

$$\left|\int_0^t h(s)\mathrm{e}^{\mathrm{i}\omega s}\mathrm{d}s - \int_0^t p(s)\mathrm{e}^{\mathrm{i}\omega s}\mathrm{d}s\right| \le C\frac{1}{\omega^{N+1}},$$

where constant C is independent of ω [13]. This means that the Filon method is as efficient as the asymptotic method for highly oscillatory integrals. In addition, for small values of ω it behaves similarly to standard quadrature rules.

In the same way, we approximate a multivariate highly oscillatory integral. Function $h : \mathbb{R}^d \to \mathbb{R}$ is interpolated by the corresponding polynomial p, and then integral $\int_{\sigma(t)} p(\boldsymbol{s})\mathrm{e}^{\mathrm{i}\omega \boldsymbol{n}^T\boldsymbol{s}}\mathrm{d}\boldsymbol{s}$ is computed explicitly. We have

$$\int_{\sigma(t)} h(\boldsymbol{s})\mathrm{e}^{\mathrm{i}\omega \boldsymbol{n}^T\boldsymbol{s}}\mathrm{d}\boldsymbol{s} \approx \int_{\sigma(t)} p(\boldsymbol{s})\mathrm{e}^{\mathrm{i}\omega \boldsymbol{n}^T\boldsymbol{s}}\mathrm{d}\boldsymbol{s}.$$

In order to approximate the solution of a partial differential equation of type (1.1), we need to approximate the integrals appearing in the Neumann series in which the non-oscillatory functions are vector values. This greatly complicates the calculations. In our approach, to expand asymptotically a multivariate highly oscillatory integral of vector-valued function over a d-dimensional simplex, we will repeatedly exploit Fubini's theorem, properties of the semigroup operator, and integration by parts. In this section, we provide an example of the asymptotic expansion for univariate and bivariate integrals appearing in the Neumann series. The general results involving integrals over a d-dimensional simplex will be presented in Chapter 3 and in Appendix A.1. We need the following

Lemma 1. *Let $\alpha \in D(\mathcal{L}^k)$, where $D(\mathcal{L}^k) = \{u \in D(\mathcal{L}^{k-1}) : \mathcal{L}^{k-1}u \in D(\mathcal{L})\}$ and let $\mathcal{L}$ be the infinitesimal generator of a strongly continuous semigroup $\{\mathrm{e}^{t\mathcal{L}}\}_{t\geq 0}$. The k-th time derivative of expression $\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha\mathrm{e}^{\tau\mathcal{L}}$ is [4]*

$$\partial_\tau^k \left(\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha\mathrm{e}^{\tau\mathcal{L}}\right) = \mathrm{e}^{(t-\tau)\mathcal{L}} \underbrace{\Big[\ldots[[\alpha,\mathcal{L}],\mathcal{L}],\ldots\Big]}_{\mathcal{L}\ appears\ k\ times} \mathrm{e}^{\tau\mathcal{L}} = (-1)^k \mathrm{e}^{(t-\tau)\mathcal{L}} ad_{\mathcal{L}}^k(\alpha)\mathrm{e}^{\tau\mathcal{L}}, \tag{2.27}$$

where $ad_{\mathcal{L}}^0(\alpha) = \alpha,\ ad_{\mathcal{L}}^k(\alpha) = \left[\mathcal{L}, ad_{\mathcal{L}}^{k-1}(\alpha)\right]$ and $[X,Y] \equiv XY - YX$ is the commutator of X and Y.

Theorem 9. *For the infinitesimal generator $\mathcal{L}$ of strongly continuous semigroup and function $\alpha \in D(\mathcal{L}^r),\ r \in \mathbb{N}$, the following identity holds*

$$\begin{aligned}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau}\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha\mathrm{e}^{\tau\mathcal{L}}\mathrm{d}\tau = &\sum_{m=0}^{r-1}\frac{1}{(\mathrm{i}\omega)^{m+1}}\left[\mathrm{e}^{\mathrm{i}\omega t}ad_{\mathcal{L}}^m(\alpha)\mathrm{e}^{t\mathcal{L}} - \mathrm{e}^{t\mathcal{L}}ad_{\mathcal{L}}^m(\alpha)\right] \\ &+ \frac{1}{(\mathrm{i}\omega)^r}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^r(\alpha)\mathrm{e}^{\tau\mathcal{L}}\mathrm{d}\tau.\end{aligned} \tag{2.28}$$

Proof. The assertion follows immediately by using Lemma 1 and formula (2.25) applied to function $h(\tau) = \mathrm{e}^{(t-\tau)\mathcal{L}}\alpha\mathrm{e}^{\tau\mathcal{L}}$. ☐

Consider now the following bivariate integral

$$\int_0^t \mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}\mathrm{e}^{\mathrm{i}\omega n_2\tau_2}\int_0^{\tau_2}\mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}}\alpha_{n_1}\mathrm{e}^{\tau_1\mathcal{L}}\mathrm{e}^{\mathrm{i}\omega n_1\tau_1}\mathrm{d}\tau_1\mathrm{d}\tau_2. \tag{2.29}$$

We assume that each appearing expressions $\mathcal{L}^k\alpha_{n_j},\ j = 1,2$ are well defined, and numbers $n_1,\ n_2$ satisfy $n_1 > 0,\ n_2 > 0$. The domain of the integral is a two dimensional simplex

$$\sigma_2(t) = \{\boldsymbol{\tau} := (\tau_1,\tau_2) \in \mathbb{R}^2 : t \geq \tau_2 \geq \tau_1 > 0\}.$$

By employing Fubini's theorem, Theorem 9, and Lemma 1, we expand the integral (2.29) with accuracy $\mathcal{O}(\omega^{-r})$ in the spirit of the expansion (2.28).

$$\int_0^t \mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}\mathrm{e}^{\mathrm{i}\omega n_2\tau_2}\int_0^{\tau_2}\mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}}\alpha_{n_1}\mathrm{e}^{\tau_1\mathcal{L}}\mathrm{e}^{\mathrm{i}\omega n_1\tau_1}\mathrm{d}\tau_1\mathrm{d}\tau_2 =$$

$$\sum_{k_1=0}^{r-1}\frac{1}{(\mathrm{i}\omega n_1)^{k_1+1}}\int_0^t \mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}\mathrm{e}^{\mathrm{i}\omega n_2\tau_2}\left[\mathrm{e}^{\mathrm{i}\omega n_1\tau_2}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\mathrm{e}^{\tau_2\mathcal{L}} - \mathrm{e}^{\tau_2\mathcal{L}}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right]\mathrm{d}\tau_2 +$$

$$\frac{1}{(\mathrm{i}\omega n_1)^r}\int_0^t \mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}\mathrm{e}^{\mathrm{i}\omega n_2\tau_2}\int_0^{\tau_2}\mathrm{e}^{\mathrm{i}\omega n_1\tau_1}\mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}}ad_{\mathcal{L}}^r(\alpha_{n_1})\mathrm{e}^{\tau_1\mathcal{L}}\mathrm{d}\tau_1\mathrm{d}\tau_2 =$$
$$\sum_{k_1=0}^{r-1}\frac{1}{(\mathrm{i}\omega n_1)^{k_1+1}}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_2(n_1+n_2)}\mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\mathrm{e}^{\tau_2\mathcal{L}} - \mathrm{e}^{\mathrm{i}\omega n_2\tau_2}\mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}\mathrm{e}^{\tau_2\mathcal{L}}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\mathrm{d}\tau_2 +$$
$$\frac{1}{(\mathrm{i}\omega n_1)^r}\int_0^t \mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}\mathrm{e}^{\mathrm{i}\omega n_2\tau_2}\int_0^{\tau_2}\mathrm{e}^{\mathrm{i}\omega n_1\tau_1}\mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}}ad_{\mathcal{L}}^r(\alpha_{n_1})\mathrm{e}^{\tau_1\mathcal{L}}\mathrm{d}\tau_1\mathrm{d}\tau_2.$$

Now for each index k_1, we integrate by parts $r-1-k_1$ times the two integrals, which appear in the penultimate line.

$$\sum_{k_1=0}^{r-1}\frac{1}{(\mathrm{i}\omega n_1)^{k_1+1}}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_2(n_1+n_2)}\mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\mathrm{e}^{\tau_2\mathcal{L}}\mathrm{d}\tau_2 =$$
$$\sum_{k_1=0}^{r-2}\frac{1}{(\mathrm{i}\omega n_1)^{k_1+1}}\sum_{k_2=0}^{r-2-k_1}\frac{1}{(\mathrm{i}\omega(n_1+n_2))^{k_2+1}}\left[\mathrm{e}^{\mathrm{i}\omega t(n_1+n_2)}ad_{\mathcal{L}}^{k_2}\left(\alpha_{n_2}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right)\mathrm{e}^{t\mathcal{L}} - \mathrm{e}^{t\mathcal{L}}ad_{\mathcal{L}}^{k_2}\left(\alpha_{n_2}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right)\right] +$$
$$\sum_{k_1=0}^{r-1}\frac{1}{(\mathrm{i}\omega n_1)^{k_1+1}}\frac{1}{(\mathrm{i}\omega(n_1+n_2))^{r-1-k_1}}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_2(n_1+n_2)}\mathrm{e}^{(t-\tau_2)\mathcal{L}}ad_{\mathcal{L}}^{r-1-k_1}\left(\alpha_{n_2}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right)\mathrm{e}^{\tau_2\mathcal{L}}\mathrm{d}\tau_2 = (\star).$$

Due to simple relations $\sum_{k_1=0}^r\sum_{k_2=0}^{r-k_1}a_{k_1}b_{k_2} = \sum_{k_1+k_2=0}^r a_{k_1}b_{k_2}$, $\sum_{k_1=0}^r a_{k_1,r-k_1} = \sum_{k_1+k_2=r}a_{k_1,k_2}$ and by simplifying expressions where necessary, we obtain

$$(\star) =$$
$$\sum_{k_1+k_2=0}^{r-2}\frac{1}{(\mathrm{i}\omega)^{k_1+k_2+2}}\frac{1}{n_1^{k_1+1}(n_1+n_2)^{k_2+1}}\left[\mathrm{e}^{\mathrm{i}\omega t(n_1+n_2)}ad_{\mathcal{L}}^{k_2}\left(\alpha_{n_2}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right)\mathrm{e}^{t\mathcal{L}} - \mathrm{e}^{t\mathcal{L}}ad_{\mathcal{L}}^{k_2}\left(\alpha_{n_2}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right)\right] +$$
$$\frac{1}{(\mathrm{i}\omega)^r}\sum_{k_1+k_2=0}^{r-1}\frac{1}{n_1^{k_1+1}}\frac{1}{(n_1+n_2)^{k_2}}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_2(n_1+n_2)}\mathrm{e}^{(t-\tau_2)\mathcal{L}}ad_{\mathcal{L}}^{k_2}\left(\alpha_{n_2}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right)\mathrm{e}^{\tau_2\mathcal{L}}\mathrm{d}\tau_2.$$

In a similar way, we expand asymptotically the remaining integrals

$$\sum_{k_1=0}^{r-1}\frac{1}{(\mathrm{i}\omega n_1)^{k_1+1}}\int_0^t \mathrm{e}^{\mathrm{i}\omega n_2\tau_2}\mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}\mathrm{e}^{\tau_2\mathcal{L}}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\mathrm{d}\tau_2 =$$
$$\sum_{k_1+k_2=0}^{r-2}\frac{1}{(\mathrm{i}\omega)^{k_1+k_2+2}}\frac{1}{n_1^{k_1+1}n_2^{k_2+1}}\left[\mathrm{e}^{\mathrm{i}\omega tn_2}ad_{\mathcal{L}}^{k_2}(\alpha_{n_2})\mathrm{e}^{t\mathcal{L}}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1}) - \mathrm{e}^{t\mathcal{L}}ad_{\mathcal{L}}^{k_2}(\alpha_{n_2})ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right] +$$
$$\frac{1}{(\mathrm{i}\omega)^r}\sum_{k_1+k_2=0}^{r-1}\frac{1}{n_1^{k_1+1}}\frac{1}{n_2^{k_2}}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_2n_2}\mathrm{e}^{(t-\tau_2)\mathcal{L}}ad_{\mathcal{L}}^{k_2}(\alpha_{n_2})\mathrm{e}^{\tau_2\mathcal{L}}ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\mathrm{e}^{\tau_2\mathcal{L}}\mathrm{d}\tau_2.$$

To sum up the above calculation, the approximation of integral (2.29) by the partial sum of the asymptotic expansion is as follows

$$\int_0^t \mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}\mathrm{e}^{\mathrm{i}\omega n_2\tau_2}\int_0^{\tau_2}\mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}}\alpha_{n_1}\mathrm{e}^{\tau_1\mathcal{L}}\mathrm{e}^{\mathrm{i}\omega n_1\tau_1}\mathrm{d}\tau_1\mathrm{d}\tau_2 = \mathcal{S}_r^2(t) + E_r^2(t),$$

where sum $\mathcal{S}_r^2(t)$ and error of the expansion $E_r^2(t)$ are equal to

$$\mathcal{S}_r^2(t) =$$
$$\sum_{k_1+k_2=0}^{r-2} \frac{1}{(\mathrm{i}\omega)^{k_1+k_2+2}} \Bigg(\frac{1}{n_1^{k_1+1}(n_1+n_2)^{k_2+1}} \left[\mathrm{e}^{\mathrm{i}\omega t(n_1+n_2)} ad_{\mathcal{L}}^{k_2}\left(\alpha_{n_2} ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right) \mathrm{e}^{t\mathcal{L}} - \mathrm{e}^{t\mathcal{L}} ad_{\mathcal{L}}^{k_2}\left(\alpha_{n_2} ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right)\right]$$
$$+ \frac{1}{n_1^{k_1+1} n_2^{k_2+1}} \left[\mathrm{e}^{\mathrm{i}\omega t n_2} ad_{\mathcal{L}}^{k_2}(\alpha_{n_2}) \mathrm{e}^{t\mathcal{L}} ad_{\mathcal{L}}^{k_1}(\alpha_{n_1}) - \mathrm{e}^{t\mathcal{L}} ad_{\mathcal{L}}^{k_2}(\alpha_{n_2}) ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right] \Bigg),$$

$$E_r^2(t) =$$
$$\frac{1}{(\mathrm{i}\omega n_1)^r} \int_0^t \mathrm{e}^{(t-\tau_2)\mathcal{L}} \alpha_{n_2} \mathrm{e}^{\mathrm{i}\omega n_2 \tau_2} \int_0^{\tau_2} \mathrm{e}^{\mathrm{i}\omega n_1 \tau_1} \mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}} ad_{\mathcal{L}}^{r}(\alpha_{n_1}) \mathrm{e}^{\tau_1\mathcal{L}} \mathrm{d}\tau_1 \mathrm{d}\tau_2 +$$
$$\frac{1}{(\mathrm{i}\omega)^r} \sum_{k_1+k_2=0}^{r-1} \frac{1}{n_1^{k_1+1}} \frac{1}{(n_1+n_2)^{k_2}} \int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_2(n_1+n_2)} \mathrm{e}^{(t-\tau_2)\mathcal{L}} ad_{\mathcal{L}}^{k_2}\left(\alpha_{n_2} ad_{\mathcal{L}}^{k_1}(\alpha_{n_1})\right) \mathrm{e}^{\tau_2\mathcal{L}} \mathrm{d}\tau_2 +$$
$$+ \frac{1}{(\mathrm{i}\omega)^r} \sum_{k_1+k_2=0}^{r-1} \frac{1}{n_1^{k_1+1}} \frac{1}{n_2^{k_2}} \int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_2 n_2} \mathrm{e}^{(t-\tau_2)\mathcal{L}} ad_{\mathcal{L}}^{k_2}(\alpha_{n_2}) \mathrm{e}^{\tau_2\mathcal{L}} ad_{\mathcal{L}}^{k_1}(\alpha_{n_1}) \mathrm{e}^{\tau_2\mathcal{L}} \mathrm{d}\tau_2.$$

It can be observed that the calculation becomes tedious and complicated even for a bivariate integral. For obvious reasons, the computations involving the asymptotic expansions of higher-dimensional integrals tend to be even more complex. Fortunately, as our numerical experiments demonstrate, a few initial terms of the Neumann series allow us to approximate the solution of the highly oscillatory differential equation with high accuracy.

The above calculations demonstrate our approach to approximating highly oscillatory integrals over a d-dimensional simplex. For each integral, we apply Fubini's theorem, and then, by using integration by parts, we expand asymptotically univariate integrals. The general result for an integral over a d-dimensional simplex will be presented in Chapter 3 and proven in Appendix A.1. The sum $\mathcal{S}_r^2(t)$ satisfies $\mathcal{S}_r^2(t) \sim \mathcal{O}(\omega^{-2})$. In bivariate integral of the form (2.29) we assumed that numbers $n_1 > 0$ and $n_2 > 0$. If n_1 and n_2 satisfy $n_1 + n_2 = 0$, we cannot perform the integration by parts for the outer integral, because the frequency exponent would vanish, i.e. $\mathrm{e}^{\mathrm{i}\omega t(n_1+n_2)} = 1$. In this case, (n_1, n_2) is orthogonal to the boundary of the simplex $\sigma_2(t)$ and we only have $\mathcal{S}_r^2 \sim \mathcal{O}(\omega^{-1})$. This makes the asymptotic expansion of integrals even more complicated. In such a situation, (n_1, n_2) is called a resonance point.

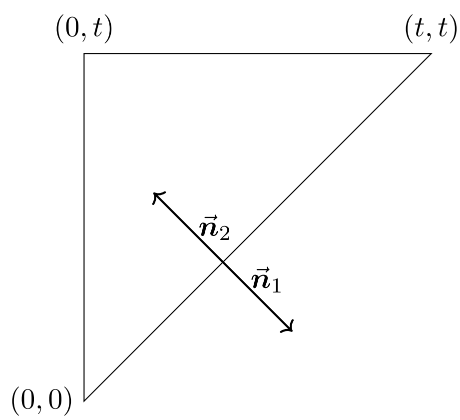


Figure 2.3: Simplex $\sigma_2(t)$ and two vectors $\vec{\boldsymbol{n}}_1 = (n, -n)$ and $\vec{\boldsymbol{n}}_2 = (-n, n)$ orthogonal to the boundary of $\sigma_2(t)$.

Chapter 3

Asymptotic expansions for the solution of a linear PDE with a multifrequency highly oscillatory potential

This chapter is written based on the article [28]. Let us recall the problem under consideration – we study the following highly oscillatory partial differential equation

$$\begin{aligned} &\partial_t u(x,t) = \mathcal{L}u(x,t) + f(x,t)u(x,t), \qquad t \in [0,t^\star], \quad x \in \Omega \subset \mathbb{R}^m, \\ &u(x,0) = u_0(x), \end{aligned} \tag{3.1}$$

with zero boundary conditions, where Ω is an open and bounded subset of $\mathbb{R}^m$ with smooth boundary $\partial\Omega$, $t^\star > 0$ and $\mathcal{L}$ is a linear differential operator of degree $2p$, $p \in \mathbb{N}$, defined by the formula

$$\mathcal{L} = \sum_{|\boldsymbol{p}|\le 2p} a_{\boldsymbol{p}}(x) D^{\boldsymbol{p}}, \qquad D^{\boldsymbol{p}} = \frac{\partial^{p_1}}{\partial x_1^{p_1}} \frac{\partial^{p_2}}{\partial x_2^{p_2}} \cdots \frac{\partial^{p_m}}{\partial x_m^{p_m}}, \quad x \in \Omega \subset \mathbb{R}^m. \tag{3.2}$$

Multi-index $\boldsymbol{p}$ is an m-tuple of nonnegative integers $\boldsymbol{p} = (p_1, p_2, \ldots, p_m)$ and $a_{\boldsymbol{p}}(x)$ are smooth, complex-valued functions of $x \in \bar{\Omega}$. We assume that function $f(x,t)$ in equation (3.1) is a highly oscillatory of type

$$f(x,t) = \sum_{n=1}^{N} \alpha_n(x) e^{in\omega t}, \quad \omega \gg 1, \quad N \in \mathbb{N}, \tag{3.3}$$

where α_n are complex-valued, sufficiently smooth functions. The proposed method can be efficiently applied also in the case of functions α_n depending on the time variable t. This will be demonstrated in numerical experiments. We aim to express the solution of (3.1) as the following partial sum of the asymptotic expansion

$$u(x,t) = p_{0,0}(x,t) + \sum_{r=1}^{R} \frac{1}{\omega^r} \sum_{s=0}^{S} p_{r,s}(x,t) e^{is\omega t} + \frac{1}{\omega^{R+1}} E_{R,S}(x,t), \quad t \in [0,t^\star], \quad x \in \Omega \subset \mathbb{R}^m, \tag{3.4}$$

where coefficients $p_{r,s}$ and the magnitude of error $E_{R,S}$ are independent of parameter ω.

Needless to say, the general form of equation (3.1) encompasses many important equations from both classical and quantum physics. The most important examples include the heat equation and the Schrödinger equation. We demonstrate that our methodology is also applicable to equations with second-order time derivatives, such as the wave equation and the Klein-Gordon equation. Highly oscillatory differential equations of type (3.1) arise in various fields, including electronic engineering [8, 10], when computing scattering frequencies [11], and in quantum mechanics [12, 21].

The research presented in this chapter is inspired by the article [12], in which the authors use a series of type (3.4) as ansatz to approximate the solution of the Klein–Gordon equation. After incorporating such ansatz to the equation, coefficients $p_{r,s}$ are determined either recursively or numerically by solving the non-oscillatory differential equations. The method turned out to be particularly effective for large oscillatory parameter ω, for which the standard numerical schemes were very expensive and inaccurate. This motivated us to take a closer look at the issue of asymptotic expansion of solution to a highly oscillatory equation. However, it is important to answer the following questions:

1. How to prove, that the solution of equation (3.1) indeed can be presented as the asymptotic series of type (3.4)?
2. Is it possible to obtain coefficients $p_{r,n}$ purely analytically (not by solving numerically differential equations)?
3. How to derive the error bound of the method?
4. Is the series (3.4) convergent?
5. Our numerical experiments regarding the paper [12] show that for small parameter ω, adding subsequent terms of series (3.4) make the approximation worse. Why is this happening?

This chapter partially answers the above questions.

In our approach, instead of employing an ansatz, we derive the partial sum of the asymptotic expansion (3.4) purely analytically. This approach enables us to obtain formulas for the coefficients $p_{r,n}$ of sum (3.4), eliminating the need to determine them by solving a system of differential equations. Furthermore, this approach allows us to derive a formula for the error in the approximation by the asymptotic sum (3.4).

To express the solution of equation (3.1) as the asymptotic series, we take advantage of the methodology proposed for computing highly oscillatory integrals. To find the approximate solution, firstly, we show that the Neumann series – in other words, a series of multivariate integrals – converges to the solution of equation (3.1) in the Sobolev space $H^{2p}(\Omega)$, where $2p$ is the order of the differential operator $\mathcal{L}$ defined in (3.2). Then, by using integration by parts and the theory of semigroups, we expand asymptotically each of these integrals into a sum of known coefficients. This is the most complicated and technical part at this stage, since the domain of each integral is a d-dimensional simplex, $d = 1, 2, \ldots$ and, as a result, the number of terms in the asymptotic expansion grows exponentially when d increases. Fortunately, our numerical experiments show that one can achieve a small enough error even for not large values of d. By organizing terms appropriately with respect to magnitudes ω^{-r} and frequencies $\mathrm{e}^{\mathrm{i}s\omega t}$, we obtain sum (3.4). Given that the Neumann series converges for any time variable t, we attain a long-time behavior of the highly oscillatory solution of equation.

The solution to equation (3.1), after spatial discretization, can also be expressed as the Magnus series [4]. The Magnus expansion is particularly important in approximating the solution of the Schrödinger equation, since any truncation of the Magnus series preserves unitarity. However, to the best of the author's knowledge, the convergence of the Magnus series has been proven only for sufficiently small time variables $t > 0$ and only for bounded operators [18, 26]. Representing the solution of equation (3.1) as the Neumann series allows its approximation for any large time variable t.

By considering the potential function f in the form (3.3), we avoid the occurrence of resonance points in the highly oscillatory integrals comprising the Neumann series. In the paper [23], the authors present the asymptotic expansion of the solution of (3.1), in which function f has a single frequency $f(x,t) = \alpha(x)\mathrm{e}^{\mathrm{i}\omega t}$. Paper [28] is the next step towards approximating the solution of equation (3.1) with a more general potential of the following form

$$f(x,t) = \sum_{\substack{n=-N \\ n\neq 0}}^{N} \alpha_n(x,t)e^{in\omega t}, \quad \omega \gg 1, \quad N \in \mathbb{N}. \tag{3.5}$$

For such a function, resonance points will appear repeatedly in the integrals which constitute the Neumann series. In this context, resonance occurs when the vector $\boldsymbol{n} \in \mathbb{Z}^d$ in the frequency term $\mathrm{e}^{\mathrm{i}\boldsymbol{n}^T\boldsymbol{\tau}}$, where $\boldsymbol{\tau} \in \mathbb{R}^d$, is orthogonal to the boundary of the integral $\int_{\sigma_d(t)} f(\boldsymbol{\tau})\mathrm{e}^{\mathrm{i}\boldsymbol{n}^T\boldsymbol{\tau}}\mathrm{d}\boldsymbol{\tau}$, with $\sigma_d(t)$ representing a d-dimensional simplex. In this manuscript, we consider a special case of such a situation and demonstrate that if the vector $\boldsymbol{n}$ is orthogonal to one edge of the simplex $\sigma_d(t)$, then resonance points vanish in the sum of these integrals.

The results presented in paper [28], described in this chapter, extend those previously introduced in [23]. Specifically, we consider a potential function f with multifrequencies (3.3), rather than one with a single frequency. Furthermore, we establish the convergence of the Neumann series in the Sobolev norm, instead of the L^2 norm, namely we provide the convergence in the norm of Sobolev space $H^{2p}(\Omega)$. Additionally, we demonstrate the applicability of the proposed methodology to equations featuring second-order time derivatives. The resonance case is also considered.

The chapter is organized as follows: in Section 3.1 we show that the solution of (3.1) can be expressed as the Neumann series. In Section 3.2, we convert each term of the Neumann series into a sum of multivariate highly oscillatory integrals. Then we introduce necessary definitions which will be needed in Section 3.3 for the asymptotic expansion of each highly oscillatory integral. Section 3.4 is devoted to the error analysis of the proposed approximation. Section 3.5 concerns highly oscillatory integrals with resonance points which form the Neumann series. In Section 3.6, we show the application of the asymptotic method to the wave equation. Numerical simulations are presented in Section 3.7.

3.1 Representation of the solution as the Neumann series

In this section, we show that the solution of (3.1) can be presented as the Neumann series for any $t > 0$. For convenience, we introduce necessary notations and making a general assumption

Notations 1. *By $H^{2p}(\Omega) = W^{2p,2}(\Omega)$, where p is a nonnegative integer, we understand the Sobolev* *space equipped with standard norm* $\|\ \|_{H^{2p}(\Omega)}$, *and* $H^p_0(\Omega)$ *is the closure of* $C^\infty_0(\Omega)$ *in the space* $H^p(\Omega)$. *In this chapter, for convenience, the norm in the space* $D(\mathcal{L}) := H^p_0(\Omega) \cap H^{2p}(\Omega)$ *is denoted by* $\|\ \| := \|\ \|_{H^{2p}(\Omega)}$. *Additionally, we slightly abuse the notation and also denote* $u(t) := u(\cdot, t)$ *as an element of an appropriate Banach space.*

The following assumption will apply in this chapter.

Assumption 1. *Suppose that*

1. Ω *is an open and bounded set in* $\mathbb{R}^m$ *with smooth boundary* $\partial\Omega$.
2. *Operator* $-\mathcal{L} : D(\mathcal{L}) := H^p_0(\Omega) \cap H^{2p}(\Omega) \to L^2(\Omega)$, *where* $\mathcal{L}$ *is of form (3.2), is a strongly elliptic of order* $2p$ *and has smooth, complex-valued coefficients* $a_{\boldsymbol{p}}(x)$ *on* $\bar{\Omega}$.
3. $u_0 \in D(\mathcal{L})$ *and* $f \in C\left([0, t^\star]; H^{2p}(\Omega)\right)$.

We emphasize that the space $D(\mathcal{L})$ is the Banach space since it is a closed subspace of the Banach space $H^{2p}(\Omega)$.

Expressing the solution $u(t)$ of equation (3.1) with the highly oscillatory potential (3.3) as the Neumann series facilitates its numerical approximation. Namely, having expressed $u(t)$ as the following series

$$u(t) = \sum_{d=0}^{\infty} T^d e^{t\mathcal{L}} u_0,$$

for certain linear operator T, each term $T^d e^{t\mathcal{L}} u_0$ is actually a sum of multivariate highly oscillatory integrals. In the following, we will show that if such an integral satisfies the nonresonance condition, then $T^d e^{t\mathcal{L}} u_0 \sim \mathcal{O}(\omega^{-d})$. Intuitively, for a large parameter $\omega \gg 1$, further terms of the Neumann series become less relevant in numerical approximation.

We start by applying Duhamel's formula, and we write equation (3.1) in the integral form

$$u(t) = e^{t\mathcal{L}} u_0 + \int_0^t e^{(t-\tau)\mathcal{L}} f(\tau) u(\tau) \mathrm{d}\tau, \tag{3.6}$$

where u_0 and $f(\tau)$, $u(\tau)$ for fixed τ are elements of the appropriate Banach spaces. Assumption 1 guarantees that differential operator $\mathcal{L}$ is the infinitesimal generator of a strongly continuous semigroup $\{\mathrm{e}^{t\mathcal{L}}\}_{t\geq 0}$ on $L^2(\Omega)$ and therefore $\max_{t\in[0,t^\star]} \|\mathrm{e}^{t\mathcal{L}}\|_{L^2(\Omega)\leftarrow L^2(\Omega)} \leq C(t^\star)$, where $C(t^\star)$ is some constant independent of t [14, 27]. Moreover, since the following a priori estimate holds

$$\|u\|_{H^{2p}(\Omega)} \leq C\left(\|\mathcal{L}u\|_{L^2(\Omega)} + \|u\|_{L^2(\Omega)}\right), \tag{3.7}$$

for any $u \in D(\mathcal{L})$, where $C > 0$ is a constant [27], operator $\mathrm{e}^{t\mathcal{L}}$ is also bounded in norm $\|\ \|$ of space $D(\mathcal{L})$ for any $t \in [0, t^\star]$. Indeed, by using (3.7) we have

$$\begin{aligned}\|\mathrm{e}^{t\mathcal{L}}\|_{D(\mathcal{L})\leftarrow D(\mathcal{L})} = \sup_{\|u\|\leq 1} \|\mathrm{e}^{t\mathcal{L}}u\| \ &\leq\ C \sup_{\|u\|\leq 1} \left(\|\mathcal{L}\mathrm{e}^{t\mathcal{L}}u\|_{L^2(\Omega)} + \|\mathrm{e}^{t\mathcal{L}}u\|_{L^2(\Omega)}\right) \\ &=\ C \sup_{\|u\|\leq 1} \left(\|\mathrm{e}^{t\mathcal{L}}\mathcal{L}u\|_{L^2(\Omega)} + \|\mathrm{e}^{t\mathcal{L}}u\|_{L^2(\Omega)}\right)\end{aligned}$$

$$
\begin{aligned}
&\leq C\|\mathrm{e}^{t\mathcal{L}}\|_{L^2(\Omega)\leftarrow L^2(\Omega)} \sup_{\|u\|\leq 1} \left(\|\mathcal{L}u\|_{L^2(\Omega)} + \|u\|_{L^2(\Omega)}\right) \\
&\leq C\|\mathrm{e}^{t\mathcal{L}}\|_{L^2(\Omega)\leftarrow L^2(\Omega)} \sup_{\|u\|\leq 1} \left(C_1\|u\| + \|u\|_{L^2(\Omega)}\right) \\
&\leq C(t^\star)
\end{aligned}
$$

and again constant $C(t^\star)$ depends on coefficients $a_{\boldsymbol{p}}(x)$ of $\mathcal{L}$, but is independent of time variable t. By variation of constant representation (3.6), operator $\{\mathrm{e}^{t\mathcal{L}}\}_{t\geq 0}$ is bounded, although the subject of consideration is equation (3.1), which features unbounded operator $\mathcal{L}$ on space $L^2(\Omega)$.

We introduce sequence $\left\{u^{[n]}\right\}_{n=0}^{\infty} \subset C\left([0,t^\star]; D(\mathcal{L})\right) =: V$

$$
u^{[n]}(t) = \sum_{d=0}^{n} T^d \mathrm{e}^{t\mathcal{L}} u_0, \quad u^{[0]}(t) = \mathrm{e}^{t\mathcal{L}} u_0, \qquad t \in [0, t^\star]. \tag{3.8}
$$

Linear operator $T : V \to V$ is determined by

$$
Tu(t) = \int_0^t \mathrm{e}^{(t-\tau)\mathcal{L}} f(\tau) u(\tau) \mathrm{d}\tau, \qquad t \in [0, t^\star], \tag{3.9}
$$

where $\mathcal{L}$ is the infinitesimal generator of a strongly continuous semigroup, and function $f \in C\left([0,t^\star]; H^{2p}(\Omega)\right)$. We show that sequence (3.8) is convergent to the solution $u \in C^1([0,t^\star]; L^2(\Omega)) \cap C([0,t^\star]; D(\mathcal{L}))$ of equation (3.1). We use the estimation of a product of two functions in a Sobolev norm

$$
\|hg\|_{H^{2p}(\Omega)} \leq M \|h\|_{H^{2p}(\Omega)} \|g\|_{H^{2p}(\Omega)}, \qquad \Omega \subset \mathbb{R}^m, \qquad 2p > m/2, \tag{3.10}
$$

for $h, g \in H^{2p}(\Omega)$, where M depends only on p and m. In the beginning, we show that expression $T^d u(t)$

$$
T^d u(t) = \int_0^t \mathrm{e}^{(t-\tau_1)\mathcal{L}} f(\tau_1) \int_0^{\tau_1} \mathrm{e}^{(\tau_1-\tau_2)\mathcal{L}} f(\tau_2) \cdots \int_0^{\tau_{d-1}} \mathrm{e}^{(\tau_{d-1}-\tau_d)\mathcal{L}} f(\tau_d) u(\tau_d) \mathrm{d}\tau_d \ldots \mathrm{d}\tau_1,
$$

for fixed t, is uniformly bounded in norm $\|\ \ \|$ of space $D(\mathcal{L})$ by a constant independent of t.

Lemma 2. *Suppose that Assumption 1 is satisfied. Let $u \in V$ (V is the domain of operator T defined in (3.9)), and $2p > m/2$. Then there exist a constant M (depending only on p and m), such that*

$$
\|T^d u(t)\| \leq M^d C_1^d C_2^d C_3 \frac{(t^\star)^d}{d!}, \quad t \in [0, t^\star], \tag{3.11}
$$

where $C_1 := \max_{t\in[0,t^\star]} \|\mathrm{e}^{t\mathcal{L}}\|_{D(\mathcal{L})\leftarrow D(\mathcal{L})}$, $C_2 := \max_{t\in[0,t^\star]} \|f(t)\|$ and $C_3 := \max_{t\in[0,t^\star]} \|u(t)\|$.

Proof. By applying inequality (3.10), and using basic properties of the operator norm, we can easily estimate $\|T^d u(t)\|$ for a fixed time t.

$$
\begin{aligned}
\|T^d u(t)\| &= \left\| \int_0^t \mathrm{e}^{(t-\tau_1)\mathcal{L}} f(\tau_1) \int_0^{\tau_1} \mathrm{e}^{(\tau_1-\tau_2)\mathcal{L}} f(\tau_2) \cdots \int_0^{\tau_{d-1}} \mathrm{e}^{(\tau_{d-1}-\tau_d)\mathcal{L}} f(\tau_d) u(\tau_d) \mathrm{d}\tau_d \ldots \mathrm{d}\tau_1 \right\| \\
&= \left\| \int_0^t \int_0^{\tau_1} \cdots \int_0^{\tau_{d-1}} \mathrm{e}^{(t-\tau_1)\mathcal{L}} f(\tau_1) \mathrm{e}^{(\tau_1-\tau_2)\mathcal{L}} f(\tau_2) \ldots \mathrm{e}^{(\tau_{d-1}-\tau_d)\mathcal{L}} f(\tau_d) u(\tau_d) \mathrm{d}\tau_d \ldots \mathrm{d}\tau_1 \right\|
\end{aligned}
$$

$$
\begin{aligned}
&\leq \int_0^t \int_0^{\tau_1} \cdots \int_0^{\tau_{d-1}} \left\| e^{(t-\tau_1)\mathcal{L}} f(\tau_1) e^{(\tau_1-\tau_2)\mathcal{L}} f(\tau_2) \ldots e^{(\tau_{d-1}-\tau_d)\mathcal{L}} f(\tau_d) u(\tau_d) \right\| \mathrm{d}\tau_d \ldots \mathrm{d}\tau_1 \\
&\leq \int_0^t \int_0^{\tau_1} \cdots \int_0^{\tau_{d-1}} \left\| e^{(t-\tau_1)\mathcal{L}} \right\| \left\| f(\tau_1) e^{(\tau_1-\tau_2)\mathcal{L}} f(\tau_2) \ldots e^{(\tau_{d-1}-\tau_d)\mathcal{L}} f(\tau_d) u(\tau_d) \right\| \mathrm{d}\tau_d \ldots \mathrm{d}\tau_1 \\
&\leq C_1 C_2 M \int_0^t \int_0^{\tau_1} \cdots \int_0^{\tau_{d-1}} \left\| e^{(\tau_1-\tau_2)\mathcal{L}} f(\tau_2) \ldots e^{(\tau_{d-1}-\tau_d)\mathcal{L}} f(\tau_d) u(\tau_d) \right\| \mathrm{d}\tau_d \ldots \mathrm{d}\tau_1 =: (\star)
\end{aligned}
$$

Constant M comes from inequality (3.10). Proceeding analogously and repeatedly we obtain

$$
(\star) \leq M^d C_1^d C_2^d C_3 \int_0^t \int_0^{\tau_1} \cdots \int_0^{\tau_{d-1}} \mathrm{d}\tau_d \ldots \mathrm{d}\tau_1 \leq M^d C_1^d C_2^d C_3 \frac{(t^\star)^d}{d!}, \quad \forall t \in [0, t^\star],
$$

and the right hand side of the above inequality is independent of t, which completes the proof. □

Theorem 10. *Suppose that Assumption 1 is satisfied, $2p > m/2$ and $t \in [0, t^\star]$. Then series*

$$
\sum_{d=0}^{\infty} T^d e^{t\mathcal{L}} u_0, \quad t \in [0, t^\star],
$$

converges absolutely and uniformly to the solution $u^\star$ of equation (3.1), and $u^\star \in C^1([0, t^\star]; L^2(\Omega)) \cap C([0, t^\star]; D(\mathcal{L}))$.

Proof. Let us denote $C_1 := \max_{t\in[0,t^\star]} \|e^{t\mathcal{L}}\|_{D(\mathcal{L})\leftarrow D(\mathcal{L})}$, $C_2 := \max_{t\in[0,t^\star]} \|f(t)\|$. By (3.11), we estimate

$$
\max_{t\in[0,t^\star]} \|T^d e^{t\mathcal{L}} u_0\| \leq \underbrace{M^d C_1^{d+1} C_2^d \|u_0\| \frac{(t^\star)^d}{d!}}_{=:A_d}, \quad \forall\ d \in \mathbb{N}.
$$

Since $\sum_{d=0}^{\infty} A_d = C_1 \|u_0\| \exp(t^\star M C_1 C_2)$ and space $D(\mathcal{L})$ is the Banach space, the Weierstrass M-test provides that sequence $\left\{u^{[n]}\right\}_{n=0}^{\infty}$ is convergent absolutely and uniformly to some function $u^\star \in C([0, t^\star], D(\mathcal{L}))$. Thus, for each $t \in [0, t^\star]$ we have

$$
u^\star(t) := \lim_{n\to\infty} u^{[n]}(t) = \sum_{d=0}^{\infty} T^d e^{t\mathcal{L}} u_0, \tag{3.12}
$$

where $u^{[n]}$ is defined by (3.8). The operator $I - T$ is a bijection and function $u^\star$ is the solution of (3.6). Indeed, it is easy to observe that

$$
(I - T) \sum_{d=0}^{n} T^d = \sum_{d=0}^{n} T^d (I - T) = I - T^{n+1}.
$$

Since $\|T^{n+1}\| \to 0$ as $n \to \infty$, for each $t \in [0, t^\star]$ we obtain

$$
(I - T) u^\star(t) = e^{t\mathcal{L}} u_0,
$$

which is the equivalent form of equation (3.6). Moreover, one can observe that the mapping $t \mapsto u^\star(t)$

is differentiable for each $t > 0$, when $u_0 \in D(\mathcal{L})$ and $f \in C([0,t^\star], H^{2p}(\Omega))$. Indeed, by considering the mild formulation of (3.1), namely

$$u^\star(t) = \mathrm{e}^{t\mathcal{L}}u_0 + \int_0^t \mathrm{e}^{(t-\tau)\mathcal{L}} f(\tau)u^\star(\tau)\mathrm{d}\tau, \tag{3.13}$$

of course the first part $\mathrm{e}^{t\mathcal{L}}u_0$ is continuously differentiable, $\frac{d}{dt}\mathrm{e}^{t\mathcal{L}}u_0 = \mathcal{L}\mathrm{e}^{t\mathcal{L}}u_0$, $\forall t > 0$, and since $u^\star(\tau)$ is continuous, function $g(t)$, defined as $g(t) := \int_0^t \mathrm{e}^{(t-\tau)\mathcal{L}} f(\tau)u^\star(\tau)\mathrm{d}\tau$, is also continuously differentiable. Since $\mathcal{L}$ is a closed operator, in addition holds

$$\frac{d}{dt}u^\star(t) = \mathrm{e}^{t\mathcal{L}}\mathcal{L}u_0 + f(t)u^\star(t) + \int_0^t \mathrm{e}^{(t-\tau)\mathcal{L}}\mathcal{L}f(\tau)u^\star(\tau)\mathrm{d}\tau.$$

Each expressions on the right-hand side are well-defined as u_0, $f(t)u^\star(t) \in D(\mathcal{L})$ for any $t \in [0,t^\star]$. Thus, we showed that solution $u^\star$ of (3.13) belongs to space $C^1([0,t^\star]; L^2(\Omega)) \cap C([0,t^\star]; D(\mathcal{L}))$. □

The above convergence proof of sequence (3.8) is similar to that presented in [23]. However, to show the convergence of (3.8) to the solution of equation (3.1), one needs to provide convergence of sequence (3.8) in the appropriate Sobolev norm.

Needless to say, the existence and uniqueness of linear evolution equations is a well-known and well-established theory in mathematics. Theorem 10 is only needed to show that solution to the equation can be presented as a series of multivariate integrals. This fact we utilize in the numerical approximation a highly oscillatory solution. It is easy to notice that in the proof of Theorem 10, operator T need not be a contraction mapping, but the Neumann series is still convergent. It can be shown that for arbitrarily time variable $t > 0$, there exists number s, such that for any $d > s$, operator T^d is a contraction mapping $\|T^d\| < 1$.

Remark 1. *The mild formulation of equation (3.1) allows us to relax the assumptions on the initial condition u_0. Instead of requiring $u_0 \in D(\mathcal{L})$, let us assume for a moment that $u_0 \in L^2(\Omega)$ and additionally that f is a bounded function $\|f\|_\infty < \infty$. By following a similar approach to the proof of Theorem 10, one can also establish the convergence of the sequence (3.8) in the norm of the space $C([0,t^\star]; L^2(\Omega))$ to the mild solution $u^\star$ of equation (3.1). In this case, the additional assumption $2p > m/2$ becomes redundant.*

Series (3.12) is called the Neumann series. Equation (3.6) can be expressed symbolically as

$$u(t) = \mathrm{e}^{t\mathcal{L}}u_0 + Tu(t).$$

It can be easy verified that for each n, the term $u^{[n]}(t)$ satisfies the relation

$$u^{[n]}(t) = \mathrm{e}^{t\mathcal{L}}u_0 + Tu^{[n-1]}(t), \quad u^{[0]}(t) = \mathrm{e}^{t\mathcal{L}}u_0.$$

Therefore, in the remaining text, we will use the terms 'n-th partial sum of the Neumann series' and 'n-th iteration of the equation' interchangeably to refer to the expression $u^{[n]}(t)$.

3.2 Presenting terms of the Neumann series as a sum of multivariate integrals

By Theorem 10, the solution to equation (3.1) can be expressed as the Neumann series $u(t) = \sum_{d=0}^{\infty} T^d \mathrm{e}^{t\mathcal{L}} u_0$. In this section, we show that for function f, defined in (3.3), each term $T^d \mathrm{e}^{t\mathcal{L}}$, $d = 1, 2, \dots$ of the Neumann series is a sum of multivariate highly oscillatory integrals. Subsequently, we will prove that each $T^d \mathrm{e}^{t\mathcal{L}}$ can be approximated by a partial sum of the asymptotic expansion. By linearity of semigroup operator $\{\mathrm{e}^{t\mathcal{L}}\}_{t\geq 0}$, we convert expression $T^d \mathrm{e}^{t\mathcal{L}}$ into a more convenient form, for function f defined in (3.3)

$$T^d \mathrm{e}^{t\mathcal{L}} = \int_0^t \int_0^{\tau_d} \cdots \int_0^{\tau_2} \mathrm{e}^{(t-\tau_d)\mathcal{L}} f(\tau_d) \mathrm{e}^{(\tau_d-\tau_{d-1})\mathcal{L}} f(\tau_{d-1}) \dots \mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}} f(\tau_1) \mathrm{e}^{\tau_1\mathcal{L}} \mathrm{d}\tau_1 \dots \mathrm{d}\tau_d =$$
$$\sum_{1\leq n_1,\dots n_d \leq N} \int_0^t \int_0^{\tau_d} \cdots \int_0^{\tau_2} \mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} \mathrm{e}^{(\tau_d-\tau_{d-1})\mathcal{L}} \alpha_{n_{d-1}} \dots \mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}} \alpha_{n_1} \mathrm{e}^{\tau_1\mathcal{L}} \mathrm{e}^{\mathrm{i}\omega(\tau_1 n_1+\cdots+\tau_d n_d)} \mathrm{d}\tau_1 \dots \mathrm{d}\tau_d =$$
$$\sum_{\boldsymbol{n}\in\{1,\dots,N\}^d} \int_{\sigma_d(t)} F_{\boldsymbol{n}}(t,\boldsymbol{\tau}) \mathrm{e}^{\mathrm{i}\omega\boldsymbol{n}^T\boldsymbol{\tau}} \mathrm{d}\boldsymbol{\tau} = \sum_{\boldsymbol{n}\in\{1,\dots,N\}^d} I[F_{\boldsymbol{n}}, \sigma_d(t)],$$

where

$$\boldsymbol{\tau} = (\tau_1, \tau_2, \dots, \tau_d),$$
$$F_{\boldsymbol{n}}(t,\boldsymbol{\tau}) = \mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} \mathrm{e}^{(\tau_d-\tau_{d-1})\mathcal{L}} \alpha_{n_{d-1}} \dots \mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}} \alpha_{n_1} \mathrm{e}^{\tau_1\mathcal{L}}, \tag{3.14}$$
$$I[F_{\boldsymbol{n}}, \sigma_d(t)] = \int_{\sigma_d(t)} F_{\boldsymbol{n}}(t,\boldsymbol{\tau}) \mathrm{e}^{\mathrm{i}\omega\boldsymbol{n}^T\boldsymbol{\tau}} \mathrm{d}\boldsymbol{\tau} \tag{3.15}$$

and $\sigma_d(t)$ denotes a d-dimensional simplex

$$\sigma_d(t) = \{\boldsymbol{\tau} := (\tau_1, \tau_2, \dots, \tau_d) \in \mathbb{R}^d : t \geq \tau_d \geq \tau_{d-1} \geq \cdots \geq \tau_2 \geq \tau_1 \geq 0\}.$$

Using the above notation, solution $u(t)$ of (3.6) can be written as

$$u(t) = \mathrm{e}^{t\mathcal{L}} u_0 + \sum_{d=1}^{\infty} \sum_{\boldsymbol{n}\in\{1,\dots,N\}^d} I[F_{\boldsymbol{n}}, \sigma_d(t)] u_0.$$

Each $F_{\boldsymbol{n}}(t,\boldsymbol{\tau})$ is a linear operator, $F_{\boldsymbol{n}}(t,\boldsymbol{\tau}) : \mathcal{D}(\mathcal{L}) \to \mathcal{D}(\mathcal{L})$ and $\boldsymbol{n} \in \mathbb{N}^d$ is a vector corresponding to $F_{\boldsymbol{n}}$ in the sense that $\boldsymbol{n}$ appears in the frequency exponent of integral (3.15).

In our approach, to expand asymptotically multivariate highly oscillatory integral of type (3.15), we will exploit repeatedly Fubini's theorem, properties of the semigroup operator and integration by parts. Therefore one should be able to compute successive partial derivatives of the expression of type (3.14). We use the identity (2.27) from Lemma 1

$$\partial_\tau^k \left(\mathrm{e}^{(t-\tau)\mathcal{L}} \alpha \mathrm{e}^{\tau\mathcal{L}} \right) = \mathrm{e}^{(t-\tau)\mathcal{L}} \underbrace{\Big[\dots [[\alpha, \mathcal{L}], \mathcal{L}], \dots \Big]}_{\mathcal{L} \textit{ appears } k \text{ times}} \mathrm{e}^{\tau\mathcal{L}} = (-1)^k \mathrm{e}^{(t-\tau)\mathcal{L}} ad_{\mathcal{L}}^k(\alpha) \mathrm{e}^{\tau\mathcal{L}},$$

where recall $ad_{\mathcal{L}}^0(\alpha) = \alpha$, $\quad ad_{\mathcal{L}}^k(\alpha) = \left[\mathcal{L}, ad_{\mathcal{L}}^{k-1}(\alpha)\right]$ and $[X,Y] \equiv XY - YX$ is the commutator of X and Y.

Unless otherwise stated, we assume that each appearing expression of type $\mathcal{L}^k\alpha_n$ is well defined for any functions $\alpha_n, n = 1, \ldots, N$.

In the asymptotic expansion of integral of type (3.15), the number of terms in a partial sum of the asymptotic series grows exponentially as the dimension d of the domain increases, therefore to facilitate the notation and keep the whole terms of the sum under control, we introduce the following definitions.

Definition 6. *By $\boldsymbol{v}_\ell^d \in \{0,1\}^d$, $\ell = 0, 1, \ldots d$ we denote the vertices of simplex $\sigma_d(1)$*

$$\begin{aligned} \boldsymbol{v}_0^d &= (1, 1, 1, \ldots, 1, 1); \\ \boldsymbol{v}_1^d &= (0, 1, 1, \ldots, 1, 1); \\ &\vdots \\ \boldsymbol{v}_\ell^d &= (\underbrace{0, \ldots, 0}_{\ell \text{ zeros}}, 1, \ldots, 1). \end{aligned}$$

Definition 7. *Let Φ_ℓ^d, $\ell = 0, 1, \ldots, d$, be a family of points such that*

$$\Phi_0^d = \{(1, 1, \ldots, 1)\},$$

$$\Phi_\ell^d = \{\boldsymbol{\phi} \in \{0,1\}^d : \boldsymbol{\phi} = (\phi_1, \phi_2, \ldots, \phi_d),\ \phi_\ell = 0,\ \phi_j = 1,\ \text{for } j > \ell\}$$

In other words, $\boldsymbol{\phi} \in \Phi_\ell^d$ if the last zero is at ℓ-th coordinate of $\boldsymbol{\phi}$, next coordinates are ones only.

Definition 8. *For $\boldsymbol{\phi} = (\phi_1, \phi_2, \ldots, \phi_d) \in \{0,1\}^d$ and multi-index $\boldsymbol{k} = (k_1, \ldots, k_d)$, we define the sequence of partial derivatives of $F(t, \tau_1, \tau_2, \ldots, \tau_d)$*

$$F^{\boldsymbol{k}}[\boldsymbol{\phi}](t) = \partial_{\tau_d}^{k_d} \left(\ldots \partial_{\tau_2}^{k_2} \left(\partial_{\tau_1}^{k_1} F(t, \tau_1, \tau_2, \ldots, \tau_d) \Big|_{\tau_1 = \phi_1 \tau_2} \right) \Big|_{\tau_2 = \phi_2 \tau_3} \cdots \right) \Big|_{\tau_d = \phi_d t}$$

Definition 8 we understand as follows: first, we compute the k_1-th partial derivative for variable τ_1. Then we substitute in place of τ_1 variable τ_2 or 0. Subsequently, we compute the k_2-th partial derivative with respect to variable τ_2 and then again we substitute $\tau_2 = \tau_3$ or $\tau_2 = 0$ and so on. We proceed in this manner until we compute the k_d-th partial derivative with respect to τ_d and substitute $\tau_d = \phi_d t$, where $\phi_d = 0$ or $\phi_d = 1$. We introduce the above definition as the order of partial derivatives at points is significant for operator defined in (3.14).

Example 4. *To present how Definition 8 operates for $F_{\boldsymbol{n}}$ definied in (3.14), we compute the first few expressions $F_{\boldsymbol{n}}^{\boldsymbol{k}}[\boldsymbol{\phi}](t)$ for $d = 1, 2$. We assume that α_n, $n = 1, \ldots, N$ are sufficiently smooth functions.*

$$\begin{aligned} F_{n_1}^{k_1}[1](t) &= \partial_{\tau_1}^{k_1} \left(\mathrm{e}^{(t-\tau_1)\mathcal{L}} \alpha_{n_1} \mathrm{e}^{\tau_1 \mathcal{L}} \right) \Big|_{\tau_1 = t} = (-1)^{k_1} ad_{\mathcal{L}}^{k_1}(\alpha_{n_1}) \mathrm{e}^{t\mathcal{L}}, \\ F_{n_1}^{k_1}[0](t) &= \partial_{\tau_1}^{k_1} \left(\mathrm{e}^{(t-\tau_1)\mathcal{L}} \alpha_{n_1} \mathrm{e}^{\tau_1 \mathcal{L}} \right) \Big|_{\tau_1 = 0} = (-1)^{k_1} \mathrm{e}^{t\mathcal{L}} ad_{\mathcal{L}}^{k_1}(\alpha_{n_1}), \\ F_{\boldsymbol{n}}^{\boldsymbol{k}}[(1,1)](t) &= \partial_{\tau_2}^{k_2} \left(\partial_{\tau_1}^{k_1} \left(\mathrm{e}^{(t-\tau_2)\mathcal{L}} \alpha_{n_2} \mathrm{e}^{(\tau_2 - \tau_1)\mathcal{L}} \alpha_{n_1} \mathrm{e}^{\tau_1 \mathcal{L}} \right) \Big|_{\tau_1 = \tau_2} \right) \Big|_{\tau_2 = t} = (-1)^{|\boldsymbol{k}|} ad_{\mathcal{L}}^{k_2} \left(\alpha_{n_2} ad_{\mathcal{L}}^{k_1}(\alpha_{n_1}) \right) \mathrm{e}^{t\mathcal{L}}, \\ F_{\boldsymbol{n}}^{\boldsymbol{k}}[(1,0)](t) &= \partial_{\tau_2}^{k_2} \left(\partial_{\tau_1}^{k_1} \left(\mathrm{e}^{(t-\tau_2)\mathcal{L}} \alpha_{n_2} \mathrm{e}^{(\tau_2 - \tau_1)\mathcal{L}} \alpha_{n_1} \mathrm{e}^{\tau_1 \mathcal{L}} \right) \Big|_{\tau_1 = \tau_2} \right) \Big|_{\tau_2 = 0} = (-1)^{|\boldsymbol{k}|} \mathrm{e}^{t\mathcal{L}} ad_{\mathcal{L}}^{k_2} \left(\alpha_{n_2} ad_{\mathcal{L}}^{k_1}(\alpha_{n_1}) \right), \\ F_{\boldsymbol{n}}^{\boldsymbol{k}}[(0,1)](t) &= \partial_{\tau_2}^{k_2} \left(\partial_{\tau_1}^{k_1} \left(\mathrm{e}^{(t-\tau_2)\mathcal{L}} \alpha_{n_2} \mathrm{e}^{(\tau_2 - \tau_1)\mathcal{L}} \alpha_{n_1} \mathrm{e}^{\tau_1 \mathcal{L}} \right) \Big|_{\tau_1 = 0} \right) \Big|_{\tau_2 = t} = (-1)^{|\boldsymbol{k}|} ad_{\mathcal{L}}^{k_2}(\alpha_{n_2}) \mathrm{e}^{t\mathcal{L}} ad_{\mathcal{L}}^{k_1}(\alpha_{n_1}), \end{aligned}$$

$$F_{\boldsymbol{n}}^{\boldsymbol{k}}[(0,0)](t) \quad = \quad \partial_{\tau_2}^{k_2}\left(\partial_{\tau_1}^{k_1}\left(\mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{n_2}\mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}}\alpha_{n_1}\mathrm{e}^{\tau_1\mathcal{L}}\right)\Big|_{\tau_1=0}\right)\Big|_{\tau_2=0} = (-1)^{|\boldsymbol{k}|}\mathrm{e}^{t\mathcal{L}}ad_{\mathcal{L}}^{k_2}(\alpha_{n_2})ad_{\mathcal{L}}^{k_1}(\alpha_{n_1}).$$

It can be shown that expression $F_{\boldsymbol{n}}^{\boldsymbol{k}}[\boldsymbol{\phi}]$, for operator $F_{\boldsymbol{n}}$ defined in (3.14), takes the following form

$$F_{\boldsymbol{n}}^{\boldsymbol{k}}[\boldsymbol{\phi}](t) = \sum_{\boldsymbol{m}\le\boldsymbol{k}}\binom{\boldsymbol{k}}{\boldsymbol{m}}(-1)^{|\boldsymbol{m}|+|\boldsymbol{k}|}\mathcal{L}^{r_{d+1}}\alpha_{n_d}\mathcal{L}^{r_d}\alpha_{n_{d-1}}\dots\mathcal{L}^{r_{\ell+1}}\alpha_{n_{\ell+1}}\mathrm{e}^{t\mathcal{L}}\mathcal{L}^{r_\ell}\alpha_{n_\ell}\dots\mathcal{L}^{r_2}\alpha_{n_1}\mathcal{L}^{r_1},$$

for certain vector $\boldsymbol{\phi}\in\Phi_\ell^d$, sufficiently smooth functions α_n, $n=1,\dots,N$ and multi-indexes $\boldsymbol{k}=(k_1,\dots.k_d)$, $\boldsymbol{m}=(m_1,\dots,m_d)$. Numbers $r_1,\dots r_{d+1}$ satisfy $r_1+\dots+r_{d+1}=|\boldsymbol{k}|$ and $\boldsymbol{m}\le\boldsymbol{k}$ means $m_i\le k_i$ for $i=1,2,\dots,d$.

3.3 Asymptotic expansion of a highly oscillatory integral subject to nonresonance condition

Let $\boldsymbol{n}=(n_1,\dots,n_d)\in\mathbb{N}^d$ be a vector. In this section, we assume that the coordinates of $\boldsymbol{n}$ satisfy the nonresonance condition:

$$n_j+n_{j-1}+\dots+n_{r+1}+n_r\neq 0, \tag{3.16}$$

for each $1\le j\le r\le d$. This condition implies that $\boldsymbol{n}$ is not orthogonal to the faces of the simplex $\sigma_d(t)$. This case encompasses situations where the highly oscillatory potential f takes the form (3.3). In this section, we shows that the integral $I[F_{\boldsymbol{n}},\sigma_d(t)]$ defined in (3.15) can be expressed as a partial sum of the asymptotic series. Let us start with the first term of the Neumann series. By applying integration by parts, the integral $[F_{n_1},(0,t)]$ can be presented as the following sum:

$$\begin{aligned}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau n_1}\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha_{n_1}\mathrm{e}^{\tau\mathcal{L}}u_0\mathrm{d}\tau = \sum_{k=0}^{r-1}\frac{1}{(\mathrm{i}\omega n_1)^{k+1}}\left[\mathrm{e}^{\mathrm{i}\omega t n_1}ad_{\mathcal{L}}^{k}(\alpha_{n_1})\mathrm{e}^{t\mathcal{L}}-\mathrm{e}^{t\mathcal{L}}ad_{\mathcal{L}}^{k}(\alpha_{n_1})\right]u_0 \\ +\frac{1}{(\mathrm{i}\omega n_1)^r}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau n_1}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{r}(\alpha_{n_1})\mathrm{e}^{\tau\mathcal{L}}u_0\mathrm{d}\tau,\end{aligned} \tag{3.17}$$

and the above expansion approximates the integral with error $\mathcal{O}(\omega^{-r-1})$. The general formula for the integral $I[F_{\boldsymbol{n}},\sigma_d(t)]$ over a d-dimensional simplex is unfortunately much more complicated. However, equation (3.17) shows the main idea of our considerations. In the later derivation, we will use simple tools, including induction, Fubini's theorem and identity (3.17).

The following definition determines coefficients that will appear as a result of integrating by parts in highly oscillatory integrals.

Definition 9. *For vector $\boldsymbol{\phi}\in\Phi_\ell^d$, vertex $\boldsymbol{v}_\ell^d$ of simplex $\sigma_d(1)$, $\ell=0,1,\dots,d$, multi-indexes $\boldsymbol{k}=(k_1,\dots,k_{d+1})$, $\tilde{\boldsymbol{k}}=(k_1,\dots,k_d)$ and vector $\boldsymbol{n}=(n_1,\dots,n_d)\in\mathbb{N}^d$ satisfying condition (3.16), we introduce the following rational numbers*

$$A_{k_1}[\phi_1](n_1)=\frac{(-1)^{\phi_1+1}}{n_1^{k_1+1}},$$

$$A_{\boldsymbol{k}}[(\boldsymbol{\phi},\phi_{d+1})]((\boldsymbol{n},n_{d+1})) = A_{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\boldsymbol{n})\frac{(-1)^{\phi_{d+1}+1}}{[(\boldsymbol{v}_\ell^d,1)\cdot(\boldsymbol{n},n_{d+1})]^{k_{d+1}+1}}.$$

One can express terms $A_{\boldsymbol{k}}[\boldsymbol{\phi}](\boldsymbol{n})$ explicitly, namely for $\boldsymbol{\phi} = (\phi_1, \phi_2, \dots \phi_d) \in \Phi_\ell^d$ we have

$$A_{\boldsymbol{k}}[\boldsymbol{\phi}](\boldsymbol{n}) = \frac{(-1)^{\phi_1+1}}{n_1^{k_1+1}}\frac{(-1)^{\phi_2+1}}{(n_1\phi_1+n_2)^{k_2+1}}\frac{(-1)^{\phi_3+1}}{((n_1\phi_1+n_2)\phi_2+n_3)^{k_3+1}}\cdots\frac{(-1)^{\phi_d+1}}{(\dots((n_1\phi_1+n_2)\phi_2+n_3)\,\phi_3+\dots+n_d)^{k_d+1}} \tag{3.18}$$

yet recursive definition will be needed later in the proof of Theorem 11. Due to assumption (3.16), we never divide by zero in the above expressions.

Example 5. *For $d = 3$ we compute coefficients $A_{\boldsymbol{k}}[\boldsymbol{\phi}](\boldsymbol{n})$ for different $\phi \in \Phi_\ell^3$, $\ell = 0, 1, 2, 3$.*

$$\begin{aligned}
\ell = 0,\ A_{\boldsymbol{k}}[(1,1,1)](\boldsymbol{n}) &= \frac{1}{n_1^{k_1+1}(n_1+n_2)^{k_2+1}(n_1+n_2+n_3)^{k_3+1}},\\
\ell = 1,\ A_{\boldsymbol{k}}[(0,1,1)](\boldsymbol{n}) &= \frac{-1}{n_1^{k_1+1}(n_2)^{k_2+1}(n_2+n_3)^{k_3+1}},\\
\ell = 2,\ A_{\boldsymbol{k}}[(0,0,1)](\boldsymbol{n}) &= \frac{1}{n_1^{k_1+1}n_2^{k_2+1}n_3^{k_3+1}},\\
\ell = 2,\ A_{\boldsymbol{k}}[(1,0,1)](\boldsymbol{n}) &= \frac{-1}{n_1^{k_1+1}(n_1+n_2)^{k_2+1}n_3^{k_3+1}},\\
\ell = 3,\ A_{\boldsymbol{k}}[(0,0,0)](\boldsymbol{n}) &= \frac{-1}{n_1^{k_1+1}n_2^{k_2+1}n_3^{k_3+1}},\\
\ell = 3,\ A_{\boldsymbol{k}}[(1,1,0)](\boldsymbol{n}) &= \frac{-1}{n_1^{k_1+1}(n_1+n_2)^{k_2+1}(n_1+n_2+n_3)^{k_3+1}},\\
\ell = 3,\ A_{\boldsymbol{k}}[(0,1,0)](\boldsymbol{n}) &= \frac{1}{n_1^{k_1+1}n_2^{k_2+1}(n_2+n_3)^{k_3+1}},\\
\ell = 3,\ A_{\boldsymbol{k}}[(1,0,0)](\boldsymbol{n}) &= \frac{1}{n_1^{k_1+1}(n_1+n_2)^{k_2+1}n_3^{k_3+1}}.
\end{aligned}$$

Coefficients $A_{\boldsymbol{k}}[\boldsymbol{\phi}](\boldsymbol{n})$ appear is the asymptotic expansion of integral (3.15). They play a fundamental role in our research in the asymptotic analysis of highly oscillatory integrals with resonance points.

Remark 2. *In the subsequent part of the paper, we employ the following notation: If $\boldsymbol{n} = (n_1, \dots, n_m) \in \mathbb{Z}^m$ is an m-dimensional vector, then $\tilde{\boldsymbol{n}} = (n_1, n_2, \dots, n_{m-1}) \in \mathbb{Z}^{m-1}$ represents a $(m-1)$-dimensional vector obtained by excluding the last coordinate n_m from $\boldsymbol{n}$.*

To simplify complex notation in the proof Theorem 11, we will also write $F := F_{\boldsymbol{n}}$ for the operator defined in (3.14), if vector $\boldsymbol{n}$ corresponding to F is clear from the context.

Theorem 11. *Let F be the operator defined in (3.14), and let $\boldsymbol{n}$ be the vector corresponding to F that satisfies the nonresonance condition (3.16). Integral (3.15) can be expressed as the r-partial sum $\mathcal{S}_r^{(d)}(t)$ of the asymptotic series with error $E_r^{(d)}(t)$*

$$I[F,\sigma_d(t)] = \int_{\sigma_d(t)} F(t,\boldsymbol{\tau})\mathrm{e}^{\mathrm{i}\omega\boldsymbol{n}^T\boldsymbol{\tau}}\mathrm{d}\boldsymbol{\tau} = \mathcal{S}_r^{(d)}(t) + E_r^{(d)}(t), \tag{3.19}$$

where

$$\mathcal{S}_r^{(d)}(t) = \sum_{|\boldsymbol{k}|=0}^{r-d} \frac{(-1)^{|\boldsymbol{k}|}}{(\mathrm{i}\omega)^{d+|\boldsymbol{k}|}} \sum_{\ell=0}^{d} \mathrm{e}^{\mathrm{i}\omega t \boldsymbol{n}^T \boldsymbol{v}_\ell^d} \sum_{\boldsymbol{\phi}\in\Phi_\ell^d} A_{\boldsymbol{k}}[\boldsymbol{\phi}](\boldsymbol{n}) F^{\boldsymbol{k}}[\boldsymbol{\phi}](t) \tag{3.20}$$

and error $E_r^{(d)}(t)$ *of the expansion is in recursive form*

$$\begin{aligned} E_r^{(1)}(t) &= \frac{(-1)^r}{(\mathrm{i}\omega)^r} \frac{1}{n_1^r} \int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_1 n_1} \partial_{\tau_1}^r F(t,\tau_1) \mathrm{d}\tau_1, \qquad (3.21)\\ E_r^{(d)}(t) &= \frac{(-1)^{r-d+1}}{(\mathrm{i}\omega)^r} \sum_{|\boldsymbol{k}|=r-d+1} \sum_{\ell=0}^{d-1} \sum_{\boldsymbol{\phi}\in\Phi_\ell^{d-1}} \frac{1}{\left(\boldsymbol{n}^T \boldsymbol{v}_\ell^d\right)^{k_d}} A_{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tilde{\boldsymbol{n}}) \int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_d \boldsymbol{n}^T \boldsymbol{v}_\ell^d} \partial_{\tau_d}^{k_d} \left(\mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} F^{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tau_d)\right) \mathrm{d}\tau_d \\ &+ \int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} E_r^{(d-1)}(\tau_d) \mathrm{e}^{\mathrm{i}\omega n_d \tau_d} \mathrm{d}\tau_d, \ \text{for } d \geq 2. \end{aligned}$$

Proof of the Theorem 11 can be found in Appendix A.1.

Let us note that we cannot consider an infinite expansion in (3.19) because $\mathcal{S}_r^{(d)}(t)$ may not converge to $I[F, \sigma_d(t)]$ as $r \to \infty$, even if $\omega \gg 1$.

Theorem 11 states that the integral $I[F, \sigma_d(t)] \sim \mathcal{O}(\omega^{-d})$ can be approximated by the sum (3.20), with an error $\mathcal{O}(\omega^{-r})$ as given by the form (3.21). A similar result was first obtained in [22], where the authors provide the asymptotic expansion of a multivariate highly oscillatory integral over a regular simplex. However, our result differs in that the integrand is a vector-valued function, instead of a real-valued function, which makes the formulas for the asymptotic expansion of highly oscillatory integrals more complicated. In addition, for our further considerations, the coefficients $A_{\boldsymbol{k}}[\boldsymbol{\phi}](\boldsymbol{n})$ and the error $E_r^{(d)}(t)$ of the expansion must be explicitly derived.

3.4 Error analysis. First four terms of the Modulated Fourier expansion

In this section, we provide the error analysis of the approximation of the solution to equation (3.1) using the sum (3.4). Additionally, we furnish ready-to-use formulas for the first four terms of the partial sum (3.4) of the asymptotic expansion.

By Theorem 11, each integral $I[F_{\boldsymbol{n}}, \sigma_d(t)]$, for vector $\boldsymbol{n}$ satisfying the nonresonance condition (3.16), and for sufficiently smooth functions α_n, $n = 1, \ldots, N$, can be expressed as a partial sum of the asymptotic expansion

$$I[F_{\boldsymbol{n}}, \sigma_d(t)] = S_{r,\boldsymbol{n}}^{(d)}(t) + E_{r,\boldsymbol{n}}^{(d)}(t),$$

where $\mathcal{S}_{r,\boldsymbol{n}}^{(d)}(t)$ is the sum corresponding to operator $F_{\boldsymbol{n}}$ and $S_{r,\boldsymbol{n}}^{(d)}(t) \sim \mathcal{O}(\omega^{-d})$. Moreover, for the r-th partial sum of the Neumann series holds

$$u^{[r]}(t) = \sum_{d=0}^{r} T^d \mathrm{e}^{t\mathcal{L}} u_0 = \mathrm{e}^{t\mathcal{L}} u_0 + \sum_{d=1}^{r} \sum_{\boldsymbol{n}\in\{1,\ldots,N\}^d} I[F_{\boldsymbol{n}}, \sigma_d(t)] u_0.$$

Therefore, it is possible to approximate the solution $u(t)$ of equation (3.1) by a sum of type (3.4). Furthermore, since the Neumann series converges for any time t, the asymptotic expansion is well-defined without the need for time steps.

We prove that the sum consists of terms of $\mathcal{S}^{(d)}_{r,\boldsymbol{n}}(t)u_0,\ d=1,2,\dots,r$

$$U^{[r]}_{as}(t)=\mathrm{e}^{t\mathcal{L}}u_0+\sum_{d=1}^{r}\sum_{\boldsymbol{n}\in\{1,\dots,N\}^d}\mathcal{S}^{(d)}_{r,\boldsymbol{n}}(t)u_0.$$

approximates the solution of (3.1) with error $\mathcal{O}(\omega^{-r-1})$.

Theorem 12. *Let $u(t)$ be the solution of (3.1) and $u^{[r]}(t)=\sum_{d=0}^{r}T^d\mathrm{e}^{t\mathcal{L}}u_0$ be the $r-$th partial sum of the Neumann series. We denote $\|\ \|_2:=\|\ \|_{L^2(\Omega)}$ and $\|\ \|_{q,2}:=\|\ \|_{H^{2p(r+1)}(\Omega)}$, where $q:=2p(r+1)$. By $\boldsymbol{T}$ we mean the operator $\boldsymbol{T}=\sum_{d=0}^{\infty}T^d$. For $t>0$, the following error estimations hold*

(1) $\|u(t)-u^{[r]}(t)\|_2\le\sup\limits_{\|v(t)\|_2\le1}\|\mathbf{T}v(t)\|_2\|T^{r+1}\mathrm{e}^{t\mathcal{L}}u_0\|_2=\mathcal{O}(\omega^{-r-1})$,

(2) $\|u(t)-U^{[r]}_{as}(t)\|_2\le\sup\limits_{\|v(t)\|_2\le1}\|\mathbf{T}v(t)\|_2\|T^{r+1}\mathrm{e}^{t\mathcal{L}}u_0\|_2+\sum\limits_{d=1}^{r}\sum\limits_{\boldsymbol{n}\in\{1,\dots,N\}^d}\|E^{(d)}_{r,\boldsymbol{n}}(t)u_0\|_2=\mathcal{O}(\omega^{-r-1})$.

Proof. Let $t>0$. According to Theorem 10, solution $u(t)$ of (3.1) can be expressed as the Neumann series $u(t)=\sum_{d=0}^{\infty}T^d\mathrm{e}^{t\mathcal{L}}u_0$. Therefore we have

$$\|u(t)-u^{[r]}(t)\|_2=\left\|\sum_{d=r+1}^{\infty}T^d\mathrm{e}^{t\mathcal{L}}u_0\right\|_2=\left\|\sum_{d=0}^{\infty}T^dT^{r+1}\mathrm{e}^{t\mathcal{L}}u_0\right\|_2\le\sup_{\|v(t)\|_2\le1}\|\mathbf{T}v(t)\|_2\|T^{r+1}\mathrm{e}^{t\mathcal{L}}u_0\|_2.$$

By Theorem 11, we have $\|T^{r+1}\mathrm{e}^{t\mathcal{L}}u_0\|_2\le\sum_{\boldsymbol{n}\in\{1,\dots,N\}^d}\left(\|\mathcal{S}^{(r+1)}_{r+1,\boldsymbol{n}}(t)u_0\|_2+\|E^{(r+1)}_{r+1,\boldsymbol{n}}(t)u_0\|_2\right)=\mathcal{O}(\omega^{-r-1})$. To show (2) we use the triangle inequality

$$\begin{aligned}\|u(t)-U^{[r]}_{as}(t)\|_2&\le\|u(t)-u^{[r]}(t)\|_2+\|u^{[r]}(t)-U^{[r]}_{as}(t)\|_2\\&\le\sup_{\|v(t)\|_2\le1}\|\mathbf{T}v(t)\|_2\|T^{r+1}\mathrm{e}^{t\mathcal{L}}u_0\|_2+\sum_{d=1}^{r}\sum_{\boldsymbol{n}\in\{1,\dots,N\}^d}\|E^{(d)}_{r,\boldsymbol{n}}(t)u_0\|_2,\end{aligned}$$

and for each $\boldsymbol{n}\in\{1,\dots,N\}^d$, in fact we have $\|E^{(d)}_{r,\boldsymbol{n}}(t)u_0\|_2=\mathcal{O}(\omega^{-r-1})$. Indeed, each integral that forms error $E^{(d)}_{r,\boldsymbol{n}}(t)u_0$ is, of course, highly oscillatory, and integrating by parts each of them results in (3). □

Expression $\boldsymbol{T}v(t)$, where $\|v(t)\|_2\le1$ is the solution of the integral equation

$$\psi(t)=v(t)+\int_0^t\mathrm{e}^{(t-\tau)\mathcal{L}}f(\tau)\psi(\tau)\mathrm{d}\tau. \tag{3.22}$$

Suppose that f is a bounded function on $[0,t^\star]$, $\|f\|_\infty<\infty$, and let $C_1:=\max_{t\in[0,t^\star]}\|\mathrm{e}^{t\mathcal{L}}\|_{L^2(\Omega)\leftarrow L^2(\Omega)}$. By Grönwall's inequality, solution of (3.22) can be estimated in L^2 norm

$$\|\mathbf{T}v(t)\|_2=\|\psi(t)\|_2\le\exp(tC_1\|f\|_\infty). \tag{3.23}$$

Remark 3. *The upper bound (3.23) of constant $\|\mathbf{T}v(t)\|_2$ may be large, especially for a big magnitude* *of $\|f\|_\infty$. Therefore, let us also consider a different approach to this issue. In the proof of inequality (1) of Theorem 12, we estimate the truncation of the Neumann series*

$$\|u(t) - u^{[r]}(t)\|_2 = \left\| \sum_{d=0}^{\infty} T^d T^{r+1} \mathrm{e}^{t\mathcal{L}} u_0 \right\|_2 . \tag{3.24}$$

Let now $v(t) = T^{r+1}\mathrm{e}^{t\mathcal{L}}u_0$. It is straightforward to verify that $\psi(t) = \sum_{d=0}^{\infty} T^d v(t)$ is the solution of the following non-homogeneous equation

$$\begin{aligned} \psi'(t) &= \mathcal{L}\psi(t) + f(t)\psi(t) + v'(t) - \mathcal{L}v(t), \\ \psi(0) &= v(0). \end{aligned} \tag{3.25}$$

From the form of function $v(t)$ we have

$$v'(t) - \mathcal{L}v(t) = f(t)T^r \mathrm{e}^{t\mathcal{L}}u_0 + \mathcal{L}T^{r+1}\mathrm{e}^{t\mathcal{L}}u_0 - \mathcal{L}T^{r+1}\mathrm{e}^{t\mathcal{L}}u_0 = f(t)T^r\mathrm{e}^{t\mathcal{L}}u_0$$

and $v(0) \equiv 0$. Therefore, equation (3.25) reads

$$\begin{aligned} \psi'(t) &= (\mathcal{L} + f(t))\psi(t) + f(t)T^r\mathrm{e}^{t\mathcal{L}}u_0, \\ \psi(0) &= 0, \end{aligned} \tag{3.26}$$

and $f(t)T^r\mathrm{e}^{t\mathcal{L}}u_0 = \mathcal{O}(\omega^{-r})$. Moreover, for a sufficiently small time variable t, the solution of (3.26) can be written as

$$\psi(t) = \int_0^t \Phi(t,s) f(s) T^r \mathrm{e}^{s\mathcal{L}} u_0 \mathrm{d}s,$$

where $\Phi(t,s)$ is the solution of the homogeneous problem

$$\Phi'(t,s) = (\mathcal{L} + f(s))\Phi(t,s), \qquad \Phi(s,s) = 1,$$

and $\Phi(t,s) = \exp(\Omega(t,s))$, where $\Omega(t,s)$ is the Magnus expansion. If, for example, (3.1) is the Schrödinger equation with a time dependent potential, then $\|\Phi(t,s)\|_2 \equiv 1$ and therefore the truncation (3.24) can be estimated in a different manner

$$\left\| \sum_{d=0}^{\infty} T^d T^{r+1} \mathrm{e}^{t\mathcal{L}} u_0 \right\|_2 = \|\psi(t)\|_2 \le t\|f\|_\infty \max_{s\in[0,t]} \|T^r \mathrm{e}^{s\mathcal{L}} u_0\|_2.$$

This provides a different estimate of the error constant $\|\mathbf{T}v(t)\|_2$.

Now we provide a ready-made formula for the sum (3.4) for $R = 3$, which approximates the solution $u(t)$ of problem (3.1) with error $\mathcal{O}(\omega^{-4})$. Solution $u(t)$ can be written as

$$u(t) = \mathrm{e}^{t\mathcal{L}}u_0 + T^1\mathrm{e}^{t\mathcal{L}}u_0 + T^2\mathrm{e}^{t\mathcal{L}}u_0 + T^3\mathrm{e}^{t\mathcal{L}}u_0 + \boldsymbol{T}T^4\mathrm{e}^{t\mathcal{L}}u_0,$$

where $\boldsymbol{T} = \sum_{d=0}^{\infty} T^d$, and the magnitude of the truncation of the Neumann series $\|\boldsymbol{T}T^4\mathrm{e}^{t\mathcal{L}}u_0\|_2 = \mathcal{O}(\omega^{-4})$.

Each term $T^1 \mathrm{e}^{t\mathcal{L}} u_0$, $T^2 \mathrm{e}^{t\mathcal{L}} u_0$ and $T^3 \mathrm{e}^{t\mathcal{L}} u_0$ we expand as follows to obtain the error of the approximation $\mathcal{O}(\omega^{-4})$

$$\begin{aligned}
T^1 \mathrm{e}^{t\mathcal{L}} u_0 &= \sum_{n_1 \in \{1,\ldots,N\}} \left(\mathcal{S}^{(1)}_{3,n_1}(t) + E^{(1)}_{3,n_1}(t) \right) u_0, \\
T^2 \mathrm{e}^{t\mathcal{L}} u_0 &= \sum_{\boldsymbol{n} \in \{1,\ldots,N\}^2} \left(\mathcal{S}^{(2)}_{3,\boldsymbol{n}}(t) + E^{(2)}_{3,\boldsymbol{n}}(t) \right) u_0, \\
T^3 \mathrm{e}^{t\mathcal{L}} u_0 &= \sum_{\boldsymbol{n} \in \{1,\ldots,N\}^3} \left(\mathcal{S}^{(3)}_{3,\boldsymbol{n}}(t) + E^{(3)}_{3,\boldsymbol{n}}(t) \right) u_0.
\end{aligned}$$

The partial sum of the asymptotic expansion that approximates solution $u(t)$ is equal to

$$U^{[3]}_{as}(t) = \mathrm{e}^{t\mathcal{L}} u_0 + \sum_{n_1 \in \{1,\ldots,N\}} \mathcal{S}^{(1)}_{3,n_1}(t) u_0 + \sum_{\boldsymbol{n} \in \{1,\ldots,N\}^2} \mathcal{S}^{(2)}_{3,\boldsymbol{n}}(t) u_0 + \sum_{\boldsymbol{n} \in \{1,\ldots,N\}^3} \mathcal{S}^{(3)}_{3,\boldsymbol{n}}(t) u_0,$$

where $\mathcal{S}^{(1)}_{3,n_1}(t) u_0$, $\mathcal{S}^{(2)}_{3,\boldsymbol{n}}(t) u_0$ and $\mathcal{S}^{(3)}_{3,\boldsymbol{n}}(t) u_0$, by identity (3.20), are of the following form

$$\begin{aligned}
\mathcal{S}^{(1)}_{3,n_1}(t) u_0 &= \frac{1}{\mathrm{i} n_1 \omega} \left(\mathrm{e}^{\mathrm{i} n_1 \omega t} \alpha_{n_1} \mathrm{e}^{t\mathcal{L}} - \mathrm{e}^{t\mathcal{L}} \alpha_{n_1} \right) u_0 + \frac{1}{(\mathrm{i} n_1 \omega)^2} \left(\mathrm{e}^{\mathrm{i} n_1 \omega t} ad^1_{\mathcal{L}}(\alpha_{n_1}) \mathrm{e}^{t\mathcal{L}} - \mathrm{e}^{t\mathcal{L}} ad^1_{\mathcal{L}}(\alpha_{n_1}) \right) u_0 \\
&+ \frac{1}{(\mathrm{i} n_1 \omega)^3} \left(\mathrm{e}^{\mathrm{i} n_1 \omega t} ad^2_{\mathcal{L}}(\alpha_{n_1}) \mathrm{e}^{t\mathcal{L}} - \mathrm{e}^{t\mathcal{L}} ad^2_{\mathcal{L}}(\alpha_{n_1}) \right) u_0,
\end{aligned}$$

$$\begin{aligned}
\mathcal{S}^{(2)}_{3,\boldsymbol{n}}(t) u_0 &= \frac{1}{(\mathrm{i}\omega)^2} \left(\mathrm{e}^{\mathrm{i}\omega t(n_1+n_2)} \frac{1}{n_1(n_1+n_2)} \alpha_{n_2} \alpha_{n_1} \mathrm{e}^{t\mathcal{L}} - \mathrm{e}^{\mathrm{i}\omega t n_2} \frac{1}{n_1 n_2} \alpha_{n_2} \mathrm{e}^{t\mathcal{L}} \alpha_{n_1} + \frac{1}{n_2(n_1+n_2)} \mathrm{e}^{t\mathcal{L}} \alpha_{n_2} \alpha_{n_1} \right) u_0 \\
&+ \frac{1}{(\mathrm{i}\omega)^3} \Bigg(\mathrm{e}^{\mathrm{i}\omega t(n_1+n_2)} \left(\frac{1}{n_1^2(n_1+n_2)} \alpha_{n_2} ad^1_{\mathcal{L}}(\alpha_{n_1}) \mathrm{e}^{t\mathcal{L}} + \frac{1}{n_1(n_1+n_2)^2} ad^1_{\mathcal{L}}(\alpha_{n_2} \alpha_{n_1}) \mathrm{e}^{t\mathcal{L}} \right) \\
&+ \mathrm{e}^{\mathrm{i}\omega t n_2} \left(\frac{-1}{n_1^2 n_2} \alpha_{n_2} \mathrm{e}^{t\mathcal{L}} ad^1_{\mathcal{L}}(\alpha_{n_1}) - \frac{1}{n_1 n_2^2} ad^1_{\mathcal{L}}(\alpha_{n_2}) \mathrm{e}^{t\mathcal{L}} \alpha_{n_1} \right) + \frac{1}{n_1 n_2 (n_1+n_2)} \mathrm{e}^{t\mathcal{L}} \alpha_{n_2} ad^1_{\mathcal{L}}(\alpha_{n_1}) \\
&+ \frac{-1}{n_1(n_1+n_2)^2} \mathrm{e}^{t\mathcal{L}} ad^1_{\mathcal{L}}(\alpha_{n_2} \alpha_{n_1}) + \frac{1}{n_1 n_2^2} \mathrm{e}^{t\mathcal{L}} ad^1_{\mathcal{L}}(\alpha_{n_2}) \alpha_{n_1} \Bigg) u_0,
\end{aligned}$$

$$\begin{aligned}
S^{(3)}_{3,\boldsymbol{n}}(t) u_0 &= \frac{1}{(\mathrm{i}\omega)^3} \Bigg(\frac{\mathrm{e}^{\mathrm{i}\omega t(n_1+n_2+n_3)}}{n_1(n_1+n_2)(n_1+n_2+n_3)} \alpha_{n_3} \alpha_{n_2} \alpha_{n_1} \mathrm{e}^{t\mathcal{L}} - \frac{\mathrm{e}^{\mathrm{i}\omega t(n_2+n_3)}}{n_1 n_2 (n_2+n_3)} \alpha_{n_3} \alpha_{n_2} \mathrm{e}^{t\mathcal{L}} \alpha_{n_1} \\
&+ \frac{\mathrm{e}^{\mathrm{i}\omega t n_3}}{n_2 n_3 (n_1+n_2)} \alpha_{n_3} \mathrm{e}^{t\mathcal{L}} \alpha_{n_2} \alpha_{n_1} - \frac{1}{(n_1+n_2+n_3)(n_2+n_3) n_3} \mathrm{e}^{t\mathcal{L}} \alpha_{n_3} \alpha_{n_2} \alpha_{n_1} \Bigg) u_0.
\end{aligned}$$

Expressions of type $\mathrm{e}^{t\mathcal{L}} u_0$, $\mathrm{e}^{t\mathcal{L}} \alpha_{n_j} u_0$, $\mathrm{e}^{t\mathcal{L}} ad^1_{\mathcal{L}}(\alpha_{n_j}) u_0$, etc. can be computed either explicitly, or very efficiently and accurately by using the spectral methods [33] and/or the splitting methods [25].

To summarize, each terms of the Neumann series $T^d \mathrm{e}^{t\mathcal{L}} u_0$ can be written as the following sum together with the error

$$T^d \mathrm{e}^{t\mathcal{L}} u_0 = \frac{1}{\omega^d} \sum_{s=0}^{dN} \mathrm{e}^{\mathrm{i}\omega s} P^d_{d,s} + \frac{1}{\omega^{d+1}} \sum_{s=0}^{dN} \mathrm{e}^{\mathrm{i}\omega s} P^d_{d+1,s} + \cdots + \frac{1}{\omega^r} \sum_{s=0}^{dN} \mathrm{e}^{\mathrm{i}\omega s} P^d_{r,s} + \frac{1}{\omega^{r+1}} \boldsymbol{E}^d_r.$$

$P^d_{j,s}$ consists of terms of $\mathcal{S}^d_{r,\boldsymbol{n}}(t)u_0$, independent of ω, which stand next to frequency $\mathrm{e}^{\mathrm{i}\omega s}$ and magnitude $\frac{1}{\omega^j}$. $\boldsymbol{E}^d_r$ is the whole error associated with the approximation of $T^d\mathrm{e}^{t\mathcal{L}}u_0$ by the partial sum of the asymptotic series.

It is very convenient to present the idea of the asymptotic expansion in the following table

$$\begin{array}{llllllll}
T^1\mathrm{e}^{t\mathcal{L}}u_0 = & \frac{1}{\omega}\sum_{s=0}^{N}\mathrm{e}^{\mathrm{i}\omega s}P^1_{1,s} & +\frac{1}{\omega^2}\sum_{s=0}^{N}\mathrm{e}^{\mathrm{i}\omega s}P^1_{2,s} & +\frac{1}{\omega^3}\sum_{s=0}^{N}\mathrm{e}^{\mathrm{i}\omega s}P^1_{3,s}+ & \dots & +\frac{1}{\omega^r}\sum_{s=0}^{N}\mathrm{e}^{\mathrm{i}\omega s}P^1_{r,s} & +\frac{1}{\omega^{r+1}}\boldsymbol{E}^1_r \\
T^2\mathrm{e}^{t\mathcal{L}}u_0 = & & \frac{1}{\omega^2}\sum_{s=0}^{2N}\mathrm{e}^{\mathrm{i}\omega s}P^2_{2,s} & +\frac{1}{\omega^3}\sum_{s=0}^{2N}\mathrm{e}^{\mathrm{i}\omega s}P^2_{3,s}+ & \dots & +\frac{1}{\omega^r}\sum_{s=0}^{2N}\mathrm{e}^{\mathrm{i}\omega s}P^2_{r,s} & +\frac{1}{\omega^{r+1}}\boldsymbol{E}^2_r \\
T^3\mathrm{e}^{t\mathcal{L}}u_0 = & & & \frac{1}{\omega^3}\sum_{s=0}^{3N}\mathrm{e}^{\mathrm{i}\omega s}P^3_{3,s}+ & \dots & +\frac{1}{\omega^r}\sum_{s=0}^{3N}\mathrm{e}^{\mathrm{i}\omega s}P^3_{r,s} & +\frac{1}{\omega^{r+1}}\boldsymbol{E}^3_r \\
\vdots & & & & \ddots & \vdots & \\
T^r\mathrm{e}^{t\mathcal{L}}u_0 = & & & & & \frac{1}{\omega^r}\sum_{s=0}^{rN}\mathrm{e}^{\mathrm{i}\omega s}P^r_{r,s} & +\frac{1}{\omega^{r+1}}\boldsymbol{E}^r_r
\end{array}$$

The error of the method consists of truncating the Neumann series and truncating the asymptotic expansion each term $T^d\mathrm{e}^{t\mathcal{L}}u_0,\ d = 1,\dots r$.

3.5 Asymptotic expansion – integrals with resonance points

Theorem 11 allows for the asymptotic expansion of integral $I[F_{\boldsymbol{n}},\sigma_d(t)]$ provided that vector $\boldsymbol{n}$ satisfies the nonresonance condition (3.16). However, given the potential function of a more general form (3.5) with negative frequencies, solution of problem (3.1) can be presented as

$$u(t) = \mathrm{e}^{t\mathcal{L}}u_0 + \sum_{d=1}^{\infty}\sum_{\boldsymbol{n}\in\boldsymbol{N}^d} I[F_{\boldsymbol{n}},\sigma_d(t)]u_0,$$

where $\boldsymbol{N}^d$ is a set of all possible vectors $\boldsymbol{n}$

$$\boldsymbol{N}^d := \{-N,\dots,-2,-1,1,2,\dots,N\}^d. \tag{3.27}$$

Set $\boldsymbol{N}^d$ comprises vectors $\boldsymbol{n}$ which are orthogonal to the simplex $\sigma_d(t)$ or its boundary. Coordinates of such $\boldsymbol{n}$ satisfy

$$n_j + n_{j-1} + \cdots + n_{r+1} + n_r = 0,$$

for certain $1 \le j < r \le d$. For those vectors we cannot apply Theorem 11 since otherwise we would divide by zero in expressions (3.18). Our advantage is, however, that instead of one integral with resonance points, we are to deal with a sum of such integrals. In Theorem 11, an increase in the dimension of integral results in an increase in the rate of decay – while $I[F,\sigma_{d-1}(t)] \sim \mathcal{O}(\omega^{-d+1})$, $I[F,\sigma_d(t)] \sim \mathcal{O}(\omega^{-d})$. This is because at any step of the proof we could integrate by parts each integral since, due to non-resonance assumption, the argument of frequency exponent $\boldsymbol{n}^T\boldsymbol{v}^d_\ell \neq 0$ and then $\mathrm{e}^{\mathrm{i}\omega t\boldsymbol{n}^T\boldsymbol{v}^d_\ell}$ never vanish.

At this stage we consider integral $I[F_{\boldsymbol{n}},\sigma_d(t)]$ with vector $\boldsymbol{n} = (n_1,n_2,n_3,\dots,n_d) \in \boldsymbol{N}^d$ whose coordinates satisfy

$$n_1 + \cdots + n_d = 0 \quad \text{and} \quad n_j + n_{j+1} + \cdots + n_{j+r} \neq 0 \quad \text{for} \qquad j = 1, \ldots, d, \quad 1 \leq j + r \leq d. \quad (3.28)$$

In other words, $\boldsymbol{n}$ is orthogonal only to the edge of simplex $\sigma_d(t)$ contained in line $\{(x_1, x_2, \ldots, x_d) \in \mathbb{R}^d : x_1 = x_2 = \cdots = x_d\}$. In such a situation, we have $\boldsymbol{n}^T \boldsymbol{v}_0^d = n_1 + \cdots + n_d = 0$ and therefore in the proof of Theorem 11 we cannot integrate by parts the last, outer integral with $\mathrm{e}^{\mathrm{i}\omega\tau_d \boldsymbol{n}^T \boldsymbol{v}_0^d}$. The general case involving the whole set (3.27) is a matter of further research.

Let $\boldsymbol{n}_j \in \mathbb{N}^d,\ j = 1, \ldots, d$ be vectors satisfying (3.28), such that

$$\begin{aligned}
\boldsymbol{n}_1 &= (n_1, n_2, n_3, \ldots, n_{d-1}, n_d), \\
\boldsymbol{n}_2 &= (n_2, n_3, n_4, \ldots, n_d, n_1), \\
&\vdots \\
\boldsymbol{n}_j &= (n_j, n_{j+1}, \ldots, n_d, n_1, \ldots, n_{j-1}), \\
&\vdots \\
\boldsymbol{n}_d &= (n_d, n_1, n_2, \ldots, n_{d-2}, n_{d-1}).
\end{aligned}$$

If $\boldsymbol{n}_1 \in \boldsymbol{N}^d$, then vectors $\boldsymbol{n}_j,\ j = 2, \ldots d$ belong to set $\boldsymbol{N}^d$ as well. Because of assumption (3.28), for each $j = 1, \ldots, d$ we have $\sum_{j=1}^d \boldsymbol{n}_j = 0$. From the coordinates of vectors $\boldsymbol{n}_j$ we form the following fractional numbers

$$\begin{aligned}
A[\tilde{\boldsymbol{n}}_1] &= \frac{1}{n_1(n_1+n_2)(n_1+n_2+n_3)\ldots(n_1+n_2+n_3+\cdots+n_{d-1})}, \\
A[\tilde{\boldsymbol{n}}_2] &= \frac{1}{n_2(n_2+n_3)(n_2+n_3+n_4)\ldots(n_2+n_3+n_4+\cdots+n_d)}, \\
&\vdots \\
A[\tilde{\boldsymbol{n}}_{k+1}] &= \frac{1}{n_{k+1}(n_{k+1}+n_{k+2})\ldots(n_{k+1}+n_{k+2}+\cdots+n_d+n_1+\cdots+n_{k-1})}, \\
&\vdots \\
A[\tilde{\boldsymbol{n}}_d] &= \frac{1}{n_d(n_d+n_1)(n_d+n_1+n_2)\ldots(n_d+n_1+n_2\cdots+n_{d-3}+n_{d-2})}.
\end{aligned}$$

(We use cyclic notation $n_s = n_{s+d}$ for $s \in \mathbb{Z}$).

Lemma 3. *Let $\boldsymbol{n}_j,\ j = 1, \ldots, d$ be vectors which satisfy condition (3.28). Then*

$$\sum_{j=1}^{d} A[\tilde{\boldsymbol{n}}_j] = 0.$$

Proof. It is sufficient to apply the partial fraction decomposition to $A[\tilde{\boldsymbol{n}}_1]$, by treating n_1 as a variable and other numbers $n_r,\ r \neq 1$ as constants. We aim to express $A[\tilde{\boldsymbol{n}}_1]$ as

$$A[\tilde{\boldsymbol{n}}_1] = \sum_{j=1}^{d-1} \frac{N_j}{n_1 + \cdots + n_j}, \tag{3.29}$$

for certain numbers $N_j,\ j = 1, \ldots d-1$. Let us fix index j. To determine coefficient N_j, we use Heaviside's Cover-up Method. Substituting $n_1 = -(n_2 + \cdots + n_j)$ we have

$$\begin{aligned} N_j &= \left. \frac{1}{n_1(n_1+n_2)\ldots(n_1+\cdots+n_{j-1})(n_1+\cdots+n_{j+1})\ldots(n_1+\cdots+n_{d-1})} \right|_{n_1=-(n_2+\cdots+n_j)} \\ &= \frac{(-1)^{j-1}}{(n_2+\cdots+n_j)\ldots n_j n_{j+1}(n_{j+1}+n_{j+2})\ldots(n_{j+1}+\cdots+n_{d-1})} \\ &= \frac{1}{(n_{j+1}+\cdots+n_1)\ldots(n_{j+1}+n_{j+2}+\cdots+n_{j-1})n_{j+1}(n_{j+1}+n_{j+2})\ldots(n_{j+1}+\ldots n_{d-1})} \\ &= \frac{n_{j+1}+\cdots+n_d}{n_{j+1}(n_{j+1}+n_{j+2})\ldots(n_{j+1}+\cdots+n_{d-1})(n_{j+1}+\cdots+n_d)(n_{j+1}+\cdots+n_1)\ldots(n_{j+1}+\cdots+n_{j-1})} \end{aligned}$$

(in the penultimate equality we used assumption (3.28)). Now since $n_{j+1}+\cdots+n_d = -(n_1+\cdots+n_j)$, substituting N_j into (3.29) we obtain

$$A[\tilde{\boldsymbol{n}}_1] = \sum_{j=1}^{d-1} \frac{-1}{n_{j+1}(n_{j+1}+n_{j+2})\ldots(n_{j+1}+\cdots+n_{j-1})} = -\sum_{j=1}^{d-1} A[\tilde{\boldsymbol{n}}_{j+1}],$$

which completes the proof. □

Now let us notice, that if multi-index $\tilde{\boldsymbol{k}} = (k_1, \ldots, k_{d-1})$ satisfy $|\tilde{\boldsymbol{k}}| = 0$ and $\boldsymbol{\phi} = (1, \ldots, 1) \in \Phi_0^{d-1}$, then $A_{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tilde{\boldsymbol{n}}_j) = A[\tilde{\boldsymbol{n}}_j]$, where $A_{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tilde{\boldsymbol{n}}_j)$ are the coefficients from Definition 9. In other words, numbers $A[\tilde{\boldsymbol{n}}_j],\ j = 1, \ldots, d$ appear with the first term $\frac{1}{(\mathrm{i}\omega)^{d-1}}$ of the asymptotic expansion of integral $I[F_{\tilde{\boldsymbol{n}}_j}, \sigma_{d-1}(t)]$.

Theorem 13. *Let $\boldsymbol{n}_j \in \boldsymbol{N}^d$ be vector which satisfies (3.28) and let $F_{\boldsymbol{n}_j}$ be the operator defined in (3.14) with corresponding vector $\boldsymbol{n}_j,\ j = 1, \ldots, d$. Then*

$$\sum_{j=1}^{d} \int_{\sigma_d(t)} F_{\boldsymbol{n}_j}(t, \boldsymbol{\tau}) \mathrm{e}^{\mathrm{i}\omega \boldsymbol{n}_j^T \boldsymbol{\tau}} \mathrm{d}\boldsymbol{\tau} \sim \mathcal{O}(\omega^{-d}).$$

In other words, the sum of these integrals with resonance points over a simplex $\sigma_d(t)$ decays in the same manner as an integral over the same domain without resonance points.

Proof. Let $F_{\boldsymbol{n}_j}(t, \boldsymbol{\tau}) = \mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_{d,j}} \mathrm{e}^{(\tau_d - \tau_{d-1})\mathcal{L}} \alpha_{n_{d-1,j}} \ldots \mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}} \alpha_{n_{1,j}} \mathrm{e}^{\tau_1 \mathcal{L}}$ be the operator with corresponding vector $\boldsymbol{n}_j = (n_{1,j}, n_{2,j}, \ldots, n_{d,j})$, and let $\mathcal{S}^{(d-1)}_{r, \tilde{\boldsymbol{n}}_j}, E^{(d-1)}_{r, \tilde{\boldsymbol{n}}_j}$ be the partial sum of the asymptotic series and the error of approximation of integral $I[F_{\tilde{\boldsymbol{n}}_j}, \sigma_{d-1}(t)]$. We use Fubini's theorem and then we apply Theorem 11 to expand asymptotically $I[F_{\tilde{\boldsymbol{n}}_j}, \sigma_{d-1}(t)]$. It is possible since the nonresonance condition is violated only for the vectors $\boldsymbol{n}_j \in \mathbb{N}^d,\ j = 1, \ldots, d$.

$$\sum_{j=1}^{d} \int_{\sigma_d(t)} F_{\boldsymbol{n}_j}(t, \boldsymbol{\tau}) \mathrm{e}^{\mathrm{i}\omega \boldsymbol{n}_j^T \boldsymbol{\tau}} \mathrm{d}\boldsymbol{\tau} =$$

$$\sum_{j=1}^{d}\int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_{d,j}} I[F_{\tilde{\boldsymbol{n}}_j},\sigma_{d-1}(\tau_d)]\mathrm{e}^{\mathrm{i}\omega\tau_d n_{d,j}}\mathrm{d}\tau_d =$$

$$\sum_{j=1}^{d}\int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_{d,j}} \left(\mathcal{S}^{(d-1)}_{r,\tilde{\boldsymbol{n}}_j}(\tau_d)+E^{(d-1)}_{r,\tilde{\boldsymbol{n}}_j}(\tau_d)\right)\mathrm{e}^{\mathrm{i}\omega\tau_d n_{d,j}}\mathrm{d}\tau_d =$$

$$\underbrace{\sum_{j=1}^{d}\sum_{|\tilde{\boldsymbol{k}}|=0}^{r-d+1}\frac{(-1)^{|\tilde{\boldsymbol{k}}|}}{(\mathrm{i}\omega)^{d-1+|\tilde{\boldsymbol{k}}|}}\sum_{\ell=1}^{d-1}\sum_{\boldsymbol{\phi}\in\Phi_\ell^{d-1}}A_{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tilde{\boldsymbol{n}}_j)\int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_{d,j}}F^{\tilde{\boldsymbol{k}}}_{\tilde{\boldsymbol{n}}_j}[\boldsymbol{\phi}](\tau_d)\mathrm{e}^{\mathrm{i}\omega\tau_d\boldsymbol{n}_j^T\boldsymbol{v}_\ell^d}\mathrm{d}\tau_d}_{=:P_1(t)}+$$

$$\underbrace{\sum_{j=1}^{d}\sum_{|\tilde{\boldsymbol{k}}|=0}^{r-d+1}\frac{(-1)^{|\tilde{\boldsymbol{k}}|}}{(\mathrm{i}\omega)^{d-1+|\tilde{\boldsymbol{k}}|}}A_{\tilde{\boldsymbol{k}}}[(1,\ldots,1)](\tilde{\boldsymbol{n}}_j)\int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_{d,j}}\boldsymbol{F}^{\tilde{\boldsymbol{k}}}_{\tilde{\boldsymbol{n}}_j}[(1,\ldots,1)](\tau_d)\mathrm{e}^{\mathrm{i}\omega\tau_d\boldsymbol{n}_j^T\boldsymbol{v}_0^d}\mathrm{d}\tau_d}_{=:P_2(t)}+$$

$$\sum_{j=1}^{d}\int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_{d,j}}E^{(d-1)}_{r,j}(\tau_d)\mathrm{e}^{\mathrm{i}\omega\tau_d n_{d,j}}\mathrm{d}\tau_d.$$

Now since vectors $\boldsymbol{n}_j,\ j=1,\ldots,d$ satisfy (3.28), we have $\boldsymbol{n}_j^T\boldsymbol{v}_0^d=0$, so $\mathrm{e}^{\mathrm{i}\omega\tau_d\boldsymbol{n}_j^T\boldsymbol{v}_0^d}=1$ and therefore we cannot expand asymptotically expression $P_2(t)$. However, if $|\tilde{\boldsymbol{k}}|=0$ then for each j holds $\mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_{d,j}}F^{\tilde{\boldsymbol{k}}}_{\tilde{\boldsymbol{n}}_j}[(1,\ldots,1)](\tau_d)=\mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_1\alpha_2\ldots\alpha_d\mathrm{e}^{\tau_d\mathcal{L}}$ since functions α_j commute with each other. As a consequence, in expression P_2 , by Lemma 3, terms with $|\tilde{\boldsymbol{k}}|=0$ vanish, so P_2 is equal to

$$P_2(t)=\sum_{j=0}^{d}\sum_{|\tilde{\boldsymbol{k}}|=1}^{n-d+1}\frac{(-1)^{|\tilde{\boldsymbol{k}}|}}{(\mathrm{i}\omega)^{d-1+|\tilde{\boldsymbol{k}}|}}A_{\tilde{\boldsymbol{k}}}[(1,\ldots,1)](\tilde{\boldsymbol{n}}_j)\int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_{d,j}}F^{\tilde{\boldsymbol{k}}}_{\tilde{\boldsymbol{n}}_j}[(1,\ldots,1)](\tau_d)\mathrm{d}\tau_d$$

and thus $P_2(t)\sim\mathcal{O}(\omega^{-d})$. Expression $P_1(t)$ we integrate by parts according to Theorem 11 since each integrals of expressions $P_1(t)$ has no resonance points, therefore $P_1(t)\sim\mathcal{O}(\omega^{-d})$ and consequently $P_1+P_2\sim\mathcal{O}(\omega^{-d})$. □

In the asymptotic series of $\sum_{j=0}^{d}I[F_{n_j},\sigma_d(t)]$, in expressions which were denoted by P_2 in the proof of Theorem 13, appear terms with integral

$$\int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_{d,j}}F^{\tilde{\boldsymbol{k}}}_{\tilde{\boldsymbol{n}}_j}[(1,\ldots,1)](\tau_d)\mathrm{d}\tau_d$$

yet they are not highly oscillatory, so we expect we can approximate them effortlessly and effectively, for example by Gauss-Legendre quadrature.

Example 6. *Consider set* $\boldsymbol{N}^2=\{\boldsymbol{n}_1=(-1,1),\boldsymbol{n}_2=(1,-1)\}$ *and two integrals*

$$I[F_{\boldsymbol{n}_1},\sigma_2(t)]\quad \textit{and}\quad I[F_{\boldsymbol{n}_2},\sigma_2(t)].$$

Then $I[F_{\boldsymbol{n}_1},\sigma_2(t)]+I[F_{\boldsymbol{n}_2},\sigma_2(t)]\sim\mathcal{O}(\omega^{-2})$ *and the first term of the asymptotic expansion of* $I[F_{\boldsymbol{n}_1},\sigma_2(t)]+$

$I[F_{\boldsymbol{n}_2}, \sigma_2(t)]$ *is equal to*

$$\frac{1}{(\mathrm{i}\omega)^2}\left(\alpha_1 \mathrm{e}^{t\mathcal{L}}\alpha_{-1}\mathrm{e}^{\mathrm{i}\omega t} + \alpha_{-1}\mathrm{e}^{t\mathcal{L}}\alpha_1 \mathrm{e}^{-\mathrm{i}\omega t} - 2\mathrm{e}^{t\mathcal{L}}\alpha_1\alpha_{-1} + \int_0^t \mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_{-1} ad^1_{\mathcal{L}}(\alpha_1)\mathrm{e}^{\tau_2\mathcal{L}}\mathrm{d}\tau_2 + \int_0^t \mathrm{e}^{(t-\tau_2)\mathcal{L}}\alpha_1 ad^1_{\mathcal{L}}(\alpha_{-1})\mathrm{e}^{\tau_2\mathcal{L}}\mathrm{d}\tau_2\right).$$

Occurring integrals are not highly oscillatory and can be computed, for example, by Gauss-Legendre quadrature with high accuracy.

To summarise this section, it is much more difficult to provide formulas for coefficients of the asymptotic expansion for integrals with resonance points. However, Theorem 13 describes the asymptotic behaviour of terms from the Neumann series, and it seems possible to use this fact to construct quadrature rules based on the Filon method.

3.6 Application of the method to the wave equation

As an example of the application of the asymptotic method, we consider the following second-order PDE

$$\begin{aligned}
&\partial^2_{tt}u = \mathcal{L}u(x,t) + f(x,t)u(x,t), \qquad t \in [0,t^\star],\ x \in \Omega \subset \mathbb{R}^m, \\
&u(x,0) = u_1(x), \quad \partial_t u(x,0) = u_2(x), \\
&u = 0 \text{ on } \partial\Omega \times [0,t^\star],
\end{aligned} \tag{3.30}$$

with function f given in (3.3). We write (3.30) as a first-order system

$$\partial_t \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 & \mathcal{I} \\ \mathcal{L} & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + f \begin{bmatrix} 0 & 0 \\ \mathcal{I} & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix},$$

where $v = \partial_t u$. Thus

$$\partial_t \underbrace{\begin{bmatrix} u \\ v \end{bmatrix}}_{\varphi} = \underbrace{\begin{bmatrix} 0 & \mathcal{I} \\ \mathcal{L} & 0 \end{bmatrix}}_{A} \begin{bmatrix} u \\ v \end{bmatrix} + \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}n\omega t} \underbrace{\begin{bmatrix} 0 & 0 \\ \alpha_n & 0 \end{bmatrix}}_{\beta_n} \begin{bmatrix} u \\ v \end{bmatrix}$$

and therefore

$$\partial_t\varphi = A\varphi + h\varphi, \quad \varphi(x,0) = [u_1(x), u_2(x)], \quad A[u,v]^T = [v, \mathcal{L}u]^T, \quad \beta_n[u,v]^T = [0, \alpha_n u]^T, \tag{3.31}$$

where $h(x,t) = \sum_{n=1}^{N} \mathrm{e}^{\mathrm{i}n\omega t}\beta_n(x)$ is a highly oscillatory function and φ is a vector valued function. Suppose that $\mathcal{L}$ is a second-order differential operator which has symmetric form

$$\mathcal{L}u = \sum_{i,j=0}^{m} \partial_{x_j}\left(a_{ij}\partial_{x_i}u\right) - cu,$$

where $a_{ij} = a_{ji},\ i,j = 1,\dots,m$ and $c \geq 0$. For simplicity, assume that $\|\alpha_n\|_\infty < \infty,\ \forall n = 1,\dots,N$. By applying Duhamel's formula, we write (3.31) as

$$\varphi(t) = \mathrm{e}^{tA}\varphi_0 + \int_0^t \mathrm{e}^{(t-\tau)A} h(\tau)\varphi(\tau)\mathrm{d}\tau. \tag{3.32}$$

Operator $A : D(A) := \left[H^2(\Omega) \cap H_0^1(\Omega)\right] \times H_0^1(\Omega) \to H_0^1(\Omega) \times L^2(\Omega)$ is the infinitesimal generator of a C_0-semigroup $\{\mathrm{e}^{tA}\}$ on $H_0^1(\Omega) \times L^2(\Omega)$ [14]. Using the same arguments as in the proof of Theorem 10, one can show that the Neumann series converges absolutely and uniformly in the norm of space $H_0^1(\Omega) \times L^2(\Omega)$ to the solution of equation (3.32).

It is worth mentioning that the structure of the terms β_n causes certain terms in the asymptotic expansion to vanish. We obtain even more zeros when we allow negative frequencies $\mathrm{e}^{-\mathrm{i}n\omega t}$ and when the coefficients α_n satisfy the condition $\alpha_{-n} = \alpha_n$. This facilitates the derivation of the coefficients in the asymptotic expansion, reduces the computational time, and enhances more the accuracy of the method. This suggests that the asymptotic expansion works particularly well for equations with the second time derivative in the form of (3.30).

3.7 Numerical examples

In this section, we present the application of the method to various equations of type (3.1) with parameter $\omega \gg 1$. For each of the equations, it is possible to find an analytical solution to compare them accurately with a numerical approximation. The L^2 norm of the error is considered in any presented example. For each equation, the solution is approximated by partial sum of the asymptotic expansion

$$u(x,t) \approx p_{0,0}(x,t) + \sum_{r=1}^{R} \frac{1}{\omega^r} \sum_{s=0}^{S} p_{r,s}(x,t) e^{is\omega t}, \tag{3.33}$$

for different R and ω.

Example 1.

We first consider the following equation

$$\begin{aligned} &\partial_t u = (1-x^2)^4 \partial_{xx}^2 u + f(x,t)u(x,t), \qquad t \in [0,3],\ x \in (-1,1), \\ &u(x,0) = u_0(x), \\ &u(-1,t) = 0 = u(1,t), \end{aligned} \tag{3.34}$$

where initial condition u_0 and highly oscillatory potential f take the forms

$$u_0(x) = \begin{cases} \mathrm{e}^{-\frac{1}{1-x^2}} & \text{if } x \in (-1,1), \\ 0 & \text{otherwise,} \end{cases}$$

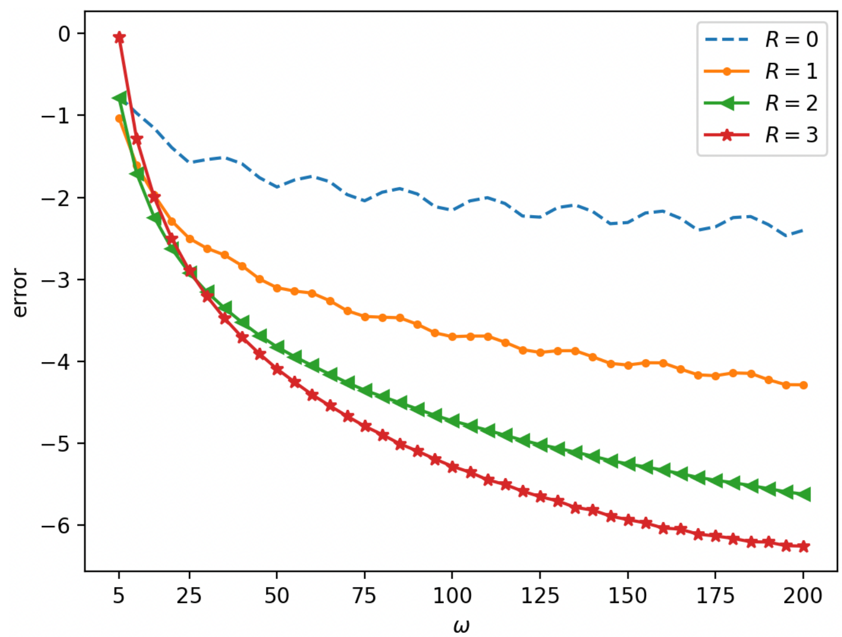


Figure 3.1: L^2 norm of the error of the method for the equation (3.34) for $t = 3$. We use a base–10 log scale.

$$\begin{aligned} f(x,t) &= \underbrace{\frac{1}{\omega^2}\left((1-x^2)^4 + 4\mathrm{i}\omega x(1-x^2)^2 + 2\omega^2(1-3x^4)\right)}_{\alpha_0(x)} + \mathrm{e}^{\mathrm{i}\omega t}\underbrace{\frac{1}{\omega^2}\left(-2(1-x^2)^4 - 4\mathrm{i}x\omega(1-x^2)^2 + x\omega^2\right)}_{\alpha_1(x)} \\ &+ \mathrm{e}^{2\mathrm{i}\omega t}\underbrace{\frac{1}{\omega^2}(1-x^2)^4}_{\alpha_2(x)}. \end{aligned}$$

The solution of (3.34) is

$$u(x,t) = \mathrm{e}^{-\frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\omega t}x}{\omega} + \frac{\mathrm{i}x}{\omega}} u_0(x)$$

and differential operator $\mathcal{L}$ is of the form

$$\mathcal{L} = (1-x^2)^4\partial^2_{xx} + \alpha_0.$$

To approximate the solution we take the first four terms of the Neumann series (the third iteration)

$$u^{[3]}(t) = \mathrm{e}^{t\mathcal{L}}u_0(x) + T^1\mathrm{e}^{t\mathcal{L}}u_0 + T^2\mathrm{e}^{t\mathcal{L}}u_0 + T^3\mathrm{e}^{t\mathcal{L}}u_0.$$

Subsequently, we expand asymptotically $T^1\mathrm{e}^{t\mathcal{L}}u_0$, $T^2\mathrm{e}^{t\mathcal{L}}u_0$ and $T^3\mathrm{e}^{t\mathcal{L}}u_0$ with error $\mathcal{O}(\omega^{-4})$. In other words, we approximate the solution of (3.34) by the partial sum of asymptotic expansion (3.4) with the first four terms. Figure 3.1 and Table 3.1 present the approximation error of the solution $u(x,3)$ for different values of ω and different lengths R of the partial sum of the Neumann series.

Example 2.
As mentioned, the method is also applicable to the potential with time–dependent functions $\alpha_n(x,t)$.

	$R=0$	$R=1$	$R=2$	$R=3$
$\omega=10$	1.12e-01	3.17e-02	2.75e-02	7.38e-02
$\omega=100$	1.23e-02	3.06e-04	2.68e-05	7.36e-06
$\omega=1000$	1.27e-03	3.15e-06	2.68e-08	1.76e-09

Table 3.1: Error of the method – equation (3.34)

	$R=0$	$R=1$	$R=2$
$\omega=10$	9.33e-03	5.28e-03	5.55e-05
$\omega=100$	5.33e-04	4.87e-05	4.94e-08
$\omega=1000$	4.96e-05	7.64e-08	4.86e-11

Table 3.2: Error of the method – equation (3.35)

Indeed, consider the following equation

$$\begin{aligned} &\partial_t u = \partial^2_{xx} u + \mathrm{e}^{\mathrm{i}\omega t}\sin(t)u(x,t), \qquad t\in[0,5],\ x\in(0,2\pi),\\ &u(x,0)=\sin(x),\\ &u(0,t)=0=u(2\pi,t). \end{aligned} \tag{3.35}$$

The solution of (3.35) equals

$$u(x,t)=\mathrm{e}^{-t-1/(\omega^2-1)+\mathrm{e}^{\mathrm{i}\omega t}\cos(t)/(\omega^2-1)-\mathrm{i}\mathrm{e}^{\mathrm{i}\omega t}\omega\sin(t)/(\omega^2-1)}\sin(x).$$

Operator $\mathcal{L}=\partial^2_{xx}$ and the potential f is $f(x,t)=\mathrm{e}^{\mathrm{i}\omega t}\alpha(x,t)$, where $\alpha(x,t)=\sin(t)$ is time–dependent function. We approximate the solution by taking the first three terms of the Neumann series

$$u^{[2]}(t)=\mathrm{e}^{t\mathcal{L}}u_0+T^1\mathrm{e}^{t\mathcal{L}}u_0+T^2\mathrm{e}^{t\mathcal{L}}u_0.$$

To expand asymptotically integrals $T^1\mathrm{e}^{t\mathcal{L}}u_0$ and $T^2\mathrm{e}^{t\mathcal{L}}u_0$ we utilize the following generalization of Lemma 1.

Lemma 4. *Let $\alpha(\tau)\in C^k([0,t^\star],D(\mathcal{L}^k))$. Then the k-th time derivative of expression $\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha(\tau)\mathrm{e}^{\tau\mathcal{L}}$ is equal to*

$$\partial^k_\tau\left(\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha(\tau)\mathrm{e}^{\tau\mathcal{L}}\right)=\sum_{\ell=0}^{k}(-1)^\ell\binom{k}{\ell}\mathrm{e}^{(t-\tau)\mathcal{L}}ad^\ell_{\mathcal{L}}\big(\alpha^{(k-\ell)}(\tau)\big)\mathrm{e}^{\tau\mathcal{L}}.$$

The proof of Lemma 4 can be found in Appendix A.2. Table 3.2 presents the error of the method up to the second iteration.

	$R=0$	$R=1$	$R=2$
$\omega=10$	3.17e-02	3.17e-02	1.71e-03
$\omega=100$	5.45e-04	5.45e-04	2.00e-07
$\omega=1000$	5.54e-06	5.54e-06	1.98e-11

Table 3.3: Error of the method – equation (3.36)

	$R=0$	$R=1$	$R=2$	$R=3$
$\omega=10$	3.58e-00	3.47e-01	2.22e-02	1.07e-03
$\omega=100$	1.00e-01	2.64e-04	4.62e-07	6.07e-10
$\omega=1000$	1.80e-02	8.41e-06	2.62e-09	6.14e-13

Table 3.4: Error of the method – equation (3.37)

Example 3.
Consider now the wave equation with potential with negative frequencies

$$\begin{aligned} &\partial_{tt}u = \partial_{xx}u + f(x,t)u(x,t), \qquad t \in [0,1],\ x \in (-L,L), \quad L = 10,\\ &u(x,0) = \mathrm{e}^{-x^2(1/2+1/\omega^2)}, \quad \partial_t u(x,0) = 0,\\ &u(-L,t) = u(L,t),\\ &\partial_t u(-L,t) = \partial_t u(L,t), \end{aligned} \tag{3.36}$$

where function f takes the form

$$f(x,t) = \left(1 - x^2 + \frac{(2 + x^2\omega^2 - 4x^2)\cos(\omega t)}{\omega^2} - \frac{4x^2\cos^2(\omega t)}{\omega^4} + \frac{x^4\sin^2(\omega t)}{\omega^2}\right).$$

The solution of (3.36) is equal to

$$u(x,t) = \mathrm{e}^{-\cos(\omega t)x^2/\omega^2}\mathrm{e}^{-x^2/2}.$$

Due to the presence of the resonance points, we do not have a general formula for the asymptotic expansion of the integrals that form the Neumann series in this case. Nevertheless, we can employ Theorem 11 and Theorem 13 to approximate only terms $T^1\mathrm{e}^{tA}$ and $T^2\mathrm{e}^{tA}$, where A is the linear operator of form (3.31). Table 3.3 presents the error of the method for a different oscillatory parameter ω.

Example 4.
In the last example, we consider the equation with the biharmonic operator

$$\begin{aligned} &\partial_t u(x,t) = \partial^4_{xxxx}u(x,t) + \mathrm{e}^{\mathrm{i}\omega t}u(x,t), \quad x \in (0,\pi), \quad t \in [0,1],\\ &u(x,0) = u_0(x) = \sin(x)\exp\left(-\frac{\mathrm{i}}{\omega}\right),\\ &u(0,t) = u(\pi,t) = 0, \end{aligned} \tag{3.37}$$

with periodic boundary conditions. The solution is

$$u(x,t) = \mathrm{e}^{t - \mathrm{i}\mathrm{e}^{\mathrm{i}\omega t}/\omega}\sin(x).$$

Table 3.4 presents the error of the method for different parameter ω and different partial sums of the asymptotic expansion.

Remark 4. *One can notice that equations (3.34), (3.36) and (3.37) do not fully satisfy Assumption 1. Indeed, linear operator $\mathcal{L}$ form equation (3.34) does not satisfy strong ellipticity condition for x near -1 or 1, and solutions $u(x,t)$ of equations (3.36) and (3.37) does not satisfy the zero boundary conditions. These are just examples to illustrate the proposed methodology and suggest that the method can probably be applied to a broader class of differential equations.*

Chapter 4

Numerical integrator for highly oscillatory differential equations based on the Neumann series

This chapter is based on an article [29]. We consider the following PDE

$$\begin{aligned} &\partial_t u(x,t) = \mathcal{L}u(x,t) + f(x,t)u(x,t), \qquad t\in[0,t^\star], \quad x\in\Omega\subset\mathbb{R}^m,\\ &u(x,0) = u_0(x), \end{aligned} \tag{4.1}$$

with zero boundary conditions, where Ω is an open and bounded subset of $\mathbb{R}^m$ with smooth boundary $\partial\Omega$, $t^\star > 0$ and $\mathcal{L}$ is a linear differential operator of degree $2p$, $p\in\mathbb{N}$, defined in 3.2. We assume that function $f(x,t)$ from the equation (4.1) is a highly oscillatory of type

$$f(x,t) = \sum_{\substack{n=-N\\ n\neq 0}}^{N} \alpha_n(x,t)e^{in\omega t}, \quad \omega \gg 1, \quad N\in\mathbb{N}, \tag{4.2}$$

where α_n are sufficiently smooth, complex-valued functions. This chapter aims to introduce a numerical integrator designed for highly oscillatory equations of type (4.1). Given the generality of equations (4.1), the proposed numerical scheme can be effectively applied to a range of linear partial differential equations, including the heat equation and the wave equation.

The motivation for the research presented in this chapter is that the method for highly oscillatory equations based on the Modulated Fourier expansion described in Chapter 3 may not converge to a solution. This means that it is only effective for equations with large oscillatory parameter ω. In this chapter, we present a third-order method whose accuracy improves with increasing parameter ω and decreasing time step h. Furthermore, the proposed approach allows for easy improvement of the convergence order of the proposed numerical integrator.

In paper [28], discussed in Chapter 3, it was shown that the solution to equation (4.1) can be presented as the Neumann series. Subsequently, by expanding asymptotically each integral in the Neumann series, it was demonstrated that the solution of the equation can be expressed as the Modulated Fourier expansion. In this chapter, instead of employing an asymptotic expansion for the integrals from the Neumann series (which is effective only in cases of large oscillations), we approximate them using quadrature rules designed for highly oscillatory integrals, such as Filon-type methods. By this approach, we can provide that the local error of the presented numerical scheme can be estimated by Ch^4, where constant C is independent of time step h and parameter ω. Furthermore, when considering a potential function f with only positive frequencies, i.e. when only numbers $n > 0$ appear in formula (4.2), one can show that the local error is bounded by $C \min\left\{h^4, h^2\omega^{-2}, \omega^{-3}\right\}$, where again the constant C is independent of both h and ω.

The convergence rate of the method can be easily improved by approximating a greater number of integrals from the Neumann series. However, this enhancement comes at the cost of requiring better regularity for both the initial condition u_0 and the functions α_n, and also leads to increased computational complexity.

Computational methods dedicated to equations of type (3.1) are presented for example in [2, 3, 35]. In this chapter, we present a complementary approach as discussed in the aforementioned papers. Our approach is distinguished by the following properties:

- the general form of the problem (4.1) allows our method to be applied to a variety of equations, including the heat equation, Schrödinger equation, and the wave equation;
- the presented approach allows easy improvement of the order of convergence of the proposed numerical integrator;
- ease of estimating the error of the method.

The chapter is organized as follows. Section 4.1 provides the derivation of the proposed numerical integrator. Section 4.2 is dedicated to the error analysis of the method, while Section 4.3 presents the results of numerical experiments.

4.1 Derivation of the method

For the convenience of presenting the method, we introduce the necessary notation and make the following general assumption, which will be used throughout this chapter.

Notations 2. *By $H^{2p}(\Omega) = W^{2p,2}(\Omega)$, where p is a nonnegative integer, we understand the Sobolev space equipped with standard norm $\| \ \|_{H^{2p}(\Omega)}$. By $u[t](\tau)$ we understand function u such that $u[t](\tau) = u(t+\tau)$. We slightly abuse the notation and also denote $u(t) := u(\cdot, t)$ as an element of an appropriate Banach space. In this chapter, for convenience, by $\| \ \| := \| \ \|_{L^2(\Omega)}$ we denote the standard norm of $L^2(\Omega)$ space.*

Assumption 2. *Suppose that*

1. *Ω is an open and bounded set in $\mathbb{R}^m$ with smooth boundary $\partial\Omega$.*
2. *Operator $-\mathcal{L} : D(\mathcal{L}) := H_0^p(\Omega) \cap H^{2p}(\Omega) \to L^2(\Omega)$, where $\mathcal{L}$ is of form (3.2), is a strongly elliptic of order $2p$ and has smooth, complex-valued coefficients $a_{\boldsymbol{p}}(x)$. Moreover $2p > m/2$.*

3. $u_0 \in D(\mathcal{L}^4)$ *and* $\alpha_n \in C^4\left([0,t^\star], H^{8p}(\Omega)\right)$, $n=-N,\dots,-1,1,\dots,N$, *where* $D(\mathcal{L}^k)=\{u\in D(\mathcal{L}^{k-1}) : \mathcal{L}^{k-1}u \in D(\mathcal{L})\}$, $k=2,\dots$

The assumed regularity of functions u_0 and α_n is related to the accuracy of the method. Recall that assumption 2 guaranties that differential operator $\mathcal{L}$ is the infinitesimal generator of a strongly continuous semigroup $\{\mathrm{e}^{t\mathcal{L}}\}_{t\geq 0}$ on $L^2(\Omega)$ and therefore $\max_{t\in[0,t^\star]}\|\mathrm{e}^{t\mathcal{L}}\|_{L^2(\Omega)\leftarrow L^2(\Omega)} \leq C(t^\star)$, where $C(t^\star)$ is some constant independent of t.

We wish to build the method based on time steps. Therefore, based on the semigroup property, we can modify equation (4.1) and express it as follows

$$\begin{aligned} &\partial_s u[t](x,s) = \mathcal{L}u[t](x,s) + f[t](x,s)u[t](x,s), \qquad s\in[0,h], \quad x\in\Omega\subset\mathbb{R}^m, \\ &u[t](x,0)=u(x,t), \end{aligned} \tag{4.3}$$

where $t\geq 0$ and $h>0$ is a small time step. By $u[t](x,s)$ we understand $u[t](x,s)=u(x,t+s)$. By applying Duhamel formula to (4.3), we obtain

$$u[t](s) \;=\; \mathrm{e}^{s\mathcal{L}}u[t](0) + \int_0^s \mathrm{e}^{(s-\tau)\mathcal{L}} f[t](\tau)u[t](\tau)\mathrm{d}\tau. \tag{4.4}$$

We could simply write $u[t](s)=u(t+s)$, but the above notation helps avoid misunderstandings in subsequent formulas.

Let V_t denotes the following space

$$V_t := C\left([t,t+h], L^2(\Omega)\right), \quad t\geq 0, \quad h>0.$$

Define the linear operator $T_t : V_t \to V_t$

$$T_t u[t](s) = \int_0^s \mathrm{e}^{(s-\tau)\mathcal{L}} f[t](\tau)u[t](\tau)\mathrm{d}\tau, \quad s\in[0,h],$$

where function f is defined in (4.2). The Neumann series for equation (4.4) reads

$$u[t](h) = \sum_{d=0}^{\infty} T_t^d \mathrm{e}^{h\mathcal{L}} u[t](0). \tag{4.5}$$

Expression $T_t^d\mathrm{e}^{h\mathcal{L}}u[t](0)$, $d=1,2,\dots$, from (4.5) is equal to

$$T_t^d\mathrm{e}^{h\mathcal{L}}u[t](0) = \int_0^h \mathrm{e}^{(h-\tau_d)\mathcal{L}} f[t](\tau_d)\int_0^{\tau_d}\mathrm{e}^{(\tau_d-\tau_{d-1})\mathcal{L}}f[t](\tau_{d-1})\cdots\int_0^{\tau_2}\mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}}f[t](\tau_1)\mathrm{e}^{\tau_1\mathcal{L}}u[t](0)\mathrm{d}\tau_1\dots\mathrm{d}\tau_d.$$

It can be shown that the series (4.5) converges in the norms $\|\ \|_{L^2(\Omega)}$ and $\|\ \|_{H^{2p}(\Omega)}$ to the solution of equation (4.4), where $2p>m/2$, for arbitrary time variable $h>0$ [28]. The idea for finding an approximate solution to equation (4.1) involves approximating the first r terms of the Neumann series (4.5) using quadrature methods designated to highly oscillatory integrals. For convenience, we introduce a set

$$\boldsymbol{N}^d := \{-N,-N+1,\dots,-1,1,\dots,N-1,N\}^d \subset \mathbb{N}^d, \tag{4.6}$$

where $2N$ is a number of terms in sum (4.2). Using definition (4.2) of the function f and the linearity of semigroup operator, we can write each term of the Neumann series $T_t^d \mathrm{e}^{h\mathcal{L}} u[t](0)$, $\mathrm{d} = 1, 2, \ldots$ in a more convenient form for our considerations

$$\begin{aligned} T_t^d \mathrm{e}^{h\mathcal{L}} u[t](0) &= \sum_{n_1,\ldots,n_d \in \boldsymbol{N}^1} \int_{\sigma_d(h)} F_{\boldsymbol{n}}(h, \tau_1, \ldots, \tau_d) \mathrm{e}^{\mathrm{i}\omega(n_1(\tau_1+t)+\cdots+n_d(\tau_d+t))} \mathrm{d}\tau_1 \ldots \tau_d \\ &= \sum_{\boldsymbol{n} \in \boldsymbol{N}^d} \mathrm{e}^{\mathrm{i}\omega t \boldsymbol{n}^T \boldsymbol{1}} I[F_{\boldsymbol{n}}, \sigma_d(h)], \end{aligned}$$

where

$$\begin{aligned} F_{\boldsymbol{n}}(h, \tau_1, \ldots \tau_d) &= \mathrm{e}^{(h-\tau_d)\mathcal{L}} \alpha_{n_d}[t](\tau_d) \mathrm{e}^{(\tau_d-\tau_{d-1})\mathcal{L}} \alpha_{n_{d-1}}[t](\tau_{d-1}) \ldots \mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}} \alpha_{n_1}[t](\tau_1) \mathrm{e}^{\tau_1 \mathcal{L}} u[t](0), \quad (4.7) \\ I[F_{\boldsymbol{n}}, \sigma_d(h)] &= \int_{\sigma_d(h)} F_{\boldsymbol{n}}(h, \boldsymbol{\tau}) \mathrm{e}^{\mathrm{i}\omega \boldsymbol{n}^T \boldsymbol{\tau}} \mathrm{d}\boldsymbol{\tau}, \\ \boldsymbol{\tau} &= (\tau_1, \tau_2, \ldots, \tau_d), \quad \boldsymbol{1} = (1, 1, \ldots, 1), \end{aligned}$$

and $\sigma_d(h)$ denotes a d-dimensional simplex

$$\sigma_d(h) = \{\boldsymbol{\tau} := (\tau_1, \tau_2, \ldots, \tau_d) \in \mathbb{R}^d : h \geq \tau_d \geq \tau_{d-1} \geq \cdots \geq \tau_2 \geq \tau_1 \geq 0\}.$$

Using the above notation, solution u of (4.4) can be written as

$$u(t+h) = u[t](h) = \mathrm{e}^{h\mathcal{L}} u[t](0) + \sum_{d=1}^{\infty} \mathrm{e}^{\mathrm{i}\omega t \boldsymbol{n}^T \boldsymbol{1}} \sum_{\boldsymbol{n} \in \boldsymbol{N}^d} I[F_{\boldsymbol{n}}, \sigma_d(h)]. \quad (4.8)$$

In the proposed numerical scheme, for each time step h we take the first four terms of the above series that approximate the function $u(t+h)$

$$u(t+h) \approx \mathrm{e}^{h\mathcal{L}} u[t](0) + \sum_{d=1}^{3} \sum_{\boldsymbol{n} \in \boldsymbol{N}^d} \mathrm{e}^{\mathrm{i}\omega t \boldsymbol{n}^T \boldsymbol{1}} I[F_{\boldsymbol{n}}, \sigma_d(h)].$$

Then, we approximate each integral $I[F_{\boldsymbol{n}}, \sigma_d(h)]$ in the above sum by applying the Filon quadrature. As a result, we derive a fourth-order local method. By employing Filon quadrature, the method's error converges to zero both as $h \to 0$ and as $\omega \to \infty$. Our decision to consider only the first four terms in the Neumann expansion is rather arbitrary. The method can be enhanced to achieve a higher level of accuracy, albeit with increased computational costs and the requirement of better regularity for functions u_0 and α_n.

Consider function $F(\tau) := F_{n_1}(h, \tau)$ from the second term of the Neumann series and the following univariate integral

$$\int_0^h F(\tau) \mathrm{e}^{n_1 \mathrm{i}\omega\tau} \mathrm{d}\tau,$$

where $n_1 = -N, -N+1, \ldots, -1, 1, \ldots, N$. Let $p(\tau)$ be a cubic Hermite interpolating polynomial

$$F(\tau) \approx p(\tau) = F(0) + a_{1,1}\tau + a_{1,2}\tau^2 + a_{1,3}\tau^3,$$

which satisfy the conditions: $p(0) = F(0)$, $p(h) = F(h)$, $p'(0) = F'(0)$, $p'(h) = F'(h)$. We have

$$\int_0^h F(\tau)\mathrm{e}^{\mathrm{i}n_1\omega\tau}\mathrm{d}\tau \approx \int_0^h p(\tau)\mathrm{e}^{\mathrm{i}n_1\omega\tau}\mathrm{d}\tau,$$

and the moments

$$\int_0^h \tau^k \mathrm{e}^{\mathrm{i}n_1\omega\tau}\mathrm{d}\tau, \quad k = 0,1,2,3,$$

can be calculated explicitly. Let now $F(\tau_1,\tau_2) := F_{\boldsymbol{n}}(h,\tau_1,\tau_2)$, $\boldsymbol{n} \in \boldsymbol{N}^2$, and consider a bivariate integral

$$\int_0^h \int_0^{\tau_2} F(\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\omega(n_1\tau_1+n_2\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2. \tag{4.9}$$

We approximate function $F(\tau_1,\tau_2)$ in points $(0,0)$, $(0,h)$ and (h,h), the vertices of the simplex $\sigma_2(h)$, by linear function $p(\tau_1,\tau_2)$,

$$F(\tau_1,\tau_2) \approx p(\tau_1,\tau_2) = F(0,0) + a_{2,1}\tau_1 + a_{2,2}\tau_2.$$

The approximation of integral (4.9) by the Filon quadrature rule reads

$$\int_0^h \int_0^{\tau_2} F(\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\omega(n_1\tau_1+n_2\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2 \approx \int_0^h \int_0^{\tau_2} p(\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\omega(n_1\tau_1+n_2\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2,$$

and the integral on the right-hand side can be computed explicitly. Similarly, we proceed with the triple integral. Function $F(\tau_1,\tau_2,\tau_3) := F_{\boldsymbol{n}}(h,\tau_1,\tau_2,\tau_3)$, $\boldsymbol{n} \in \boldsymbol{N}^3$ is approximated by linear function p at the vertices of the simplex $\sigma_3(h)$: $(0,0,0)$, $(0,0,h)$, $(0,h,h)$, (h,h,h),

$$F(\tau_1,\tau_2,\tau_3) \approx p(\tau_1,\tau_2,\tau_3) = F(0,0,0) + a_{3,1}\tau_1 + a_{3,2}\tau_2 + a_{3,3}\tau_3.$$

Then we have

$$\int_0^h \int_0^{\tau_3} \int_0^{\tau_2} F(\tau_1,\tau_2,\tau_3)\mathrm{e}^{\mathrm{i}\omega(n_1\tau_1+n_2\tau_2+n_3\tau_3)}\mathrm{d}\tau_1\mathrm{d}\tau_2\mathrm{d}\tau_3 \approx \int_0^h \int_0^{\tau_3} \int_0^{\tau_2} p(\tau_1,\tau_2,\tau_3)\mathrm{e}^{\mathrm{i}\omega(n_1\tau_1+n_2\tau_2+n_3\tau_3)}\mathrm{d}\tau_1\mathrm{d}\tau_2\mathrm{d}\tau_3.$$

The precise formulas for determining the coefficients $a_{i,j}$ are presented in the Appendix A.3.

The proposed algorithm for computing the successive approximation of the solution u can be expressed in the following form:

$$\begin{aligned}
u^{k+1} &= \Bigg(\mathrm{e}^{h\mathcal{L}} + \sum_{n_1}\int_0^h \left(a_{1,0} + a_{1,1}\tau + a_{1,2}\tau^2 + a_{1,3}\tau^3\right)\mathrm{e}^{n_1\mathrm{i}\omega(\tau+t_k)}\mathrm{d}\tau \\
&+ \sum_{n_1,n_2}\int_0^h \int_0^{\tau_2} (a_{2,0} + a_{2,1}\tau_1 + a_{2,2}\tau_2)\mathrm{e}^{\mathrm{i}\omega(n_1(\tau_1+t_k)+n_2(\tau_2+t_k))}\mathrm{d}\tau_1\mathrm{d}\tau_2 \\
&+ \sum_{n_1,n_2,n_3}\int_0^h \int_0^{\tau_3} \int_0^{\tau_2} (a_{3,0} + a_{3,1}\tau_1 + a_{3,2}\tau_2 + a_{3,3}\tau_3)\mathrm{e}^{\mathrm{i}\omega(n_1(\tau_1+t_k)+n_2(\tau_2+t_k)+n_3(\tau_3+t_k))}\mathrm{d}\tau_1\mathrm{d}\tau_2\mathrm{d}\tau_3\Bigg)u^k \\
t_{k+1} &= t_k + h, \quad k = 0,1,\ldots,K-1,
\end{aligned} \tag{4.10}$$

where $u^0 = u_0$, $t_0 = 0$, $t_K = t^\star$, $n_1,n_2,n_3 \in \{-N,-N+1,\ldots,-1,1,\ldots,N\}$ and the coefficients $a_{i,j}$

are chosen so that the corresponding polynomial satisfies the Hermite interpolation conditions. Each of the integrals appearing in the scheme is computed explicitly. Furthermore, the expression $\mathrm{e}^{h\mathcal{L}}$ and the coefficients $a_{i,j}$ of the interpolating polynomials, after spatial discretization, can be computed very efficiently and accurately using spectral method or splitting methods.

As we will see in the numerical examples, the proposed numerical scheme can be successfully applied to partial differential equations with the second-time derivative. For details, we refer to Chapter 3, Section 3.6.

4.2 Local error analysis

The entire error of the method comes from two sources: the approximation of each integral from the partial sum of the Neumann series, and the error associated with the truncation of the Neumann expansion. In [28], the authors provide the asymptotic expansion of integral $I[F_{\boldsymbol{n}}, \sigma_d(h)]$ from the Neumann series (4.8), where $F_{\boldsymbol{n}}$ is the function of the form (4.7), for the special case when the potential function f has positive frequencies, specifically when f takes the form

$$f(x,t) = \sum_{n=1}^{N} \alpha_n(x,t) e^{in\omega t}, \quad \omega \gg 1, \quad N \in \mathbb{N}. \tag{4.11}$$

In such a situation, each integral $I[F_{\boldsymbol{n}}, \sigma_d(h)]$ satisfies the nonresonance condition and therefore can be approximated by the partial sum $\mathcal{S}_r^{(d)}(h)$ of the asymptotic expansion

$$I[F_{\boldsymbol{n}}, \sigma_d(h)] = \int_{\sigma_d(h)} F(h, \boldsymbol{\tau}) \mathrm{e}^{\mathrm{i}\omega \boldsymbol{n}^T \boldsymbol{\tau}} \mathrm{d}\boldsymbol{\tau} = \mathcal{S}_r^{(d)}(h) + E_r^{(d)}(h), \quad r \geq d,$$

where $E_r^{(d)}(h) = \mathcal{O}(\omega^{-r-1})$ is the error related to approximation of integral $I[F_{\boldsymbol{n}}, \sigma_d(h)]$ by sum $\mathcal{S}_r^{(d)}(h) \sim \mathcal{O}(\omega^{-d})$. A similar result was first obtained in [22], where the authors provided the asymptotic expansion of a multivariate highly oscillatory integral over a regular simplex. However, in our analysis, the non-oscillatory function $F_{\boldsymbol{n}}$ is vector-valued rather than real-valued. We begin the error analysis of the proposed numerical method by considering function f from equation (4.1) in the form (4.11). Recall that $\| \ \|$ denotes the standard norm of $L^2(\Omega)$ space. In the following estimations, C is a constant that depends on functions α_n, initial condition $u[t](0)$ of equation (4.3), their derivatives, solution u, differential operator $\mathcal{L}$ and $t^\star$, but it is independent of the time step h and the oscillatory parameter ω. Let us also note that since by Assumption 2, the function $f \in C^4\left([0,t^\star], H^{8p}(\Omega)\right)$, we can apply the Sobolev embedding theorem to conclude that $\|f(s)\|_\infty < \infty$ for all $s \in [0, t^\star]$. Therefore, the norm of product of two functions f and u can easily be estimated as $\|f(s)u(s)\| \leq \|f(s)\|_\infty \|u(s)\|$, $\forall s \in [0, t^\star]$.

4.2.1 Positive frequencies

Lemma 5. *Let $F(\tau)$ be a 4 times continuously differentiable, vector-valued function, and let $p(\tau)$ be a cubic Hermite interpolation polynomial such that $p(0) = F(0)$, $p(h) = F(h)$, $p'(0) = F'(0)$,*

$p'(h) = F'(h)$. *Then the error of the Filon method satisfies*

$$\left\| \int_0^h (F-p)(\tau) e^{\mathrm{i} n_1 \omega \tau} \mathrm{d}\tau \right\| \leq C \min\left\{ h^5, \frac{1}{\omega^3}, \frac{h^3}{\omega^2} \right\}.$$

Proof. The estimation that the error is bounded by $C\omega^{-3}$ directly follows from well-known results concerning Filon quadrature, as described in [22]. By using the Taylor series with the remainder in integral form, one can show that $\|F(\tau) - p(\tau)\| \leq Ch^4$ and $\|F''(\tau) - p''(\tau)\| \leq Ch^2$. Therefore, by using integration by parts, we have

$$\left\| \int_0^h (F(\tau) - p(\tau)) e^{\mathrm{i} n_1 \omega \tau} \mathrm{d}\tau \right\| = \frac{1}{(n_1\omega)^2} \left\| \int_0^h (F''(\tau) - p''(\tau)) e^{\mathrm{i} n_1 \omega \tau} \mathrm{d}\tau \right\| \leq C\frac{h^3}{\omega^2},$$

which completes the proof. □

Lemma 6. *Let $F(\tau_1, \tau_2)$ be a vector-valued function of class C^2 and $p(\tau_1, \tau_2)$ be a linear function that satisfies the conditions: $p(0,0) = F(0,0)$, $p(0,h) = F(0,h)$, $p(h,h) = F(h,h)$. Let numbers $n_1 > 0$, $n_2 > 0$. Then*

$$\left\| \int_0^h \int_0^{\tau_2} (F-p)(\tau_1,\tau_2) e^{\mathrm{i}\omega(n_1\tau_1 + n_2\tau_2)} \mathrm{d}\tau_1 \mathrm{d}\tau_2 \right\| \leq C \min\left\{ h^4, \frac{h^2}{\omega^2}, \frac{1}{\omega^3} \right\}.$$

Proof. Since vector (n_1, n_2) satisfies the nonresonance condition, the integral $I[F, \sigma_2(h)]$ can be expanded asymptotically $I[F, \sigma_2(h)] \sim \mathcal{O}(\omega^{-2})$, and therefore the Filon method provides that the error satisfy $I[(F-p), \sigma_2(h)] = \mathcal{O}(\omega^{-3})$. As in the case in the proof of Lemma 5, by using the Taylor series with the remainder in integral form, we have the estimations $\|F(\tau_1,\tau_2) - p(\tau_1,\tau_2)\| \leq Ch^2$ and $\|\partial^1_{\tau_1} (F(\tau_1,\tau_2) - p(\tau_1,\tau_2))\| \leq Ch$. For simplicity, let us assume that $n_1 = n_2 = 1$. Using integration by parts, we get

$$\begin{aligned}
\left\| \int_0^h \int_0^{\tau_2} (F-p)(\tau_1,\tau_2) e^{\mathrm{i}\omega(\tau_1+\tau_2)} \mathrm{d}\tau_1 \mathrm{d}\tau_2 \right\| \leq\ & \frac{1}{\omega} \left\| \int_0^h (F-p)(\tau_2,\tau_2) e^{2\mathrm{i}\omega\tau_2} - (F-p)(0,\tau_2) e^{\mathrm{i}\omega\tau_2} \mathrm{d}\tau_2 \right\| \\
+\ & \frac{1}{\omega^2} \left\| \int_0^h \partial^1_{\tau_1}(F-p)(\tau_2,\tau_2) e^{2\mathrm{i}\omega\tau_2} - \partial^1_{\tau_1}(F-p)(0,\tau_2) e^{\mathrm{i}\omega\tau_2} \mathrm{d}\tau_2 \right\| \\
+\ & \frac{1}{\omega^2} \left\| \int_0^h \int_0^{\tau_2} \partial^2_{\tau_1}(F-p)(\tau_1,\tau_2) e^{\mathrm{i}\omega(\tau_1+\tau_2)} \mathrm{d}\tau_1 \mathrm{d}\tau_2 \right\|.
\end{aligned}$$

The second and third term on the right side of the above inequality are bounded by $Ch^2\omega^{-2}$, where C is some constant independent of h and ω. In the case of the first expression, we again apply integration by parts and the definition of the polynomial p, and thus get the following

$$\begin{aligned}
&\frac{1}{\omega} \left\| \int_0^h (F-p)(\tau_2,\tau_2) e^{2\mathrm{i}\omega\tau_2} - (F-p)(0,\tau_2) e^{\mathrm{i}\omega\tau_2} \mathrm{d}\tau_2 \right\| \leq \\
&\frac{1}{2\omega^2} \left\| \int_0^h \partial^1_{\tau_2}(F-p)(\tau_2,\tau_2) e^{2\mathrm{i}\omega\tau_2} \mathrm{d}\tau_2 \right\| + \frac{1}{\omega^2} \left\| \int_0^h \partial^1_{\tau_2}(F-p)(0,\tau_2) e^{\mathrm{i}\omega\tau_2} \mathrm{d}\tau_2 \right\| \leq C\frac{h^2}{\omega^2},
\end{aligned}$$

which concludes the proof. □

In a similar vein, we estimate the error of the Filon method for the triple integral

Lemma 7. *Let $F(\tau_1,\tau_2,\tau_3)$ be a vector valued function of class C^2 and $p(\tau_1,\tau_2,\tau_3)$ be a linear function approximating F such that $p(0,0,0) = F(0,0,0)$, $p(0,0,h) = F(0,0,h)$, $p(0,h,h) = F(0,h,h)$, $p(h,h,h) = F(h,h,h)$. Let numbers $n_1,n_2,n_3 > 0$. Then the error of the Filon method can be estimated as follows*

$$\left\|\int_0^h\int_0^{\tau_3}\int_0^{\tau_2}(F-p)(\tau_1,\tau_2,\tau_3)\mathrm{e}^{\mathrm{i}\omega(n_1\tau_1+n_2\tau_2+n_3\tau_3)}\mathrm{d}\tau_1\mathrm{d}\tau_2\mathrm{d}\tau_3\right\| \le C\min\left\{h^5,\frac{h^3}{\omega^2},\frac{1}{\omega^4}\right\}.$$

To complete the analysis of the local error, we need to estimate the truncation error of the Neumann series. We write the solution of (4.4) as

$$u[t](h) \;=\; \underbrace{\sum_{d=0}^{r}T_t^d\mathrm{e}^{h\mathcal{L}}u[t](0)}_{=:u^{[r]}[t](h)}+\underbrace{\sum_{d=r+1}^{\infty}T_t^d\mathrm{e}^{h\mathcal{L}}u[t](0)}_{=:\mathcal{R}^{[r+1]}[t](h)} = u^{[r]}[t](h)+\mathcal{R}^{[r+1]}[t](h),$$

where, in our considerations, we take $r = 3$.

Lemma 8. *Let the function f from equation (4.4) be of the form (4.11). Then the remainder $\mathcal{R}^{[4]}[t](h)$ of the Neumann series (4.5) satisfied the following estimate*

$$\|\mathcal{R}^{[4]}[t](h)\| \le C\min\left\{h^4,\frac{h^2}{\omega^2},\frac{1}{\omega^4}\right\},$$

where constant C depends on functions α_n, $u[t](0)$ their derivatives, solution u, operator $\mathcal{L}$ and $t^\star$, but is independent of time step h and parameter ω.

Proof. By using the basic properties of the operator norm and the fact that $\|f\|_\infty < \infty$ we have

$$\left\|\mathcal{R}^{[4]}[t](h)\right\| \;=\; \left\|\sum_{d=4}^{\infty}T_t^d\mathrm{e}^{h\mathcal{L}}u[t](0)\right\| = \left\|T_t^4\sum_{d=0}^{\infty}T_t^d\mathrm{e}^{h\mathcal{L}}u[t](0)\right\| = \|T_t^4u[t](h)\| \le Ch^4\sup_{s\in[0,h]}\|u[t](s)\|.$$

Let us now denote by $\boldsymbol{T}_t$ the operator $\boldsymbol{T}_t = \sum_{d=0}^{\infty}T_t^d$. On the other hand, we estimate

$$\begin{aligned}\left\|\mathcal{R}^{[4]}[t](h)\right\| &= \left\|\sum_{d=4}^{\infty}T_t^d\mathrm{e}^{h\mathcal{L}}u[t](0)\right\| = \left\|\sum_{d=0}^{\infty}T_t^dT_t^4\mathrm{e}^{h\mathcal{L}}u[t](0)\right\| = \left\|\mathbf{T}_tT_t^4\mathrm{e}^{h\mathcal{L}}u[t](0)\right\|\\ &\le \sup_{\|v[t](h)\|\le1}\|\mathbf{T}_tv[t](h)\|\|T_t^{4-k}T_t^k\mathrm{e}^{h\mathcal{L}}u[t](0)\|.\end{aligned}$$

Expression $T_t^4\mathrm{e}^{h\mathcal{L}}u[t](0)$ is a sum of highly oscillatory integrals over a 4-dimensional simplex which satisfy the nonresonance condition and therefore $\|T_t^4\mathrm{e}^{h\mathcal{L}}u[t](0)\| = \mathcal{O}(\omega^{-4})$. In addition, by using basic properties of the operator norm and the simple inequality $\|uv\|_{L^2} \le \|u\|_{L^2}\|v\|_\infty$, we have

$$\begin{aligned}\|T_t^4\mathrm{e}^{h\mathcal{L}}u[t](0)\| &= \left\|\int_0^h\mathrm{e}^{(h-\tau_4)\mathcal{L}}f[t](\tau_4)\int_0^{\tau_4}\mathrm{e}^{(\tau_4-\tau_3)\mathcal{L}}f[t](\tau_3)T^2\mathrm{e}^{\tau_3\mathcal{L}}u[t](0)\mathrm{d}\tau_3\mathrm{d}\tau_4\right\|\\ &\le \int_0^h\left\|\mathrm{e}^{(h-\tau_4)\mathcal{L}}f[t](\tau_4)\int_0^{\tau_4}\mathrm{e}^{(\tau_4-\tau_3)\mathcal{L}}f[t](\tau_3)T^2\mathrm{e}^{\tau_3\mathcal{L}}u[t](0)\mathrm{d}\tau_3\right\|\mathrm{d}\tau_4\end{aligned}$$

$$
\begin{aligned}
&\leq \; C_1 \int_0^h \left\| \int_0^{\tau_4} \mathrm{e}^{(\tau_4-\tau_3)\mathcal{L}} f[t](\tau_3) T^2 \mathrm{e}^{\tau_3 \mathcal{L}} u[t](0) \mathrm{d}\tau_3 \right\| \mathrm{d}\tau_4 \\
&\leq \; C_1 \int_0^h \int_0^{\tau_4} \left\| \mathrm{e}^{(\tau_4-\tau_3)\mathcal{L}} f[t](\tau_3) T^2 \mathrm{e}^{\tau_3 \mathcal{L}} u[t](0) \right\| \mathrm{d}\tau_3 \mathrm{d}\tau_4 \\
&\leq \; C_1^2 \int_0^h \int_0^{\tau_4} \left\| T^2 \mathrm{e}^{\tau_3 \mathcal{L}} u[t](0) \right\| \mathrm{d}\tau_3 \mathrm{d}\tau_4,
\end{aligned}
$$

where the constant $C_1 > 0$ depends on the norm of the semigroup operator $\{\mathrm{e}^{t\mathcal{L}}\}_{t\in[0,t^\star]}$ and the supremum norm of the function f. Since term $T^2\mathrm{e}^{\tau_3\mathcal{L}}u[t](0)$ satisfies $\left\|T^2\mathrm{e}^{\tau_3\mathcal{L}}u[t](0)\right\| = \mathcal{O}(\omega^{-2})$, we obtain the estimate

$$
\|T_t^4 \mathrm{e}^{h\mathcal{L}} u[t](0)\| \leq C\frac{h^2}{\omega^2}.
$$

Moreover, it can be observed that expression $\boldsymbol{T}_t v[t](h)$, where $\|v[t](h)\|_2 \leq 1$ is the solution of the integral equation

$$
\psi[t](h) = v[t](h) + \int_0^h \mathrm{e}^{(h-\tau)\mathcal{L}} f[t](\tau)\psi[t](\tau)\mathrm{d}\tau.
$$

By Grönwall's inequality, expression $\psi = \boldsymbol{T}_t v[t](h)$ is also bounded in L^2 norm for any function $v[t](h)$ such that $\|v[t](h)\|_2 \leq 1$. Using the boundedness of operator $\boldsymbol{T}_t$, we can estimate

$$
\left\| \sum_{d=4}^{\infty} T_t^d \mathrm{e}^{h\mathcal{L}} u[t](0) \right\| \leq C\frac{h^{4-k}}{\omega^k}, \quad k = 1, 2, 3, 4,
$$

which completes the proof. □

Let us emphasize that the time derivatives of the solution of the highly oscillatory equation (4.4) do not appear in the above estimates, which means that the constant C is independent of the parameter ω.

By collecting the estimations of integrals presented in Lemmas 5, 6, 7, and estimation of the remainder of the Neumann series in Lemma 8, one can provide the following local error bound of the scheme.

Theorem 14. *Let Assumption 2 be satisfied and let the potential function f be of the form (4.11). Then the local error of the numerical scheme (4.10) satisfies the following estimate in the L^2 norm*

$$
\|u(t_0 + h) - u^1\| \leq C \min\left\{h^4, \frac{h^2}{\omega^2}, \frac{1}{\omega^3}\right\},
$$

where constant C is independent of time step h and parameter ω.

4.2.2 The case involving negative frequencies

The situation becomes more complicated when we perform the error analysis of the proposed numerical integrator for potential function f in the general form (4.2). Let $\boldsymbol{n} = (n_1, \ldots, n_d) \in \boldsymbol{N}^d$, where set

$\boldsymbol{N}^d$ is defined in (4.6). Coordinates of $\boldsymbol{n}$ may satisfy

$$n_j + n_{j-1} + \cdots + n_{r+1} + n_r = 0,$$

for certain $1 \le j < r \le d$, and therefore $\boldsymbol{n}$ is orthogonal to the boundary of simplex $\sigma_d(h)$. Vector $\boldsymbol{n}$ does not satisfy the nonresonance condition, and, as a result, simple integration by parts does not yield error estimates similar to those presented in Lemmas 5, 6, and 7. In this case, we still obtain the fourth-order local error estimate of the numerical scheme $\|u(t_0+h)-u^1\| \le Ch^4$, where C is independent of ω and h, but we wish to derive a numerical scheme whose accuracy improves significantly with increasing ω.

At this stage, we consider two bivariate integrals from the Neumann series, $I[F_{\boldsymbol{n}_1}, \sigma_2(h)]$ and $I[F_{\boldsymbol{n}_2}, \sigma_2(h)]$, where $\boldsymbol{n}_1 = (-n, n)$ and $\boldsymbol{n}_2 = (n, -n)$. Vectors $\boldsymbol{n}_1, \boldsymbol{n}_2 \in \boldsymbol{N}^2$ are orthogonal to the boundary of simplex $\sigma_2(h)$. By integration by parts one can show that $I[F_{\boldsymbol{n}_1}, \sigma_2(h)] \sim \mathcal{O}(\omega^{-1})$, $I[F_{\boldsymbol{n}_2}, \sigma_2(h)] \sim \mathcal{O}(\omega^{-1})$ but sum of the integrals satisfies $(I[F_{\boldsymbol{n}_1}, \sigma_2(h)] + [F_{\boldsymbol{n}_2}, \sigma_2(h)]) \sim \mathcal{O}(\omega^{-2})$ [28]. We exploit this fact by imposing an additional interpolation condition to construct Filon's quadrature rule for the sum of two bivariate integrals that do not satisfy the nonresonance condition. We also assume that coefficients of function f satisfy $\alpha_{-n} = \alpha_n$, $\forall n \in \boldsymbol{N}^1$, therefore $F_{\boldsymbol{n}_1} = F_{\boldsymbol{n}_2} =: F_{\boldsymbol{n}}$.

Theorem 15. *Let coefficients $\alpha_{-n} = \alpha_n$, $\forall n \in \boldsymbol{N}^1$ and consider function $F_{\boldsymbol{n}}$ of the form (4.7), i.e. $F_{\boldsymbol{n}}(\tau_1, \tau_2) = \mathrm{e}^{(h-\tau_2)\mathcal{L}}\alpha_n[t](\tau_2)\mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}}\alpha_n[t](\tau_1)\mathrm{e}^{\tau_1\mathcal{L}}u[t](0)$. Let polynomial $p(\tau_1, \tau_2) = b_0 + b_1\tau_1 + b_2\tau_2 + b_3\tau_1\tau_2$ satisfies the following interpolation conditions*

$$p(0,0) = F_{\boldsymbol{n}}(0,0), \quad p(0,h) = F_{\boldsymbol{n}}(0,h), \quad p(h,h) = F_{\boldsymbol{n}}(h,h),$$

and

$$\int_0^h \partial^1_{\tau_1} p(\tau_2, \tau_2)\mathrm{d}\tau_2 = \int_0^h \partial^1_{\tau_1} F_{\boldsymbol{n}}(\tau_2, \tau_2)\mathrm{d}\tau_2. \tag{4.12}$$

Then

$$\left\| \int_0^h \int_0^{\tau_2} (F_{\boldsymbol{n}} - p)(\tau_1, \tau_2)\mathrm{e}^{\mathrm{i}\omega n(\tau_1-\tau_2)} + (F_{\boldsymbol{n}} - p)(\tau_1, \tau_2)\mathrm{e}^{\mathrm{i}\omega n(-\tau_1+\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2 \right\| \le C \min\left\{ h^4, \frac{h^2}{\omega^2}, \frac{1}{\omega^3} \right\}.$$

Proof. For simplicity, we can assume $n = 1$. It follows from the previous considerations that $(F_{\boldsymbol{n}} - p) = \mathcal{O}(h^2)$, $\partial^1_{\tau_1}(F_{\boldsymbol{n}} - p) = \mathcal{O}(h)$ and $\partial^1_{\tau_2}(F_{\boldsymbol{n}} - p) = \mathcal{O}(h)$. Integration by parts and application of interpolation conditions gives

$$\begin{aligned}
&\left\| \int_0^h \int_0^{\tau_2} (F_{\boldsymbol{n}} - p)(\tau_1, \tau_2)\mathrm{e}^{\mathrm{i}\omega(\tau_1-\tau_2)} + (F_{\boldsymbol{n}} - p)(\tau_1, \tau_2)\mathrm{e}^{\mathrm{i}\omega(-\tau_1+\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2 \right\| \le \\
&\frac{1}{\omega}\left(\left\| \int_0^h (F_{\boldsymbol{n}} - p)(\tau_2, \tau_2) - (F_{\boldsymbol{n}} - p)(0, \tau_2)\mathrm{e}^{-\mathrm{i}\omega\tau_2}\mathrm{d}\tau_2 - \int_0^h (F_{\boldsymbol{n}} - p)(\tau_2, \tau_2) - (F_{\boldsymbol{n}} - p)(0, \tau_2)\mathrm{e}^{\mathrm{i}\omega\tau_2}\mathrm{d}\tau_2 \right\| \right) + \\
&\frac{1}{\omega^2}\left\| \int_0^h \partial^1_{\tau_1}((F_{\boldsymbol{n}} - p)(\tau_2, \tau_2))\mathrm{d}\tau_2 \right\| + \frac{1}{\omega^2}\left\| \int_0^h \partial^1_{\tau_1}((F_{\boldsymbol{n}} - p)(0, \tau_2))\mathrm{e}^{-\mathrm{i}\omega\tau_2}\mathrm{d}\tau_2 \right\| + \\
&\frac{1}{\omega^2}\left\| \int_0^h \partial^1_{\tau_1}((F_{\boldsymbol{n}} - p)(\tau_2, \tau_2))\mathrm{d}\tau_2 \right\| + \frac{1}{\omega^2}\left\| \int_0^h \partial^1_{\tau_1}((F_{\boldsymbol{n}} - p)(0, \tau_2))\mathrm{e}^{\mathrm{i}\omega\tau_2}\mathrm{d}\tau_2 \right\| + \\
&\frac{1}{\omega^2}\left\| \int_0^h \int_0^{\tau_2} \partial^2_{\tau_1}(F_{\boldsymbol{n}} - p)(\tau_1, \tau_2)\mathrm{e}^{\mathrm{i}\omega(\tau_1-\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2 \right\| + \frac{1}{\omega^2}\left\| \int_0^h \int_0^{\tau_2} \partial^2_{\tau_1}(F_{\boldsymbol{n}} - p)(\tau_1, \tau_2)\mathrm{e}^{\mathrm{i}\omega(-\tau_1+\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2 \right\| \le
\end{aligned}$$

$$\frac{1}{\omega^2}\left\|\int_0^h \partial^1_{\tau_2}(F_{\boldsymbol{n}}-p)(0,\tau_2)\mathrm{e}^{-\mathrm{i}\omega\tau_2}\mathrm{d}\tau_2\right\| + \frac{1}{\omega^2}\left\|\int_0^h \partial^1_{\tau_2}(F_{\boldsymbol{n}}-p)(0,\tau_2)\mathrm{e}^{\mathrm{i}\omega\tau_2}\mathrm{d}\tau_2\right\| + C\min\left\{\frac{h^2}{\omega^2},\frac{1}{\omega^3}\right\} \leq$$
$$C\min\left\{\frac{h^2}{\omega^2},\frac{1}{\omega^3}\right\},$$

which completes the proof. □

Since the function $F_{\boldsymbol{n}}$ is non-oscillatory, we can compute the integral (4.12) efficiently and effortlessly, using methods such as Gauss-Legendre quadrature.

In the case when function f is of the form (4.2), and the coefficients of f satisfy $\alpha_{-n} = \alpha_n$, $\forall n \in \boldsymbol{N}^1$, the improved scheme reads

$$\begin{aligned}
u^{k+1} &= \Bigg(\mathrm{e}^{h\mathcal{L}} + \sum_{n_1}\int_0^h \left(a_{1,0}+a_{1,1}\tau+a_{1,2}\tau^2+a_{1,3}\tau^3\right)\mathrm{e}^{n_1\mathrm{i}\omega(\tau+t_k)}\mathrm{d}\tau \\
&+ \sum_{n_1+n_2\neq 0}\int_{\sigma_2(h)}(a_{2,0}+a_{2,1}\tau_1+a_{2,2}\tau_2)\mathrm{e}^{\mathrm{i}\omega(n_1(\tau_1+t_k)+n_2(\tau_2+t_k))}\mathrm{d}\tau_1\mathrm{d}\tau_2 \\
&+ \sum_{n=1}^{N}\int_{\sigma_2(h)}(b_0+b_1\tau_1+b_2\tau_2+b_3\tau_1\tau_2)(\mathrm{e}^{\mathrm{i}\omega n(\tau_1-\tau_2)}+\mathrm{e}^{\mathrm{i}\omega n(-\tau_1+\tau_2)})\mathrm{d}\tau_1\mathrm{d}\tau_2 \\
&+ \sum_{n_1,n_2,n_3}\int_{\sigma_3(h)}(a_{3,0}+a_{3,1}\tau_1+a_{3,2}\tau_2+a_{3,3}\tau_3)\mathrm{e}^{\mathrm{i}\omega(n_1(\tau_1+t_k)+n_2(\tau_2+t_k)+n_3(\tau_3+t_k))}\mathrm{d}\tau_1\mathrm{d}\tau_2\mathrm{d}\tau_3\Bigg)u^k, \\
t_{k+1} &= t_k + h.
\end{aligned}$$

4.3 Numerical examples

In this section, we employ the proposed numerical integrator to solve highly oscillatory heat equations and wave equations. The L^2 norm of the error is considered in any presented example. In our numerical experiments, to find an approximate solution, we use the Fourier and Chebyshev spectral methods, as described in [32, 33]. In Examples 1, 3 and 4 we used $M = 100$ spatial grid points. Example 2 concerns a two-dimensional case, in which we used $M = 20$ grid points.

Example 1. The heat equation.
Consider the equation

$$\begin{aligned}
&\partial_t u = \partial^2_{xx}u + f(x,t)u(x,t), \qquad t\in[0,1],\ x\in(0,2\pi), \\
&u(x,0) = u_0(x), \\
&u(0,t) = 0 = u(2\pi,t),
\end{aligned} \tag{4.13}$$

with initial condition u_0

$$u_0(x) = \sin(x),$$

and function f

$$f(x,t) = 1 - \underbrace{\frac{(-\mathrm{i}+t(\omega-3\mathrm{i}))\cos(x)}{\omega}}_{\alpha_1}\mathrm{e}^{\mathrm{i}\omega t} + \underbrace{\frac{\sin(x)^2t^2}{\omega^2}}_{\alpha_2}\mathrm{e}^{2\mathrm{i}\omega t}.$$

The potential function f involves time-dependent coefficients α_1 and α_2 The solution to (4.13) is

$$u(x,t) = \mathrm{e}^{\mathrm{i}\mathrm{e}^{\mathrm{i}\omega t}\cos(x)t/\omega}\sin(x).$$

Figure 4.1 displays the error of the method for equation (4.13).

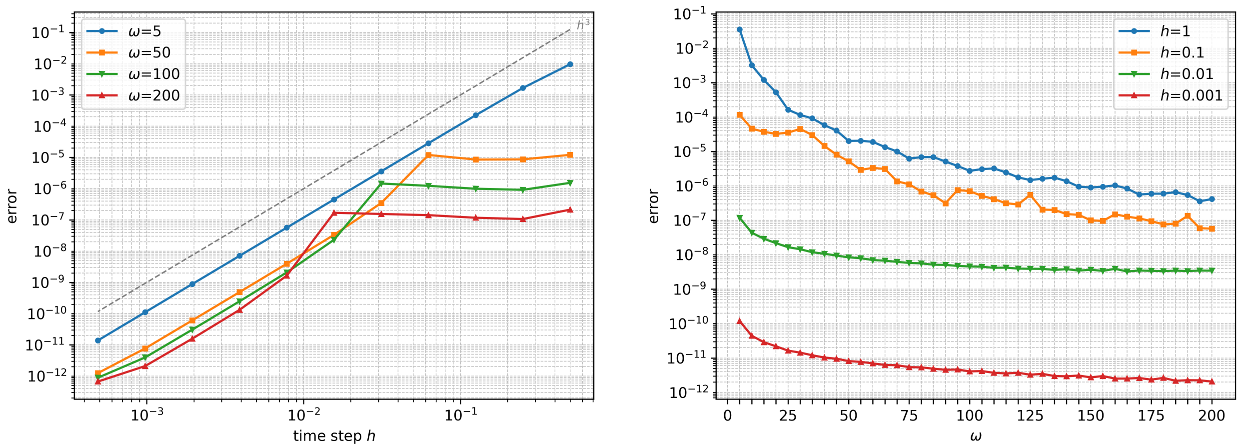


Figure 4.1: Numerical approximation of the solution to equation (4.13). Error versus time step (left graph) and error versus parameter ω (right graph).

Example 2. Two-dimensional heat equation.

$$\begin{aligned}
&\partial_t u(x,y,t) = \partial^2_{xx}u(x,y,t) + \partial^2_{yy}u(x,y,t) + f(x,y,t)u(x,y,t), \qquad t \in [0,1],\ x \in \Omega,\\
&u(x,y,0) = u_0(x,y), \\
&u(x,y,t) = 0 \quad \text{on } \partial\Omega,
\end{aligned} \tag{4.14}$$

where domain $\Omega = [-1,1]\times[-1,1]$. The initial condition u_0 is

$$u_0(x,y) = \sin(\pi x)\sin(\pi y)\mathrm{e}^{\cos(\pi x)\cos(\pi y)/\omega},$$

and function f

$$f(x,y,t) = 2\pi^2 + \underbrace{\frac{(6\pi^2 + \mathrm{i}\omega)\cos(\pi x)\cos(\pi y)}{\omega}}_{\alpha_1}\mathrm{e}^{\mathrm{i}\omega t} + \underbrace{\frac{0.5\pi^2(-1+\cos(2\pi x)\cos(2\pi y))}{\omega^2}}_{\alpha_2}\mathrm{e}^{2\mathrm{i}\omega t}.$$

The solution to equation (4.14) reads

$$u(x,y,t) = \sin(\pi x)\sin(\pi y)\exp(\exp(\mathrm{i}\omega t)\cos(\pi x)\cos(\pi y)/\omega).$$

Figure 4.2 presents the error of the proposed method applied to equation (4.14).

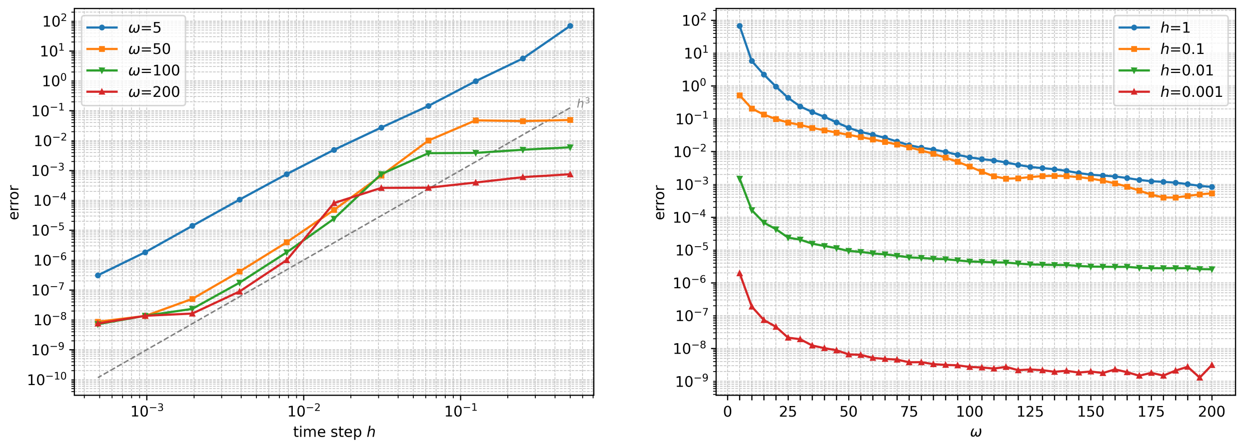


Figure 4.2: Numerical approximation of the solution to equation (4.14). Error versus time step (left graph) and error versus parameter ω (right graph).

Example 3. The wave equation with nonresonance points.

$$
\begin{aligned}
&\partial_{tt}^2 u = \partial_{xx}^2 u + f(x,t)u(x,t), \qquad t \in [0,1],\ x \in (-L,L), \quad L = 10,\\
&u(x,0) = u_0(x), \quad \partial_t u(x,0) = v_0(x),\\
&u(-L,t) = u(L,t),\\
&\partial_t u(-L,t) = \partial_t u(L,t),
\end{aligned} \tag{4.15}
$$

where initial conditions

$$u_0(x) = \mathrm{e}^{-x^2(1/2+1/\omega^2)}, \quad v_0(x) = -\frac{\mathrm{i}x^2}{\omega}u_0(x),$$

and function f

$$f(x,t) = 1 - x^2 + \frac{2 + x^2(-4+\omega^2)}{\omega^2}\mathrm{e}^{\mathrm{i}\omega t} - \frac{x^2(4 + x^2\omega^2)}{\omega^4}\mathrm{e}^{2\mathrm{i}\omega t}.$$

The solution to (4.15) is

$$u(x,t) = \mathrm{e}^{-x^2/2}\mathrm{e}^{-\mathrm{e}^{\mathrm{i}t\omega}x^2/\omega^2}.$$

Figure 4.3 illustrates the error associated with the approximation of the solution to equation (4.15).

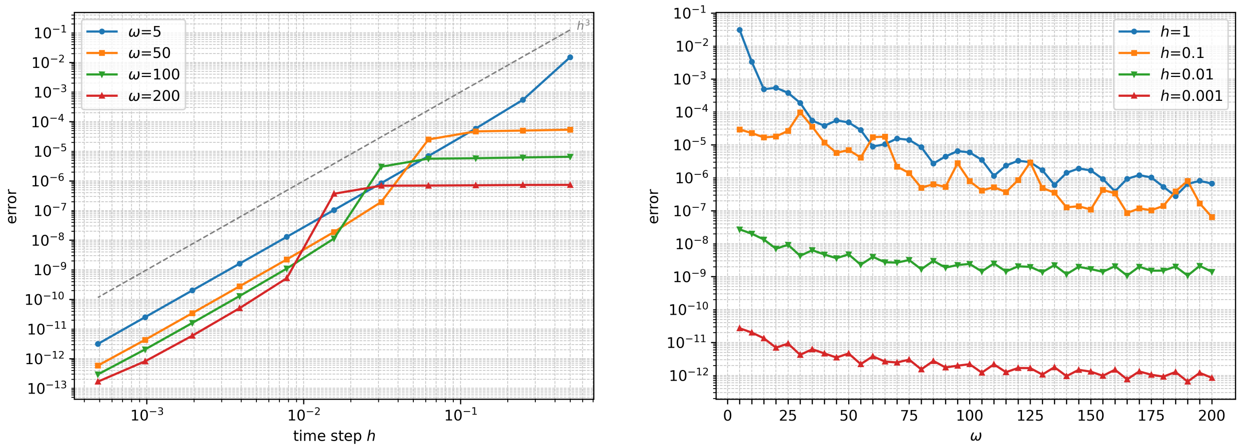


Figure 4.3: Numerical approximation of the solution to equation (4.15). Error versus time step (left graph) and error versus ω (right graph).

Example 4. The wave equation with resonance points.
In the last example, consider now the wave equation with potential function f with negative frequencies

$$
\begin{aligned}
&\partial_{tt}^2 u = \partial_{xx}^2 u + f(x,t)u(x,t), \qquad t \in [0,1],\ x \in (-L, L), \quad L = 10,\\
&u(x,0) = \mathrm{e}^{-x^2(1/2+1/\omega^2)}, \quad \partial_t u(x,0) = 0,\\
&u(-L,t) = u(L,t),\\
&\partial_t u(-L,t) = \partial_t u(L,t),
\end{aligned}
\tag{4.16}
$$

where function f takes the form

$$f(x,t) = 1 - x^2 + \frac{(2 + x^2\omega^2 - 4x^2)\cos(\omega t)}{\omega^2} - \frac{4x^2\cos^2(\omega t)}{\omega^4} + \frac{x^4\sin^2(\omega t)}{\omega^2}.$$

The solution of (4.16) is equal to

$$u(x,t) = \mathrm{e}^{-\cos(\omega t)x^2/\omega^2}\mathrm{e}^{-x^2/2}.$$

Figure 4.4 presents the error of the proposed method for equation (4.16).

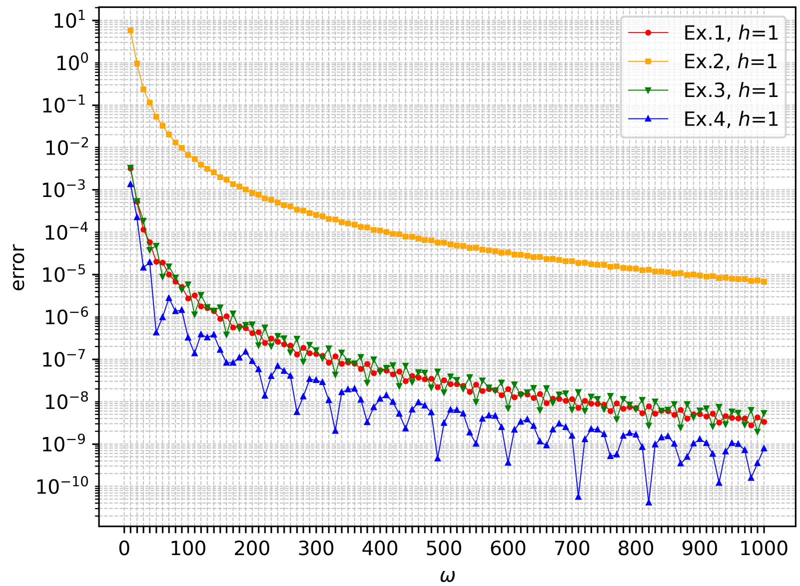


Figure 4.5: The error of approximating the solutions of equations (4.13), (4.14), (4.15), and (4.16), for ω ranging from 5 to 1000, with step size $h = 1$.

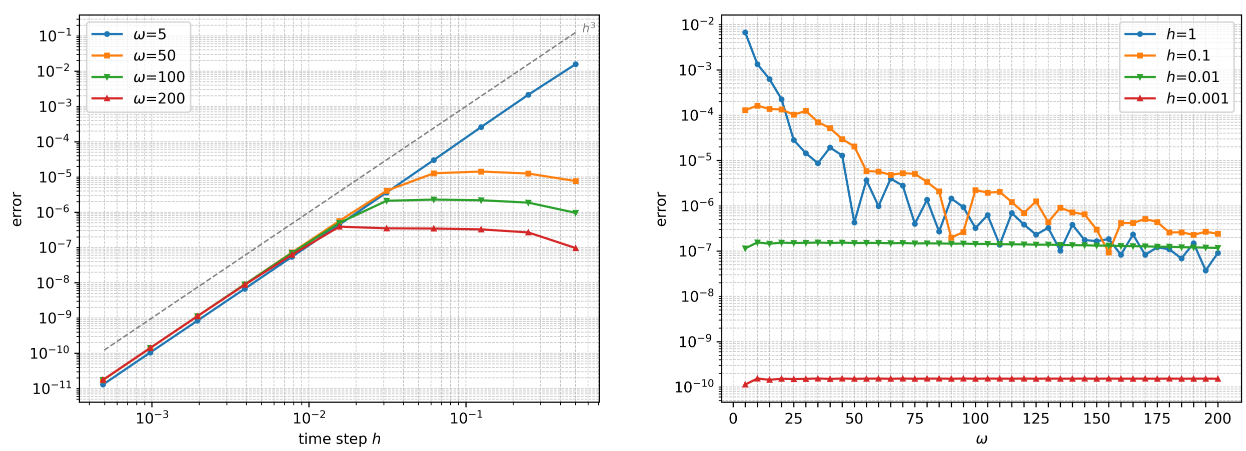
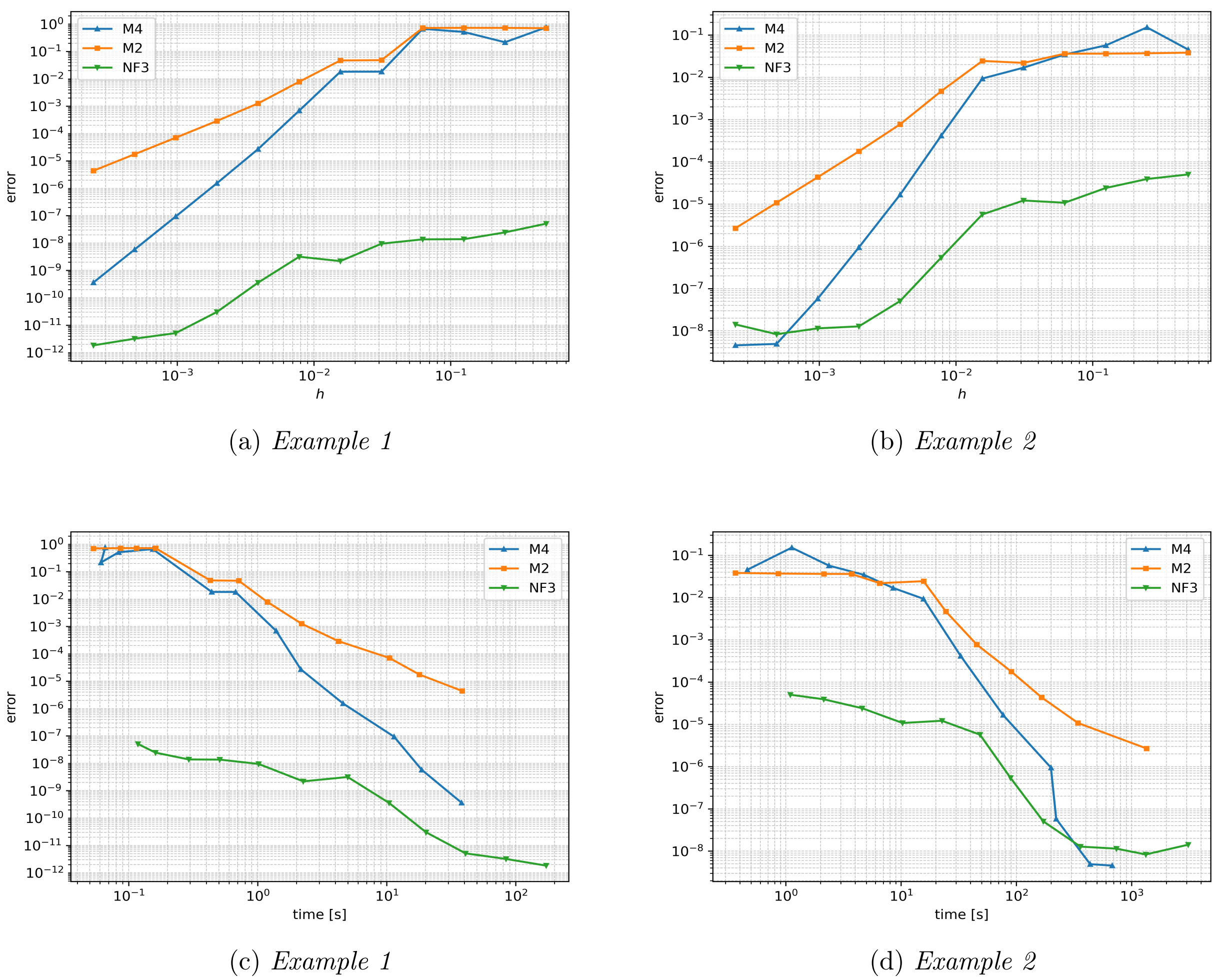


Figure 4.4: Numerical approximation of the solution to equation (4.16). Error versus time step (left figure) and error versus ω (right figure) .

The Neumann series converges for all variables t, unlike the Magnus expansion, which converges only locally. Therefore, in the proposed scheme, any time step can be taken to find an approximate solution. In Figure 4.5, we illustrate the error of the method for all four examples with step size $h = 1$, where ω ranges from 5 to 1000. In each graph of error versus time step h, it can be observed that the proposed method is effective for both small ($\omega = 5$) and large ($\omega = 200$) oscillatory parameter ω.

4.3.1 Comparison with other methods

In this section, we compare the proposed numerical method (denoted as $NF3$) with selected existing methods. For this purpose, we used schemes based on the Magnus expansion: the exponential fourth-order method (denoted as $M4$) and the exponential midpoint method of order two (denoted as $M2$). Both integrators are described in detail in [18]. Each scheme was applied to equations (4.13), (4.14), and (4.15), where in each case the parameter $\omega = 500$. As is well known, the methods $M4$ and $M2$ are very effective for nonoscillatory equations. However, for a large parameter ω which accounts for the oscillation of the equation, their effectiveness is limited. The proposed $NF3$ method performs particularly well in a highly oscillatory regime. The results of the comparisons are shown in Figures 4.6 and 4.7.



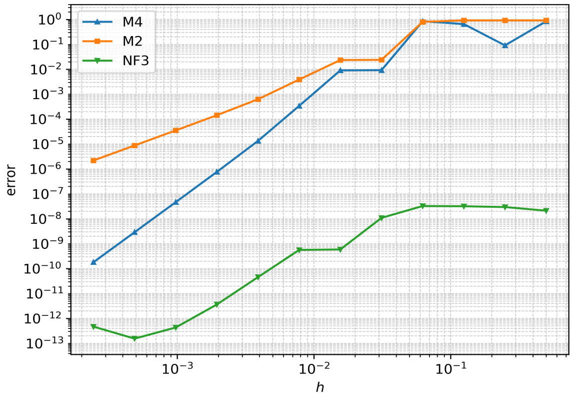
(a) *Example 1*

(b) *Example 2*

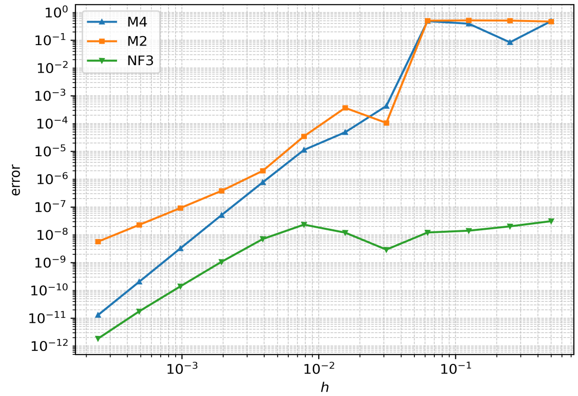
(c) *Example 1*

(d) *Example 2*

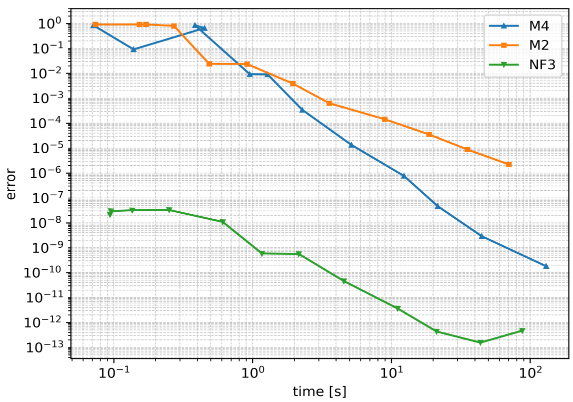
Figure 4.6: Comparison of the proposed method $NF3$ with the exponential 4th order method (M4) and the exponential 2nd order midpoint method (M2). The numerical schemes have been applied to the equations (4.13) and (4.14), where $\omega = 500$. Top row presents accuracy of schemes and the bottom row time of computation in seconds.



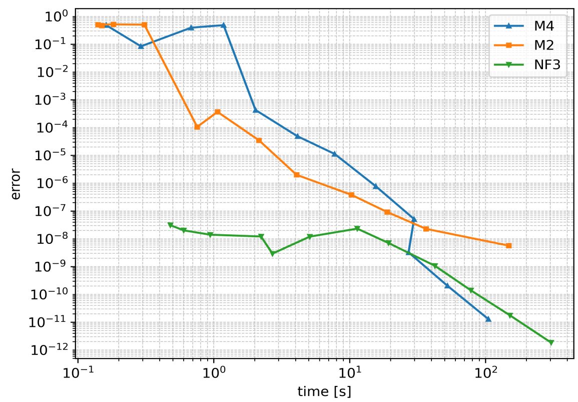
(a) *Example 3*



(b) *Example 4*



(c) *Example 3*



(d) *Example 4*

Figure 4.7: Same as Figure 4.6 for equations 4.15 and 4.16.

Chapter 5

Conclusion – summary and plans for future research

In this dissertation, we have proposed two computational methods for approximating the highly oscillatory solution of equation (1.1). In the first method, we analytically derived the Modulated Fourier expansion and then employed it to find an approximate solution (MFE). In the second method, we approximated highly oscillatory integrals from the Neumann series by using quadrature rules for highly oscillatory integrals. The second method converges to the solution as $\omega \to \infty$ or time step $h \to 0$. There are several plans for extending the proposed approach.

1. The primary concern is to establish rigorous estimations for the error formulas that arise in the asymptotic expansion of highly oscillatory integrals in (3.19). This task is particularly challenging, especially when we consider a general differential operator $\mathcal{L}$ in the form (3.2). It should be noted that the partial sum $\mathcal{S}_r^{(d)}(t)$, used to approximate the integral $I[F_{\boldsymbol{n}}, \sigma_d(t)]$, may be divergent as $r \to \infty$. A significant advancement in the approximation of highly oscillatory PDEs would involve determining the maximum value of $r^\star$, beyond which the method's error begins to increase.

2. The next step could involve deriving methods for equations with a more general strongly oscillatory potential f, as given by the formula

$$f(x,t) = \sum_{n=1}^{N} \alpha_n(x,t) \mathrm{e}^{\mathrm{i}\omega g_n(t)}, \quad \omega \gg 1, \quad N \in \mathbb{N},$$

   where α_n and g_n are sufficiently smooth real or complex valued functions. This requires the use of appropriate modifications of the Filon methods.

3. As mentioned earlier, the MFE is a widely employed tool in computational mathematics for analyzing highly oscillatory differential equations. To the best of the author's knowledge, it has so far been used as an ansatz, assuming that the solution to a highly oscillatory equation can be represented as an asymptotic series of the form (1.6). In articles [23, 28] the MFE is analytically derived for linear partial differential equations. An ambitious goal would be to derive analytically

MFE for the nonlinear highly oscillatory equations, for example for the problem (1.3) described in Chapter 1.

4. There are possible modifications of the integrator proposed in Chapter 4. For integrals which appears in the Neumann series, different extensions of the Filon method can be applied. For example, the nonoscillatory integrands can be approximated not only at points that are the ends of the integration interval but also at the intermediate points. This should further improve the accuracy of the method.

Appendix A

A.1

Theorem 16. *Let F be the operator defined in (3.14), and let $\boldsymbol{n}$ be the vector corresponding to F that satisfies the nonresonance condition (3.16). Integral (3.15) can be expressed as r-partial sum $\mathcal{S}_r^{(d)}(t)$ of the asymptotic series with error $E_r^{(d)}(t)$*

$$I[F,\sigma_d(t)] = \int_{\sigma_d(t)} F(t,\boldsymbol{\tau})\mathrm{e}^{\mathrm{i}\omega \boldsymbol{n}^T\boldsymbol{\tau}}\mathrm{d}\boldsymbol{\tau} = \mathcal{S}_r^{(d)}(t) + E_r^{(d)}(t), \tag{A.1}$$

where

$$\mathcal{S}_r^{(d)}(t) = \sum_{|\boldsymbol{k}|=0}^{r-d} \frac{(-1)^{|\boldsymbol{k}|}}{(\mathrm{i}\omega)^{d+|\boldsymbol{k}|}} \sum_{\ell=0}^{d} \mathrm{e}^{\mathrm{i}\omega t\boldsymbol{n}^T\boldsymbol{v}_\ell^d} \sum_{\boldsymbol{\phi}\in\Phi_\ell^d} A_{\boldsymbol{k}}[\boldsymbol{\phi}](\boldsymbol{n})F^{\boldsymbol{k}}[\boldsymbol{\phi}](t) \tag{A.2}$$

and error $E_r^{(d)}(t)$ of the expansion is in recursive form

$$\begin{aligned} E_r^{(1)}(t) &= \frac{(-1)^r}{(\mathrm{i}\omega)^r}\frac{1}{n_1^r}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_1 n_1}\partial_{\tau_1}^r F(t,\tau_1)\mathrm{d}\tau_1, \qquad (A.3)\\ E_r^{(d)}(t) &= \frac{(-1)^{r-d+1}}{(\mathrm{i}\omega)^r} \sum_{|\boldsymbol{k}|=r-d+1}\sum_{\ell=0}^{d-1}\sum_{\boldsymbol{\phi}\in\Phi_\ell^{d-1}} \frac{1}{\left(\boldsymbol{n}^T\boldsymbol{v}_\ell^d\right)^{k_d}} A_{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tilde{\boldsymbol{n}}) \int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_d\boldsymbol{n}^T\boldsymbol{v}_\ell^d}\partial_{\tau_d}^{k_d}\left(\mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_d}F^{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tau_d)\right)\mathrm{d}\tau_d\\ &+ \int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_d}E_r^{(d-1)}(\tau_d)\mathrm{e}^{\mathrm{i}\omega n_d\tau_d}\mathrm{d}\tau_d, \ \textit{for } d\geq 2. \end{aligned}$$

Proof. We show the statement by induction on d. For $d=1$ we integrate by parts r times integral $I[F,(0,t)]$ and thus we obtain

$$\begin{aligned} I[F,(0,t)] &= \int_0^t F(t,\tau_1)\mathrm{e}^{\mathrm{i}\omega n_1\tau_1}\mathrm{d}\tau_1\\ &= \sum_{k_1=0}^{n-1}\frac{(-1)^{k_1}}{(\mathrm{i}\omega)^{1+k_1}}\left(\mathrm{e}^{\mathrm{i}\omega n_1}\frac{1}{n_1^{k_1+1}}\partial_{\tau_1}^{k_1}F(t,\tau_1)\Big|_{\tau_1=t} + \frac{-1}{n_1^{k_1+1}}\partial_{\tau_1}^{k_1}F(t,\tau_1)\Big|_{\tau_1=0}\right)\\ &+ \frac{(-1)^r}{(\mathrm{i}\omega)^r}\frac{1}{n_1^r}\int_0^t \mathrm{e}^{\mathrm{i}\omega\tau_1 n_1}\partial_{\tau_1}^r F(t,\tau_1)\mathrm{d}\tau_1\\ &= \sum_{k_1=0}^{r-1}\frac{(-1)^{k_1}}{(\mathrm{i}\omega)^{1+k_1}}\sum_{\ell=0}^{1}\mathrm{e}^{\mathrm{i}\omega v_\ell^1 n_1}\sum_{\phi\in\Phi_\ell^1}A_{k_1}[\phi](n_1)F^{k_1}[\phi](t) + E_r^{(1)}(t)\\ &= \mathcal{S}_r^{(1)}(t) + E_r^{(1)}(t). \end{aligned}$$

Let $\tilde{\boldsymbol{n}} = (n_1, \ldots, n_{d-1})$, $\tilde{\boldsymbol{k}} = (k_1, \ldots, k_{d-1}) \in \mathbb{N}^{d-1}$ and $\boldsymbol{n} = (n_1, \ldots, n_d)$, $\boldsymbol{k} = (k_1, \ldots, k_d) \in \mathbb{N}^d$. Suppose now the formula (A.1) is true for $I[F, \sigma_{d-1}(t)] = \int_{\sigma_{d-1}(t)} F(\boldsymbol{\tau}) \mathrm{e}^{\mathrm{i}\omega \tilde{\boldsymbol{n}}^T \boldsymbol{\tau}} \mathrm{d}\boldsymbol{\tau}$.

$$
\begin{aligned}
&\int_{S_d(t)} F(t, \boldsymbol{\tau}) \mathrm{e}^{\mathrm{i}\omega \boldsymbol{n}^T \boldsymbol{\tau}} \mathrm{d}\boldsymbol{\tau} \overset{(1)}{=} \\
&\int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} I[F, \sigma_{d-1}(\tau_d)] \mathrm{e}^{\mathrm{i}\omega \tau_d n_d} \mathrm{d}\tau_d \overset{(2)}{=} \int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} \left(\mathcal{S}_r^{(d-1)}(\tau_d) + E_r^{(d-1)}(\tau_d) \right) \mathrm{e}^{\mathrm{i}\omega \tau_d n_d} \mathrm{d}\tau_d \overset{(3)}{=} \\
&\sum_{|\tilde{\boldsymbol{k}}|=0}^{r-d+1} \frac{(-1)^{|\tilde{\boldsymbol{k}}|}}{(\mathrm{i}\omega)^{d-1+|\tilde{\boldsymbol{k}}|}} \sum_{\ell=0}^{d-1} \sum_{\boldsymbol{\phi} \in \Phi_\ell^{d-1}} A_{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tilde{\boldsymbol{n}}) \int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} F^{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tau_d) \mathrm{e}^{\mathrm{i}\omega \tau_d \boldsymbol{n}^T \boldsymbol{v}_\ell^d} \mathrm{d}\tau_d + \\
&\int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} E_r^{(d-1)}(\tau_d) \mathrm{e}^{\mathrm{i}\omega \tau_d n_d} \mathrm{d}\tau_d \overset{(4)}{=} \\
&\sum_{|\tilde{\boldsymbol{k}}|=0}^{r-d+1} \frac{(-1)^{|\tilde{\boldsymbol{k}}|}}{(\mathrm{i}\omega)^{d-1+|\tilde{\boldsymbol{k}}|}} \sum_{\ell=0}^{d-1} \sum_{\boldsymbol{\phi} \in \Phi_\ell^{d-1}} A_{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tilde{\boldsymbol{n}}) \Bigg\{ \sum_{k_d=0}^{r-d-|\tilde{\boldsymbol{k}}|} \frac{(-1)^{k_d}}{(\mathrm{i}\omega)^{k_d+1}} \frac{1}{(\boldsymbol{n}^T \boldsymbol{v}_\ell^d)^{k_d+1}} \cdot \\
&\quad \cdot \left(\mathrm{e}^{\mathrm{i}\omega t \boldsymbol{n}^T \boldsymbol{v}_\ell^d} \partial_{\tau_d}^{k_d} \left[\mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} F^{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tau_d) \right] \Big|_{\tau_d = t} - \partial_{\tau_d}^{k_d} \left[\mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} F^{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tau_d) \right] \Big|_{\tau_d = 0} \right) + \\
&\frac{(-1)^{r-d-|\tilde{\boldsymbol{k}}|+1}}{(\mathrm{i}\omega)^{r-d-|\tilde{\boldsymbol{k}}|+1}} \frac{1}{(\boldsymbol{n}^T \boldsymbol{v}_\ell^d)^{r-d-|\tilde{\boldsymbol{k}}|+1}} \int_0^t \partial_{\tau_d}^{r-d-|\tilde{\boldsymbol{k}}|+1} \left(\mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} F^{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tau_d) \right) \mathrm{e}^{\mathrm{i}\omega \tau_d \boldsymbol{n}^T \boldsymbol{v}_\ell^d} \mathrm{d}\tau_d \Bigg\} + \\
&\int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} E_r^{(d-1)}(\tau_d) \mathrm{e}^{\mathrm{i}\omega \tau_d n_d} \mathrm{d}\tau_d \overset{(5)}{=} \\
&\sum_{|\boldsymbol{k}|=0}^{r-d} \frac{(-1)^{|\boldsymbol{k}|}}{(\mathrm{i}\omega)^{d+|\boldsymbol{k}|}} \sum_{\ell=0}^{d-1} \sum_{\phi \in \Phi_\ell^{d-1}} A_{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tilde{\boldsymbol{n}}) \frac{1}{(\boldsymbol{n}^T \boldsymbol{v}_\ell^d)^{k_d+1}} \Bigg[\\
&\mathrm{e}^{\mathrm{i}\omega t \boldsymbol{n}^T \boldsymbol{v}_\ell^d} \partial_{\tau_d}^{k_d} \left[\mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} F^{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tau_d) \right] \Big|_{\tau_d = 1 \cdot t} - \mathrm{e}^{\mathrm{i}\omega t \boldsymbol{n}^T \boldsymbol{v}_d^d} \partial_{\tau_d}^{k_d} \left[\mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} F^{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tau_d) \right] \Big|_{\tau_d = t \cdot 0} \Bigg] + \\
&\frac{(-1)^{r-d+1}}{(\mathrm{i}\omega)^r} \sum_{|\boldsymbol{k}|=r-d+1} \sum_{\ell=0}^{d-1} \sum_{\boldsymbol{\phi} \in \Phi_\ell^{d-1}} A_{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tilde{\boldsymbol{n}}) \frac{1}{(\boldsymbol{n}^T \boldsymbol{v}_\ell^d)^{k_d}} \int_0^t \partial_{\tau_d}^{k_d} \left(\mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} F^{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tau_d) \right) \mathrm{e}^{\mathrm{i}\omega \tau_d \boldsymbol{n}^T \boldsymbol{v}_\ell^d} \mathrm{d}\tau_d \\
&+ \int_0^t \mathrm{e}^{(t-\tau_d)\mathcal{L}} \alpha_{n_d} E_r^{(d-1)}(\tau_d) \mathrm{e}^{\mathrm{i}\omega \tau_d n_d} \mathrm{d}\tau_d \overset{(6)}{=} \\
&\sum_{|\boldsymbol{k}|=0}^{r-d} \frac{(-1)^{|\boldsymbol{k}|}}{(\mathrm{i}\omega)^{d+|\boldsymbol{k}|}} \sum_{\ell=0}^{d-1} \mathrm{e}^{\mathrm{i}\omega t \boldsymbol{n}^T \boldsymbol{v}_\ell^d} \sum_{\boldsymbol{\phi} \in \Phi_\ell^d} A_{\boldsymbol{k}}[\boldsymbol{\phi}](\boldsymbol{n}) F^{\boldsymbol{k}}[\boldsymbol{\phi}](t) + \\
&+ A_{\boldsymbol{k}}[(\phi_1, \ldots, \phi_{d-1}, 0)](\boldsymbol{n}) F^{\boldsymbol{k}}[(\phi_1, \ldots, \phi_{d-1}, 0)](t) + E_r^{(d)}(t) = \\
&\sum_{|\boldsymbol{k}|=0}^{r-d} \frac{(-1)^{|\boldsymbol{k}|}}{(\mathrm{i}\omega)^{d+|\boldsymbol{k}|}} \sum_{\ell=0}^{d} \mathrm{e}^{\mathrm{i}\omega t \boldsymbol{n}^T \boldsymbol{v}_\ell^d} \sum_{\boldsymbol{\phi} \in \Phi_\ell^d} A_{\boldsymbol{k}}[\boldsymbol{\phi}](\boldsymbol{n}) F^{\boldsymbol{k}}[\boldsymbol{\phi}](t) + E_r^{(d)}(t)
\end{aligned}
$$

(we assume that $\sum_{k=0}^{-1} a_k = 0$). Throughout the above inductive proof we utilize properties of integral $I[F, \sigma_d(t)]$, operator F, and simple summation identities. More precisely, where necessary, in the above identities we have used:

(1) form (3.14) of function F and Fubini's theorem,

(2) induction hypothesis,

(3) formula for asymptotic expansion of $I[F,\sigma_{d-1}(t)]$ and identity $\tilde{\boldsymbol{n}}^T\boldsymbol{v}_\ell^{d-1}+n_d=\boldsymbol{n}^T(\boldsymbol{v}_\ell^{d-1},1)$,

(4) integration by parts $r-d-|\tilde{\boldsymbol{k}}|+1$ times and the nonresonance condition (3.16),

(5) summation identity $\sum_{|\tilde{\boldsymbol{k}}|=0}^{r+1}\sum_{k_d=0}^{r-|\tilde{\boldsymbol{k}}|}a_{k_1,\ldots,k_{d-1},k_d}=\sum_{|\boldsymbol{k}|=0}^{r}a_{k_1,\ldots,k_d}$ and identity $\sum_{|\tilde{\boldsymbol{k}}|=0}^{r-d+1}a_{k_1,\ldots,k_{d-1},r-d-|\tilde{\boldsymbol{k}}|+1}=\sum_{|\boldsymbol{k}|=r-d+1}a_{k_1,\ldots,k_d}$,

(6) Definition 8, according to which $\partial_{\tau_d}\left[\mathrm{e}^{(t-\tau_d)\mathcal{L}}\alpha_{n_d}F^{\tilde{\boldsymbol{k}}}[\boldsymbol{\phi}](\tau_d)\right]\Big|_{\tau_d=\phi_d t}=F^{\boldsymbol{k}}[\boldsymbol{\phi}](t)$, and Definition 9.

We have proved that the integral $I[F,\sigma_d(t)]\sim\mathcal{O}(\omega^{-d})$ can indeed be approximated by the sum (A.2), with an error $\mathcal{O}(\omega^{-r})$ as given by the form (A.3). ☐

A.2

Lemma 9. *The k-th time derivative of expression* $\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha(\tau)\mathrm{e}^{\tau\mathcal{L}}$ *is*

$$\partial_\tau^k\left(\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha(\tau)\mathrm{e}^{\tau\mathcal{L}}\right)=\sum_{\ell=0}^{k}(-1)^\ell\binom{k}{\ell}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell}\big(\alpha^{(k-\ell)}(\tau)\big)\mathrm{e}^{\tau\mathcal{L}}. \tag{A.4}$$

Proof. We prove the statement by induction on k. Let $k=1$.

$$\begin{aligned}\partial_\tau^1\left(\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha(\tau)\mathrm{e}^{\tau\mathcal{L}}\right) &= \partial_\tau^1\left(\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha(\tau)\right)\mathrm{e}^{\tau\mathcal{L}}+\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha(\tau)\mathcal{L}\mathrm{e}^{\tau\mathcal{L}}\\ &= (-1)\mathcal{L}\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha(\tau)\mathrm{e}^{\tau\mathcal{L}}+\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha'(\tau)\mathrm{e}^{\tau\mathcal{L}}+\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha(\tau)\mathcal{L}\mathrm{e}^{\tau\mathcal{L}}\\ &= (-1)\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^1(\alpha(\tau))\mathrm{e}^{\tau\mathcal{L}}+\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha'(\tau)\mathrm{e}^{\tau\mathcal{L}}\\ &= \sum_{\ell=0}^{1}(-1)^\ell\binom{1}{\ell}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell}\big(\alpha^{(1-\ell)}(\tau)\big)\mathrm{e}^{\tau\mathcal{L}}.\end{aligned}$$

Suppose now the formula (A.4) is valid for $k-1,\ k>1$. Then, by induction, we have

$$\begin{aligned}&\partial_\tau^k\left(\mathrm{e}^{(t-\tau)\mathcal{L}}=\alpha(\tau)\mathrm{e}^{\tau\mathcal{L}}\right)=\\ &\partial_\tau^1\left(\partial_\tau^{k-1}\left(\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha(\tau)\mathrm{e}^{\tau\mathcal{L}}\right)\right)=\\ &\sum_{\ell=0}^{k-1}(-1)^\ell\binom{k-1}{\ell}\partial_\tau^1\left(\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell}\big(\alpha^{(k-1-\ell)}(\tau)\big)\mathrm{e}^{\tau\mathcal{L}}\right)=\\ &\sum_{\ell=0}^{k-1}(-1)^\ell\binom{k-1}{\ell}\left((-1)\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell+1}(\alpha^{(k-1-\ell)}(\tau))\mathrm{e}^{\tau\mathcal{L}}+\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell}\big(\alpha^{(k-\ell)}(\tau)\big)\mathrm{e}^{\tau\mathcal{L}}\right)=\\ &\sum_{\ell=0}^{k-2}(-1)^{\ell+1}\binom{k-1}{\ell}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell+1}(\alpha^{(k-(\ell+1))}(\tau))\mathrm{e}^{\tau\mathcal{L}}+(-1)^k\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{k}(\alpha(\tau))\mathrm{e}^{\tau\mathcal{L}}\\ &+\sum_{\ell=1}^{k-1}(-1)^\ell\binom{k-1}{\ell}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell}\big(\alpha^{(k-\ell)}(\tau)\big)\mathrm{e}^{\tau\mathcal{L}}+\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha^{(k)}(\tau)\mathrm{e}^{\tau\mathcal{L}}=\end{aligned}$$

$$\sum_{\ell=1}^{k-1}(-1)^{\ell}\binom{k-1}{\ell-1}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell}(\alpha^{(k-\ell)}(\tau))\mathrm{e}^{\tau\mathcal{L}}+(-1)^{k}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{k}(\alpha(\tau))\mathrm{e}^{\tau\mathcal{L}}$$
$$+\sum_{\ell=1}^{k-1}(-1)^{\ell}\binom{k-1}{\ell}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell}\big(\alpha^{(k-\ell)}(\tau)\big)\mathrm{e}^{\tau\mathcal{L}}+\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha^{(k)}(\tau)\mathrm{e}^{\tau\mathcal{L}}=$$
$$\sum_{\ell=1}^{k-1}(-1)^{\ell}\binom{k}{\ell}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell}(\alpha^{(k-\ell)}(\tau))\mathrm{e}^{\tau\mathcal{L}}$$
$$+\mathrm{e}^{(t-\tau)\mathcal{L}}\alpha^{(k)}(\tau)\mathrm{e}^{\tau\mathcal{L}}+(-1)^{k}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{k}(\alpha(\tau))\mathrm{e}^{\tau\mathcal{L}}=$$
$$\sum_{\ell=0}^{k}(-1)^{\ell}\binom{k}{\ell}\mathrm{e}^{(t-\tau)\mathcal{L}}ad_{\mathcal{L}}^{\ell}(\alpha^{(k-\ell)}(\tau))\mathrm{e}^{\tau\mathcal{L}}.$$

In the penultimate equality we used the identity $\binom{k}{\ell}=\binom{k-1}{\ell}+\binom{k-1}{\ell-1}$. □

A.3

We provide precise calculations for approximating by the Filon method highly oscillatory integrals: univariate, bivariate, and trivariate, from the Neumann series. The calculations are used in Chapter 4

Univariate integral
Consider the following integral

$$\int_0^h \mathrm{e}^{(h-\tau)\mathcal{L}}\alpha_{n_1}[t](\tau)\mathrm{e}^{\tau\mathcal{L}}u[t](0)\mathrm{e}^{n_1\mathrm{i}\omega\tau}\mathrm{d}\tau.$$

We denote $F(\tau):=\mathrm{e}^{(h-\tau)\mathcal{L}}\alpha_{n_1}[t](\tau)\mathrm{e}^{\tau\mathcal{L}}u[t](0)$. Function F is approximated by using Hermite interpolation $F(0)=p(0)$, $F(h)=p(h)$, $F'(0)=p'(0)$, $F'(h)=p'(h)$. The polynomial p approximating function F is equal to

$$\begin{aligned} p(\tau) &= F(0)+\tau F'(0)+\frac{\tau^2}{h^2}(3F(h)-3F(0)-2hF'(0)-hF'(h)) \\ &\quad +\frac{\tau^3}{h^3}(hF'(h)-2F(h)+2F(0)+hF'(0)), \\ &= F(0)+a_{1,1}\tau+a_{1,2}\tau^2+a_{1,3}\tau^3, \end{aligned}$$

where

$$\begin{aligned} a_{1,1} &= F'(0), \\ a_{1,2} &= \frac{1}{h^2}(3F(h)-3F(0)-2hF'(0)-hF'(h)), \\ a_{1,3} &= \frac{1}{h^3}(hF'(h)-2F(h)+2F(0)+hF'(0)). \end{aligned}$$

If function α_{n_1} is dependent on time, then

$$F(0)=\mathrm{e}^{h\mathcal{L}}\alpha_{n_1}[t](0)u[t](0),\qquad F'(0)=\Big(-\mathrm{e}^{h\mathcal{L}}ad_{\mathcal{L}}^{1}(\alpha_{n_1}[t](0))+\mathrm{e}^{h\mathcal{L}}\alpha_{n_1}[t]'(0)\Big)\,u[t](0),$$

$$F(h) = \alpha_{n_1}[t](h)\mathrm{e}^{h\mathcal{L}}u[t](0), \qquad F'(h) = \left(-ad^1_{\mathcal{L}}(\alpha_{n_1}[t](h))\mathrm{e}^{h\mathcal{L}} + \alpha_{n_1}[t]'(h)\mathrm{e}^{h\mathcal{L}}\right)u[t](0),$$

where $ad^1_{\mathcal{L}}(\alpha) = [\mathcal{L}, \alpha]$ and $[X, Y] \equiv XY - YX$ is the commutator of X and Y. Approximation of the univariate integral is as follows

$$\int_0^h F(\tau)\mathrm{e}^{n_1 \mathrm{i}\omega\tau}\mathrm{d}\tau \approx \int_0^h \left(F(0) + a_{1,1}\tau + a_{1,2}\tau^2 + a_{1,3}\tau^3\right)\mathrm{e}^{n_1\mathrm{i}\omega\tau}\mathrm{d}\tau.$$

Bivariate integral with nonresonnce points

We approximate the following bivariate integral

$$\int_0^h\int_0^{\tau_2} F(\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\omega(n_1+n_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2,$$

where $F(\tau_1, \tau_2) := \mathrm{e}^{(h-\tau_2)\mathcal{L}}\alpha_{n_2}[t](\tau_2)\mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}}\alpha_{n_1}[t](\tau_1)\mathrm{e}^{\tau_1\mathcal{L}}u[t](0)$. Function F is interpolated in the nodes $(0,0)$, (h,h), $(0,h)$, and $F(0,0) = p(0,0)$, $F(0,h) = p(0,h)$, $F(h,h) = p(h,h)$, where $p(\tau_1,\tau_2)$ is a linear polynomial that approximate function F

$$F(\tau_1,\tau_2) = \underbrace{F(0,0) + a_{2,1}\tau_1 + a_{2,2}\tau_2}_{p(\tau_1,\tau_2)} + \mathcal{O}(h^2),$$

where

$$a_{2,1} = \frac{1}{h}(F(h,h) - F(0,h)), \quad a_{2,2} = \frac{1}{h}(F(0,h) - F(0,0)),$$

and

$$\begin{aligned} F(0,0) &= \mathrm{e}^{h\mathcal{L}}\alpha_{n_2}[t](0)\alpha_{n_1}[t](0)u[t](0), \quad F(0,h) = \alpha_{n_2}[t](h)\mathrm{e}^{h\mathcal{L}}\alpha_{n_1}[t](0)u[t](0),\\ F(h,h) &= \alpha_{n_2}[t](h)\alpha_{n_1}[t](h)\mathrm{e}^{h\mathcal{L}}u[t](0). \end{aligned}$$

Approximation of the bivariate integral reads

$$\int_0^h\int_0^{\tau_2} F(\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\omega(n_1\tau_1+n_2\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2 \approx \int_0^h\int_0^{\tau_2}(F(0,0) + a_{2,1}\tau_1 + a_{2,2}\tau_2)\mathrm{e}^{\mathrm{i}\omega(n_1\tau_1+n_2\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2.$$

Bivariate integrals with resonnce points

Consider the following sum of two integrals with resonnce points $(n,-n)$ and $(-n,n)$

$$\int_0^h\int_0^{\tau_2} F(\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\omega n(\tau_1-\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2 + \int_0^h\int_0^{\tau_2} F(\tau_1,\tau_2)\mathrm{e}^{\mathrm{i}\omega n(-\tau_1+\tau_2)}\mathrm{d}\tau_1\mathrm{d}\tau_2,$$

where $F(\tau_1,\tau_2) := \mathrm{e}^{(h-\tau_2)\mathcal{L}}\alpha_n[t](\tau_2)\mathrm{e}^{(\tau_2-\tau_1)\mathcal{L}}\alpha_n[t](\tau_1)\mathrm{e}^{\tau_1\mathcal{L}}u[t](0)$. The bivariate integrals with resonance points necessitate the imposition of an additional interpolating condition. Let $p(\tau_1,\tau_2) = F(0,0) +$

$b_1\tau_1 + b_2\tau_2 + b_3\tau_1\tau_2$, be a polynomial with coefficients b_j defined by the formulas

$$\begin{aligned} b_1 &= \frac{1}{h}(F(0,h) - F(0,0)), \\ b_2 &= \frac{1}{h}(2X + F(0,h) - F(h,h)), \\ b_3 &= \frac{2}{h^2}(F(h,h) - F(0,h) - X), \end{aligned}$$

where

$$X = \int_0^h \partial^1_{\tau_1} F(\tau_2,\tau_2)\mathrm{d}\tau_2 = \int_0^h \mathrm{e}^{(h-\tau_2)\mathcal{L}}\alpha_n[t](\tau_2)\left(-ad^1_{\mathcal{L}}(\alpha_n[t](\tau_2)) + \alpha_n[t]'(\tau_2)\right)\mathrm{e}^{\tau_2\mathcal{L}}u[t](0)\mathrm{d}\tau_2.$$

Polynomial p satisfies the conditions

$$\begin{aligned} p(0,0) &= F(0,0), \\ p(0,h) &= F(0,h), \\ p(h,h) &= F(h,h), \\ \int_0^h \partial^1_{\tau_1} p(\tau_2,\tau_2)\mathrm{d}\tau_2 &= \int_0^h \partial^1_{\tau_1} F(\tau_2,\tau_2)\mathrm{d}\tau_2. \end{aligned}$$

The Filon quadrature reads

$$\int_0^h\int_0^{\tau_2} F(\tau_1,\tau_2)\left(\mathrm{e}^{\mathrm{i}\omega n(\tau_1-\tau_2)} + \mathrm{e}^{\mathrm{i}\omega n(-\tau_1+\tau_2)}\right)\mathrm{d}\tau_1\mathrm{d}\tau_2 \approx \int_0^h\int_0^{\tau_2} p(\tau_1,\tau_2)\left(\mathrm{e}^{\mathrm{i}\omega n(\tau_1-\tau_2)} + \mathrm{e}^{\mathrm{i}\omega n(-\tau_1+\tau_2)}\right)\mathrm{d}\tau_1\mathrm{d}\tau_2.$$

Trivariate integral

The last integral to be approximated is

$$\int_0^h\int_0^{\tau_3}\int_0^{\tau_2} F(\tau_1,\tau_2,\tau_3)\mathrm{e}^{\mathrm{i}\omega(\tau_1 n_1+\tau_2 n_2+\tau_3 n_3)}\mathrm{d}\tau_1\mathrm{d}\tau_2\mathrm{d}\tau_3,$$

where $F(\tau_1,\tau_2,\tau_3) = \mathrm{e}^{(h-\tau_3)\mathcal{L}}\alpha_{n_3}[t](\tau_3)\mathrm{e}^{(\tau_3-\tau_2)\mathcal{L}}\alpha_{n_2}[t](\tau_2)\mathrm{e}^{(\tau_2-\tau_1)}\alpha_{n_1}[t](\tau_1)\mathrm{e}^{\tau_1\mathcal{L}}u[t](0)$. Function F is interpolated in the nodes $(0,0,0)$, $(0,0,h)$, $(0,h,h)$, (h,h,h) and $F(0,0,0) = p(0,0,0)$, $F(0,0,h) = p(0,0,h)$, $F(0,h,h) = p(0,h,h)$, $F(h,h,h) = p(h,h,h)$.

$$F(\tau_1,\tau_2,\tau_3) \approx p(\tau_1,\tau_2,\tau_3) = F(0,0,0) + a_{3,1}\tau_1 + a_{3,2}\tau_2 + a_{3,3}\tau_3,$$

where

$$\begin{aligned} a_{3,3} &= \frac{1}{h}(F(0,0,h) - F(0,0,0)), \\ a_{3,2} &= \frac{1}{h}(F(0,h,h) - F(0,0,h)), \\ a_{3,1} &= \frac{1}{h}(F(h,h,h) - F(0,h,h)), \end{aligned}$$

and

$$
\begin{aligned}
F(0,0,0) &= \mathrm{e}^{h\mathcal{L}}\alpha_{n_3}[t](0)\alpha_{n_2}[t](0)\alpha_{n_1}[t](0)u[t](0),\\
F(0,0,h) &= \alpha_{n_3}[t](h)\mathrm{e}^{h\mathcal{L}}\alpha_{n_2}[t](0)\alpha_{n_1}[t](0)u[t](0),\\
F(0,h,h) &= \alpha_{n_3}[t](h)\alpha_{n_2}[t](h)\mathrm{e}^{h\mathcal{L}}\alpha_{n_1}[t](0)u[t](0),\\
F(h,h,h) &= \alpha_{n_3}[t](h)\alpha_{n_2}[t](h)\alpha_{n_1}[t](h)\mathrm{e}^{h\mathcal{L}}u[t](0).
\end{aligned}
$$

Approximation of the trivariate integral is

$$
\int_0^h\int_0^{\tau_3}\int_0^{\tau_2} F(\tau_1,\tau_2,\tau_3)\mathrm{e}^{\mathrm{i}\omega(\tau_1 n_1+\tau_2 n_2+\tau_3 n_3)}\mathrm{d}\tau_1\mathrm{d}\tau_2\mathrm{d}\tau_3 \approx
$$
$$
\int_0^h\int_0^{\tau_3}\int_0^{\tau_2}(F(0,0,0)+a_{3,1}\tau_1+a_{3,2}\tau_2+a_{3,3}\tau_3)\mathrm{e}^{\mathrm{i}\omega(\tau_1 n_1+\tau_2 n_2+\tau_3 n_3)}\mathrm{d}\tau_1\mathrm{d}\tau_2\mathrm{d}\tau_3.
$$

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