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Randomness, structure preservation, and low-regularity numerical approximations for nonlinear dispersive equations

Yvonne Alama Bronsard

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SORBONNE UNIVERSITÉ
LJLL

École doctorale **Sciences Mathématiques de Paris Centre**
Unité de recherche **Laboratoire Jacques-Louis Lions**

Thèse présentée par **Yvonne ALAMA BRONSARD**

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Spécialité **Analyse numérique**

**Schémas numériques pour les équations
dispersives non linéaires : analyse à faible
régularité, cadre aléatoire et préservation de
symétries**

**Randomness, structure preservation, and low-regularity numerical
approximations for nonlinear dispersive equations**

Thèse dirigée par Katharina SCHRATZ

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À Lia, Stan, Sylvie, et Camille

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Gens du pays, c'est votre tour
De vous laisser parler d'amour

Gilles Vignault, 1975

nous te ferons, Terre de Québec
lit des résurrections
et des mille fulgurances de nos métamorphoses
de nos levains où lève le futur
de nos volontés sans concessions
les hommes entendront ton pouls dans l'histoire
c'est nous ondulant dans l'automne d'octobre
c'est le bruit roux de chevreuils d'automne
l'avenir dégagé

l'avenir engagé

Gaston Miron, 1970, l'Hexagone

Contraste

Et ronronnait le réfrigérateur
Dans le silence du matin

Les deux petits enfants
Et leur grand-père
Ouvrirent sa porte

Il y avait là
Dans le réfrigérateur
La moitié d'un Saint-Honoré
Ce gâteau à la crème
Entouré de choux à la crème
Et recouvert de miel

Il y avait là des confitures
De la confiture de rhubarbe
De la confiture de cassis
De la confiture de framboise
Et même de la gelée de coings
Mère de toutes les confitures

Il y avait là
Deux morceaux de fromage
Une motte de beurre
Des œufs
Du beurre d'arachide
Et la moitié
D'un gigot d'agneau

Les deux petits enfants
Qui étaient ravissants
Étaient ravis

Le vieux grand-père
Était un vieux grognon
Il n'était ni ravi ni ravissant

Il referma la porte du réfrigérateur
« Qu'allons-nous manger ? »
Dit le vieux grand-père

*Camille Bronsard,
Au jour J du mois M de l'an A,
Les carnets de Dame Plume, 2011*

1976

Tu es au carrefour des Cultures anciennes

Tu as vu
Le tombeau de Khéops
Celui d'Agamemnon celui de Clytemnestre

Tu as vu
Les pierres du défi de maintes acropoles
Les marbres raffinés de maintes agoras

Et du mont Palatin
tu as vu
Les pierres du défi de Rome l'Éternelle

Séduit par Andrinople
Ébloui par Grenade
Tu as vu
Les étoiles mourir
Sur les blancs minarets des mosquées de Sinan
Et le soleil mourir
Sur les murs cramois du divin Alhambra

L'Histoire est passée par ici
Elle qui ne passe pas chez toi
Elle qui ne veut pas de toi

Terrassier sous Khéops
Potier sous Périclès
Eunuque sous Soliman

Toi tu veux un pays que chacun te refuse
Tu habites aujourd'hui une terre sans promesse
Tu voudrais un destin
pour ton peuple et pour toi

Esclave
Esclave d'âge en âge
Tu appelles ta Revanche

Tu recherches l'Esprit qui vibrait en ces terres

Tu ne peux rien sauver de ce peuple qui meurt
Au choc le plus léger ton empreinte s'efface
Tu ne peux rien sauver de ta vie qui s'envole
Par ce peuple qui meurt tu ne peux te survivre

Antigone mourante en un désert futur
Tu ne peux qu'amuser la galerie française
Funambule immobile entre des pics sublimes
Tu ne peux qu'épater ceux qui ont réussi

Renié par tes dieux dont triomphe Athéna
Tu ne peux plus changer ton échec en victoire
Condamné au succès par tous les dieux anciens
Tu ne peux réussir sans être mercenaire

Seul et désemparé tu reviens en ces lieux
Et promènes sans fin ta lamentable errance
Ton désespoir est laid tu maudis tous les dieux

Tu recherches l'Esprit qui vibrait en ces terres

Il ne peut rien pour toi
Ta quête est sans objet

Tu es seul
 ironiquement apatride
 comiquement cénobite
 superbement citoyen du monde
Tu réalises tous les rêves fous

Ceux qui ont réussi les ont rêvés pour toi

Tu es seul
 et tu penses à ton coin de terre
À ton peuple lassé pourtant si près du but
Doucement
Tristement
Bêtement
Dans une euthanasie finement programmée

Tu es seul et tu sais que tu ne peux déchoir

Condamné au succès il te faut comploter
Contre les dieux contre les faits contre l'Histoire
Condamné au succès tu ne peux que lutter
Avec des plans nouveaux et des trames nouvelles

Tu maudissais l'Histoire
Trouves-y une faille

Tu dois vaincre l'Esprit qui vibrait en ces terres

*Camille Bronsard,
Au jour J du mois M de l'an A,
Les carnets de Dame Plume, 2011*

SCHÉMAS NUMÉRIQUES POUR LES ÉQUATIONS DISPERSIVES NON LINÉAIRES : ANALYSE À FAIBLE RÉGULARITÉ, CADRE ALÉATOIRE ET PRÉSERVATION DE SYMÉTRIES

Randomness, structure preservation, and low-regularity numerical approximations for nonlinear dispersive equations

Résumé

Le travail présenté dans cette thèse relève du domaine de l'analyse numérique et s'appuie sur des outils issus de l'étude des équations aux dérivées partielles (EDP). Nous nous concentrons sur les discrétisations temporelles des équations dispersives non linéaires. L'objectif est de réduire les hypothèses de régularité nécessaires lors de la conception et de l'analyse des méthodes numériques, afin de traiter les dynamiques à faible régularité.

La partie I de la thèse introduit de nouveaux schémas à faible régularité, adaptés à des domaines bornés génériques. Le chapitre 2 présente des résultats de convergence au premier et au second ordre pour l'approximation de l'équation de Gross-Pitaevskii, lorsque la donnée initiale et le potentiel sont peu réguliers. Le chapitre 3 généralise la construction de ces schémas aux ordres supérieurs, et pour une classe générale d'équations d'évolution non linéaires.

La partie II est constituée du chapitre 4, qui génère des constructions d'ordre élevé dans le cadre de conditions initiales aléatoires.

Finalement, la partie III se consacre à l'étude en temps long d'équations dispersives, et de leurs invariants, en considérant des schémas préservant leur structure. Elle débute avec le chapitre 5, qui introduit un nouvel intégrateur symétrique pour l'équation de Schrödinger non linéaire, et démontre des résultats de convergence à des taux fractionnaires, en fonction de la régularité de Sobolev de la donnée initiale. Par la suite, le chapitre 6 étend cette construction symétrique aux ordres supérieurs et pour la résolution numérique d'une classe générale d'équations dispersives. Des simulations numériques montrent que ces nouveaux schémas symétriques présentent d'excellentes propriétés de préservation de la structure.

Les extensions aux ordres supérieurs développées aux chapitres 3, 4, et 6 se fondent sur de nouvelles techniques d'arbres décorés, inspirées par le champ des EDP stochastiques singulières, via la théorie des structures de régularité.

Mots clés : équations dispersives non linéaires, faible régularité, schémas préservant la structure, arbres décorés

Abstract

The work presented in this thesis belongs to the field of numerical analysis, and builds on tools stemming from the study of partial differential equations (PDEs). We focus on time discretizations to nonlinear dispersive equations. The aim is to reduce the *smoothness* assumptions on the design and analysis of numerical methods, in order to treat *low-regularity* dynamics.

Part I of the thesis develops novel low-regularity schemes, suited for general bounded domains. Chapter 2 presents first and second order convergence results for the Gross-Pitaevskii equation, when both the initial data and the potential are non-smooth. Chapter 3 generalizes the construction of these schemes to higher order and to a general class of nonlinear evolution equations with potentials.

Part II of the thesis consists of Chapter 4, which considers higher-order constructions for *randomized* initial conditions. Part III of the thesis considers the long-time properties and invariants of the equation, and deals with *structure-preserving* schemes. We first introduce in Chapter 5 a novel symmetric time integrator for the nonlinear Schrödinger equation. We give fractional convergence rates as a function of the Sobolev regularity of the initial data. Chapter 6 extends the latter work by constructing higher order symmetric integrators for a general class of dispersive equations. All these new symmetric schemes exhibit excellent structure preservation and convergence properties, which are witnessed in numerical experiments.

The higher order extensions of Chapters 3, 4, 6 follow new techniques based on decorated tree series, inspired by singular stochastic PDEs via the theory of Regularity Structures.

Keywords: nonlinear dispersive equations, low-regularity, structure preserving schemes, decorated trees

Chapter 1

Introduction

The study of nonlinear partial differential equations (PDEs), and more specifically those modeling non-smooth phenomena, arising in nonlinear optics, shallow water waves, and wave turbulence, is at the heart of an intense international activity. While linear problems or smooth solutions are generally well understood, a reliable description of *nonlinear* and *non-smooth* phenomena remains an important challenge in computational mathematics today. This is especially the case when studying nonlinear dispersive equations, since one cannot expect the smoothing effects that are present in parabolic equations. The lack of smoothness in the solution leads to large errors in numerical simulations, massive computational costs and ultimately causes the failure of classical schemes. Yet many interesting physical phenomena exhibit non-smooth behavior. An essential task is thus to develop and study suitable numerical schemes for approximating such non-smooth behavior. To this end, we will be interested in constructing and analyzing numerical approximations to the following class of dispersive equations

$$\begin{cases} \partial_t u(t, x) - \mathcal{L}u(t, x) = p(u(t, x)), & (t, x) \in \mathbb{R} \times \mathbb{T}^d, \quad d \in \{1, 2, 3\} \\ u(0, x) = u_0(x), \end{cases} \quad (1.1)$$

where $p(u(t, x))$ is a polynomial in $u(t, x)$, its conjugate $\bar{u}(t, x)$, and their spatial derivatives, see (6.5) for more detail. We ask \mathcal{L} to be a linear operator which generates a strongly continuous *group* $\{e^{t\mathcal{L}}\}_{t \in \mathbb{R}}$ of contractions on L^2 , and require \mathcal{L} to involve only polynomials in the frequencies when mapped in Fourier space. Namely, we denote $P(k)$ the Fourier multiplier of \mathcal{L} and require $P(k)$ to be polynomial in k . We give two prototypical examples of nonlinear dispersive equations belonging to the above class (1.1).

Example 1 A classical model in quantum mechanics and a natural starting point for the study of dispersive equations is the (cubic) nonlinear Schrödinger equation (NLS), which corresponds to taking $\mathcal{L} = i\Delta$, $P(k) = -i|k|^2$, and $p(u) = -i|u|^2u$:

$$\partial_t u(t, x) - i\Delta u(t, x) = -i|u(t, x)|^2 u(t, x). \quad (1.2)$$

Example 2 Another example is the Korteweg–de Vries equation (KdV), which serves as a model for waves in shallow waters, and corresponds to the case $\mathcal{L} = -\partial_x^3$, $P(k) = ik^3$, and $p(u) = \frac{1}{2}\partial_x(u^2)$:

$$\partial_t u(t, x) + \partial_x^3 u(t, x) = \frac{1}{2}\partial_x(u^2(t, x)). \quad (1.3)$$

Throughout this manuscript I have been interested in developing new techniques to obtain computational schemes for approximating *in time* low regularity solutions to such equations, with an emphasis on what can be rigorously proven to guarantee their reliability. Numerically approximating low regularity solutions is a challenge since classical approximation techniques require smoothness. As an illustration, in the case of the NLS equation (1.2), both classical finite differences or splitting methods require at least H^2 -solutions for L^2 -convergence at first order, and H^4 -solutions for L^2 -convergence at second order [Lub08, BBD02, SS84, BDDL21, HP17]. On the other hand, the equation is locally well-posed (LWP) for solutions in $H^\alpha(\mathbb{T}^d)$, with $\alpha \geq 0$, $\alpha > 0$, and $\alpha > 1/2$ for $d = 1, 2$ and 3 respectively. A question I have investigated is how to reduce the gap between the degree of regularity required by the numerical approximation and the regularity needed for the local well-posedness theory.

The numerical challenges of discretizing such equations are in part governed by the theoretical challenges in proving their well-posedness. We quote Daniel Tataru [Tat04] introducing well-posedness results for the wave map equation :

The initial work in this field was mostly devoted to the local study of problems with reasonably smooth initial data. Often this reduces to analyzing linear problems. The well-posedness questions becomes harder to answer when one considers either problems with less regular data or solutions which exist for a larger time. Then one needs to gain a better and better understanding of the nonlinear wave interactions.

The same can be said in the discrete setting. The goal of this manuscript is to deepen our understanding on both aspects, by constructing and analyzing new schemes which converge under *less regular data* and which have a good *long-time* behavior. Parts I and II of this manuscript focus on obtaining schemes that converge under less regular data, in deterministic and randomized settings. Part III deals with long-time behavior of the schemes.

Remark 1.0.1 (From semi-discrete to fully discrete approximations) Throughout this manuscript we will focus on building and analyzing novel approximations in *time*. Going from the semi-discretization in time to the fully discrete problem is an important step. We refer for instance to the works [LW21, OY22, CLR20, LMS21, LW21, BMW23, BW23b] which explore fully discrete low-regularity settings.

We begin with a comparison between *classical* approximation techniques and novel *low-regularity* approaches.

1.1 A scheme at first order: classical versus low-regularity approaches

A large toolbox of numerical schemes for dispersive equations has been developed, based on different discretization techniques. *Exponential integrators* and *Lawson methods* rely on discretizing Duhamel's formula, otherwise called the variation-of-constants formula. *Finite difference* schemes directly discretize the underlying equation (1.1) via explicit or implicit Taylor approximations. *Splitting methods* are based upon splitting the full equation into a series of simpler subproblems. The above classical schemes often allow for a precise and efficient approximation, but are designed for *smooth* solutions, requiring high regularity assumptions. To illustrate this, we will construct and compare first order time-approximations to the class of dispersive equations (1.1). We start by writing *Duhamel's formula* for $u(t)$:

$$u(t) = e^{t\mathcal{L}}u_0 + \int_0^t e^{(t-s)\mathcal{L}}p(u(s))ds \quad (1.4)$$

and iterate Duhamel's formula for $u(s)$ inside $p(u(s))$ to obtain the next iterate

$$u(t) = e^{t\mathcal{L}}u_0 + \int_0^t e^{(t-s)\mathcal{L}}p(e^{s\mathcal{L}}u_0)ds + \int_0^t \int_0^s \dots ds_1 ds. \quad (1.5)$$

Namely, the above equality (1.5) follows by Taylor expanding the nonlinearity p appearing in (1.4) around the linear flow: $p(u(s)) = p(e^{s\mathcal{L}}u_0) + \int_0^s \dots ds_1$, with an integral remainder. We search an approximation over one time step $t = \tau$. In order to obtain a first order approximation in *time*, we neglect the double integral in (1.5), which corresponds to the second order term:

$$u(\tau) = e^{\tau\mathcal{L}}u_0 + \int_0^\tau e^{(\tau-s)\mathcal{L}}p(e^{s\mathcal{L}}u_0)ds + O(\tau^2). \quad (1.6)$$

If we suppose that $p(u)$ is locally Lipschitz, as defined in (2.11), neglecting the $O(\tau^2)$ -term does not require any additional regularity, see for example (2.25). As we are considering time approximations, the main challenge is to replace the integrand

$$e^{-s\mathcal{L}}p(e^{s\mathcal{L}}u_0) \quad (1.7)$$

by an approximation which can be integrated explicitly on $[0, \tau]$. Classical methods are based upon Taylor expanding in time the exponentials appearing in the above equation (1.7) as follows: $e^{s\mathcal{L}}u = 1 + O(s\mathcal{L}u)$. Hence, they are based upon linear frequency approximations. We give the example of a first order exponential integrator.

Example 3 (The Euler exponential method) A first order exponential integrator consists in Taylor expanding the exponential appearing inside the nonlinearity :

$$e^{-s\mathcal{L}}p(e^{s\mathcal{L}}u_0) \approx e^{-s\mathcal{L}}p(u_0). \quad (1.8)$$

The scheme after one time-step, which expresses u^{n+1} in terms of u^n , is then obtained by integrating exactly the remaining term $e^{(\tau-s)\mathcal{L}}$:

$$u^{n+1} = e^{\tau\mathcal{L}}u^n + \tau\varphi_1(\tau\mathcal{L})p(u^n) \quad \text{with} \quad \varphi_1(z) = \frac{e^z - 1}{z}. \quad (1.9)$$

It remains to quantify the local error induced by the approximation (1.8). For the NLS equation (1.2), following the reference [HO10], the local error has the following explicit form:

$$|u|^4u - 2|u|^2\Delta u + u^2\overline{\Delta u}. \quad (1.10)$$

First order convergence of this method thus requires two additional derivatives on the solution, and more specifically requires H^2 -solutions when measuring the error in L^2 . If the solution is however not sufficiently smooth, the local error becomes unbounded and the exponential integrator fails to converge at first order, see Figure 1.1.

A new discretization technique was introduced in the works [HS17b, OS18] in the case of the KdV equation (1.3) and the NLS equation (1.2). The idea is based on a new nonlinear approach, and a refined analysis made in Fourier space. Instead of linearizing the frequency interactions in the central oscillatory term (1.7), the nonlinear frequency interactions between the linear flow $e^{-s\mathcal{L}}$ and the nonlinear factor $p(e^{s\mathcal{L}}u_0)$ are incorporated into the numerical discretization. This allows for the convergence of novel time discretizations under lower regularity assumptions on the solution.

In the following section we illustrate the new discretization technique of [OS18] for the NLS equation (1.2), and compare it with classical approaches.

1.1.1 Illustration on the nonlinear Schrödinger equation

We propose in this section a method of construction introduced in [AB23b] for the NLS equation (1.2), which offers a framework for the derivation of different classes of schemes: the previous scheme of [OS18] built at low-regularity, newly designed ones presented in this manuscript, and classical integrators. We recall that $p(u) = -i|u|^2u$ and let $t_n = n\tau$, with τ the time step.

We start by making a change of variables. Instead of working with the equation (1.2) in u , we twist the variables with respect to the leading differential operator $\mathcal{L} = i\Delta$:

$$e^{it\Delta}v = u, \quad (1.11)$$

and work with the equation in v :

$$\partial_t v = e^{-it\Delta}p(e^{it\Delta}v), \quad v(0) = u_0, \quad (1.12)$$

as well as its integral form (obtained by integrating on $[t_n, t_n + s]$):

$$v(t_n + s) = v(t_n) + e^{-it_n\Delta} \int_0^s e^{-is_1\Delta} p(e^{i(t_n+s_1)\Delta} v(t_n + s_1)) ds_1. \quad (1.13)$$

This change of variables is a well-known approach in the theoretical analysis of dispersive equations in low regularity spaces [Bou93], in rough path theory [Gub12], as well as in numerical analysis for constructing Lawson methods [Law67, HLO20] and resonance-based schemes [HS17b, OS18].

Remark 1.1.1 (The advantage of twisting the variable) The equation (1.2) for u is driven by the differential operator $i\Delta$, an unbounded operator on L^2 . This is not the case for the equation (1.12) in v , which is written in terms of the nonlinearity and the free Schrödinger group, a bounded operator in L^2 . The numerical advantage thus lies in the fact that the approximation

$$v(t_n + s) \approx v(t_n), \quad |s| \leq \tau, \quad (1.14)$$

does not require additional regularity on the solution v . Indeed, it follows from equation (1.13) that for $\sigma > d/2$

$$\|v(t_n + s) - v(t_n)\|_{H^\sigma} \leq \int_0^s \|p(e^{i(t_n+s_1)\Delta} v(t_n + s_1))\|_{H^\sigma} ds_1 \leq \left(\sup_{0 \leq s_1 \leq s} \|v(t_n + s_1)\|_{H^\sigma}^3 \right) s.$$

The same analysis would yield in the untwisted variable the approximation $u(t_n + s) \approx e^{is\Delta}u(t_n)$, $|s| \leq \tau$. Obtaining the approximation $u(t_n + s) \approx u(t_n)$ requires Taylor expanding at first order the linear flow $e^{is\Delta}$, and hence two additional derivative on the solution.

Next, we map Duhamel's formula (1.13) in Fourier space, with $s = \tau$ the time step. Expanding v in Fourier series $v(t, x) = \sum_{k \in \mathbb{Z}} v_k(t) e^{ikx}$, allows to express the action of the linear Schrödinger flow on v , $e^{\pm it\Delta} v(t, x) = \sum_{k \in \mathbb{Z}} v_k(t) e^{\mp itk^2} e^{ikx}$. We note that the upcoming derivation can analogously be obtained in higher dimensions with $\mathbf{k} = (k^1, \dots, k^d) \in \mathbb{Z}^d$. The k -th Fourier coefficient of $v(t_{n+1})$ reads

$$v_k(t_{n+1}) = v_k(t_n) - i \sum_{k=-k_1+k_2+k_3} e^{it_n R(k)} \int_0^\tau e^{isR(k)} \bar{v}_{k_1}(t_n+s) v_{k_2}(t_n+s) v_{k_3}(t_n+s) ds, \quad (1.15)$$

where we collected all the frequency interactions into the *resonance structure* $R(k)$:

$$R(k) = k^2 + k_1^2 - k_2^2 - k_3^2 = 2k_1^2 - 2k_1(k_2 + k_3) + 2k_2k_3, \quad k = -k_1 + k_2 + k_3. \quad (1.16)$$

The goal is to approximate in time the integrand in equation (1.15). The idea behind the novel nonlinear approach in [OS18], is to base the approximation on the specific form of the resonance structure (1.16). We illustrate this approach with the general decomposition presented in [AB23b], which improves on the scheme of [OS18]. Namely, we decompose the integrand in (1.15) into three factors:

$$I_\tau = \int_0^\tau e^{isR_{\text{dom}}(k)} e^{isR_{\text{low}}(k)} g(s) ds \quad (1.17)$$

with

$$\begin{aligned} R(k) &= R_{\text{dom}}(k) + R_{\text{low}}(k), & g(s) &= \bar{v}_{k_1}(t_n+s) v_{k_2}(t_n+s) v_{k_3}(t_n+s), \\ R_{\text{dom}} &= 2k_1^2, & R_{\text{low}} &= -2k_1(k_2 + k_3) + 2k_2k_3. \end{aligned} \quad (1.18)$$

The choice of the above decomposition (1.17) is dictated by the regularity assumptions needed to approximate each of the factors. Using Duhamel's formula (1.13) we can approximate $g(s)$ at its left end point: $g(s) \approx g(0)$ with a local error in $O(s)$ *without additional regularity requirements*, see equation (1.14). It remains to treat the oscillatory term:

$$e^{isR_{\text{dom}}(k)} e^{isR_{\text{low}}(k)} g(0), \quad (1.19)$$

which corresponds to the term (1.7), when mapped in Fourier space. A second approximation step is necessary to obtain a practical implementation of the scheme, see Remark (1.1.2). We observe that approximating the factor $e^{isR_{\text{low}}(k)}$ asks for *less* regularity than approximating $e^{isR_{\text{dom}}(k)}$. Indeed, the terms $k_l k_j$ (for $l \neq j$) appearing in $R_{\text{low}}(k)$ correspond to products of first order derivatives. Hence, by denoting $v = v(t_n)$, a formal first-order Taylor expansion yields

$$e^{isR_{\text{low}}} = 1 + O(sR_{\text{low}}), \quad \text{with} \quad R_{\text{low}}g(0) \sim -2(|\nabla v|^2 \bar{v} + 2v \nabla v \cdot \nabla \bar{v}), \quad (1.20)$$

after mapping back from frequency to spatial variables. If we tried to approximate the dominant factor $e^{isR_{\text{dom}}(k)}$, as $2k_1^2$ corresponds to second order derivatives in Fourier space, we would require more regularity:

$$e^{isR_{\text{dom}}} = 1 + O(sR_{\text{dom}}), \quad \text{with} \quad R_{\text{dom}}g(0) \sim 2v^2 \Delta \bar{v}. \quad (1.21)$$

Therefore, we choose to Taylor expand the lower term (1.20), making the approximation $R(k) \approx R_{\text{dom}}(k)$, and *integrate exactly* the dominant term:

$$I_\tau \approx \int_0^\tau e^{isR_{\text{dom}}(k)} ds g(0) = \frac{e^{2i\tau k_1^2} - 1}{2ik_1^2} g(0),$$

in order to obtain a scheme whose local error requires the least regularity. We finally map back in physical space, and in the untwisted variables. We thereby obtain the so-called first-order *resonance-based* integrator

$$u^{n+1} = e^{i\tau\Delta} u^n - i\tau e^{i\tau\Delta} ((u^n)^2 \varphi_1(-2i\tau\Delta) \bar{u}^n), \quad \varphi_1(z) = \frac{e^z - 1}{z}. \quad (1.22)$$

The local error of the scheme is governed by the approximation made in (1.20) and is of the form:

$$-2(|\nabla v|^2 \bar{v} + 2v \nabla v \cdot \nabla \bar{v}), \quad (1.23)$$

which only requires the boundedness of one, instead of two, additional derivatives on the solution. For a discussion on the practical implementation of the above scheme we again refer to Remark 1.1.2, and for the terminology *resonance-based* integrator to Remark 1.1.3.

Remark 1.1.2 (An interplay between efficient implementation and proximity to the solution) Ideally, once

the first approximation step $g(s) \approx g(0)$ is performed, one would hope to integrate the remaining oscillations (1.19) exactly in time (on $[0, \tau]$). While this can be done analytically:

$$\int_0^\tau e^{iR(k)s} ds = \frac{e^{i\tau R(k)} - 1}{iR(k)}, \quad R(k) = 2k_1^2 - 2k_1(k_2 + k_3) + 2k_2k_3, \quad (1.24)$$

it does not yield a practical implementation, as it results in a generalized convolution (of Coifman-Meyer type [CM75]) which cannot be mapped back to physical space, due to the factor $(2k_1^2 - 2k_1(k_2 + k_3) + 2k_2k_3)^{-1} \bar{v}_{k_1} v_{k_2} v_{k_3}$. Hence, the computations would need to be fully made in Fourier space. Carrying this out in higher spatial dimensions d would cause large memory and computational efforts of order $O(|K|^{d-\ell})$, where K denotes the highest frequency in the discretization and ℓ is the number of factors in the nonlinearity. For practical computations, we want to be able to express the discretization also in physical space in order to use the Fast Fourier Transform (FFT) which is of computational effort of order $O(|K|^d \log |K|^d)$. Therefore, we choose an approximation of the integrand (1.19) which allows for a practical implementation (by not performing exact integration), while optimizing the local error to require the least regularity. The latter dictates the choice of the decomposition (1.18). If one was not concerned with the lack of regularity of the solution, but for example the conservation of a certain quantity of interest, then the choice of the frequency decomposition (1.18) could be taken differently.

Remark 1.1.3 (The scheme entitled “resonance-based integrator”) The terminology *resonance-based* integrator comes from the fact that the scheme is based upon the resonance structure (1.16) of the underlying PDE. Another name used is *Fourier* integrator. Further on, we will discuss extensions to these results which are suited on more general domains. These integrators will then be termed *low regularity* integrators.

We would like to address a common misconception. The construction of these resonance-based integrators are not based on the resonant case $R(k) = 0$. From a numerical point of view, the resonant case $R(k) = 0$ is trivial given that there are no oscillations to approximate; the discretization of Duhamel’s integral would simply amount to $\tau p(u^n)$. However, the case $R(k) \neq 0$ is more subtle as one needs to capture the oscillations $e^{isR(k)}$ also in the numerical approximation. We note that interestingly, the difficulties are reversed when working in the theoretical analysis of dispersive equations, since in the resonant case $R(k) = 0$ we do not gain the decay $\frac{1}{R(k)}$ in the frequencies when integrating (see equation (1.24)).

The above scheme (1.22) was first obtained by [OS18], using slightly different steps. The authors of [OS18] do not pass directly in Fourier space – as in (1.15) – and first approximate $v(t_n + s_1) \approx v(t_n)$ in Duhamel’s integral (1.13), as this does not require additional regularity (see (1.14)). However, making this first approximation ($v(t_n + s) \approx v(t_n)$ or in Fourier space $g(s) \approx g(0)$) breaks the symmetric structure of the underlying PDE (1.2) and leads to loss of structure preservation. We will see in Section 1.6 that to obtain schemes which have good structure-preserving properties we need to make a different approximation to $v(t_n + s)$ (or in Fourier $g(s)$) and should consider the general form (1.17). This approach was first taken in [AB23b].

We refer to Figure 1.1a where first order convergence of the resonance-based scheme (1.22) in L^2 norm and for H^1 solutions is observed in numerical experiments. In Section 1.2.1 rigorous convergence results of the scheme are discussed.

We next compare this resonance-based discretization with classical time integrators.

Comparison with classical approximation techniques. The Euler exponential method corresponds to making the approximation $R(k) \approx k^2$ recovering the scheme (1.9) with local error (1.10).

Another quite popular method of approximation are splitting methods ([MQ02, Fao12, BBD02, Lub08]). We recall that splitting methods consists in separating the linear $\mathcal{L} = i\Delta$ and nonlinear part $p(u) = -i|u|^2u$ and composing the exact flows of the differential equations:

$$\partial_t u = i\Delta u, \quad \text{and} \quad \partial_t u = -i|u|^2 u. \quad (1.25)$$

The first-order Lie splitting scheme is then given by:

$$\begin{aligned} u^{n+1/2} &= e^{-i\tau|u^n|^2} u^n, \\ u^{n+1} &= e^{i\tau\Delta} u^{n+1/2}, \end{aligned} \quad (1.26)$$

with the explicit local error

$$2(2|\nabla u|^2 u + \bar{u}(\nabla u \cdot \nabla u) + u^2 \Delta \bar{u}),$$

see for example [Lub08, Section 4.2]. Because of the last term $u^2 \Delta \bar{u}$ in the above formula, the Lie splitting method requires two additional derivatives on the solution, as does the Euler exponential method.

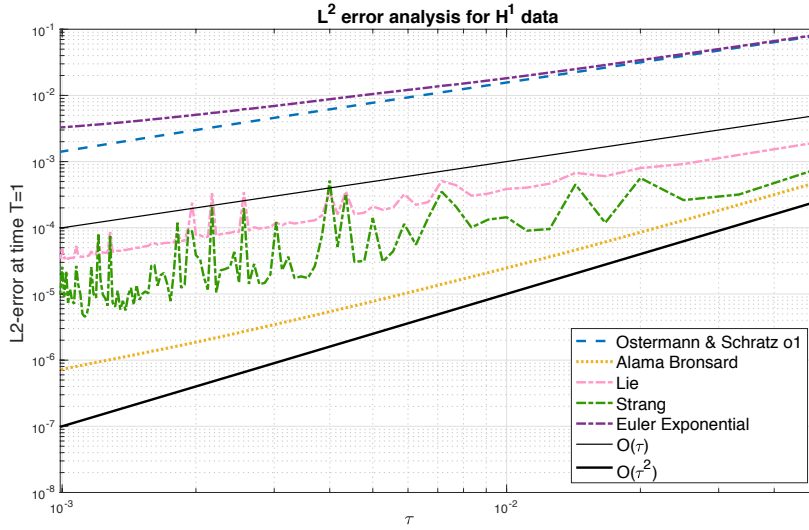
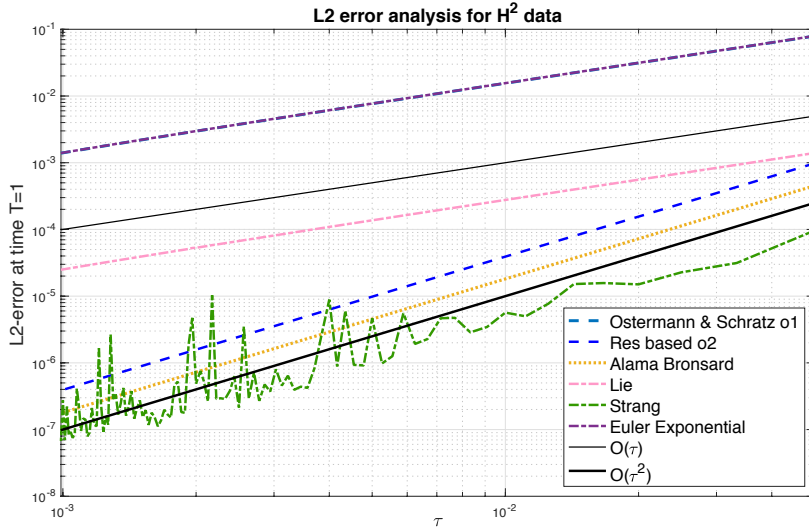
(a) H^1 data.(b) H^2 data.

Figure 1.1 – Convergence plots taken from [AB23b], for classical integrators (green, pink, purple) versus integrators suited for low-regularity solutions (light blue, dark blue, yellow). The Euler exponential method (1.9) in purple, and the first order Lie splitting (1.26) in pink do not converge at first order in Plot 1.1a. The second order Strang splitting in green oscillates erratically in both plots, due to the lack of regularity. The first order resonance-based scheme in light blue (Osterman & Schratz o1) is given by (1.22) and was derived in [OS18]. Its extension to second order (Res based o2, dark blue) is derived for instance in [BS22]. The symmetric scheme in yellow (Alama Bronsard) is given by (1.49) and introduced in Section 1.6.1.

To understand the difference behind this splitting approximation 1.26 and the resonance-based approach (1.17), we formally Taylor expand the nonlinear part in (1.26): $e^{-i\tau|u|^2} = 1 - i\tau|u|^2 + O(\tau^2)$. This does not require additional regularity assumptions since the error term in $O(\tau^2)$ only involves a polynomial of u . The local error analysis is then dominated by the remainder

$$u(t_{n+1}) - \left(e^{i\tau\Delta} u(t_n) - i\tau e^{i\tau\Delta} (|u(t_n)|^2 u(t_n)) \right). \quad (1.27)$$

In the frequency variables, the above corresponds to taking $R(k) \approx 0$ (and $g(s) \approx g(0)$), thereby neglecting all the oscillations in (1.19). Equivalently, by recalling Duhamel's integral (1.6) written in the spatial variables, the splitting method corresponds to the approximation

$$e^{-s\mathcal{L}} p(e^{s\mathcal{L}} u_0) \approx p(u_0), \quad (1.28)$$

which treats the problem as a linear one. Such linearized frequency approximations are computational very convenient,

since the oscillations in (1.28) no longer appear in the approximation. However, the method does not resolve the nonlinear frequency interactions of the system and treats the resolution of the linear $i\Delta$ and the nonlinear term $p(u)$ independently.

In conclusion, these classical approximation techniques do not take into account the interactions between the frequencies from the linear and nonlinear term. The idea behind the resonance-based schemes is to do so, while maintaining a scheme that can be efficiently implemented at the same computational cost as classical schemes. In the course of this manuscript, we will build on this nonlinear approach to obtain both novel low-regularity approximations and better structure preserving schemes.

The next section is devoted to a discussion on prior rigorous convergence results and on the spaces in which they are obtained, both for time integrators as well as finite difference methods in time.

1.2 Explicit convergence rates

An important part of this manuscript (i.e. Chapters 2 and 5) deals with obtaining explicit convergence rates of order τ^ν , which are quantified as a function of the Sobolev regularity of the solution, $u \in C([0, T], H^\alpha)$, and the Sobolev norm H^σ in which we measure the error. We let $\nu > 0$ and $\alpha \geq \sigma \geq 0$ and consider the error:

$$\|u(t_n) - u^n\|_{H^\sigma} \leq C_T \left(\sup_{[0, T]} \|u(t)\|_{H^\alpha} \right) \tau^\nu, \quad 0 \leq t_n = n\tau \leq T. \quad (1.29)$$

Throughout this thesis we denote $C_T(\cdot)$ a generic constant which depends continuously on its arguments, and exponentially on the final time T . These error analysis results are thereby *local in time*, see Remark 1.6.2. Unless stated otherwise we set ourselves on \mathbb{T}^d , with $d \in \{1, 2, 3\}$. We present two different perspectives when exploring the interplay between ν , α and σ :

1. *Full order of convergence.* We fix the desired order of convergence $\nu = m \in \mathbb{N}$, and search for the optimal regularity $\alpha = \alpha(d, \sigma, \nu)$ which is needed for the convergence of the method to order ν . The required regularity $\alpha(d, \sigma, \nu)$ depends on the spatial dimension d , the norm H^σ , and the order of convergence ν . This approach is the most common one in the literature, and Chapter 2 presents results of this type.
2. *Fractional order of convergence.* We fix the H^σ -norm, and assume the regularity $u \in C([0, T], H^\alpha)$. One cannot hope to obtain full order of convergence when the boundedness of the local error term requires higher regularity assumptions than what is assumed on the solution $u(t)$. Fractional convergence rates are then expected, with the rate as a function of the regularity α . This approach is more general, since we recover the full-order convergence result, when enough regularity is assumed. The results of Chapter 5 go in this direction.

The choice of the regularity parameters α and σ strongly influences the complexity of the analysis to obtain a convergence result of type (1.29). We distinguish three categories, from easiest to most challenging :

- *Case $\sigma > d/2$.* We need $\alpha \geq \sigma$ and hence also $\alpha > d/2$. In this case we have that $H^\sigma \hookrightarrow L^\infty$, and by using the Kato-Ponce estimate it follows that H^σ forms an algebra: $\|uv\|_{H^\sigma} \leq C_\sigma \|u\|_{H^\sigma} \|v\|_{H^\sigma}$. Both the local error and stability analysis follow easily for a polynomial nonlinearity, and applying Lady Windermere's fan argument allows to conclude global convergence, see Chapter 2.
- *Case $0 \leq \sigma \leq d/2$ and $\alpha > d/2$.* We have $u(t) \in L^\infty$, however the space H^σ does not form an algebra, and hence one needs refined bilinear estimates (see 2.10, 5.14, 5.15). In particular, for the stability of the scheme the following estimate is crucial for bounding the nonlinear terms:

$$\|wz\|_{H^\sigma} \leq C_{\sigma, d} \|w\|_{\frac{d}{2} + \epsilon} \|z\|_{H^\sigma}, \quad 0 \leq \sigma \leq d/2, \quad \epsilon > 0. \quad (1.30)$$

Using a refined global error analysis, one can still push the error analysis down to H^σ through a Lady-Windermere's fan argument, by first proving fractional convergence of the scheme in a suitable higher order Sobolev space. This is presented in Chapters 2 and 5.

- *Case $0 \leq \sigma \leq d/2$ and $0 < \alpha \leq d/2$.* Given that an estimate of the form (1.30) is out of reach in this rough setting, we cannot obtain the global convergence by combining a local error and stability analysis through Lady Windermere's fan argument. As in the theoretical analysis of PDEs at low regularity, in order to consider very rough solutions $u(t) \in H^\alpha$ with $\alpha \leq d/2$, one needs to call upon more refined tools such as Strichartz estimates and Bourgain spaces [Bou93, BGT04, Tao06].

The above cases are particularly relevant when the nonlinearity is a polynomial in u and \bar{u} , such as for the NLS equation (1.2), which is discussed next.

In the following Sections 1.2.1 and 1.2.2, we discuss the state of the art regarding convergence results for the NLS and KdV equations, before introducing new research directions in Section 1.3, which are explored in the rest of the manuscript.

1.2.1 Comparing convergence results for the nonlinear Schrödinger equation

Resonance-based schemes. We expect resonance-based schemes to have the following convergence rates:

Convergence in H^σ at order τ^ν for $u_0 \in H^\alpha$, with $\alpha = \sigma + \nu$ and $\sigma > d/2$.

We refer to [OS18] in the case $0 < \nu \leq 1$, and [OWY22] in the case $\nu = 2$. In these results the analysis is restrained to the torus using Fourier series and the frequency decomposition (1.19).

In the case $0 \leq \sigma \leq d/2$ more regularity assumptions are needed and we refer to the work [AB23a] presented in Chapter 2, which treats the cases $\sigma \geq 0$, $\nu = 1, 2$ and $\alpha > d/2$.

Finally, the authors of [ORS22b] introduce discrete Bourgain spaces allowing them to consider the rough case of $0 < \alpha \leq 1/2$ on the one-dimensional torus \mathbb{T} . They show fractional convergence in L^2 of order τ^ν for $u_0 \in H^\alpha(\mathbb{T})$ with $0 < \alpha \leq 1$ and $\nu < 1$.

When set on the one-dimensional torus \mathbb{T} , several recent results build on the approach of making a decomposition in Fourier space and use the resonance structure (1.16), either for coupling the time integrator with a spectral spatial discretization, or for designing schemes under even lower regularity assumptions, see [WY22, LW21, OY22, CLL23].

Splitting and exponential integrators. In general, the order of convergence of these integrators behaves as follows:

Convergence in H^σ of order τ^ν for $u_0 \in H^\alpha$, with $\alpha = \sigma + 2\nu$ and $\sigma \geq 0$.

In the case $u_0 \in H^\alpha$ with $\alpha > d/2$, we refer to the works of [BBD02, Lub08, Gau11, Fao12, Tha12, ESS16] for convergence of Lie and Strang splitting methods, and to [Duj09, HO10, HLO20] for exponential integrators. In the more subtle case $\alpha \leq d/2$, we refer to [ORS22a] and [JO23], which show fractional rates up to first order with $\sigma = 0$, $\nu = \frac{\alpha}{2}$, and $0 < \alpha \leq 2$, of a filtered version of the Lie splitting method.

Finite difference approximations in time. For an overview on these methods (with a comparison to splitting techniques) we refer to [ABB13]. The convergence of these methods requires at least as much regularity as splitting or exponential methods. For example, second-order convergence of a leap-frog and relaxation type finite difference schemes are obtained in [SS84] and [BDDL21], respectively. They require at least four additional derivatives on the solution, as is the case of exponential and splitting methods.

Type	Reference	Domain	Order ν	Error norm σ	Relation $\frac{\alpha-\sigma}{\nu}$
Resonance based and low-regularity schemes	[OS18]	\mathbb{T}^d	$\in (0, 1]$	$> d/2$	1
	[OWY22]	\mathbb{T}^d	2	$> d/2$	1
	Chapter 2	$\Omega \subset \mathbb{R}^d$	1 & 2	$> d/2$	1
	Chapter 2	$\Omega \subset \mathbb{R}^d$	1 & 2	$\in [0, d/2)$	$1 + (d/2 - \sigma)/2\nu$
Splitting or Exponential Integrators	[BBD02]	\mathbb{R}^2	1 & 2	0	2
	[Lub08]	\mathbb{R}^3	2	0	2
	[Tha12], etc.	\mathbb{R}^d	$\in \mathbb{N}$	0	2
Finite differences	[BDDL21]	\mathbb{R}^d	2	$> d/2$	2

Table 1.1 – Convergence results of the form (1.29) for the NLS equation (1.2). The interplay between the error norm σ , the convergence rate γ , and the regularity assumption α , is expressed by the value of $\frac{\alpha-\sigma}{\nu}$, that is, by the additional regularity requirement per order of convergence.

To give some perspective, we take a step back from the NLS equation and compare the regularity requirements for the approximation to the KdV equation (1.3), which is posed in dimension $d = 1$.

1.2.2 Comparing convergence results for the Korteweg-de Vries equation

Two effects are present in the KdV equation: Burger’s nonlinearity $\partial_x(u^2)$, which set alone forms shocks in finite time, and Airy’s dispersive term ∂_x^3 , whose linear evolution $\partial_t u + \partial_x^3 u = 0$ preserves all Sobolev norms. In the error analysis, the challenge lays in the stability bound due to the derivative appearing in the nonlinearity. Indeed, given that the nonlinearity is not locally Lipschitz, the bilinear estimates of the form (1.30) do not suffice to obtain stability.

Type	Reference	Order ν	Error norm σ	Relation $\frac{\alpha-\sigma}{\nu}$
Resonance based schemes or Fourier integrators	[HS17b]	1	1	2
	[WZ21]	2	≥ 0	2
	[WZ22b]	1	$> 1/2$	1
	[WZ22b]	2	≥ 0	3/2
	[LW22]	$\in (0, 1]$	0	1
Splitting or Exponential Integrators	[RS22]	$\in [0, 1]$	0	3
	[HKRT11]	2	≥ 8	9/2
	[HLR13]	2	≥ 1	5/2
Fully discrete schemes	[CLR20]	$\in [1/14, 1]$	0	$6/\min(1, \nu + 1/2)$
	[OS20]	1	0	3

Table 1.2 – Convergence results of the form (1.29) for the KdV equation (1.3).

Resonance-based schemes: For the KdV equation, mapping Duhamel’s iterate in Fourier space as in (1.15), we obtain

$$R(k) = k_1^3 + k_2^3 - k^3 = -3kk_1k_2, \quad k = k_1 + k_2. \quad (1.31)$$

The first resonance-based scheme was introduced for the KdV equation in the work [HS17b], where the design of first and second order schemes is presented. A convergence analysis using energy estimates allows to show first-order convergence in H^1 for solutions in H^3 , thereby requiring two additional derivatives. Constructing the first-order resonance-based scheme for the KdV equation is simpler than for the NLS equation, as one can integrate exactly all of the resonance structure $R(k)$ into the numerical discretisation, as opposed to the NLS equation, see Remark 1.1.2. On the other hand, the stability analysis, and hence the global error analysis, is more intricate. The authors of [WZ21] offer a convergence result for the second-order resonance based scheme of [HS17b], in the case $\nu = 2$, $\alpha = \sigma + 4$, and $\sigma \geq 0$.

A further improvement on these results is given in [WZ22b] which introduces new first and second order integrators converging in the case $\nu = 1$, $\alpha = \sigma + 1$, $\sigma > 1/2$ and $\nu = 2$, $\alpha = \sigma + 3$, $\sigma \geq 0$, respectively. A first order (unfiltered) integrator requiring even less regularity is then analyzed in [LW22] with $\nu = \alpha$, $0 < \alpha \leq 1$, $\sigma = 0$.

Splitting and exponential integrators: For filtered versions of the Lie splitting and Euler exponential methods the authors of [RS22] shows the following fractional convergence result:

Convergence in H^σ of order τ^ν , for $u_0 \in H^\alpha$, with $\alpha = \sigma + 3\nu$ and $\nu \leq 1$.

For an analysis at second order of the Strang splitting method we cite [HKRT11] and [HLR13], which show convergence in the case $\nu = 2$, $\alpha = \sigma + 5$, $\sigma \geq 1$, under the assumption that the nonlinear part, i.e., Burgers equation $\partial_t u = -\frac{1}{2}\partial_x u^2$, is solved exactly. Applying the same analysis on the Lie splitting method would yield first-order convergence ($\nu = 1$) for $\alpha = \sigma + 3$, coinciding with the result of [RS22].

Fully-discrete schemes when coupled with a finite difference method in space. We refer to [CLR20], where a fully discrete convergence analysis of a finite difference (FD) scheme for the KdV equation with explicit rates up to first order is introduced for the first time. The authors discretize this equation with a Rusanov scheme for the nonlinear part, which corresponds to introducing a linear and explicit diffusion effect. This allows them to handle the derivative in the Burger’s nonlinearity and to show first-order convergence in $L^2(\mathbb{R})$ for $u_0 \in H^6(\mathbb{R})$, together with fractional convergence rates up to first order in the case $\nu \leq 1$, $3/4 \leq \alpha \leq 6$, $\sigma = 0$ (when the dispersive term ∂_x^3 is treated in an implicit manner). They work on the real line \mathbb{R} and obtain convergence rates for non-smooth initial data (down to $\alpha = 3/4$) by making use of the dispersive smoothing effects of the underlying equation on \mathbb{R} .

We also mention the work of [OS20] which couples the space-discretization used in [CLR20], based on the Rusanov correction for the Burgers nonlinearity, with an exponential integrator in time. They show first order convergence of the explicit scheme in L^2 for $u_0 \in H^3$, and with the CFL condition $\tau = O(h)$. We notice that coupling the FD Rusanov discretization in space with an exponential integrator in time ([OS20]) requires less regularity than if a FD time approximation is considered ([CLR20]).

1.3 Branching out in new directions

Following this introduction to resonance-based integrators, many questions remain.

1. **General domains.** The construction of these resonance-based schemes entirely relies on decomposing the solution on its Fourier basis, and thereby on imposing periodic boundary conditions. A first natural question is whether one can generalize the construction of these schemes from the torus \mathbb{T}^d to more general domains, such as smooth bounded domains $\Omega \subset \mathbb{R}^d$ with homogeneous Dirichlet boundary conditions.
2. **Higher order.** Up to now we have only constructed the first order resonance-based scheme (1.22), and discussed results of order at most two. A next question is whether we can push the design up to (arbitrarily) high order.
3. **Unifying approach.** These resonance-based schemes are built on the resonance structure of the underlying equation, see (1.16) for NLS and (1.31) for KdV. Can one build an algorithmic procedure to construct these schemes for a class of equations, such as for the class (1.1), without the need of analyzing one equation at a time?
4. **Structure preservation.** Finally, we are interested in obtaining schemes which exhibit good long-time behavior, preserving – up to a certain extent – the conserved quantities of the equation on the discrete level. The resonance-based scheme (1.22) unfortunately does not have good *structure-preserving* properties. Is it possible to construct schemes at low-regularity which also preserves the geometric structure of the equation?

This manuscript is divided into three parts, that address the above topics.

Part I answers questions regarding topics 1, 2 and 3, by offering in Chapter 3, an algorithmic way to construct higher-order schemes to a class of nonlinear evolution equations (with potentials) set on general domains. This is based on the article [ABBS22b]. This latter work generalizes the construction of the schemes made in the article [AB23a] presented in Chapter 2, which designs and analyses schemes for the Gross-Pitaevskii equation in low-regularity regimes.

Part II pursues in the direction of topics 2 and 3 in a randomized setting, inspired by the works in probabilistic well-posedness and in Wave Turbulence theory. The single work [ABBS22a] is presented in Chapter 4.

Part III focusses on topic 4 and introduces schemes which are advantageous both in non-smooth *and* smooth settings. We first introduce in Chapter 5 the work [AB23b] which presents a novel time integrator for the NLS equation (1.2). The integrator is *symmetric*, provably converges at low-regularity, and exhibits in numerical experiments remarkable long-time near-preservation of the mass and energy, without any CFL type conditions. This chapter also addresses topic 1. We then present the work [ABBMS23] which combines the topics 2, 3, and 4, by generalizing the latter work to the class of dispersive equations (1.1) up to high orders. In numerical simulations, we witness better structure preserving properties of these new symmetric integrators compared to classical splitting schemes, even in the smooth setting of C^∞ -solutions.

We begin with the state of the art regarding Part I of this manuscript, and more specifically topic 1.

1.4 A brief introduction to Part I

1.4.1 Beyond periodic boundary conditions

Our starting point is the work [RS21], which overcomes the necessity of Fourier-based expansions, and hence of periodic boundary conditions, by introducing new filtering techniques and a functional setting based on semi-group theory. The authors introduce a framework allowing for the construction and analysis of first and second order *low-regularity integrators* on more general domains and to the following class of nonlinear evolution equations:

$$\begin{cases} \partial_t u - \mathcal{L}u = f(u, \bar{u}), & (t, x) \in \mathbb{R} \times \Omega, \\ u(0, x) = u_0(x), & x \in \Omega, \end{cases} \quad (1.32)$$

with Ω either equal to the full space \mathbb{R}^d , the torus \mathbb{T}^d , or a smooth bounded domain $\Omega \subset \mathbb{R}^d$. In the case of a smooth bounded domain, the problem is equipped with homogeneous boundary conditions, which are encoded in the choice of the domain of the operator \mathcal{L} . The main assumptions on \mathcal{L} are the following:

- i) \mathcal{L} is a linear operator defined on a Hilbert space X of complex valued functions $u \in \mathbb{C}$;
- ii) \mathcal{L} generates a strongly continuous semigroup $\{e^{t\mathcal{L}}\}_{t \geq 0}$ of contractions on X ;
- iii) $\mathcal{A} = -\mathcal{L} + \bar{\mathcal{L}}$ generates a group $\{e^{t\mathcal{A}}\}_{t \in \mathbb{R}}$ of unitary operators on X ;
- iv) \mathcal{L} and $\bar{\mathcal{L}}$ commute: $[\mathcal{L}, \bar{\mathcal{L}}] = 0$.

Example 4 Admissible operators \mathcal{L} include the heat operator Δ , the Schrödinger operator $i\Delta$, the half wave operator $i|\nabla|$, and the Klein-Gordon and wave type operators $i\sqrt{-\Delta + m^2}$, with mass $m \geq 0$.

In addition, it is assumed that the nonlinearity f is tensorized under the form

$$f(v, w) = \mathcal{B}(F(v) \cdot G(w)), \quad F, G : \mathbb{C} \rightarrow \mathbb{C}^J, \quad (1.33)$$

where \mathcal{B} is a linear operator. It is also assumed that f is locally Lipschitz and maps a ball into itself, as defined for example in equations (5.18).

The class of evolution equations (1.32) encompasses the class of dispersive equations (1.1). Indeed, with the above framework, the authors of [RS21] can deal in a unified way with parabolic, hyperbolic, dispersive as well as mixed type equations. However, an important class of equations is missing, namely equations with a *potential*. The goal of the work [AB23a] presented in Chapter 2, is to close this gap and propose a novel low regularity integrator for the Gross Pitaevskii (GP) equation,

$$i\partial_t u(t, x) = -\Delta u(t, x) + V(x)u(t, x) + |u(t, x)|^2 u(t, x), \quad (t, x) \in \mathbb{R} \times \Omega, \quad (1.34)$$

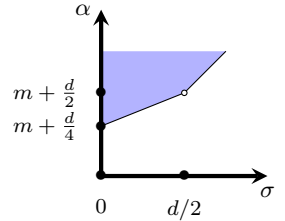
with a non-smooth potential $V(x)$. In this work first and second order integrators are constructed and are proven to converge at integer order $\nu = m \in \{1, 2\}$, under low-regularity assumptions both on the solution $u(t)$ and on the potential V . We denote by $u^n = \Phi_m^\tau(u^{n-1})$ the low-regularity integrators of order m , given at equation (2.5) and (2.7) respectively. Set on the d -dimensional torus \mathbb{T}^d , the convergence result reads as follows:

Theorem 1.4.1 (Theorems 2.1.1 and 2.1.2) *Let $d \in \{1, 2, 3\}$, $\sigma \geq 0$, $T > 0$, $m \in \{1, 2\}$ and*

$$\alpha := \begin{cases} m + \sigma, & \text{if } \sigma > \frac{d}{2}, \\ m + \frac{\sigma}{2} + \frac{d}{4}, & \text{if } 0 \leq \sigma < \frac{d}{2}. \end{cases}$$

For every $u_0 \in H^\alpha$ and $V \in H^\alpha$, there exists $\tau_{\min} > 0$ and $C_T > 0$ such that for every $\tau \leq \tau_{\min}$:

$$\|u(t_n) - u^n\|_{H^\sigma} \leq C_T \tau^m, \quad 0 \leq t_n = n\tau \leq T.$$



For simplicity, the error analysis was made on the torus \mathbb{T}^d . Nevertheless, the tools involved are inspired by the filtering techniques of [RS21], which do not use Fourier-based expansions and hence can be extended to more general domains. We refer to the work [AB23b], presented in Part III of this manuscript, which introduces a functional framework yielding convergence result both on the torus and on smooth bounded domains with homogeneous Dirichlet boundary conditions. Finally, for an explanation on the filtering techniques used, we refer to equation (5.31) and Section 2.3.2.

The work of Chapter 2 motivated the second result of this manuscript, presented in Chapter 3, which generalizes the construction of low-regularity schemes *up to arbitrary order* and for a class of nonlinear evolution equations with potentials.

In the next section we discuss topics 2 and 3, and present the results of Chapter 3.

1.4.2 Higher order approximations

In order to obtain more precise approximations, which are also computationally efficient, one needs to construct higher order methods. Developing such methods requires involved nontrivial calculations, especially when made at low regularity or in high dimensions, and is very laborious when the schemes are constructed one equation at a time.

Based on iterating Duhamel's formula (1.4) once, we constructed in Section 1.1 the *first* order resonance-based integrator (1.22) as well as the Euler exponential method (1.9). In order to obtain higher-order schemes one needs to include the approximation to higher-order Duhamel iterates:

$$\begin{aligned} u(t) &= e^{t\mathcal{L}} u_0 + \int_0^t e^{(t-s_1)\mathcal{L}} p(e^{s_1\mathcal{L}} u_0) ds_1 \\ &+ \int_0^t e^{(t-s_1)\mathcal{L}} \left[p'(e^{s_1\mathcal{L}} u_0) \int_0^{s_1} e^{(s_1-s_2)\mathcal{L}} p(e^{s_2\mathcal{L}} u_0) ds_2 \right] ds_1 + \dots \end{aligned} \quad (1.35)$$

In the above we approximated p at $u(s_j)$ by its Taylor expansion about the linear flow $e^{s_j\mathcal{L}} u_0$, $j \in \mathbb{N}$:

$$p(u(s_j)) = p(e^{s_j\mathcal{L}} u_0) + p'(e^{s_j\mathcal{L}} u_0) \int_0^{s_j} e^{(s_j-s_{j+1})\mathcal{L}} p(e^{s_{j+1}\mathcal{L}} u_0) ds_{j+1} + \dots$$

We note that Taylor expanding $p(u(s_j))$ in the time variable was avoided, as this would require additional regularity on the solution.

We let $r + 1$ be the desired order of the scheme. To obtain a scheme of order $r + 1$, we need to consider the terms in the above formula (1.35) that contain up to $r + 1$ integrals in time, and approximate them suitably.

We start by discussing higher-order approximations to the class of dispersive equations (1.1). For an approximation at low-regularity using resonance-based schemes, the idea is to map the Duhamel iterates into Fourier space. The k -th Fourier coefficient of $u(t)$ is denote by:

$$\begin{aligned} u_k(t) &= e^{tP(k)}u_k(0) + e^{tP(k)} \int_0^t e^{-s_1P(k)} p_k(e^{s_1P(k)}u_k(0)) ds_1 \\ &+ e^{tP(k)} \int_0^t e^{-s_1P(k)} \left[p'_k(e^{s_1P(k)}u_k(0)) e^{s_1P(k)} \int_0^{s_1} e^{-s_2P(k)} p_k(e^{s_2P(k)}u_k(0)) ds_2 \right] ds_1 + \dots \end{aligned} \quad (1.36)$$

where the Fourier multiplier of \mathcal{L} is denoted by $P(k)$. For instance, for the Schrödinger equation we have $\mathcal{L} = i\Delta$ and $P(k) = -ik^2$. With a slight abuse of notation, we denoted by k all of the frequencies in Fourier, instead of k_1, k_2, k_3 , etc.

At higher order, the resonance structure of the iterated integrals becomes very intricate, and it is a complicated task to choose a suitable resonance-based discretization. In the following, we discuss new techniques allowing for higher order constructions.

Decorated trees

We first present the work [BS22], which introduces an algorithmic approach to building resonance-based schemes up to arbitrary order and to the class of dispersive equations (1.1) on the d -dimensional torus. Generally speaking, the work [BS22] develops an algebraic framework – inspired by those in SPDEs via regularity structures [CK99, Hai14] – to systematize a new analytical idea. Namely, they encode the scheme using combinatorial structure called *decorated trees*, allowing to systematize the approximation of the Duhamel iterates. We divide the idea behind the work [BS22] into two steps:

- a.) *On the continuous level.* We encode each of the Duhamel iterates in (1.36) by a decorated tree. In the case of the NLS equation (1.2), we have:

$$\begin{aligned} u_k(t) &= \underbrace{e^{tP(k)}}_{\Pi\left(\begin{array}{c} \textcircled{k} \\ \downarrow \\ \bullet \end{array}\right)(t)} u_k(0) + \underbrace{e^{tP(k)} \int_0^t e^{-s_1P(k)} p_k(e^{s_1P(k)}u_k(0)) ds_1}_{\Pi\left(\begin{array}{c} \textcircled{k} \\ \downarrow \\ \textcircled{k_1} \\ \downarrow \\ \textcircled{k_2} \\ \downarrow \\ \bullet \end{array}\right)(t)} \\ &+ \underbrace{e^{tP(k)} \int_0^t e^{-s_1P(k)} \left[p'_k(e^{s_1P(k)}u_k(0)) e^{s_1P(k)} \int_0^{s_1} e^{-s_2P(k)} p_k(e^{s_2P(k)}u_k(0)) ds_2 \right] ds_1 + \dots}_{\Pi\left(\begin{array}{c} \textcircled{k} \\ \downarrow \\ \textcircled{k_1} \\ \downarrow \\ \textcircled{k_2} \\ \downarrow \\ \textcircled{k_3} \\ \downarrow \\ \bullet \end{array}\right)(t)} \end{aligned}$$

where Π maps *decorated trees* to *Duhamel iterates*. The edges encode the operators in Duhamel's formula. Namely, the brown edge \downarrow encodes the linear flow $e^{tP(k)}$, and the blue edge \downarrow encodes the time integral $\int_0^t e^{-s_1P(k)} \dots ds_1$. A dotted edge corresponds to taking the complex conjugate of the expressions. For example, we have

$$\Pi\left(\begin{array}{c} \textcircled{k} \\ \downarrow \\ \bullet \end{array}\right)(t) = e^{tP(k)}, \quad \Pi\left(\begin{array}{c} \textcircled{k} \\ \downarrow \\ \bullet \end{array}\right)(t) = e^{-tP(k)}.$$

Lastly, the node decoration encodes the frequencies. This approach of encoding Duhamel's iterates in Fourier using decorated trees is also widely used in the theoretical study of dispersive equations. We discuss this further in Section 1.5.

The character Π , called a *pre-model* or *Feynman rule*, separates the algebraic level from the analytical one, and allows to expand the solution as a tree series expansion. We let $r+1$ denote the order of the scheme, and \mathcal{V}_k^r the set of trees of size $r+1$, encoding an iterated integral with up to $r+1$ integrals. We can expand the solution (truncated at order $r+1$) as the following Butcher-type tree series:

$$u_k^r(t) = \sum_{T \in \mathcal{V}_k^r} \frac{\Upsilon^P(T)}{S(T)} \Pi(T)(t), \quad (1.37)$$

where $S(T) \in \mathbb{N}$ is the symmetry factor associated to the tree T , $\Upsilon^P(T)$ is the elementary differential which depends on $u_k(0)$ and encodes the coefficient appearing in the iteration of Duhamel's formulation, and $\Pi(T)(t)$ represents a

Fourier iterated integral. In their article, the authors denote the above expansion (1.37) by $U_k^r(t, u_0)$. Lastly, we give an example of the set \mathcal{V}_k^r : for a first order scheme we fix $r = 0$ and obtain

$$\mathcal{V}_k^0 = \{T_0, T_1\}, \text{ with } T_0 = \begin{array}{c} \circlearrowleft k \\ | \\ \bullet \end{array}, \quad T_1 = \begin{array}{c} \circlearrowleft k_2 \\ | \\ \circlearrowleft k_1 \cdots \circlearrowleft k_3 \\ | \\ \bullet \end{array}. \quad (1.38)$$

The above tree based formalism is inspired by the works of [BCCH20] and [Hai14]. There, this formalism is used to derive a general framework for solving a large class of singular SPDEs in subcritical-regimes, via the theory of Regularity Structures.

- b.) *On the discrete level.* The second step is to approximate each Duhamel integral $\Pi(T)(\tau)$, where τ denotes the time step. The approximation of each Duhamel integral is made using the resonance-based approach detailed previously (see Section 1.1.1). The discretization is automated via a notion of high and lower parts (1.18) dictated by the resonance structure $R(k)$ of the underlying equation. This automatization is led by the approximation operator

$$\Pi^{r,n} : \mathcal{V}_k^r \rightarrow \text{approximate iterated integral},$$

which is a resonance-based approximation of Π . Namely, given a decorated tree T , $\Pi^{r,n}(T)$ is a resonance-based approximation of the iterated integral encoded by the tree T . The index n corresponds to a formal a priori assumption on the regularity required on the initial data, and allows to make simple Taylor expansions when sufficient regularity is assumed. The mapping $\Pi^{r,n}$ expresses in Fourier space the numerical scheme after one time step, denoted by $U_k^{n,r}(\tau)$, as the following tree series:

$$U_k^{n,r}(\tau) = \sum_{T \in \mathcal{V}_k^r} \frac{\Upsilon^p(T)}{S(T)} \Pi^{n,r}(T)(\tau). \quad (1.39)$$

The main theorem of the work [BS22] is the following formal local error expansion, which sums all the the local error made by the approximation of each iterated integral:

$$U_k^{n,r}(\tau) - u_k^r(\tau) = \sum_{T \in \mathcal{V}_k^r} \mathcal{O}_{\|\cdot\|}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T, n) \Upsilon^p(T)), \quad (1.40)$$

where $\mathcal{L}_{\text{low}}^r$ involves all lower order frequency interactions neglected during the resonance-based approximation. The global order of the scheme is $r + 1$, and hence the local error is of order $r + 2$. We now give the author's definition of the big-O notation in (1.40) to express the local error term.

Definition 1.4.1 Let $\Phi^\tau(u_0) = u^1 \approx u(\tau)$ denote the numerical solution at time $t = \tau$. We write

$$u(\tau) - \Phi^\tau(u_0) = \mathcal{O}_{\|\cdot\|}(\tau^m \tilde{\mathcal{L}}u_0) \quad (1.41)$$

if in a suitable norm $\|\cdot\|$, it holds that

$$\|u(\tau) - \Phi^\tau(u_0)\| \leq C(T, d) \tau^m \sup_{0 \leq t \leq \tau} \|q(\tilde{\mathcal{L}}u(t))\|, \quad (1.42)$$

for some polynomial q , differential operator $\tilde{\mathcal{L}}$, and constant C independent of τ .

If (1.41) holds, it is said that the numerical solution u^1 approximates the exact solution $u(t)$ at time $t = \tau$ with a local error of order $\mathcal{O}_{\|\cdot\|}(\tau^m \tilde{\mathcal{L}}u_0)$.

Example 5 (First order scheme for NLS) For the first order low-regularity approximation to the NLS equation, we fix $r = 0$ and $n = 1$ in equation (1.39). The scheme after one time step is given by

$$U_k^{1,0}(\tau) = e^{-i\tau k^2} u_k(0) - i\tau e^{-i\tau k^2} \sum_{k=-k_1+k_2+k_3} \bar{u}_{k_1}(0) u_{k_2}(0) u_{k_3}(0) \varphi_1(2i\tau k_1^2),$$

and coincides with the first order resonance-based scheme (1.22). The only approximation made is on the integral $\Pi(T_1)$, where T_1 is given in (1.38). Moreover, $\mathcal{L}_{\text{low}}^0(T_1, n = 1)$ is given in Fourier by $R_{\text{low}} = -2k_1(k_2 + k_3) + 2k_2k_3$, and can be mapped in physical space to (1.23). In [BS22, Corollary 5.1] the authors write that the local error is of order $\mathcal{O}_{\|\cdot\|}(\tau^2 |\nabla|u)$, meaning that one obtains a local error of order τ^2 in a suitable norm $\|\cdot\|$, if one can bound the term (1.23) in this norm.

The choice of the norm $\|\cdot\|$ dictates the regularity assumptions needed on the solution to obtain global convergence, see Remark 1.4.2. Fixing the regularity index n to one, allows to construct a scheme whose local error only involves differential operators of order one. By taking $n = 2$, one recovers the classical Euler exponential method (1.9), whose local error is of order $\mathcal{O}_{\|\cdot\|}(\tau^2 \Delta u)$, involving differential operators of order two.

Obtaining the formal local error term (1.40) is an important first step towards obtaining convergence of the scheme. However, to obtain a global convergence result, one needs to fix the space and norm $\|\cdot\|$ in which to work with, rigorously bound the local error term in this norm (as in (1.42)) and couple this with a stability argument to conclude. Deducing the global error from the local error is in general non trivial for PDE problems. The two articles [AB23a, AB23b] deal with this rigorous analysis, and are presented in Chapters 2 and 5 respectively.

Remark 1.4.2 (Rigorous regularity assumptions) The choice of norm taken in Definition 1.4.1 is important and determines the regularity needed to bound the local error term (1.42), and hence for the convergence of the scheme. We illustrate this on the first order approximation to the NLS equation, by taking two different choices of norms and quantifying the regularity assumptions thereby required.

When measuring in L^2 -norm: one needs to bound the local error term (1.23) in L^2 , which by using classical Sobolev embedding require $u_0 \in H^{1+\frac{d}{4}}$. Indeed, for each of the terms in (1.23), we have that for $d \leq 3$:

$$\|u \nabla u \cdot \nabla u\|_{L^2} \leq C_d \|u\|_{L^\infty} \|\nabla u\|_{L^4}^2 \leq C_d \|u\|_{H^{\frac{d}{2}+\epsilon}} \|\nabla u\|_{H^{\frac{d}{4}}}^2 \leq C_d \|u\|_{H^{1+\frac{d}{4}}}^3,$$

where we used the Sobolev embeddings $H^{\frac{d}{4}} \hookrightarrow L^4$ and $H^\sigma \hookrightarrow L^\infty$, $\sigma > d/2$.

We make the important point that even though the formal local error term in [BS22, Corollary 5.1] reads $\mathcal{O}_{\|\cdot\|}(\tau^2 |\nabla| u)$, one cannot bound this local error term in L^2 while only asking for H^1 -solutions. This is due to the polynomial q appearing in (1.42).

When measuring in H^σ , $\sigma > d/2$: using the fact that the space is an algebra we can bound the local error term (1.23) for $u_0 \in H^{\sigma+1}$:

$$\|u \nabla u \cdot \nabla u\|_{H^\sigma} \leq C_d \|u\|_{H^\sigma} \|\nabla u\|_{H^\sigma}^2 \leq C_d \|u\|_{H^{\sigma+1}}^3.$$

This analysis is made more generally in H^σ -norm for $\sigma \geq 0$ in Chapter 2, where first and second order convergence results are obtained.

We finish by discussing a limitation of the work [BS22]. Given that their algorithm heavily relies on expansions made in Fourier space, the method is restricted to spatial domains which are periodic and to dispersive equations with polynomial nonlinearities. We overcome this limitation in the work [ABBS22b], presented next. We introduce a nested commutator structure to pull out the oscillatory phases, which replaces and generalizes the Fourier-based constructions. This work extends the tools presented in Section 1.4.1 to higher-order.

Introducing Chapter 3

In this chapter, we use an algebraic framework, to systematically derive low-regularity integrators on the general domains of Section 1.4.1. We consider the approximation, up to arbitrary order, to the following class of evolution equations:

$$\begin{cases} \partial_t u(t, x) - \mathcal{L}u(t, x) = \sum_l f_l(u(t, x), \bar{u}(t, x)) V_l(x), & (t, x) \in \mathbb{R} \times \Omega, \Omega \subseteq \mathbb{R}^d, \\ u(0, x) = u_0(x). \end{cases} \quad (1.43)$$

Here, \mathcal{L} and f_l satisfy the same hypotheses as \mathcal{L} and f in equation (1.32) of Section 1.4.1. We recognize the GP equation (1.34) in the case where $V_0 = 1, V_1 = V, f_0(u, \bar{u}) = \bar{u}u^2, f_1(u, \bar{u}) = u$. The above class of evolution equations is more general than both (1.1) and (1.32).

In order to obtain higher-order approximations we consider the Duhamel's iterates (1.35) where we replace the nonlinearity $p(u)$ by $\sum_l f_l(u, \bar{u}) V_l$. We obtain a scheme by discretizing each iterated integral, as detailed below.

- a.) *On the continuous level.* This time we encode by decorated trees the Duhamel iterates (1.35) in the physical variables. We generalize the decorated trees in [BS22] which relied on Fourier-based expansions, to consider more general domains and equations. We let the brown edge encode the integral of the linear flow :

$$\int_0^t e^{(t-s)\mathcal{L}} \dots ds = \text{brown edge}.$$

Each node of the tree encodes a term in the nonlinearity, and the decoration on the l -th node encodes the potential V_l (and possible monomials). For example, for the GP equation there are two nodes corresponding to the two nonlinear terms ($f_l, l = \{0, 1\}$):

$$\circ \equiv (e^{is\Delta} u_0^2)(e^{-is\Delta} \bar{u}_0), \quad \bullet \equiv (e^{is\Delta} u_0)V.$$

Incoming edges to a node induce derivatives on f_t , allowing to encode Duhamel iterates with more than one integral in time. This allows to iteratively define a set of trees \mathcal{T}^r encoding – through the mapping Π – each Duhamel iterate consisting of $r + 1$ integrals in time. We can thus express $u(t)$ truncated at order $r + 1$, as the tree series expansion:

$$u^r(t) = e^{t\mathcal{L}}u_0 + \sum_{T \in \mathcal{T}^r} \Pi(T)(t).$$

We note that the symmetry factor $S(T)$ and elementary differential $\Upsilon^p(T)$ previously appearing in (1.37), are directly included in $\Pi(T)$, see Remark 3.3.1.

- b.) *On the discrete level.* We define a new operator Π_A^r mapping a decorated tree in \mathcal{T}^r to an *approximate Duhamel iterate*. The map Π_A^r is a discretized version of Π . The desired order of the scheme is $r + 1$ and A is a given domain of regularity of u_0 and $(V_t)_t$, reflecting the a priori regularity assumed on the initial data and the potentials. The role of A was played by the index n in the periodic setting, see (1.39). The operator Π_A^r discretizes the Duhamel iterates at low-regularity by filtering out the dominant parts, integrating them exactly, and approximating the lower order parts through commutator based expansions. The numerical scheme U_A^r , after one time step, is given by:

$$U_A^r(\tau) = e^{\tau\mathcal{L}}u_0 + \sum_{T \in \mathcal{T}^r} \Pi_A^r(T)(\tau),$$

For the sake of clarity, we have not included in the above discussion a technical preliminary step, which extracts the linear flow $e^{t\mathcal{L}}u_0$ from inside the nonlinearity $p(e^{t\mathcal{L}}u_0)$. This step gives a unified form of the Duhamel iterates, allowing to encode them using decorated trees, see Section 3.4. A comparison between the decorated trees used in [BS22] and those from the present work is given in Remark 3.2.4.

The main theorem is a formal local error expansion, measuring the error made when approximating each Duhamel iterate over one time step.

Theorem 1.4.2 (*Theorem 3.4.3 in a simplified notation*)

$$U_A^r(\tau) - u^r(\tau) = \sum_{T \in \mathcal{T}^r} \mathcal{O}_{\|\cdot\|}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T, A))$$

where the operator $\mathcal{L}_{\text{low}}^r(T, A)$, embeds the necessary regularity on the solution.

The above accounts for the local error made by the approximation in step b. In the end, we need to sum the above error terms with the error from the truncation made in step a. If the nonlinearity considered does not involve derivatives, step b is the dominant one and dictates the needed regularity, for a discussion on the subject see Remark 1.5.1.

We stress the fact that these higher-order techniques only guarantee a formal local error bound as above, where the big-O notation is to be understood in the sense of Definition 1.4.1. In order to obtain convergence of the scheme, a separate and careful analysis needs to be made: first for estimating the local error in an appropriate functional space, and secondly to obtain stability of the scheme.

For an example of this algorithmic approach, we refer to Section 3.5.1 where classical and low-regularity first and second order integrators for the GP equation are obtained, together with their formal local error expansion. To obtain a rigorous convergence result of these schemes, we once again refer to the results of Chapter 2.

We finish this section with a short historic note. The idea of using a tree-series based expansions to express the numerical scheme was heavily studied in the context of ODEs in the 70s by the pioneering works of [But72, HW74]. More precisely, it was used for the characterization of Runge-Kutta methods via Butcher series (B-series), see the reviews [But16, HLW10]. The algebraic framework used at this time was a foundation first for Gubinelli's approach to Rough Path Theory [Gub04, Gub10], and afterwards to Hairer's theory of regularity structures [Hai14], a generalization of Rough Paths. Nowadays, these ideas are making their way back to the study of numerical schemes, but for PDEs instead of ODEs.

1.5 A brief introduction to Part II

In the previous Section 1.4.2 we discussed the design to higher order of new families of numerical schemes for *deterministic* PDEs, suited for *low-regularity* initial data. Typical examples of low regularity functions are given by realizations of random fields. In the work [ABBS22a] presented in Chapter 4, we enter a probabilistic setting by considering a randomized initial condition:

$$u(0, x) = v^\eta(x) = \sum_{k \in \mathbf{Z}^d} c_k \eta_k e^{ikx}, \quad (1.44)$$

where the η_k are independent standard complex Gaussian random variables. The above expression is a Gaussian randomization of a deterministic function $\sum_k c_k e^{ikx}$. The choice of how one measures the numerical discretization in a stochastic setting can take a probabilistic form and be formulated in different ways. In Chapter 4, we choose to quantify the convergence rate of approximations of the second moment $\mathbb{E}(|u_k(t, v^n)|^2)$ of the k -th Fourier coefficient u_k of the solution u to the class of dispersive equations (1.1). We construct approximations of arbitrarily high order to the second moment $\mathbb{E}(|u_k(t, v^n)|^2)$, based upon the tree series expansions discussed in Section 1.4.2. Working with gaussian random variables and integer moments of polynomial nonlinearities of these random variables is a crucial choice that allows us to use Wick formulas and their rich algebraic structure to set up the framework. We now outline the main steps involved in Chapter 4.

Following equation (1.37), one can express the time continuous solution, truncated at order $r + 1$, as a tree series expansion:

$$u_k^r(\tau, v^n) = e^{tP(k)} \eta_k c_k + e^{tP(k)} \int_0^\tau e^{-s_1 P(k)} p_k(e^{s_1 P(k)} \eta_k c_k) ds_1 + \dots = \sum_{T \in \mathcal{V}_k^r} \frac{\Upsilon^p(T)}{S(T)} \Pi(T)(\tau),$$

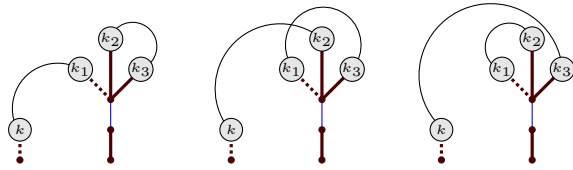
where we have taken $t = \tau$, the time step. We can thus make a first approximation, with local error in $O(\tau^{r+2})$, of the second moment $\mathbb{E}(|u_k(\tau, v^n)|^2)$ using the truncated solution u_k^r :

$$\mathbb{E}(|u_k(\tau, v^n)|^2) \approx \mathcal{Q}_{\leq r+1} \mathbb{E}(|u_k^r(\tau, v^n)|^2), \quad (1.45)$$

where $\mathcal{Q}_{\leq r+1}$ keeps only the terms of order at most $r + 1$, i.e. in $O(\tau^m)$, with $m \leq r + 1$. When computing the product $|u_k^r(\tau, v^n)|^2$, a number of terms involve products of an odd number of noise variables, that have null expectation. The other terms are even polynomials in the noise variables, whose expectation is described by Wick's formula, which states that for centered gaussian variables the expectation of the product of an even number of gaussians is given by the product of the expectations of their two-by-two product, summed over all possible pairings. For example, if u satisfies the NLS equation (1.2), one term we would want to approximate is the expectation $\mathbb{E}(\overline{\Upsilon^p(T_0)} \Pi(T_0) \Upsilon^p(T_1) \Pi(T_1))$, where T_0 and T_1 correspond to the terms of order zero and one in Duhamel's formula, see (1.38). Given that the trees T_0 and T_1 have in total four leaves, the expectation contains terms of the form:

$$\begin{aligned} \mathbb{E}(\overline{\eta_k \eta_{k_1} \eta_{k_2} \eta_{k_3}}) &= \mathbb{E}(\overline{\eta_k \eta_{k_1}}) \mathbb{E}(\eta_{k_2} \eta_{k_3}) + \mathbb{E}(\overline{\eta_k \eta_{k_2}}) \mathbb{E}(\eta_{k_1} \eta_{k_3}) + \mathbb{E}(\overline{\eta_k \eta_{k_3}}) \mathbb{E}(\eta_{k_1} \eta_{k_2}) \\ &= \delta_{k, -k_1} \delta_{k_2, -k_3} + \delta_{k, k_2} \delta_{k_1, k_3} + \delta_{k, k_3} \delta_{k_1, k_2}. \end{aligned}$$

The first line in the above uses Wick's formula, while the second line exploits the properties of the random variables $(\eta_k)_k$. We see that the above yields a nontrivial value under the following conditions on the frequencies: $(k, k_2) = (-k_1, -k_3)$ or $(k, k_1) = (k_2, k_3)$ or $(k, k_1) = (k_3, k_2)$. We can capture these conditions diagrammatically through Feynman-type diagrams:



We see that computing the expectation amounts, through Wick's formula, to pairing the leaves of the trees. We introduce for this purpose a new combinatorial structure called *paired decorated forests*, which are composed of two decorated trees whose decorations on the leaves come in pair. The expansion for $\mathbb{E}(|u_k(t, v^n)|^2)$, following the first approximation (1.45), can then be rewritten in terms of these paired decorated forests:

$$\mathbb{E}(|u_k(\tau, v^n)|^2) \approx \mathcal{Q}_{\leq r+1} \mathbb{E}(|u_k^r(\tau, v^n)|^2) = \sum_{T_1 \cdot T_2 \in \mathcal{G}_k^r} \frac{\overline{\Upsilon^p(T_1)} \Upsilon^p(T_2)}{S(T_1) S(T_2)} \overline{\Pi}(T_1)(\tau) \Pi(T_2)(\tau).$$

The set \mathcal{G}_k^r consists of all paired forests $F = T_1 \cdot T_2$ whose encoding as Duhamel iterates $\overline{\Pi}(T_1)(\tau) \Pi(T_2)(\tau)$ contains at most $r + 1$ integrals in time.

As discussed in steps b.) of Section 1.4.2, by replacing the continuous mapping Π by a discrete analogue $\Pi^{n,r}$ we obtain a tree-series expansion of our numerical approximation after one time step, which we denote by $V_k^{n,r}(\tau)$:

$$V_k^{n,r}(\tau) = \sum_{F = T_1 \cdot T_2 \in \mathcal{G}_k^r} \frac{\overline{\Upsilon^p(T_1)} \Upsilon^p(T_2)}{S(T_1) S(T_2)} \mathcal{Q}_{\leq r+1} (\overline{\Pi}^{n,r} T_1 \Pi^{n,r} T_2)(\tau). \quad (1.46)$$

The operator $\Pi^{n,r}$ is the same as the one used in the expansion (1.39) and allows for a resonance-based approximation to the Duhamel iterates. Together with the design (1.46) of higher-order approximation to the second moment $V_k(\tau) = \mathbb{E}(|u_k(\tau, v^\eta)|^2)$, we derive the following formal local error:

$$V_k^{n,r}(\tau) - V_k(\tau) = \sum_{T_1 \cdot T_2 \in \mathcal{G}_k^r} \mathcal{O}_{\|\cdot\|}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n) \tilde{\Upsilon}^p(T_1) \Upsilon^p(T_2)), \quad (1.47)$$

where the operator $\mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n)$ embeds the necessary regularity on the solution.

Remark 1.5.1 (An additional term in the local error) We note that the above equation (1.47) takes into account the second approximation step (1.46), by summing up the local errors made by $\Pi^{n,r}$ to Π , during the resonance-based approximation to each Duhamel iterate. The first approximation step made at equation (1.45) can also require additional regularity on the initial data. In most cases, the second approximation step made by $\Pi^{n,r}$ requires the most regularity. This is however not the case for instance for the KdV equation (1.3), where the leading error term stems from the first approximation (1.45). In this case one needs to look at the general form of the local error, by taking into account both approximation steps as follows:

$$\begin{aligned} V_k^{n,r}(\tau) - V_k(\tau) = & \sum_{T_1 \cdot T_2 \in \mathcal{G}_k^r} \mathcal{O}_{\|\cdot\|}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n) \tilde{\Upsilon}^p(T_1) \Upsilon^p(T_2)) \\ & + \mathcal{O}_{\|\cdot\|}(\tau^{r+2} |\nabla|^{\alpha(r+2)}(k) \mathbb{E}(\tilde{p}_k(u(t), v^\eta))), \end{aligned}$$

for some polynomial \tilde{p} . We refer to the proof of Theorem 4.4.3 for details.

While the derivation of the formal local error term (1.47) is a first important step, the next step is to rigorously prove convergence of the method through global error bounds. Contrary to the deterministic setting, no convergence results have been obtained in the probabilistic setting (1.44) with i.i.d. gaussian random initial conditions. In the theoretical analysis of PDEs, many interesting results have been established in this probabilistic setting in the last decade, see for instance [CO12, NS15] for NLS type equations, [BT08] for the cubic wave equation, [Bri20] for the derivative nonlinear wave equation, [NPS13] for the periodic Navier-Stokes equations, and more generally [BOP19] for a survey on recent developments in *probabilistic Cauchy theory*. These papers study nonlinear PDEs with random initial data in singular regimes, and establish probabilistic well-posedness results at much lower regularity regimes than what can be attained in the deterministic setting, reaching down to scaling-supercritical regularities. A question of personal interest for the future is whether one can devise discrete counterparts to these probabilistic PDE techniques to obtain improved convergence results.

Finally, this numerical probabilistic work uses tools which are similar to the ones used in the theory of *wave turbulence* for the rigorous derivation of wave kinetic equations, where the quantity $\mathbb{E}(|u_k(t, v^\eta)|^2)$ plays an important role. These recent works in wave turbulence theory also use decorated trees and construct Feynman diagrams through Wick's formula to express the second moment $\mathbb{E}(|u_k(t, v^\eta)|^2)$ as a tree series expansion. We refer for instance to [BGHS21, ACG21, DH23, DNY22, LS11] in the context of NLSEs and to [HRST22, ST21] for KdV-type systems. This active field has numerous applications in physics and applied sciences (e.g. oceanography and atmospheric sciences) and seeks a statistical description of the out-of-equilibrium dynamics of equations, ranging from the NLSE to water waves or Vlasov-Maxwell, see [ZF67]. The fundamental equation of wave turbulence theory, called the wave kinetic equation or the Kolmogorov-Zakharov equation, is used on a daily basis for wave forecasting.

The author would like to mention that the main motivation in considering the randomized initial condition (1.44) and the approximation to the second moment $\mathbb{E}(|u_k(t, v^\eta)|^2)$, came from listening to talks at a semester workshop at the ICERM and through the Simons Collaboration on Wave Turbulence, regrouping in part the *probabilistic Cauchy theory* and *wave turbulence theory* communities.

1.6 A brief introduction to Part III

Algorithms preserving the structure of the underlying equation constitute an important part of computational mathematics, see [HLW10, Fao12]. However, in general they heavily rely on highly regular solutions. For instance, for the NLS equation (1.2), we mentioned in Section 1.2.1 finite difference schemes [Bes04, BDDL21, SS84] which preserve the mass and energy, as well as the Strang splitting methods [Lub08, BBD02] which preserves the mass and nearly preserves the energy, see Remark 1.6.1. Yet, all of these schemes require at least H^4 solutions for second order convergence in L^2 .

The goal of Part III is to extend the novel nonlinear approach and low-regularity approximation techniques presented in Part I, to the construction of symmetric schemes for dispersive equations. The schemes we obtain show very good long-time behavior in numerical experiments both in the smooth and non-smooth setting. Surprisingly, even in the smooth setting, our schemes surpass the long time energy preservation properties of classical splitting methods.

1.6.1 A symmetric scheme for the nonlinear Schrödinger equation, suited for non-smooth solutions

We start by presenting the work [AB23b] on the NLS equation (1.2) contained in Chapter 5. The NLS equation is time reversible, meaning that $u(-t, x)$ is again solution of (1.2), and preserves the mass

$$\|u(t)\|_{L^2}^2 = \int |u(t, x)|^2 dx = \|u_0\|_{L^2}^2$$

and the energy

$$E(t) = \frac{1}{2} \int |\nabla u(t, x)|^2 dx + \frac{1}{4} \int |u(t, x)|^4 dx = E(0)$$

of the solution over its interval of existence in time.

Part III builds on the observation that low regularity schemes discussed in earlier sections do not preserve the invariants of the underlying equation, such as the mass and energy for the NLS equation, see Figures 5.2 and 5.3. In Chapter 5, we construct and rigorously analyze a novel scheme with strong geometric structure at low regularity, allowing for a reliable symmetric approximation to the NLS equation. Namely, the scheme preserves the time-reversibility of the equation and numerical simulations show good near-preservation of the mass and energy over long times. Moreover, we witness experimentally that the new symmetric low-regularity scheme has better long time near-preservation of the energy than classical splitting schemes. We refer to Figure 1.2 where we plot the error in the energy over time, first for a smooth initial condition $u_0 \in C^\infty$, then in the case of a rougher initial condition $u_0 \in H^2$. We notice that the first order resonance-based scheme (blue) does not preserve the energy, even over short times. In Figure 1.2a the Lie and Strang splitting (pink and green) approximatively preserves the energy up until a point ($t \sim 30$), while in the rougher case of Figure 1.2b, the energy explodes after much shorter times. This behavior is rigorously studied in the work of [Fao12] where the author shows that a CFL condition is necessary to guarantee long-time approximate energy preservation for splitting methods, see also Remark 1.6.1. Namely, if we fix the time step τ and increase the highest Fourier frequency K , thereby going from an ODE to the (desired) PDE setting, the energy ceases to be preserved at some point. In comparison, the new symmetric low-regularity scheme (yellow triangle) does not suffer from a comparable CFL condition, and performs well for both smooth and low-regularity solutions. We refer to Figures 6.5a and 6.6a for simulations over longer times ($t = 4000$).

Remark 1.6.1 (Near energy preservation of splitting methods for the NLS equation under a CFL condition)

Splitting methods preserve the symplectic structure and L^2 norm of the solution, however they do not preserve exactly the energy on the discrete level. Indeed, under suitable assumptions, the numerical approximation can be shown to solve (almost) exactly a *modified* PDE at each time step. This results in the existence of a *modified* energy which is preserved along the numerical flow, where – among other assumptions – for smooth solutions and under a CFL condition, it can be shown that the modified energy is close to the exact energy. More specifically, the CFL condition imposes that the time step size τ has to be chosen such that $\tau \lesssim K^{-2}$ where K denotes the highest frequency in the discretization, see [Fao12]. This step size restriction is not only a theoretical technicality, but also observed in numerical experiments, see Figure 1.2. We also refer to a number of important works where the near-preservation of the energy over exponentially long times is shown using modulated Fourier expansions (see [CHL08, GL10b, GL10a]) or normal form techniques ([FGP10a, FGP10b, FG11]).

We now portray the idea behind the construction of this symmetric scheme. We recall that a scheme is said to be *symmetric* or *time reversible* if it remains unchanged under the transformations $\tau \rightarrow -\tau$ and $n \leftrightarrow n + 1$.

We once again start from Duhamel's integral mapped in Fourier space (1.15), whose integrand is decomposed in (1.17) into the three factors: $e^{isR_{\text{dom}}(k)} e^{isR_{\text{low}}(k)} g(s)$, with $R(k) = R_{\text{dom}}(k) + R_{\text{low}}(k)$ given in (1.18). To construct the first-order resonance-based scheme (1.22) we simply Taylor expanded both $g(s)$ and $e^{isR_{\text{low}}(k)}$ about the left end point: $e^{isR_{\text{low}}(k)} g(s) \approx g(0)$. This however breaks the symmetric structure of the underlying PDE and leads to schemes which are not structure preserving. We thus look for a symmetric approximation of both the non-oscillatory $g(s)$ and lower part $e^{isR_{\text{low}}(k)}$. In Chapter 5 we choose the following symmetric approximation: $h(s) \approx h(0)\mathbb{1}_{[0, \tau/2]} + h(\tau)\mathbb{1}_{(\tau/2, \tau]}$, which in our context yields

$$I_\tau = \int_0^\tau e^{isR_{\text{dom}}(k)} \underbrace{e^{isR_{\text{low}}(k)} g(s)}_{\approx g(0)\mathbb{1}_{[0, \tau/2]} + e^{i\tau R_{\text{low}}(k)} g(\tau)\mathbb{1}_{(\tau/2, \tau]}} ds. \quad (1.48)$$

By integrating exactly the dominant part $e^{isR_{\text{dom}}(k)}$, mapping back to physical space and in the untwisted variable, we obtain the symmetric scheme:

$$u^{n+1} = \Phi_{-\tau/2}^{-1} \circ \Phi_{\tau/2}(u^n) = e^{i\tau\Delta} u^n - i\frac{\tau}{2} e^{i\tau\Delta} ((u^n)^2 \varphi_1(-i\tau\Delta) \bar{u}^n) - i\frac{\tau}{2} ((u^{n+1})^2 \varphi_1(i\tau\Delta) \overline{u^{n+1}}), \quad (1.49)$$

where Φ_τ is the first order resonance-based scheme (1.22) constructed in the introduction. In fact, the symmetric approximation (1.48) is chosen because it coincides with the symmetrization of the first order resonance-based scheme Φ_τ . For other choices of symmetric approximations, we refer to Section 1.6.2 and to Chapter 6.

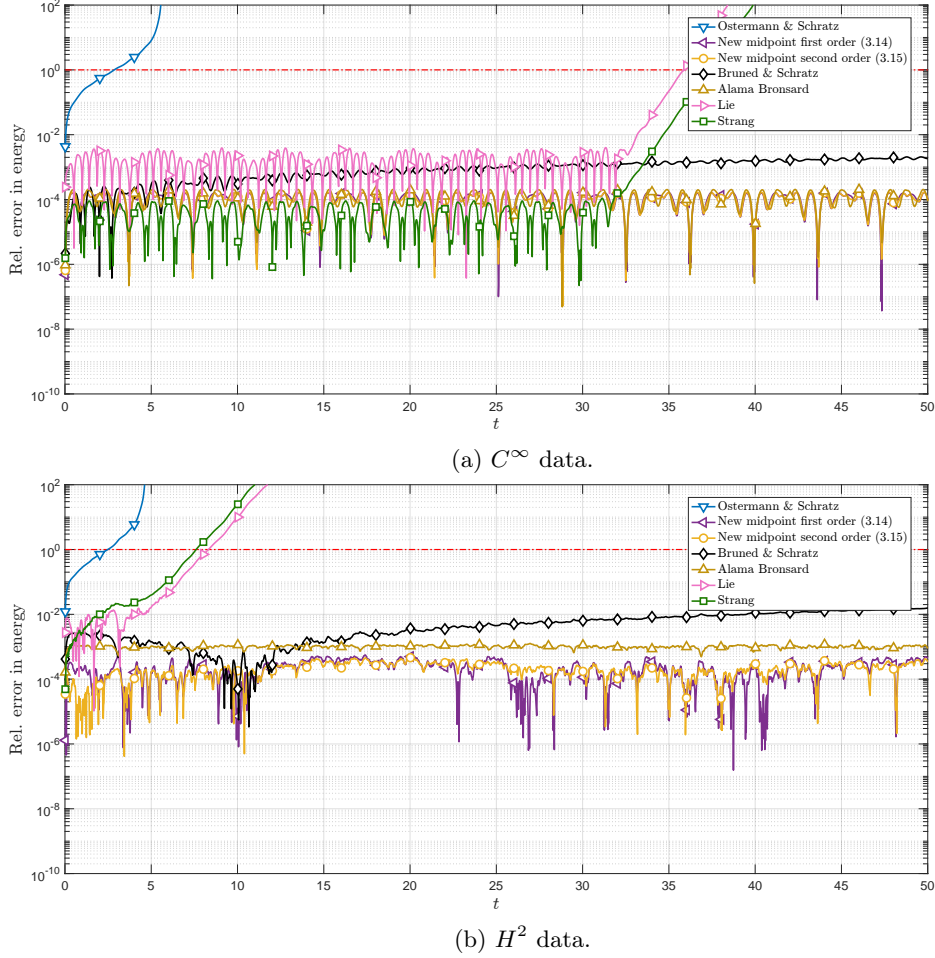


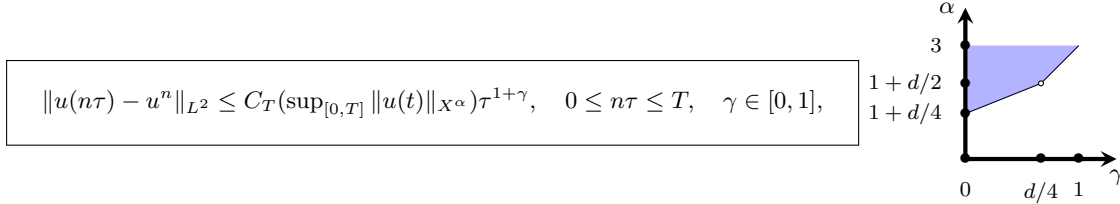
Figure 1.2 – Error in the Hamiltonian for smooth and non-smooth initial data with $t = n\tau \in [0, 50]$, $\tau = 0.02$ and $K = 1024$. The plots are taken from the work [ABBMS23], see Section 6.5.2 for further numerical experiments.

A notable difference between this symmetric scheme and previous low-regularity schemes is its *implicit* nature. We refer to Figure 5.4 which shows that the computational cost of the symmetric scheme is comparable to that of the asymmetric second order resonance-based scheme. Namely, its improved convergence properties make up for the extra cost of solving the implicit system (1.49) at each time step.

A desired property of symmetric schemes is that they are of *even order*. This however is only true under sufficient regularity assumptions of the solution. Chapter 5 focuses on obtaining the minimal regularity assumptions needed for convergence of the scheme from first to second order. The error analysis presented is suited both for periodic domains $\Omega = \mathbb{T}^d$ and smooth bounded domains $\Omega \subset \mathbb{R}^d$ with homogeneous Dirichlet boundary conditions. We choose to work in the fractional space

$$X^\sigma(\Omega) = \mathcal{D}((-\Delta)^{\sigma/2}), \quad \|u\|_{X^\sigma}^2 = \|u\|_{L^2}^2 + \|(-\Delta)^{\sigma/2} u\|_{L^2}^2.$$

In particular $X^\sigma(\mathbb{T}^d) = H^\sigma(\mathbb{T}^d)$, and in the more subtle case of a smooth bounded domain, the space $X^\sigma(\Omega)$ embeds both the regularity and the necessary boundary conditions. In this case, one is lead to characterize domains of fractional powers of the Dirichlet Laplacian, via complex interpolation spaces, see Section 5.2. We obtain the following convergence result:



where the regularity α is minimized through well-chosen bilinear estimates. The admissible values of α and γ are represented by the blue zone on the above right picture. The detailed theorems are given in Section 5.1.2, and the bilinear estimates in Section 5.2.2. We refer to Figure 1.1 where convergence plots are made for H^1 and H^2 initial data. We observe that the symmetric scheme (yellow) has a better error constant than the previous resonance-based schemes (light and dark blue), the exponential integrator (purple), and the Lie splitting method (pink).

We give a brief overview of current *local in time* results that build new bridges between structure preserving methods and low-regularity approaches. In [WY22], a first-order Fourier integrator is introduced for the NLS equation (1.2) set on the 1-dimensional torus \mathbb{T} , which almost conserves the mass. For the cubic Klein-Gordon equation set on \mathbb{T} , an explicit symmetric three time-step low-regularity integrator was obtained by [WZ22a], using Gautschi-type methods. The authors of [MS23] introduce a framework for building novel symplectic resonance-based integrators, encompassing both the KdV equation and the 1-dimensional NLS equation. A symmetrized resonance-based integrator for the Schrödinger map (SM) is obtained in [BMS22], where they relate the SM flow to the NLS equation set on 1- d torus \mathbb{T} via the Hasimoto transform. Finally, the recent work [BW23a] establishes a second-order explicit and symmetric three-time step method for the GP equation (1.34) with a low-regularity potential V , using Gautschi-type exponential wave integrators.

Remark 1.6.2 (From short to long time scales) All of these convergence results allow to rigorously prove the reliability of a numerical discretization over short times $[0, T]$, as the error constant C_T usually depends exponentially on the final time T . Pushing the analysis to obtain error estimates over longer times, or even *uniformly in time*, is thus a highly nontrivial problem.

A first step was made by the authors of [CS22b]. Using scattering theory in order to obtain quantitative time decay estimates, they show uniform in time error estimates for the NLS equation on the full space \mathbb{R}^d , for a Lie splitting discretization. Their convergence analysis is, however, limited to \mathbb{R}^d as it heavily relies on dispersive effects, which do not hold on the torus \mathbb{T}^d or more generally on compact domains. The step from the full space to the compact setting is – as in the continuous setting – nontrivial since in the latter dispersion does not translate into decay. Nevertheless, compact domains are computationally very interesting as spatial discretizations of nonlinear PDEs are in general performed in truncated domains. Hence, obtaining results uniformly in time which can also be implemented on the discrete level is a very interesting open problem.

To prove well-posedness on the theoretical level, a common approach is to either start by showing LWP over a *small* time-interval $[0, T]$, or global well-posedness with *small* initial data $\|u_0\| < \epsilon$. On the numerical level, we have previously discussed the first case; the second case is explored at low-regularity in [FMS23].

The work of Chapter 5 initiated the fruitful collaboration [ABBMS23] presented in Chapter 6, which we discuss next.

1.6.2 Symmetric higher-order extensions

Chapter 6 extends the construction of the symmetric low-regularity integrator (1.49) to higher order and for the class of dispersive equations (1.1), when set on the torus \mathbb{T}^d .

We first recall Duhamel’s formula (1.4), which, in the twisted variables (1.11) and mapped in Fourier, corresponds to

$$v_k(t) = v_k(0) + \int_0^t e^{-s_1 P(k)} p_k \left(e^{s_1 P(k)} v_k(s_1) \right) ds_1. \quad (1.50)$$

Previously, to obtain higher-order schemes we iterated Duhamel’s formula about the linear flow $e^{s_j \mathcal{L}} u_0$, yielding (1.35) and (1.36) in Fourier space. In the twisted variable, this amounts to iterating the above equation (1.50) about the left-end point $v_k(0)$. Namely, we substitute $v_k(s_1) = v_k(0) + \int_0^{s_1} \dots ds_2$ in the above equation, then use a Taylor expansion in p_k about $e^{s_1 P(k)} v_k(0)$.

In the previous Section 1.6.1, we saw that making this asymmetric approximation about the left end point $v_k(s) \approx v_k(0)$ (or equivalently $g(s) \approx g(0)$ in (1.48)) leads to schemes which are *not structure preserving*. The solution we propose is to make a symmetric approximation of the non-oscillatory part $g(s)$ (and hence $v_k(s)$), such as the approximation $v_k(s) \approx v_k(0) \mathbb{1}_{[0, \tau/2]} + v_k(\tau) \mathbb{1}_{(\tau/2, \tau]}$, which puts equal weights on both end points $s = 0$ and $s = \tau$. Hence, the first step towards obtaining higher order symmetric schemes is to iterate Duhamel’s formula in $v_k(s_j)$ in a symmetric fashion, by

putting equal weights on Duhamel's formulas centered about 0 and τ :

$$\begin{aligned} v_k(s_j) &= v_k(0) + \int_0^{s_j} e^{-s_{j+1}P(k)} p_k \left(e^{s_{j+1}P(k)} v_k(s_{j+1}) \right) ds_{j+1}, \\ v_k(s_j) &= v_k(\tau) + \int_{s_j}^{\tau} e^{-s_{j+1}P(k)} p_k \left(e^{s_{j+1}P(k)} v_k(s_{j+1}) \right) ds_{j+1}. \end{aligned}$$

In Chapter 6, we first take the mid-point rule as our symmetric approximation:

$$v_k(s_j) = \frac{v_k(0) + v_k(\tau)}{2} + O(\tau), \quad s_j \in [0, \tau]. \quad (1.51)$$

We let $r + 1$ denote the order of the scheme. We iterate the above equation (1.51) inside Duhamel's formula (1.50) and obtain an expansion of the continuous solution (written in the untwisted variables) and up to order $r + 1$ as a tree series

$$u_{\text{mid},k}^r(t) = \sum_{T \in \mathcal{V}_k^r} \frac{\Upsilon_{\text{mid}}^p(T)}{S(T)} \Pi_{\text{mid}}(T)(t). \quad (1.52)$$

The above series is of the same form as the tree-series expansion (1.37), the only difference lies in the definition of the character Π and coefficient Υ^p . Here, we encode the symmetric iterations of Duhamel's formula in Π_{mid} and Υ_{mid}^p , whereas Π and Υ^p encoded Duhamel's iterates centered about zero (see (1.36) or (1.50)). Note that in Chapter 6 everything is directly written in the untwisted variables. It is however much more intuitive to start by working in the twisted variables, and to make the decomposition (1.15) and (1.17), as presented above.

The next step is to discretize at low-regularity each Duhamel iterate $\Pi_{\text{mid}}(T)(\tau)$ in a symmetric fashion. This is to be compared with Section 1.6.1: up to this point we have approximated $g(s)$ in (1.48), and we are now ready to approximate the lower part $e^{isR_{\text{low}}(k)}$. We introduce the operator $\Pi_{\text{mid}}^{n,r}$, which based on the frequency decomposition $R(k)$ (and on the a priori degree of regularity of the solution n), gives a symmetric low-regularity approximation of the remaining oscillatory factors, based on polynomial interpolation. After one time step the scheme takes the form

$$U_{\text{mid},k}^{n,r}(\tau) = \sum_{T \in \mathcal{V}_k^r} \frac{\Upsilon_{\text{mid}}^p(T)}{S(T)} \Pi_{\text{mid}}^{n,r}(T)(\tau), \quad (1.53)$$

together with the formal local error expansion:

$$U_{\text{mid},k}^{n,r}(\tau) - u_{\text{mid},k}^r(\tau) = \sum_{T \in \mathcal{V}_k^r} \mathcal{O}_{\|\cdot\|}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T, n) \Upsilon_{\text{mid}}^p(T)). \quad (1.54)$$

This is to be compared with the tree series (1.39) and local error (1.40).

Throughout this iterative procedure of building the scheme, we choose the mid-point rule as our symmetric approximation, and obtain the class (1.53). We are also interested in obtaining a more general class of symmetric approximations encompassing the class (1.53), the previously built symmetric integrators (such as (1.49)), as well as new symmetric integrators. In Section 6.3.2 we derive a *forest formula*, which characterizes a large class of symmetric schemes. We derive a general formula (6.14) parametrizing resonance-based and classical integrators and deduce conditions on the coefficients of this formula to obtain a symmetric scheme, see Proposition 6.52 and Section 6.4.2. While the forest formula (6.14) comprises a large class of integrators, it is not defined in a recursive manner, hence obtaining a closed formula for the local error terms (such as (1.54)) is not obvious. The advantage of fixing a symmetric approximation (such as the mid-point rule (1.51)) and constructing the iterative procedure (1.52) on each tree T , is that one has a derivation of the local error terms (1.54) at hand.

We refer to Figure 1.2 where new symmetric integrators (light yellow and purple) are tested numerically, and show good near-preservation of the energy without CFL conditions.

Remark 1.6.3 (Symmetric versus symplectic schemes) The idea behind the chapters 5 and 6 is heavily based upon the decompositions (1.17) and (1.18). We first iterate Duhamel's formula in the nonlinearity in a symmetric fashion, give a symmetric approximation to the lower order parts and integrate the dominant part exactly. This yields symmetric schemes. To obtain *symplectic resonance-based schemes*, a different decomposition of the oscillatory terms $e^{isR(k)}$ must be done to ensure that the approximation originates in another Hamiltonian system with the same symplectic structure and conservation of normalization. A suitable decomposition of the frequencies $R(k)$ was recently obtained by the authors of [MS23] in the case of the KdV equation and the 1-dimensional NLS equation (see also Remark 6.2.5).

Prospects: Part III makes a first step towards obtaining reliable long-time approximations to dispersive equations, both in smooth and non-smooth regimes. An interesting next step is to see what can be rigorously proven on the

near-preservation of the mass and the energy over long times, as observed in the numerical experiments of Section 6.5.2.

Further developing these low-regularity and structure preserving techniques should enhance our understanding of the global behavior of dispersive equations, such as the existence of global solutions or quantization effects.

In contrast, for PDEs whose solution is not defined globally in time, finding reliable descriptions of blow-up phenomena, and hence describing the formation of singularities faithfully, remains a grand challenge. We refer to the major theoretical breakthroughs in this direction in the context of the NLS equation [MRS10, MRRS22]. Another interesting application is the detection of dispersive blow-ups [BS93, BS10, BPSS14], which are point-wise blow-ups preserving the global well-posedness of the solution. These mathematical phenomena may be relevant in explaining the formation of rogue waves in shallow and deep waters [KPS08, CHA11].

Part I

Beyond periodic boundary conditions and
higher-order extensions

Chapter 2

Error analysis of a class of semi-discrete schemes for solving the Gross-Pitaevskii equation at low regularity

This chapter is based on the article [AB23a] published in the Journal of Computational and Applied Mathematics.

Abstract. We analyze a class of time discretizations for solving the nonlinear Schrödinger equation with non-smooth potential and at low-regularity on an arbitrary Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d \leq 3$. We show that these schemes, together with their optimal local error structure, allow for convergence under lower regularity assumptions on both the solution and the potential than is required by classical methods, such as splitting or exponential integrator methods. Moreover, we show first and second order convergence in the case of periodic boundary conditions, in any fractional positive Sobolev space H^r , $r \geq 0$, beyond the more typical L^2 or H^σ ($\sigma > \frac{d}{2}$) -error analysis. Numerical experiments illustrate our results.

2.1 Introduction

We consider the Gross-Pitaevskii (GP) equation

$$i\partial_t u(t, x) = -\Delta u(t, x) + V(x)u(t, x) + |u(t, x)|^2 u(t, x), \quad (t, x) \in \mathbb{R} \times \Omega \quad (2.1)$$

with $\Omega \subset \mathbb{R}^d$, $d \leq 3$, and an initial condition

$$u|_{t=0} = u_0. \quad (2.2)$$

When $\partial\Omega \neq \emptyset$, we assign boundary conditions which will be encoded in the choice of the domain of the operator $\mathcal{L} = i\Delta$. We recall that the linear operator $\mathcal{L} = i\Delta$ generates a group $\{e^{t\mathcal{L}}\}_{t \in \mathbb{R}}$ of unitary operators on $L^2(\Omega)$. We will deal with mild solutions of the initial value problem (2.1) and (2.2) which are given by Duhamel's formula;

$$u(t) = e^{it\Delta} u_0 + \int_0^t e^{i(t-\zeta)\Delta} f(u, \bar{u}, V)(\zeta, x) d\zeta \quad (2.3)$$

where we denote the nonlinearity by

$$f(u, \bar{u}, V)(t, x) = -i(V(x)u(t, x) + u^2(t, x)\bar{u}(t, x)). \quad (2.4)$$

Throughout this article we will be interested in studying numerical schemes which approximate the time dynamics of (2.1) at low-regularity, by means of appropriate approximations of Duhamel's formula. Namely, we are interested in providing a reliable approximation of (2.1) (or equivalently of (2.3)) when the initial data u_0 and the potential V are non-smooth, in the sense that they belong to Sobolev spaces of low order.

One setting for the Gross-Pitaevskii equation is to describe the dynamics of Bose-Einstein condensates in a potential trap. In many physically relevant situations the potential is assumed to be rough or disordered, and hence the study of equation (2.1) in this non-smooth or low-regularity framework is of physical interest ([NBP13], [WWW⁺98]).

Recently much progress has been made in the development of low-regularity approximations to nonlinear evolution equations. First, in the case of periodic boundary conditions a class of schemes called *Fourier integrators* [ORS21] or *resonance based schemes* [BS22] were introduced to approximate the time dynamics of dispersive equations such as NLS, KdV, and Klein-Gordon (see [HS17b], [OS18], [CS22a]). Recently, higher order extensions of these *resonance based*

schemes were introduced in [BS22] for approximating in a unified fashion a large class of dispersive equations with periodic boundary conditions. These *resonance based schemes* were shown to converge in a more general setting, namely under lower regularity assumptions, than classical methods required (see [OS18], [ORS21] and references therein for a comparative analysis). The name of these schemes is due to their construction which revolves around Fourier based expansions of the solution and of the resonance structure of the equation. We explain the idea behind these resonance based schemes in detail in Section 2.3.1. These ideas were then extended in [RS21] to treat more general domains $\Omega \subset \mathbb{R}^d$ and boundary conditions and allow to deal with a class of parabolic, hyperbolic and dispersive equations in a unified fashion. The resulting schemes were termed *low-regularity integrators*, or *Duhamel's integrators* (see [RS21]). A next natural step in this study of low-regularity approximations to nonlinear PDEs is to introduce a potential term uV with minimal regularity assumptions on the solution u and the potential V . The goal of this article is to study first and second low-regularity schemes for equation (2.1), with an emphasis on the error analysis. In Chapter 3 we present a general framework for deriving low-regularity schemes up to arbitrary order, using new techniques based on decorated trees series analysis to extend the construction of the schemes presented in this article.

In this article we study a class of low-regularity integrators to solve the Gross-Pitaevskii equation (2.1) on an arbitrary domain $\Omega \subset \mathbb{R}^d$. In the case where the domain is a torus \mathbb{T}^d , we state and prove first and second order convergence in any fractional positive Sobolev space H^r , under moderate regularity assumptions on both the solution u and the potential V . These are stronger convergence results than the more typical L^2 or H^σ ($\sigma > \frac{d}{2}$) -convergence analysis, and apply to the nonlinear Schrödinger equation as an immediate consequence.

2.1.1 First-order low regularity integrator

In Section 2.3.2 we construct the following first order low-regularity integrator on Ω . For $n \geq 0$, we define,

$$u^{n+1} = \Phi_1^\tau(u^n) := e^{i\tau\Delta}(u^n - i\tau(u^n\varphi_1(-i\tau\Delta)V + (u^n)^2\varphi_1(-2i\tau\Delta)\bar{u}^n)), \quad \text{where } u^0 = u_0, \quad (2.5)$$

and $\varphi_1(z) = \frac{e^z - 1}{z}$ is a bounded operator on $i\mathbb{R}$. The construction of this scheme does not rely on Fourier based techniques, and hence one can couple the above time discretization not only with spectral methods but with more general types of spatial discretizations. Indeed, on general domains one can call upon Krylov space methods for the approximation of the matrix exponential $e^{it\Delta}$, and the action of the $\varphi_1(\cdot)$ functions (see [GRT18] and [HO10]). The fully discrete analysis on a smooth bounded domain with homogeneous Dirichlet conditions and with a finite elements space discretization, is the objective of future work.

We prove in Section 2.3.4 the following first order convergence result for the scheme (2.5), in the case of periodic boundary conditions. For the local-wellposedness result of (2.1) and (2.2) we refer to Theorem 2.2.1 given in Section 2.2.

Theorem 2.1.1 *Let $T > 0$, $r \geq 0$, and*

$$r_1 := \begin{cases} 1 + r, & \text{if } r > \frac{d}{2}, \\ 1 + \frac{r}{2} + \frac{d}{4}, & \text{if } 0 \leq r < \frac{d}{2}. \end{cases} \quad (2.6)$$

For every $u_0 \in H^{r_1}(\mathbb{T}^d)$ and $V \in H^{r_1}(\mathbb{T}^d)$, let $u \in \mathcal{C}([0, T], H^{r_1}(\mathbb{T}^d))$ be the unique solution of (2.1). Then there exists $\tau_{\min} > 0$ and $C_T > 0$ such that for every time step size $\tau \leq \tau_{\min}$ the numerical solution u^n given in equation (2.5) has the following error bound:

$$\|u^n - u(n\tau)\|_{H^r} \leq C_T\tau, \quad 0 \leq n\tau \leq T.$$

Before moving on to the second order scheme and its convergence result we make a few remarks on the regularity assumptions made in the above theorem. A consequence of Theorem 2.1.1 is that for any initial data and potential in $H^{r+1}(\Omega)$ where $r > \frac{d}{2}$ and $\Omega = \mathbb{T}^d$ (or on the full space $\Omega = \mathbb{R}^d$) we have the following global error estimate:

$$\max_{1 \leq n\tau \leq T} \|u^n - u(n\tau)\|_{H^r} \leq C(\sup_{[0, T]} \|u(t)\|_{H^{r+1}}, \|V\|_{H^{r+1}})\tau.$$

Namely we only ask one additional Sobolev derivative on the initial data u_0 and the potential V in order to obtain first-order convergence of our low-regularity scheme (2.5). This is due to the favorable local error structures that these low-regularity schemes inherit. See ([OS18], [BS22], [RS21]), and references therein for an in depth comparative analysis of these low-regularity schemes with classical methods such as splitting methods, or exponential integrator methods.

Secondly, in the case $0 < r < \frac{d}{2}$ the convergence analysis in H^r -norm of a time discretization of equation (2.1) has not to our knowledge previously been studied, and these are the first convergence results in this regime. A direct consequence of the above theorem is that in the critical case $r = \frac{d}{2}$, we obtain first order convergence in $H^{\frac{d}{2}}$ with $r_1 = 1 + \frac{d}{2} + \epsilon$, for arbitrarily small $\epsilon > 0$.

Finally, when $r = 0$, we consider the regularity assumptions required for an L^2 -error analysis, and compare them with the existing L^2 convergence results for the Gross-Pitaevskii equation (2.1). When $r = 0$, Theorem 2.1.1 states,

$$\|u^n - u(n\tau)\|_{L^2} \leq C(\sup_{[0,T]} \|u(t)\|_{H^{1+\frac{d}{4}}}, \|V\|_{H^{1+\frac{d}{4}}})\tau, \quad 0 \leq n\tau \leq T.$$

To our knowledge, this is the first convergence result of this type with low-regularity assumptions on both the solution $u(t)$ and the potential V . Indeed, in the literature L^2 -convergence results have been established for smooth potentials. See, for example [JL00], where the authors showed first-order convergence of a Lie splitting scheme for the linear Schrödinger equation with a potential term uV where they require V to be a C^5 -smooth potential. The authors of [HP17] were able to show first-order convergence to (2.1) of a Crank-Nicholson scheme for a rough, discontinuous potential V , which is of physical relevance in the context of Bose-Einstein condensates. Namely, for $V = V_d + V_s$, where $V_s \in C_0^\infty(\Omega)$ is smooth perturbation of a disordered potential $V_d \in L^\infty(\Omega)$, the authors obtained first order convergence of their scheme under -among other assumptions- $u_t \in L^2(0, T; H^2(\Omega))$, [HP17, Theorem 4.1]. Further, as detailed in [HP17, Appendix A], due to the roughness of V_d the highest regularity assumption one can hope for on the solution is $u(t) \in H^2(\Omega)$, and this regularity is required for their error analysis. In contrast to these results Theorem 2.1.1 permits low-regularity assumptions simultaneously on *both* $u(t)$ and V . Finally, we refer to [RS21, Corollary 20] where the authors show first order convergence in $L^2(\Omega)$ of a low-regularity scheme for the nonlinear Schrödinger equation (NLS) while analogously asking for $1 + \frac{d}{4}$ Sobolev regularity on the initial data.

2.1.2 Second-order low regularity integrator

In [Section 2.4, Corollary 2.4.3] we derive the following second order low-regularity integrator on Ω . For $n \geq 0$, we define,

$$\begin{aligned} u^{n+1} = \Phi_2^\tau(u^n) := & e^{i\tau\Delta}u^n - i\tau e^{i\tau\Delta}(u^n\varphi_1(-i\tau\Delta)V + (u^n)^2\varphi_1(-2i\tau\Delta)\bar{u}^n) \\ & - i\tau\left((e^{i\tau\Delta}u^n)\varphi_2(-i\tau\Delta)(e^{i\tau\Delta}V) + (e^{i\tau\Delta}u^n)^2\varphi_2(-2i\tau\Delta)e^{i\tau\Delta}\bar{u}^n\right) \\ & + i\tau e^{i\tau\Delta}(u^n\varphi_2(-i\tau\Delta)V + (u^n)^2\varphi_2(-2i\tau\Delta)\bar{u}^n) \\ & - \frac{\tau^2}{2}e^{i\tau\Delta}(|u^n|^4u^n + 3u^n|u^n|^2V - |u^n|^2u^n\bar{V} + u^nV^2), \end{aligned} \quad (2.7)$$

where $\varphi_2(z) = \frac{e^z - \varphi_1(z)}{z}$ is a bounded operator on $i\mathbb{R}$. We present in [Section 2.4.2, Corollary 2.4.8] yet another derivation of a low-regularity second order scheme for (2.1). We also offer in Chapter 3 a similar low-regularity scheme as above, using a different construction based on tree series analysis. As for the first order scheme, the above time discretization can be coupled with various spatial discretizations such as with finite elements.

We prove in Section 2.4.4 the following second order convergence result for the scheme (2.7), in the case of periodic boundary conditions.

Theorem 2.1.2 *Let $T > 0$, $r \geq 0$, and*

$$r_2 := \begin{cases} 2 + r, & \text{if } r > \frac{d}{2}, \\ 2 + \frac{r}{2} + \frac{d}{4}, & \text{if } 0 \leq r < \frac{d}{2}. \end{cases} \quad (2.8)$$

For every $u_0 \in H^{r_2}(\mathbb{T}^d)$ and $V \in H^{r_2}(\mathbb{T}^d)$, let $u \in \mathcal{C}([0, T], H^{r_2}(\mathbb{T}^d))$ be the unique solution of (2.1). Then there exists $\tau_{\min} > 0$ and $C_T > 0$ such that for every time step size $\tau \leq \tau_{\min}$ the numerical solution given in equation (2.7) has the following error bound:

$$\max_{1 \leq n \leq N} \|u^n - u(n\tau)\|_{H^r} \leq C_T \tau^2. \quad (2.9)$$

We comment on the regularity assumptions made in the above theorem. First, in the (smooth) regime $r > \frac{d}{2}$, we ask only for two additional derivatives on the initial data u_0 and the potential V . A preceding second order convergence result has been established for the NLS equation by [OWY22] in this regime. Indeed, using a resonance-based approach the authors [OWY22] showed second order convergence in H^r , for $r > \frac{d}{2}$, and $u_0 \in H^{r+2}$, of a low-regularity scheme for NLS (given by equation (2.7) with $V = 0$). Secondly, to our knowledge this is the first convergence result in H^r of a second order time discretization of equation (2.1) in the intermediate regime $0 < r < \frac{d}{2}$. In the critical case $r = \frac{d}{2}$, second order convergence directly follows from the above theorem with $r_2 = 2 + \frac{d}{2} + \epsilon$ and $\epsilon > 0$ arbitrarily small. Finally, we compare once again our result to the L^2 -convergence results obtained in the literature; we mention the authors [JL00] who show second order convergence of a Strang splitting scheme for a C^5 -smooth potential. Whereas, the authors [HP17] obtain second order convergence of a Crank-Nicholson scheme for a smooth potential V and -among other assumptions-

for $u_{tt} \in L^2(0, T; H^2(\Omega))$. As mentioned previously, we emphasize that in contrast to previous results we establish convergence under low-regularity assumptions on *both* u and V .

2.1.3 Outline of the paper

We motivate the construction of the first order low-regularity integrator in Section 2.3.1 by first deriving the scheme in the periodic setting. We then generalize to the construction of the low-regularity scheme for an arbitrary domain $\Omega \subset \mathbb{R}^d$. In Section 2.4 we introduce the second order low-regularity integrator and discuss stability issues which arise. We then propose two different approaches to guarantee the stability of our proposed scheme. Section 2.3 and 2.4 also include the local and global error analysis of the first and second low-regularity integrators. Finally, in Section 2.5 we present numerical experiments underlining our theoretical findings. In the next section we briefly introduce some notation and nonlinear estimates which are crucial for the local and global error analysis.

2.2 Notation and nonlinear estimates

We begin by establishing some notation used in the paper, starting by the definition of the norm used throughout the error analysis sections. Our analysis will be made in the periodic fractional Sobolev space,

$$H^r(\mathbb{T}^d) := \left\{ u = \sum_{k \in \mathbb{Z}^d} u_k \frac{e^{ikx}}{\sqrt{(2\pi)^d}} \in L^2(\mathbb{T}^d) : |u|_r^2 \triangleq \sum_{k \in \mathbb{Z}^d} |k|^{2r} |u_k|^2 < +\infty \right\}$$

which is endowed with the norm

$$\begin{aligned} \|u\|_{H^r}^2 &= \|u\|_{L^2(\mathbb{T}^d)}^2 + \|(-\Delta)^{r/2} u\|_{L^2(\mathbb{T}^d)}^2 \\ &= \sum_{k \in \mathbb{Z}^d} (1 + |k|^{2r}) |u_k|^2, \end{aligned}$$

where $u_k = \frac{1}{\sqrt{(2\pi)^d}} \int_{\mathbb{T}^d} u e^{-ikx} dx$.

Throughout the remainder of this section we fix $\sigma > \frac{d}{2}$, and we restrict the class of initial data and potential to belong to the Sobolev space H^σ . We now present some nonlinear estimates which will be fundamental for our analysis. We separate our H^r -error analysis into two cases: $0 \leq r \leq \frac{d}{2}$, and $r > \frac{d}{2}$. In the case where $0 \leq r \leq \frac{d}{2}$ we have,

$$\|vw\|_{H^r} \lesssim \|v\|_{H^\sigma} \|w\|_{H^r}, \quad (2.10)$$

while in the regime $r > \frac{d}{2}$ the above holds with $\sigma = r$ (see for example [HS17a, equation (2.49)]). For completeness, we provide a proof of the above inequality (2.10) in the Appendix for both regimes of r . These estimates will be used frequently throughout the error analysis sections (see Sections 2.3.3, 2.3.4, 2.4.3, 2.4.4).

One can easily deduce from the inequality (2.10) the following estimates on the nonlinearity (2.4);

$$\begin{aligned} \|f(w, \bar{w}, V)\|_{H^r} &\leq C_{r,\sigma} (\|w\|_{H^\sigma}, \|V\|_{H^\sigma}) \|w\|_{H^r} \\ \|f(w, \bar{w}, V) - f(v, \bar{v}, V)\|_{H^r} &\leq C_{r,\sigma} (\|w\|_{H^\sigma}, \|v\|_{H^\sigma}, \|V\|_{H^\sigma}) \|w - v\|_{H^r}, \end{aligned} \quad (2.11)$$

where $C_{r,\sigma}(\|u\|, \|v\|, \|w\|)$ denotes a generic constant which depends on the bounded arguments $\|u\|$, $\|v\|$, and $\|w\|$. In the regime $r > \frac{d}{2}$ the above holds with $\sigma = r$.

Remark 2.2.1 In order to deal with less smooth initial data $u_0 \in H^r$, $r \leq \frac{d}{2}$ one cannot make use of the bilinear estimate (2.10) and one would need to call upon more subtle tools to show appropriate fractional convergence of the scheme. Several works have been made when working on $\Omega = \mathbb{T}$ or $\Omega = \mathbb{R}^d$ where low-regularity estimates for very rough data $u_0 \in H^r$, $r \leq \frac{d}{2}$ could be obtained by using tools from dispersive PDE such as discrete Strichartz estimates, or Bourgain spaces, see [ORS21], [ORS22b]. This refined error analysis is out of scope for this paper.

We finish this subsection by stating the following local well-posedness result of a solution to (2.1) and (2.2) of the form (2.3). Indeed, using the estimates (2.11), one obtains from a classical Banach fixed point argument the following result:

Theorem 2.2.1 *Let $\sigma_0 > \frac{d}{2}$. Given any $u_0 \in H^{\sigma_0}(\mathbb{T}^d)$, and $V \in H^{\sigma_0}(\mathbb{T}^d)$ there exists $T > 0$ and a unique solution $u \in C([0, T], H^{\sigma_0}(\mathbb{T}^d))$ to (2.1).*

2.3 First order scheme and analysis

In this section we start by giving the main ideas behind the construction of the first order low-regularity scheme (see [RS21]). We propose a novel low-regularity integrator for the approximation of Duhamel's formula (2.3). We will approximate equation (2.3) at the time step $t_n + \tau$, where τ is the time step size. By iterating Duhamel's formula (2.3), we obtain the first order iteration

$$u(t_n + \tau) = e^{i\tau\Delta}[u(t_n) - i\mathcal{J}_1(\tau, \Delta, u(t_n))] + R_{1,0}(\tau, u) \quad (2.12)$$

where the principal oscillatory integral (at first order) is given by

$$\mathcal{J}_1(\tau, \Delta, v) = \int_0^\tau e^{-i\zeta\Delta}[V(x)(e^{i\zeta\Delta}v) + (e^{i\zeta\Delta}v)^2(e^{-i\zeta\Delta}\bar{v})]d\zeta \quad (2.13)$$

and the remainder

$$R_{1,0}(\tau, u) = \int_0^\tau e^{i(\tau-\zeta)\Delta}[f(u(t_n + \zeta), \bar{u}(t_n + \zeta), V) - f(e^{i\zeta\Delta}u(t_n), e^{-i\zeta\Delta}\bar{u}(t_n), V)]d\zeta.$$

We will construct a suitable discretization of the integral (2.13) to allow for a low-regularity approximation to the first order Duhamel iterate (2.12). The idea is to filter out the dominant parts, which we denote by \mathcal{L}_{dom} , of the nonlinear frequency interactions within the integral (2.13) and embed them in the discretization. The lower-order parts will be approximated and incorporated in the local error analysis.

First, to illustrate the underlying idea and to provide intuition behind the construction of these low-regularity integrators we start by analyzing the case of periodic boundary conditions $\Omega = \mathbb{T}$, with V a periodic potential. The ideas presented in the next section were first introduced by the authors [OS18] for solving a class of semilinear Schrödinger equations. After presenting the periodic case in a formal way, we rigorously detail in Section 2.3.2 the construction of the first order scheme in the more general case of an arbitrary domain $\Omega \subset \mathbb{R}^d$.

2.3.1 Case of periodic boundary conditions: $\Omega = \mathbb{T}$

Assuming that $v \in L^2$, we can expand v in Fourier series $v = \sum_{k \in \mathbb{Z}} \hat{v}_k e^{ikx}$. This allows us to express the action of the Schrödinger flow on v , $e^{\pm it\Delta}v(x) = \sum_{k \in \mathbb{Z}} \hat{v}_k e^{\mp itk^2} e^{ikx}$. Similarly assuming $V \in L^2$ we have $V(x) = \sum_{l \in \mathbb{Z}} \hat{V}_l e^{ilx}$. In Fourier space, the oscillatory integral (2.13) is then given by,

$$\mathcal{J}_1(\tau, \Delta, v) = \sum_{l_1+l_2=l} \hat{V}_{l_1} \hat{v}_{l_2} e^{ilx} \int_0^\tau e^{i\zeta R_2(l)} d\zeta + \sum_{-k_1+k_2+k_3=k} \bar{\hat{v}}_{k_1} \hat{v}_{k_2} \hat{v}_{k_3} e^{ikx} \int_0^\tau e^{i\zeta R_1(k)} d\zeta \quad (2.14)$$

with the resonance structure,

$$R_1(k) = 2k_1^2 - 2k_1(k_2 + k_3) + 2k_2k_3, \text{ and } R_2(l) = l_1^2 + 2l_1l_2. \quad (2.15)$$

Ideally we would like to integrate all the nonlinear frequency interactions (2.15) exactly and embed them in the discretization. This, however, would result in a generalized convolution (of Coifman-Meyer type [CM75]), which cannot be rewritten in physical space. Hence, the computations would need to be fully made in Fourier space. Carrying this out in higher spatial dimensions d would cause large memory and computational efforts of order $O(|K|^{d-\ell})$, where K denotes the highest frequency in the discretization and ℓ is the number of factors in the nonlinearity. For practical computations, we want to be able to express the discretization also in physical space in order to use the Fast Fourier Transform (FFT) which is of computational effort of order $O(|K|^d \log |K|^d)$. Therefore, we choose in the following an approximation of the integral (2.14) which allows for a practical implementation (by not performing exact integration), while optimizing the local error in the sense of regularity. We detail this procedure below.

We can extract the dominant and lower-order parts from the resonance structures (2.15) by recalling that $2k_1^2$ and l_1^2 correspond to second order derivatives in Fourier while the terms $k_m k_j$ (for $m \neq j$) correspond to product of first order derivatives. We choose,

$$R_1(k) = \mathcal{L}_{dom,1}(k_1) + \mathcal{L}_{low,1}(k_1, k_2, k_3), \quad R_2(l) = \mathcal{L}_{dom,2}(l_1) + \mathcal{L}_{low,2}(l_1, l_2)$$

with

$$\mathcal{L}_{dom,1}(k_1) = 2k_1^2, \quad \mathcal{L}_{low,1}(k_1, k_2, k_3) = -2k_1(k_2 + k_3) + 2k_2k_3, \quad \text{and}$$

$$\mathcal{L}_{dom,2}(l_1) = l_1^2, \quad \mathcal{L}_{low,2}(l_1, l_2) = 2l_1l_2.$$

From the above and from equation (2.14), by a simple Taylor's expansion on the lower-order parts we (formally) allow for the following approximation of the oscillatory integral in Fourier space,

$$\begin{aligned} \mathcal{J}_1(\tau, \Delta, v) &= \sum_{l_1+l_2=l} \hat{V}_{l_1} \hat{v}_{l_2} e^{ilx} \int_0^\tau e^{i\zeta \mathcal{L}_{dom,2}(l_1)} e^{i\zeta \mathcal{L}_{low,2}(l_1, l_2)} d\zeta \\ &\quad + \sum_{-k_1+k_2+k_3=k} \bar{\hat{v}}_{k_1} \hat{v}_{k_2} \hat{v}_{k_3} e^{ikx} \int_0^\tau e^{i\zeta \mathcal{L}_{dom,1}(k_1)} e^{i\zeta \mathcal{L}_{low,1}(k_1, k_2, k_3)} d\zeta \\ &= \sum_{l_1+l_2=l} \hat{V}_{l_1} \hat{v}_{l_2} e^{ilx} \int_0^\tau e^{i\zeta \mathcal{L}_{dom,2}(l_1)} (1 + O(\zeta \mathcal{L}_{low,2}(l_1, l_2))) d\zeta \\ &\quad + \sum_{-k_1+k_2+k_3=k} \bar{\hat{v}}_{k_1} \hat{v}_{k_2} \hat{v}_{k_3} e^{ikx} \int_0^\tau e^{i\zeta \mathcal{L}_{dom,1}(k_1)} (1 + O(\zeta \mathcal{L}_{low,1}(k_1, k_2, k_3))) d\zeta. \end{aligned}$$

Mapping back into physical space we thus have

$$\begin{aligned} \mathcal{L}_{dom,1}(v) &= -2\Delta v, \quad \mathcal{L}_{low,1}(v) = 2(2|\nabla v|^2 v - |\nabla v|^2 \bar{v}), \\ \mathcal{L}_{dom,2}(v) &= -\Delta v, \quad \mathcal{L}_{low,2}(v, V) = -2\nabla V \nabla v, \end{aligned}$$

and

$$\begin{aligned} \mathcal{J}_1(\tau, \Delta, v) &= \int_0^\tau [e^{i\zeta \mathcal{L}_{dom,2}} V] v + [e^{i\zeta \mathcal{L}_{dom,1}} \bar{v}] v^2 + O(\zeta(\mathcal{L}_{low,2}(v, V) + \mathcal{L}_{low,1}(v))) d\zeta \\ &= \tau[v\varphi_1(i\tau \mathcal{L}_{dom,2})V + v^2\varphi_1(i\tau \mathcal{L}_{dom,1})\bar{v}] + O(\tau^2(\mathcal{L}_{low,2}(v, V) + \mathcal{L}_{low,1}(v))). \end{aligned} \quad (2.16)$$

Hence, for a small time step τ , by plugging the above expression of \mathcal{J}_1 in the iterate (2.12) and ignoring the lower-order terms yields the first-order resonance based discretization

$$u^{n+1} = e^{i\tau\Delta} [u^n - i\tau(u^n \varphi_1(-i\tau\Delta)V + (u^n)^2 \varphi_1(-2i\tau\Delta)\bar{u}^n)]. \quad (2.17)$$

The above scheme (2.17) has a favorable local error structure; namely from equation (2.16) we see that (formally) this discretization only ask for *first order* derivatives on the initial data and potential.

We now place ourselves in the general framework $\Omega \subset \mathbb{R}^d$, and make use of filtering techniques to recover the first order low-regularity approximation (2.17) in this general setting. The ideas presented in the next section are inspired by the work of [RS21].

2.3.2 General boundary conditions: $\Omega \subset \mathbb{R}^d$

The goal of this section is to construct a first order discretization of the oscillatory integral (2.13) when working on a general domain Ω , and which allows for the improved local error structure (2.16) established in the preceding section. This is achieved by introducing a properly chosen filtered function which will filter out the dominant oscillatory terms $\mathcal{L}_{dom,1}, \mathcal{L}_{dom,2}$ explicitly found in the preceding section.

First, we recall the definition of the commutator-type term $\mathcal{C}[H, L]$ for $H(v_1, \dots, v_n)$, $n \geq 1$, a function and L a linear operator:

$$\mathcal{C}[H, L](v_1, \dots, v_n) = -L(H(v_1, \dots, v_n)) + \sum_{i=1}^n D_i H(v_1, \dots, v_n) \cdot L v_i.$$

We make an important note that the above differs from the well known Lie commutator used for the error analysis of classical methods, such as for splitting methods (see for example [HLW10], [JL00]).

We define the filtered function by

$$\mathcal{N}(\tau, s, \zeta, \Delta, v) = e^{-is\Delta} [e^{is\Delta} e^{-i\zeta\Delta} V(e^{is\Delta} v) + (e^{is\Delta} v)^2 (e^{is\Delta} e^{-2i\zeta\Delta} \bar{v})]. \quad (2.18)$$

The principal oscillations (2.13) can be expressed with the aid of the filter function \mathcal{N} as

$$\mathcal{J}_1(\tau, \Delta, v) = \int_0^\tau \mathcal{N}(\tau, \zeta, \zeta, \Delta, v) d\zeta.$$

By the fundamental theorem of calculus we have

$$\mathcal{J}_1(\tau, \Delta, v) = \int_0^\tau \mathcal{N}(\tau, 0, \zeta, v) d\zeta + \int_0^\tau \int_0^\zeta \partial_s \mathcal{N}(\tau, s, \zeta, v) ds d\zeta \quad (2.19)$$

where

$$\mathcal{N}(\tau, 0, \zeta, v) = [e^{i\zeta \mathcal{L}_{dom,2}} V]v + [e^{i\zeta \mathcal{L}_{dom,1}} \bar{v}]v^2 \quad (2.20)$$

and

$$\begin{aligned} \partial_s \mathcal{N}(\tau, s, \zeta, v) &= e^{-is\Delta} \mathcal{C}[f, i\Delta](e^{is\Delta} v, e^{is\Delta} e^{-2i\zeta\Delta} \bar{v}, e^{is\Delta} e^{-i\zeta\Delta} V), \\ \mathcal{C}[f, i\Delta](u, v, w) &= -2i(\nabla w \cdot \nabla u + |\nabla u|^2 v + \nabla(u^2) \cdot \nabla v). \end{aligned} \quad (2.21)$$

Hence, we recover the discretization of the oscillatory integral (2.13) together with an improved local error structure of the form (2.16);

$$\mathcal{J}_1(\tau, \Delta, v) = \tau[v\varphi_1(i\tau \mathcal{L}_{dom,2})V + v^2\varphi_1(i\tau \mathcal{L}_{dom,1})\bar{v}] + R_{1,1}(\tau)$$

where

$$R_{1,1}(\tau) = \int_0^\tau \int_0^\zeta e^{-is\Delta} \mathcal{C}[f, i\Delta](e^{is\Delta} v, e^{is\Delta} e^{-2i\zeta\Delta} \bar{v}, e^{is\Delta} e^{-i\zeta\Delta} V) ds d\zeta.$$

Corollary 2.3.1 *The exact solution u of (2.1) can be expanded as*

$$u(t_n + \tau) = e^{i\tau\Delta} [u(t_n) - i\tau(u(t_n)\varphi_1(-i\tau\Delta)V + (u(t_n))^2\varphi_1(-2i\tau\Delta)\bar{u}(t_n))] + \mathcal{R}_1(\tau, t_n)$$

where the remainder is given by

$$\begin{aligned} \mathcal{R}_1(\tau, t_n) &= \int_0^\tau e^{i(\tau-\zeta)\Delta} [f(u(t_n + \zeta), \bar{u}(t_n + \zeta), V) - f(e^{i\zeta\Delta} u(t_n), e^{-i\zeta\Delta} \bar{u}(t_n), V)] d\zeta \\ &\quad + \int_0^\tau \int_0^\zeta e^{i(\tau-s)\Delta} \mathcal{C}[f, i\Delta](e^{is\Delta} u(t_n), e^{is\Delta} e^{-2i\zeta\Delta} \bar{u}(t_n), e^{is\Delta} e^{-i\zeta\Delta} V) ds d\zeta. \end{aligned} \quad (2.22)$$

The first order low-regularity scheme (2.5) follows from the above Corollary 2.3.1 by neglecting the remainder $\mathcal{R}_1(\tau, t_n)$. We next show the first-order error estimates for the scheme (2.5) by first estimating its favorable commutator-type local error structure.

2.3.3 Local error estimates

Proposition 2.3.2 *Let $T > 0$, $r \geq 0$, and r_1 as in Theorem 2.1.1, namely*

$$r_1 = \begin{cases} 1 + r, & \text{if } r > \frac{d}{2}, \\ 1 + \frac{r}{2} + \frac{d}{4}, & \text{if } 0 \leq r \leq \frac{d}{2}. \end{cases}$$

Assume there exists $C_T > 0$ such that

$$\sup_{[0, T]} \|u(t)\|_{H^{r_1}} \leq C_T, \quad \text{and} \quad \|V\|_{H^{r_1}} \leq C_T, \quad (2.23)$$

then there exists $M_T > 0$ such that for every $\tau \in (0, 1]$,

$$\|\mathcal{R}_1(\tau, t_n)\|_{H^r} \leq M_T \tau^2, \quad 0 \leq t_n \leq T, \quad (2.24)$$

where $t_n = n\tau$ and $\mathcal{R}_1(\tau, t_n)$ is given in equation (2.22).

Proof. We write the error term $\mathcal{R}_1(\tau, t_n)$, defined in equation (2.22), as the sum of two terms, $\mathcal{R}_1(\tau, t_n) = \mathcal{G}^1(\tau, t_n) + \mathcal{G}^2(\tau, t_n)$. We begin by estimating the first term $\mathcal{G}^1(\tau, t_n)$. Using the inequalities (2.11) on f , and the boundedness of

$e^{it\Delta}$ on Sobolev spaces we have that for all $r \geq 0$ and some $\sigma > \frac{d}{2}$,

$$\begin{aligned}
\|\mathcal{G}^1(\tau, t_n)\|_{H^r} &\leq \tau \sup_{\zeta \in [0, \tau]} \|f(u(t_n + \zeta), \bar{u}(t_n + \zeta), V) - f(e^{i\zeta\Delta}u(t_n), e^{-i\zeta\Delta}\bar{u}(t_n), V)\|_{H^r} \\
&\leq \tau C_{r, \sigma} (\sup_{[0, T]} \|u(t)\|_{H^\sigma}, \|V\|_{H^\sigma}) \sup_{\zeta \in [0, \tau]} \|u(t_n + \zeta) - e^{i\zeta\Delta}u(t_n)\|_{H^r} \\
&\leq \tau C_{r, \sigma} (\sup_{[0, T]} \|u(t)\|_{H^\sigma}, \|V\|_{H^\sigma}) \sup_{\zeta \in [0, \tau]} \left\| \int_0^\zeta e^{i(\zeta-s)\Delta} f(u(t_n + s), \bar{u}(t_n + s), V) ds \right\|_{H^r} \\
&\leq \tau^2 C_{r, \sigma} (\sup_{[0, T]} \|u(t)\|_{H^\sigma}, \|V\|_{H^\sigma}) \sup_{s \in [0, \tau]} \|f(u(t_n + s), \bar{u}(t_n + s), V)\|_{H^r} \\
&\leq C_{r, \sigma} (\sup_{[0, T]} \|u(t)\|_{H^\sigma}, \sup_{[0, T]} \|u(t)\|_{H^r}, \|V\|_{H^\sigma}) \tau^2,
\end{aligned} \tag{2.25}$$

where we use Duhamel's formula to go from the third to the fourth line. First, in the regime $r > \frac{d}{2}$, the above holds with $\sigma = r$. Using the fact that $r_1 > r$ yields the desired bound $\|\mathcal{G}^1(\tau, t_n)\|_{H^r} \leq C_T \tau^2$ in this regime. When $r < \frac{d}{2}$, we will construct an appropriate $\sigma > \frac{d}{2}$ which will be used throughout the remainder of the proof when making the analysis in this non-smooth regime.

Let $0 < \epsilon < \frac{1}{4}$, and let

$$\sigma_0 = \frac{d}{2} + \frac{\epsilon}{2}. \tag{2.26}$$

For $d \leq 3$, we have that $\frac{d}{2} + \epsilon < 1 + \frac{d}{4}$, and hence σ_0 satisfies

$$\frac{d}{2} < \sigma_0 < \frac{d}{2} + \epsilon < 1 + \frac{d}{4}. \tag{2.27}$$

Consequently, by recalling the definition (2.6) of r_1 , we have that $r_1 > \sigma_0$ when $r < \frac{d}{2}$. Hence, in the regime $r < \frac{d}{2}$, since $r_1 > \sigma_0$ we obtain the desired bound $\|\mathcal{G}^1(\tau, t_n)\|_{H^r} \leq C_T \tau^2$ by taking $\sigma = \sigma_0$ in equation (2.25).

We now estimate the second term $\mathcal{G}^2(\tau, t_n)$ in the remainder (2.22), using the explicit expression of the commutator (2.21) and the nonlinear estimate (2.10). In the regime $r > \frac{d}{2}$, we have $r_1 = r + 1$ and

$$\begin{aligned}
\|\mathcal{C}[f, i\Delta](u, v, w)\|_{H^r} &\leq C_r (\|\nabla w \cdot \nabla u\|_{H^r} + \|\nabla u\|^2 v\|_{H^r} + 2\|u \nabla u \cdot \nabla v\|_{H^r}) \\
&\leq C_r (\|u\|_{r+1}, \|v\|_{r+1}, \|w\|_{r+1}) \\
&\leq C_r (\|u\|_{r_1}, \|v\|_{r_1}, \|w\|_{r_1}).
\end{aligned}$$

When $0 \leq r < \frac{d}{2}$, we will make use of the bilinear estimate

$$\|uv\|_{H^r} \leq C_{r, d} \|u\|_{H^{\frac{r}{2} + \frac{d}{4}}} \|v\|_{H^{\frac{r}{2} + \frac{d}{4}}}, \tag{2.28}$$

which is a particular case of [Hör97, Theorem 8.3.1]. It follows from the above estimate (2.28) and the inequality (2.10) with $\sigma = \sigma_0$ as defined in (2.26) that

$$\begin{aligned}
\|\mathcal{C}[f, i\Delta](u, v, w)\|_{H^r} &\leq C_{r, d} (\|\nabla w\|_{H^{\frac{r}{2} + \frac{d}{4}}}, \|\nabla u\|_{H^{\frac{r}{2} + \frac{d}{4}}}, \|v\|_{H^{\sigma_0}}, \|u\|_{H^{\sigma_0}}, \|\nabla v\|_{H^{\frac{r}{2} + \frac{d}{4}}}) \\
&\leq C_{r, d} (\|w\|_{H^{1 + \frac{r}{2} + \frac{d}{4}}}, \|u\|_{H^{1 + \frac{r}{2} + \frac{d}{4}}}, \|v\|_{H^{1 + \frac{r}{2} + \frac{d}{4}}}).
\end{aligned}$$

Hence, by definition (2.6) of r_1 , given any $r \in \mathbb{R}^+ \setminus \{\frac{d}{2}\}$, we have shown the following bound,

$$\|\mathcal{C}[f, i\Delta](u, v, w)\|_{H^r} \leq C_{r, d} (\|u\|_{r_1}, \|v\|_{r_1}, \|w\|_{r_1}). \tag{2.29}$$

Further, since $e^{is\Delta}$ is an isometry on Sobolev spaces we obtain the following estimate of \mathcal{G}^2 in H^r norm,

$$\|\mathcal{G}^2(\tau, t_n)\|_{H^r} \leq C_{r, d} (\sup_{[0, T]} \|u(t)\|_{H^{r_1}}, \|V\|_{H^{r_1}}) \tau^2, \quad r \in \mathbb{R}^+ \setminus \{\frac{d}{2}\}.$$

The local error estimate is hence demonstrated. \square

Remark 2.3.3 By following the proof of Proposition 2.3.2 one can ask for less Sobolev regularity on the potential V , while asking for more regularity on the solution $u(t)$. Indeed, for example, by making the analysis in the L^2 -norm, one can ask for $V \in H^1$, and $u(t) \in H^{1 + \frac{d}{2} + \epsilon}$, with $\epsilon > 0$ arbitrarily small.

2.3.4 Global error estimates

Using the local error estimates established in the preceding section we show global first order convergence of our scheme (2.5) under the favorable regularity assumptions on the initial condition and the potential established previously.

Proof of Theorem 2.1.1. Let $e^n = u^n - u(t_n)$, where $u^n = \Phi_1^\tau(u^{n-1})$ is given in equation (2.5). We begin by decomposing the error term as follows,

$$\|e^{n+1}\|_{H^r} \leq \|\Phi_1^\tau(u(t_n)) - u(t_{n+1})\|_{H^r} + \|\Phi_1^\tau(u^n) - \Phi_1^\tau(u(t_n))\|_{H^r}. \quad (2.30)$$

The first term of the above expression is given by the local error $\mathcal{R}_1(\tau, t_n)$ defined at equation (2.22), and which is of order τ^2 by Proposition 2.3.2. We wish to establish a stability estimate of the numerical flow Φ_1^τ to bound the second term in equation (2.30), and to conclude by a *Lady Windermere's fan* argument ([HLW10]).

By using the estimate and (2.10), together with the fact that $e^{i\xi\Delta}$ and $\varphi_1(i\xi\Delta)$ are bounded on Sobolev spaces (for all $\xi \in \mathbb{R}$), it easily follows from the definition of our scheme (2.5) that for all $r \geq 0$,

$$\|\Phi_1^\tau(u(t_n)) - \Phi_1^\tau(u^n)\|_{H^r} \leq e^{L_n\tau} \|e^n\|_{H^r}, \quad L_n := C(\|u^n\|_{H^\sigma}, \|u(t_n)\|_{H^\sigma}, \|V\|_{H^\sigma}), \quad (2.31)$$

where for $r > \frac{d}{2}$ we have $\sigma = r$, and for $r \leq \frac{d}{2}$, we have $\sigma > \frac{d}{2}$.

Using Proposition 2.3.2, and the estimate (2.31) a bound of the error term (2.30) is given by,

$$\|e^{n+1}\|_{H^r} \leq M_T\tau^2 + e^{L_n\tau} \|e^n\|_{H^r}, \quad e^0 = 0, \quad r \neq \frac{d}{2}. \quad (2.32)$$

The global error estimate then easily follows by induction on the above inequality (2.32) once the following uniform bound is obtained:

$$\sup_{n\tau \leq T} \|u^n\|_{H^\sigma} < +\infty, \quad (2.33)$$

for sufficiently small time step τ , which depends on the final time T and the norm of the initial condition $\|u_0\|_{H^\sigma}$. In the remainder of the proof we establish the bound (2.33) for appropriate choices of σ depending on the H^r -norm considered.

In the regime $r > \frac{d}{2}$ we take $\sigma = r$, and the result follows by the classical *Lady Windermere's fan* argument ([HLW10]). Indeed, the uniform bound (2.33) easily follows for sufficiently small τ by a bootstrap argument on the estimate (2.32).

Using a refined global error analysis one can push down the error analysis to the H^r -norm for $0 \leq r < \frac{d}{2}$. We take $\sigma = \sigma_0$ where σ_0 is given in equation (2.26). In order to show the uniform bound (2.33) we establish fractional convergence of the scheme (2.5) in the higher order Sobolev space H^{σ_0} . Namely, we show that there exists $\delta > 0$ such that the following estimate holds

$$\|e^{n+1}\|_{H^{\sigma_0}} \leq M_T\tau^{1+\delta} + e^{L_n\tau} \|e^n\|_{H^{\sigma_0}}. \quad (2.34)$$

where $L_n = C(\|u^n\|_{H^{\sigma_0}}, \|u(t_n)\|_{H^{\sigma_0}}, \|V\|_{H^{\sigma_0}})$. Using the decomposition (2.30), and the bound (2.31) with $r = \sigma_0$, we are left to show the following local error estimate,

$$\|\mathcal{R}_1(\tau, t_n)\|_{H^{\sigma_0}} \leq M_T\tau^{1+\delta}, \quad (2.35)$$

in order to obtain the bound (2.34). We obtain the bound (2.35) by an interpolation argument. We first show a bound on the remainder $\mathcal{R}_1(\tau, t_n)$ in H^{r_1} -norm. By using Duhamel's formula and by construction of our numerical scheme (2.5) we have

$$\mathcal{R}_1(\tau, t_n) = \int_0^\tau e^{i(\tau-s)\Delta} f(u(t_n) + s, \bar{u}(t_n) + s, V) ds - i\tau e^{i\tau\Delta} (u(t_n)\varphi_1(-i\tau\Delta)V + (u(t_n))^2\varphi_1(-2i\tau\Delta)\bar{u}(t_n)).$$

One can estimate each of the above terms separately using the first estimate in equation (2.11) with $r = \sigma = r_1$. Indeed, this yields

$$\begin{aligned} \|\mathcal{R}_1(\tau, t_n)\|_{H^{r_1}} &\leq C_{r_1}(\|u(t_n)\|_{H^{r_1}}, \|V\|_{H^{r_1}})\tau \\ &\leq C_{r_1, T}\tau, \end{aligned} \quad (2.36)$$

Finally, since $r_1 > \sigma_0 > r$ there exists $\theta \in (0, 1)$ such that

$$\|\mathcal{R}_1(\tau, t_n)\|_{H^{\sigma_0}} \leq \|\mathcal{R}_1(\tau, t_n)\|_{H^{r_1}}^\theta \|\mathcal{R}_1(\tau, t_n)\|_{H^r}^{1-\theta}.$$

Using the local error estimates (2.24) and (2.36) we have

$$\|\mathcal{R}_1(\tau, t_n)\|_{H^{\sigma_0}} \leq M_T\tau^{2-\theta}$$

where $2 - \theta > 0$. Hence we have shown the bounds (2.35) and (2.34) with $\delta = 1 - \theta$. This yields the desired bound

(2.33) with $\sigma = \sigma_0$, and for sufficiently small τ , by a classical bootstrap argument on equation (2.34). The first order convergence of the scheme (2.5) follows by induction using the global bound (2.32), with $\sigma = \sigma_0$. \square

2.4 Second order scheme and analysis

The idea to derive a higher order scheme is to iterate Duhamel's formula (2.3), and to Taylor expand f around $e^{i\tau\Delta}v$, where we let $v = u_0$. For a second order scheme this yields the following expansion,

$$\begin{aligned} u(\tau) = e^{i\tau\Delta} & \left[v - i\mathcal{J}_1(\tau, \Delta, v) - i \int_0^\tau e^{-i\zeta_1\Delta} [D_1 f(e^{i\zeta_1\Delta}v, e^{-i\zeta_1\Delta}\bar{v}, V) \cdot e^{i\zeta_1\Delta} \mathcal{J}_1(\zeta_1, \Delta, v)] d\zeta_1 \right. \\ & \left. + i \int_0^\tau e^{-i\zeta_1\Delta} [D_2 f(e^{i\zeta_1\Delta}v, e^{-i\zeta_1\Delta}\bar{v}, V) \cdot e^{-i\zeta_1\Delta} \overline{\mathcal{J}_1(\zeta_1, \Delta, v)}] d\zeta_1 \right] + O(\tau^3) \end{aligned} \quad (2.37)$$

where

$$D_1 f(v, \bar{v}, V) = -i(V + 2v\bar{v}), \text{ and } D_2 f(v, \bar{v}, V) = -iv^2, \quad (2.38)$$

and where we Taylor expanded f around $e^{i\tau\Delta}v$ up to second order in order to obtain a remainder of order three. Next, the aim is to derive a second order approximation to the integrals appearing in the above expansion (2.37).

First, we treat the iterated integrals appearing in the above expression, namely the third and fourth term in equation (2.37). By a standard Taylor expansion we linearize the exponentials appearing in these iterated integrals. For both $v, V \in H^2$, this yields

$$-ie^{i\zeta_1\Delta} \mathcal{J}_1(\zeta_1, \Delta, v) = \zeta_1 f(v, \bar{v}, V) + O(\zeta_1^2(\Delta v + \Delta V)).$$

Using the above we make the following second order approximation of the iterated integrals in equation (2.37);

$$\begin{aligned} -i \int_0^\tau e^{-i\zeta_1\Delta} [D_1 f(e^{i\zeta_1\Delta}v, e^{-i\zeta_1\Delta}\bar{v}, V) \cdot e^{i\zeta_1\Delta} \mathcal{J}_1(\zeta_1, \Delta, v)] d\zeta_1 &= \int_0^\tau \zeta_1 D_1 f(v, \bar{v}, V) \cdot f(v, \bar{v}, V) d\zeta_1 \\ &\quad + O(\tau^3(\Delta v + \Delta V)), \\ i \int_0^\tau e^{-i\zeta_1\Delta} [D_2 f(e^{i\zeta_1\Delta}v, e^{-i\zeta_1\Delta}\bar{v}, V) \cdot e^{-i\zeta_1\Delta} \overline{\mathcal{J}_1(\zeta_1, \Delta, v)}] d\zeta_1 &= \int_0^\tau \zeta_1 D_2 f(v, \bar{v}, V) \cdot \overline{f(v, \bar{v}, V)} d\zeta_1 \\ &\quad + O(\tau^3(\Delta v + \Delta V)). \end{aligned} \quad (2.39)$$

The above calculations motivate the choice of the expansion for u stated in the following lemma.

Lemma 2.4.1 *Let $v = u^0$. At second order u can be expanded as*

$$u(\tau) = u_2(\tau) + R_{2,0}(\tau)$$

with

$$u_2(\tau) = e^{i\tau\Delta}v - ie^{i\tau\Delta} \mathcal{J}_1(\tau, \Delta, v) - \frac{\tau^2}{2} e^{i\tau\Delta} (|v|^4 v + 3v|v|^2 V - |v|^2 v \bar{V} + vV^2),$$

and

$$\begin{aligned} R_{2,0}(\tau) &= \int_0^\tau e^{i(\tau-\zeta_1)\Delta} [f(u(\zeta_1), \bar{u}(\zeta_1), V) - f(e^{i\zeta_1\Delta}v, e^{-i\zeta_1\Delta}\bar{v}, V)] d\zeta_1 \\ &\quad + e^{i\tau\Delta} \int_0^\tau \zeta_1 (|v|^4 v + 3v|v|^2 V - |v|^2 v \bar{V} + vV^2) d\zeta_1. \end{aligned}$$

Proof. The result immediately follows by recalling the definition of the principal oscillations (2.13), and Duhamel's formula (2.3). Moreover, we note that by simple calculations one has

$$D_1 f(v, \bar{v}, V) \cdot f(v, \bar{v}, V) = -(V^2 v + 3v^2 \bar{v} V + 2v^3 \bar{v}^2), \quad D_2 f(v, \bar{v}, V) \cdot \overline{f(v, \bar{v}, V)} = \bar{V} \bar{v} v^2 + v^3 \bar{v}^2,$$

and hence by equation (2.38) we have,

$$D_1 f(v, \bar{v}, V) \cdot f(v, \bar{v}, V) + D_2 f(v, \bar{v}, V) \cdot \overline{f(v, \bar{v}, V)} = -(|v|^4 v + 3v|v|^2 V - |v|^2 v \bar{V} + vV^2). \quad (2.40)$$

The above calculations together with equations (2.37) and (2.39) motivates the inclusion of the last term in the expansion of $u_2(\tau)$. \square

It remains to establish a low-regularity second order approximation to the principal oscillatory integral (2.13). We first recall from Section 2.3.2 that in order to derive a low-regularity approximation of \mathcal{J}_1 at first order we used the filtered

function (2.18) and its first order Taylor expansion (2.19). Analogously, to obtain a second order approximation of \mathcal{J}_1 we Taylor expand equation (2.18) around $s = 0$ up to second order, and include the first two terms of this expansion into our scheme. This yields,

$$\mathcal{N}(\tau, \zeta, \Delta, v) = \mathcal{N}(\tau, 0, \zeta, \Delta, v) + \zeta \partial_s \mathcal{N}(\tau, 0, \zeta, \Delta, v) + \int_0^\zeta \int_0^s \partial_{s_1}^2 \mathcal{N}(\tau, s_1, \zeta, \Delta, v) ds_1 ds. \quad (2.41)$$

Equivalently, using the filtered function (2.18), the above expression is written as

$$\begin{aligned} e^{-i\zeta\Delta} f(e^{i\zeta\Delta} v, e^{-i\zeta\Delta} \bar{v}, V) &= f(v, e^{-2i\zeta\Delta} \bar{v}, e^{-i\zeta\Delta} V) + \zeta \mathcal{C}[f, i\Delta](v, e^{-2i\zeta\Delta} \bar{v}, e^{-i\zeta\Delta} V) \\ &+ \int_0^\zeta \int_0^s e^{-is_1\Delta} \mathcal{C}^2[f, i\Delta](e^{is_1\Delta} v, e^{is_1\Delta} e^{-2i\zeta\Delta} \bar{v}, e^{is_1\Delta} e^{-i\zeta\Delta} V) ds_1 ds \end{aligned} \quad (2.42)$$

where the local error structure is governed by the second-order commutator type term

$$\begin{aligned} \mathcal{C}^2[f, i\Delta](u, v, w) &:= \mathcal{C}[\mathcal{C}[f, i\Delta], i\Delta](u, v, w) \\ &= \sum_{l=1}^d (\partial_l^2 u \partial_l^2 w) + (2u + v)(\partial_l^2 u \partial_l^2 v) + (\partial_l v)^2 \partial_l^2 u + 2(\partial_l u)^2 \partial_l^2 v + \partial_l v \partial_l u (2\partial_l^2 u + \partial_l^2 v). \end{aligned} \quad (2.43)$$

In practical computations we need to address the stability issues caused by including into the scheme the second term $\mathcal{C}[f, i\Delta](v, e^{-2i\zeta\Delta} \bar{v}, e^{-i\zeta\Delta} V)$ which has the form (2.21), since it involves spatial derivatives. Different approaches can be made to treat this issue and guarantee the stability of the scheme and in what follows we offer two different approaches. The first approach is based on [RS21] and consists in first introducing a stabilization in the Taylor series expansion (2.41) based on finite difference approximations. The second approach relies on directly embedding the commutator term appearing in equation (2.42) into the discretization, and then stabilizes the scheme a posteriori by the use of a properly chosen filter function.

2.4.1 A first approach to guarantee stability

A first approach consists in stabilizing the second term of equation (2.41). This may be done by introducing the following finite difference approximation of $\partial_s \mathcal{N}(\tau, 0, \zeta, \Delta, v)$:

$$\partial_s \mathcal{N}(\tau, 0, \zeta, \Delta, v) = \frac{1}{\tau} (\mathcal{N}(\tau, \tau, \zeta, \Delta, v) - \mathcal{N}(\tau, 0, \zeta, \Delta, v)) + O(\tau \partial_s^2 \mathcal{N}(\tau, \eta, \zeta, \Delta, v)) \quad (2.44)$$

for some $\eta \in [0, \tau]$, and where

$$\partial_s^2 \mathcal{N}(\tau, \eta, \zeta, \Delta, v) = e^{-i\eta\Delta} \mathcal{C}^2[f, i\Delta](e^{i\eta\Delta} v, e^{i\eta\Delta} e^{-2i\zeta\Delta} \bar{v}, e^{i\eta\Delta} e^{-i\zeta\Delta} V). \quad (2.45)$$

The above expansion comes into play in the following lemma, where we obtain a stable second order approximation of the principal oscillation \mathcal{J}_1 .

Lemma 2.4.2 *At second order the principal oscillations can be expanded by*

$$\begin{aligned} \mathcal{J}_1(\tau, \Delta, v) &= \tau(v\varphi_1(-i\tau\Delta)V + v^2\varphi_1(-2i\tau\Delta)\bar{v}) \\ &+ \tau e^{-i\tau\Delta} \left((e^{i\tau\Delta} v)\varphi_2(-i\tau\Delta)(e^{i\tau\Delta} V) + (e^{i\tau\Delta} v)^2\varphi_2(-2i\tau\Delta)(e^{i\tau\Delta} \bar{v}) \right) \\ &- \tau(v\varphi_2(-i\tau\Delta)V + v^2\varphi_2(-2i\tau\Delta)\bar{v}) + iR_{2,1}^1(\tau) \end{aligned}$$

where $\varphi_2(z) = \frac{1}{z}(e^z - \varphi_1(z))$ and the remainder is given by

$$\begin{aligned} R_{2,1}^1(\tau) &= \int_0^\tau \int_0^\zeta \int_0^s e^{-is_1\Delta} \mathcal{C}^2[f, i\Delta](e^{is_1\Delta} v, e^{is_1\Delta} e^{-2i\zeta\Delta} \bar{v}, e^{is_1\Delta} e^{-i\zeta\Delta} V) ds_1 ds d\zeta \\ &+ \int_0^\tau \zeta \int_0^1 \int_0^{\tau s} e^{-is_1\Delta} \mathcal{C}^2[f, i\Delta](e^{is_1\Delta} v, e^{is_1\Delta} e^{-2i\zeta\Delta} \bar{v}, e^{is_1\Delta} e^{-i\zeta\Delta} V) ds_1 ds d\zeta. \end{aligned} \quad (2.46)$$

Proof. Using the filtered function (2.18), and plugging the finite difference (2.44) into the Taylor expansion (2.41) we

obtain

$$\begin{aligned}\mathcal{J}_1(\tau, \Delta, v) &= \int_0^\tau \mathcal{N}(\tau, \zeta, \zeta, \Delta, v) d\zeta \\ &= \int_0^\tau \mathcal{N}(\tau, 0, \zeta, \Delta, v) d\zeta + \frac{1}{\tau} \int_0^\tau \zeta (\mathcal{N}(\tau, \tau, \zeta, \Delta, v) - \mathcal{N}(\tau, 0, \zeta, \Delta, v)) d\zeta \\ &\quad + \int_0^\tau \zeta \int_0^1 \int_0^s \partial_{s_1}^2 \mathcal{N}(\tau, s_1, \zeta, \Delta, v) ds_1 ds d\zeta + \int_0^\tau \int_0^\zeta \int_0^s \partial_{s_1}^2 \mathcal{N}(\tau, s_1, \zeta, \Delta, v) ds_1 ds d\zeta.\end{aligned}$$

Using the filtered function (2.18), equation (2.45) and the definition (2.46) of $R_{2,1}^1(\tau)$ it follows from the above that,

$$\begin{aligned}\mathcal{J}_1(\tau, \Delta, v) &= \int_0^\tau ([e^{-i\zeta\Delta} V]v + [e^{-2i\zeta\Delta} \bar{v}]v^2) d\zeta \\ &\quad + \frac{1}{\tau} e^{-i\tau\Delta} \int_0^\tau \zeta ([e^{-i\zeta\Delta} e^{i\tau\Delta} V](e^{i\tau\Delta} v) + [e^{-2i\zeta\Delta} e^{i\tau\Delta} \bar{v}](e^{i\tau\Delta} v)^2) d\zeta \\ &\quad - \frac{1}{\tau} \int_0^\tau \zeta ([e^{-i\zeta\Delta} V]v + [e^{-2i\zeta\Delta} \bar{v}]v^2) d\zeta + iR_{2,1}^1(\tau) \\ &= \tau(v\varphi_1(-i\tau\Delta)V + v^2\varphi_1(-2i\tau\Delta)\bar{v}) \\ &\quad + \tau e^{-i\tau\Delta} \left((e^{i\tau\Delta} v)\varphi_2(-i\tau\Delta)(e^{i\tau\Delta} V) + (e^{i\tau\Delta} v)^2\varphi_2(-2i\tau\Delta)(e^{i\tau\Delta} \bar{v}) \right) \\ &\quad - \tau(v\varphi_2(-i\tau\Delta)V + v^2\varphi_2(-2i\tau\Delta)\bar{v}) + iR_{2,1}^1(\tau)\end{aligned}$$

which concludes the proof. \square

By merging the two preceding lemmas 2.4.1 and 2.4.2, we obtain the following second order low-regularity scheme for (2.1).

Corollary 2.4.3 *The exact solution u of (2.1) can be expanded as*

$$\begin{aligned}u(t_n + \tau) &= e^{i\tau\Delta} u(t_n) - i\tau e^{i\tau\Delta} (u(t_n)\varphi_1(-i\tau\Delta)V + u(t_n)^2\varphi_1(-2i\tau\Delta)\bar{u}(t_n)) \\ &\quad - i\tau \left((e^{i\tau\Delta} u(t_n))\varphi_2(-i\tau\Delta)(e^{i\tau\Delta} V) + (e^{i\tau\Delta} u(t_n))^2\varphi_2(-2i\tau\Delta)e^{i\tau\Delta}\bar{u}(t_n) \right) \\ &\quad + i\tau e^{i\tau\Delta} (u(t_n)\varphi_2(-i\tau\Delta)V + u(t_n)^2\varphi_2(-2i\tau\Delta)\bar{u}(t_n)) \\ &\quad - \frac{\tau^2}{2} e^{i\tau\Delta} (|u(t_n)|^4 u(t_n) + 3u(t_n)|u(t_n)|^2 V - |u(t_n)|^2 u(t_n)\bar{V} + u(t_n)V^2) \\ &\quad + \mathcal{R}_2^1(\tau, t_n)\end{aligned}\tag{2.47}$$

where the remainder is given by

$$\begin{aligned}\mathcal{R}_2^1(\tau, t_n) &= \int_0^\tau e^{i(\tau-\zeta)\Delta} [f(u(t_n + \zeta), \bar{u}(t_n + \zeta), V) - f(e^{i\zeta} u(t_n), e^{-i\zeta} \bar{u}(t_n), V)] d\zeta \\ &\quad + e^{i\tau\Delta} \int_0^\tau \zeta (|u(t_n)|^4 u(t_n) + 3u(t_n)|u(t_n)|^2 V - |u(t_n)|^2 u(t_n)\bar{V} + u(t_n)V^2) d\zeta \\ &\quad + \int_0^\tau \int_0^\zeta \int_0^s e^{i(\tau-s_1)\Delta} \mathcal{C}^2[f, i\Delta](e^{is_1\Delta} u(t_n), e^{is_1\Delta} e^{-2i\zeta\Delta} \bar{u}(t_n), e^{is_1\Delta} e^{-i\zeta\Delta} V) ds_1 ds d\zeta \\ &\quad + \int_0^\tau \zeta \int_0^1 \int_0^{\tau s} e^{i(\tau-s_1)\Delta} \mathcal{C}^2[f, i\Delta](e^{is_1\Delta} u(t_n), e^{is_1\Delta} e^{-2i\zeta\Delta} \bar{u}(t_n), e^{is_1\Delta} e^{-i\zeta\Delta} V) ds_1 ds d\zeta.\end{aligned}\tag{2.48}$$

and where the explicit expression for the commutator is given in equation (2.43).

2.4.2 A second approach to guarantee stability

We next present a second approach to the second order approximation of the principal oscillations \mathcal{J}_1 . In contrast to the preceding section we will first write the approximation in terms of the commutator, then stabilize the scheme by the use of a properly chosen filter function.

Lemma 2.4.4 *To second order the principal oscillations can be expanded by*

$$\begin{aligned} \mathcal{J}_1(\tau, \Delta, v) &= \tau(v\varphi_1(-i\tau\Delta)V + v^2\varphi_1(-2i\tau\Delta)\bar{v}) + \tau^2\mathcal{C}[f, i\Delta](v, \varphi_2(-2i\tau\Delta)\bar{v}, \varphi_2(-i\tau\Delta)V) \\ &\quad + iR_{2,1}^2(\tau) \end{aligned} \quad (2.49)$$

where the remainder is given by,

$$R_{2,1}^2(\tau) = \int_0^\tau \int_0^\zeta \int_0^s e^{-is_1\Delta} \mathcal{C}^2[f, i\Delta](e^{is_1\Delta}v, e^{is_1\Delta}e^{-2i\zeta\Delta}\bar{v}, e^{is_1\Delta}e^{-i\zeta\Delta}V) ds_1 ds d\zeta. \quad (2.50)$$

Proof. Using the definition of the principal oscillations (2.13) and equation (2.42) one has the following expansion,

$$\begin{aligned} \mathcal{J}_1(\tau, \Delta, v) &= \int_0^\tau f(v, e^{-2i\zeta\Delta}\bar{v}, e^{-i\zeta\Delta}V) d\zeta + \int_0^\tau \zeta \mathcal{C}[f, i\Delta](v, e^{-2i\zeta\Delta}\bar{v}, e^{-i\zeta\Delta}V) d\zeta \\ &\quad + \int_0^\tau \int_0^\zeta \int_0^s e^{-is_1\Delta} \mathcal{C}^2[f, i\Delta](e^{is_1\Delta}v, e^{is_1\Delta}e^{-2i\zeta\Delta}\bar{v}, e^{is_1\Delta}e^{-i\zeta\Delta}V) ds_1 ds d\zeta \\ &= \tau(v\varphi_1(-i\tau\Delta)V + v^2\varphi_1(-2i\tau\Delta)\bar{v}) + \tau^2\mathcal{C}[f, i\Delta](v, \varphi_2(-2i\tau\Delta)\bar{v}, \varphi_2(-i\tau\Delta)V) \\ &\quad + iR_{2,1}^2(\tau). \end{aligned}$$

where the second term could be integrated exactly using the structure of the commutator (2.21) and of the nonlinearity (2.4) \square

The following lemma provides the second order low regularity integrator up to this step.

Lemma 2.4.5 *The exact solution u of (2.1) can be expanded as*

$$\begin{aligned} u(t_n + \tau) &= e^{i\tau\Delta}u(t_n) - i\tau e^{i\tau\Delta}(u(t_n)\varphi_1(-i\tau\Delta)V + u(t_n)^2\varphi_1(-2i\tau\Delta)\bar{u}(t_n)) \\ &\quad - i\tau^2 e^{i\tau\Delta} \mathcal{C}[f, i\Delta](u(t_n), \varphi_2(-2i\tau\Delta)\bar{u}(t_n), \varphi_2(-i\tau\Delta)V) \\ &\quad - \frac{\tau^2}{2} e^{i\tau\Delta} (|u(t_n)|^4 u(t_n) + 3u(t_n)|u(t_n)|^2 V - |u(t_n)|^2 u(t_n)\bar{V} + u(t_n)V^2) \\ &\quad + R_{2,2}^2(\tau, t_n) \end{aligned} \quad (2.51)$$

where the remainder is given by

$$\begin{aligned} R_{2,2}^2(\tau) &= \int_0^\tau e^{i(\tau-\zeta)\Delta} [f(u(t_n + \zeta), \bar{u}(t_n + \zeta), V) - f(e^{i\zeta}u(t_n), e^{-i\zeta}\bar{u}(t_n), V)] d\zeta \\ &\quad + e^{i\tau\Delta} \int_0^\tau \zeta (|u(t_n)|^4 u(t_n) + 3u(t_n)|u(t_n)|^2 V - |u(t_n)|^2 u(t_n)\bar{V} + u(t_n)V^2) d\zeta \\ &\quad + \int_0^\tau \int_0^\zeta \int_0^s e^{i(\tau-s_1)\Delta} \mathcal{C}^2[f, i\Delta](e^{is_1\Delta}u(t_n), e^{is_1\Delta}e^{-2i\zeta\Delta}\bar{u}(t_n), e^{is_1\Delta}e^{-i\zeta\Delta}V) ds_1 ds d\zeta. \end{aligned}$$

To stabilize the term appearing in the second line of equation (2.51), which is of the form $\tau^2\mathcal{C}[f, i\Delta](v, \bar{v}, V)$, we introduce an appropriate filter operator which we denote by Ψ . More precisely, we will construct a filter operator of the form

$$\Psi = \psi(i\tau|\nabla|),$$

where ψ is a suitably chosen filter function which allows to stabilize the scheme while introducing an error term which only requires H^2 -regularity on the initial data and potential. Namely, we require the filter function ψ to introduce the same optimal local error of $O(\tau^3\Delta(v+V))$ as is introduced by the low-regularity second order scheme up to this step (see equations (2.39), (2.43) and Section 2.4.3 for the thorough analysis). We refer to [HLW10] for an introduction to filter functions in the ODE setting. We now present two sufficient assumptions on the filter operator which once established, guarantees the stability of the low-regularity scheme (2.51).

Assumption 1. The filter operator $\Psi = \psi(i\tau|\nabla|)$, satisfies the following bound

$$\|\tau\Psi[\mathcal{C}[f, i\Delta](v, \bar{v}, V)]\|_r \leq C_{r,d,v} \|v\|_r^m \quad (2.52)$$

for some $m = m(f) \in \mathbb{N}$ and $r = r(d) \geq 0$.

Assumption 2. The filter operator $\Psi = \psi(i\tau|\nabla|)$ satisfies the following expansion

$$\Psi[\mathcal{C}[f, i\Delta](v, \bar{v}, V)] = \mathcal{C}[f, i\Delta](v, \bar{v}, V) + O(\tau|\nabla|^2(v + V)). \quad (2.53)$$

The condition in Assumption 1 guarantees the stability of the scheme in the H^r -norm, while the condition in Assumption 2 preserves the optimal local error structure of $O(\tau^3|\nabla|^2(v + V))$ with the inclusion of the filter function ψ . This is an essential ingredient for the local and global error analysis of the scheme.

Remark 2.4.6 The stability estimate (2.52) relies on the algebraic structure of the underlying space. In the following stability analysis we will restrict our attention to sufficiently smooth Sobolev spaces H^r with $r > \frac{d}{2} + 1$. This allows us to exploit the following classical bilinear estimate,

$$\|vw\|_{s_0} \leq C\|v\|_{s_0}\|w\|_{s_0},$$

where $s_0 = r - 1$. An analysis in a lower order Sobolev space would require the use of more refined estimates on the commutator term using the generalized Leibniz rule (see [BCD11, Chapter 2]). This analysis is not detailed here, since we tackle the error analysis of the second order scheme (2.47), based upon the first approach (see Section 2.4.1).

A choice of filter operator which is well adapted for the second order scheme (2.51) is the following.

Lemma 2.4.7 *The filter operator*

$$\Psi = \varphi_1(i\tau|\nabla|) := \frac{e^{i\tau|\nabla|} - 1}{i\tau|\nabla|} \quad (2.54)$$

satisfies Assumption 1 and 2 with $r > \frac{d}{2} + 1$.

Proof. We first show how the filter function (2.54) satisfies Assumption 1 and hence guarantees the stability of the second order low-regularity scheme. By definition of the φ_1 function and using the explicit form of the commutator (2.21) together with the bilinear estimate we have,

$$\begin{aligned} \|\tau\varphi_1(i\tau|\nabla|)\mathcal{C}[f, i\Delta](v, \bar{v}, V)\|_r &\leq \|(e^{i\tau|\nabla|} - 1)|\nabla|^{-1}\mathcal{C}[f, i\Delta](v, \bar{v}, V)\|_r \\ &\leq 4\|\nabla V \cdot \nabla v + |\nabla v|^2\bar{v} + 2v\nabla v \cdot \nabla\bar{v}\|_{r-1} \\ &\leq C_{r,d}(\|\nabla V\|_{r-1}\|\nabla v\|_{r-1} + \|\nabla v\|_{r-1}^2\|v\|_{r-1} \\ &\quad + 2\|v\|_{r-1}\|\nabla v\|_{r-1}^2) \\ &\leq C_{r,d}(\|V\|_r\|v\|_r + 3\|v\|_r^3) \\ &\leq C_{r,d,V}(\|v\|_r + \|v\|_r^3). \end{aligned}$$

Furthermore, by a simple Taylor's expansion we have that,

$$\varphi_1(i\tau|\nabla|) = 1 + O(\tau|\nabla|). \quad (2.55)$$

It then follows by the form of the commutator (2.21) that the filter function (2.54) satisfies Assumption 2. Indeed, from the above equation we have,

$$\varphi_1(i\tau|\nabla|)\mathcal{C}[f, i\Delta](v, \bar{v}, V) = \mathcal{C}[f, i\Delta](v, \bar{v}, V) + O(\tau|\nabla|\mathcal{C}[f, i\Delta](v, \bar{v}, V)),$$

where by equation (2.21) we have that formally $O(\tau|\nabla|\mathcal{C}[f, i\Delta](v, \bar{v}, V)) = O(\tau|\nabla|^2(v + V))$. Hence, formally we see that the inclusion of the filter function (2.54) preserves the optimal local error, by only requiring two additional derivatives on the initial datum and the potential (see Proposition 2.4.9, in the regime $r > \frac{d}{2}$). \square

The following Corollary provides a *stable* second order low-regularity scheme for (2.1), by using the filter function (2.54).

Corollary 2.4.8 *The exact solution u of (2.1) can be expanded as*

$$\begin{aligned} u(t_n + \tau) &= e^{i\tau\Delta}u(t_n) - i\tau e^{i\tau\Delta}(u(t_n)\varphi_1(-i\tau\Delta)V + u(t_n)^2\varphi_1(-2i\tau\Delta)\bar{u}(t_n)) \\ &\quad - i\tau^2 e^{i\tau\Delta}\varphi_1(i\tau|\nabla|)\mathcal{C}[f, i\Delta](u(t_n), \varphi_2(-2i\tau\Delta)\bar{u}(t_n), \varphi_2(-i\tau\Delta)V) \\ &\quad - \frac{\tau^2}{2} e^{i\tau\Delta}(|u(t_n)|^4 u(t_n) + 3u(t_n)|u(t_n)|^2 V - |u(t_n)|^2 u(t_n)\bar{V} + u(t_n)V^2) \\ &\quad + \mathcal{R}_2^2(\tau, t_n). \end{aligned} \quad (2.56)$$

where

$$\begin{aligned} \mathcal{R}_2^2(\tau, t_n) &= \int_0^\tau e^{i(\tau-\zeta)\Delta} [f(u(t_n + \zeta), \bar{u}(t_n + \zeta), V) - f(e^{i\zeta}u(t_n), e^{-i\zeta}\bar{u}(t_n), V)] d\zeta \\ &+ e^{i\tau\Delta} \int_0^\tau \zeta (|u(t_n)|^4 u(t_n) + 3u(t_n)|u(t_n)|^2 V - |u(t_n)|^2 u(t_n)\bar{V} + u(t_n)V^2) d\zeta \\ &+ \int_0^\tau \int_0^\zeta \int_0^s e^{i(\tau-s_1)\Delta} \mathcal{C}^2[f, i\Delta](e^{is_1\Delta}u(t_n), e^{is_1\Delta}e^{-2i\zeta\Delta}\bar{u}(t_n), e^{is_1\Delta}e^{-i\zeta\Delta}V) ds_1 d\zeta ds \\ &- i\tau^2 e^{i\tau\Delta} (I - \varphi_1(i\tau\nabla)) [\mathcal{C}[f, i\Delta](u(t_n), \varphi_2(-2i\tau\Delta)\bar{u}(t_n), \varphi_2(-i\tau\Delta)V)]. \end{aligned}$$

2.4.3 Local error estimates

In this section we prove that the second order scheme (2.47) introduces a local error of order three under favorable regularity assumptions of the initial datum and potential. As was the case for the error analysis of the first-order scheme (Section 2.3.3), we make the analysis in H^r -norm where the regularity assumptions on v and V will depend on the regime of r considered.

Proposition 2.4.9 *Let $T > 0$, $r \geq 0$, and r_2 as in Theorem 2.1.2, namely*

$$r_2 = \begin{cases} 2 + r, & \text{if } r > \frac{d}{2}, \\ 2 + \frac{r}{2} + \frac{d}{4}, & \text{if } 0 \leq r < \frac{d}{2}. \end{cases}$$

Assume there exists $C_T > 0$ such that

$$\sup_{[0, T]} \|u(t)\|_{H^{r_2}} \leq C_T, \quad \text{and} \quad \|V\|_{H^{r_2}} \leq C_T,$$

then there exists $M_T > 0$ such that for every $\tau \in (0, 1]$

$$\|\mathcal{R}_2^1(\tau, t_n)\|_{H^r} \leq M_T \tau^3, \quad 0 \leq t_n \leq T,$$

where $t_n = n\tau$, and $\mathcal{R}_2^1(\tau, t_n)$ is given in equation (2.48).

Proof. We write the error term $\mathcal{R}_2^1(\tau, t_n)$, as the sum of four terms, $\mathcal{R}_2^1(\tau, t_n) = \mathcal{E}^1(\tau, t_n) + \mathcal{E}^2(\tau, t_n) + \mathcal{E}^3(\tau, t_n) + \mathcal{E}^4(\tau, t_n)$. We start by establishing the third order estimate for the two last terms \mathcal{E}^3 and \mathcal{E}^4 . These bounds are obtained using the same arguments as those made to bound the term \mathcal{G}^2 in the proof of Proposition 2.3.2, by noticing that $r_2 = r_1 + 1$. Indeed, from the explicit expression of the second-order commutator (2.43) and using the inequality (2.10), we obtain that for $r > \frac{d}{2}$,

$$\|\mathcal{C}^2[f, i\Delta](u, v, w)\|_{H^r} \leq C_r (\|w\|_{H^{r+2}}, \|u\|_{H^{r+2}}, \|v\|_{H^{r+2}}), \quad (2.57)$$

and for $0 \leq r < \frac{d}{2}$ and $l = 1, \dots, d$,

$$\begin{aligned} \|\mathcal{C}^2[f, i\Delta](u, v, w)\|_{H^r} &\leq C_{r,d} (\|\partial_l^2 w\|_{H^{\frac{r}{2} + \frac{d}{4}}}, \|\partial_l^2 u\|_{H^{\frac{r}{2} + \frac{d}{4}}}, \|\partial_l^2 v\|_{H^{\frac{r}{2} + \frac{d}{4}}}, \|u\|_{H^{\sigma_0}}, \|v\|_{H^{\sigma_0}}, \|\partial_l^2 u\|_{H^r}, \|\partial_l^2 v\|_{H^r}, \\ &\quad \|\partial_l v\|_{H^{\sigma_0}}, \|\partial_l u\|_{H^{\sigma_0}}) \\ &\leq C_{r,d} (\|w\|_{H^{2 + \frac{r}{2} + \frac{d}{4}}}, \|u\|_{H^{2 + \frac{r}{2} + \frac{d}{4}}}, \|v\|_{H^{2 + \frac{r}{2} + \frac{d}{4}}}, \|u\|_{H^{2+r}}, \|v\|_{H^{2+r}}, \|u\|_{H^{1+\sigma_0}}, \|v\|_{H^{1+\sigma_0}}) \\ &\leq C_{r,d} (\|w\|_{H^{2 + \frac{r}{2} + \frac{d}{4}}}, \|u\|_{H^{2 + \frac{r}{2} + \frac{d}{4}}}, \|v\|_{H^{2 + \frac{r}{2} + \frac{d}{4}}}), \end{aligned}$$

where we once again used the bilinear estimates (2.28) and (2.10) with $\sigma = \sigma_0$ in the first line, and in the third line the definition (2.26) of σ_0 and the fact that $r < \frac{r}{2} + \frac{d}{4}$ when $r < \frac{d}{2}$.

Next, we show that the sum of the remaining terms, $(\mathcal{E}^1 + \mathcal{E}^2)(\tau, t_n)$, of equation (2.48) is of third order. We have that $r_2 > 2$, and hence $u(t), V \in H^2$. Thereby, by Taylor expanding the exponential appearing inside the Duhamel's integral (2.3) we obtain the following expansion : $u(t_n + \zeta) = e^{i\zeta\Delta}u(t_n) + \zeta f^n + \tilde{R}(\zeta, t_n)$ where $f^n = f(u(t_n), \bar{u}(t_n), V)$ and

$$\tilde{R}(\zeta, t_n) = \int_0^\zeta e^{i(\zeta-s)\Delta} f(u(t_n + s), \bar{u}(t_n + s), V) ds - \zeta f^n. \quad (2.58)$$

Using the above expansion for u we rewrite the error term $(\mathcal{E}^1 + \mathcal{E}^2)(\tau, t_n)$ as,

$$\begin{aligned} (\mathcal{E}^1 + \mathcal{E}^2)(\tau, t_n) &= \int_0^\tau e^{i(\tau-\zeta)\Delta} [f(e^{i\zeta\Delta}u(t_n) + \zeta f^n + \tilde{R}(\zeta, t_n), e^{-i\zeta\Delta}\bar{u}(t_n) + \zeta\bar{f}^n + \overline{\tilde{R}(\zeta, t_n)}, V) \\ &\quad - f(e^{i\zeta\Delta}u(t_n), e^{-i\zeta\Delta}\bar{u}(t_n), V)] d\zeta \\ &\quad - e^{i\tau\Delta} \int_0^\tau \zeta (D_1 f^n \cdot f^n + D_2 f^n \cdot \bar{f}^n) d\zeta, \end{aligned} \quad (2.59)$$

where $D_1 f^n \cdot f^n + D_2 f^n \cdot \bar{f}^n$ is given by equation (2.40). For notational convenience we let $a_1 := e^{i\zeta\Delta}u(t_n) + \zeta f^n$. The idea in order to show that the above error term (2.59) is of third-order revolves around making three suitable Taylor expansions. By Taylor expanding f around (a_1, \bar{a}_1, V) and $(e^{i\zeta\Delta}u(t_n), e^{-i\zeta\Delta}\bar{u}(t_n), V)$ respectively we obtain,

$$\begin{aligned} f(a_1 + \tilde{R}(\zeta, t_n), \bar{a}_1 + \overline{\tilde{R}(\zeta, t_n)}, V) &= f(a_1, \bar{a}_1, V) + E_1(\zeta), \\ f(a_1, \bar{a}_1, V) &= f(e^{i\zeta\Delta}u(t_n), e^{-i\zeta\Delta}\bar{u}(t_n), V) + E_2(\zeta), \end{aligned} \quad (2.60)$$

where

$$\begin{aligned} E_1(\zeta) &= \int_0^1 D_1 f(a_1 + \theta\tilde{R}(\zeta, t_n), \bar{a}_1 + \theta\overline{\tilde{R}(\zeta, t_n)}, V) \cdot \tilde{R}(\zeta, t_n) \\ &\quad + D_2 f(a_1 + \theta\tilde{R}(\zeta, t_n), \bar{a}_1 + \theta\overline{\tilde{R}(\zeta, t_n)}, V) \cdot \overline{\tilde{R}(\zeta, t_n)} d\theta, \end{aligned} \quad (2.61)$$

$$\begin{aligned} E_2(\zeta) &= \zeta \int_0^1 [D_1 f(e^{i\zeta\Delta}u(t_n) + \theta\zeta f^n, e^{-i\zeta\Delta}\bar{u}(t_n) + \theta\zeta\bar{f}^n, V) \cdot f^n \\ &\quad + D_2 f(e^{i\zeta\Delta}u(t_n) + \theta\zeta f^n, e^{-i\zeta\Delta}\bar{u}(t_n) + \theta\zeta\bar{f}^n, V) \cdot \bar{f}^n] d\theta. \end{aligned} \quad (2.62)$$

Hence, plugging equation (2.60) into equation (2.59) yields,

$$(\mathcal{E}^1 + \mathcal{E}^2)(\tau, t_n) = \int_0^\tau e^{i(\tau-\zeta)\Delta} E_1(\zeta) d\zeta + e^{i\tau\Delta} \int_0^\tau e^{-i\zeta\Delta} E_2(\zeta) d\zeta - e^{i\tau\Delta} \int_0^\tau \zeta (D_1 f^n \cdot f^n + D_2 f^n \cdot \bar{f}^n) d\zeta. \quad (2.63)$$

In order to show that the first term in the above equation is of third-order we show the bound $\|E_1(\zeta)\|_r \leq C_T \zeta^2$. By equation (2.61) and by using the bilinear inequality (2.10) we have that for all $r \geq 0$ and some $\sigma > \frac{d}{2}$,

$$\begin{aligned} \|E_1(\zeta)\|_r &\leq \sup_{\theta \in [0,1]} \left(\|D_1 f(a_1 + \theta\tilde{R}(\zeta, t_n), \bar{a}_1 + \theta\overline{\tilde{R}(\zeta, t_n)}, V)\|_\sigma \right. \\ &\quad \left. + \|D_2 f(a_1 + \theta\tilde{R}(\zeta, t_n), \bar{a}_1 + \theta\overline{\tilde{R}(\zeta, t_n)}, V)\|_\sigma \right) \|\tilde{R}(\zeta, t_n)\|_r \\ &\leq C_r \left(\|V\|_\sigma, \sup_{t \in [0,T]} \|u(t)\|_\sigma, \sup_{(\zeta,t) \in [0,\tau] \times [0,T]} \|\tilde{R}(\zeta, t)\|_\sigma \right) \|\tilde{R}(\zeta, t_n)\|_r \end{aligned} \quad (2.64)$$

where the last inequality follows by using the explicit form of the derivatives (2.38), the first estimation of equation (2.11), and the fact that $e^{i\zeta\Delta}$ is an isometry on Sobolev spaces. When $r > \frac{d}{2}$, the above holds for $\sigma = r$. Next, we show that,

$$\sup_{(\zeta,t) \in [0,\tau] \times [0,T]} \|\tilde{R}(\zeta, t)\|_{\sigma_0} < +\infty, \quad \text{and} \quad \|\tilde{R}(\zeta, t_n)\|_r \leq C_T \zeta^2, \quad (2.65)$$

where σ_0 is given by equation (2.26). We obtain the first bound by using the first estimate of equation (2.11) on f with $r = \sigma_0$,

$$\sup_{(\zeta,t) \in [0,\tau] \times [0,T]} \|\tilde{R}(\zeta, t)\|_{\sigma_0} \leq \tau C_{\sigma_0} \left(\sup_{t \in [0,T]} \|u(t)\|_{\sigma_0}, \|V\|_{\sigma_0} \right) < +\infty.$$

Next, we obtain the second estimate in equation (2.65) using the Fundamental Theorem of Calculus. By letting

$u = u(t_n + s_1)$ we have,

$$\begin{aligned}\tilde{R}(\zeta, t_n) &= \int_0^\zeta \int_0^s \partial_{s_1} \left(e^{i(\zeta-s_1)\Delta} f(u, \bar{u}, V) \right) ds_1 ds + \zeta e^{i\zeta\Delta} f^n - \zeta f^n \\ &= \int_0^\zeta \int_0^s e^{i(\zeta-s_1)\Delta} \left(i\Delta f(u, \bar{u}, V) + D_1 f(u, \bar{u}, V)(i\Delta u + f(u, \bar{u}, V)) \right. \\ &\quad \left. + D_2 f(u, \bar{u}, V)(-i\overline{\Delta u} + \overline{f(u, \bar{u}, V)}) \right) ds_1 ds + i\zeta^2 \varphi_1(i\zeta\Delta)\Delta f(u, \bar{u}, V),\end{aligned}\tag{2.66}$$

where to obtain the second line we used equation (2.1), and for the last term we used the definition of the φ_1 operator. The second estimate of equation (2.65) then follows immediately from equation (2.66) by observing that,

$$\|\Delta f(v, \bar{v}, V)\|_r + \|D_i f(v, \bar{v}, V)\Delta u\|_r \leq C_r(\|v\|_{r_2}, \|V\|_{r_2}), \quad i = 1, 2.$$

It remains to show that the difference of the second and third term in equation (2.63) is of third-order. Formally, this directly follows by making a Taylor expansion of $e^{i\zeta\Delta}u(t_n) + \theta\zeta f^n$ around $\zeta = 0$: $e^{i\zeta\Delta}u(t_n) + \theta\zeta f^n = u(t_n) + O(\zeta\Delta u(t_n))$. By using the same application of the Fundamental Theorem of Calculus as done in equation (2.66) one obtains this third order bound. This concludes the proof. \square

2.4.4 Global error estimate

Using the local error estimates established in the preceding section together with a stability argument we show global second order convergence of our low regularity integrator under the regularity assumptions established in Proposition 2.4.9.

Proof of Theorem 2.1.2. We let $u^{n+1} = \Phi_2^\tau(u^n)$ be the numerical scheme defined in equation (2.7). The outline of the proof of this second-order convergence result follows exactly the same lines as the first order convergence result given in Theorem 2.1.1. Indeed, in the case where $r > \frac{d}{2}$ the global error estimate follows by a classical *Lady Windermere's argument* ([HLW10]). In the regime $r < \frac{d}{2}$, by exploiting the same interpolation argument as made in the proof of Theorem 2.1.1, and by using definition (2.48) of \mathcal{R}_2^1 we have that there exists an $\delta > 0$ such that

$$\|\mathcal{R}_2^1(\tau, t_n)\|_{H^{\sigma_0}} \leq M_T \tau^{1+\delta},$$

where σ_0 is defined in equation (2.26). From the above we obtain the bound (2.34) and hence the apriori H^{σ_0} -bound on the iterates: $\sup_{n\tau \leq T} \|u^n\|_{H^{\sigma_0}} < +\infty$, for τ sufficiently small. Using the local error analysis given in Proposition 2.4.9 we obtain second order convergence of the scheme (2.7) by performing an inductive argument with

$$\|e^{n+1}\|_{H^r} \leq M_T \tau^3 + e^{L_n \tau} \|e^n\|_{H^r}, \quad e^0 = 0,\tag{2.67}$$

since $\sup_{n\tau \leq T} L_n \leq C_{T,r}(\|u^n\|_{H^{\sigma_0}}) < +\infty$. This concludes the proof. \square

2.5 Numerical Experiments

In this section we provide some numerical experiments to support our theoretical convergence results. We consider the Gross-Pitaevskii equation (2.1) with an initial data of the form

$$u_0(x) = \sum_{k \in \mathbb{Z}} (1 + |k|)^{-\vartheta - \frac{1}{2}} a_k e^{ikx},\tag{2.68}$$

where the coefficients $(a_k)_{k \in \mathbb{Z}}$ are chosen as uniformly distributed random complex numbers in $[0, 1] + i[0, 1]$, using the matlab function `rand`. The parameter $\vartheta \geq 0$ dictates the regularity assumption on the above function (2.68), namely it insures that $u_0 \in H^{\vartheta - \epsilon}$. We choose the potential V to have the same form (2.68), as the initial condition.

For the space discretization, we couple the first and second order low-regularity time integrators (2.5) and (2.7) with a standard Fourier pseudo-spectral method. We take the largest Fourier mode as $K = 2^{10}$, yielding a spatial mesh size of $\Delta x = 0.0061$.

In order to test our convergence result, we choose to measure the error in the (discrete) L^2 , $H^{\frac{1}{2}}$, and H^1 norms. For each of these three norms we plot the first and second order low regularity integrators given in equations (2.5) and (2.7) for $u_0, V \in H^{r_1}$ and $u_0, V \in H^{r_2}$ respectively (see equations (2.6) and (2.8)). The error at time $T = 1$ are given in Figure (2.1). The results of our numerical experiments agree with the corresponding theoretical convergence results: we observed first and second order convergence for the regularity assumptions given in Theorem 2.1.1 and 2.1.2. We recall that in the

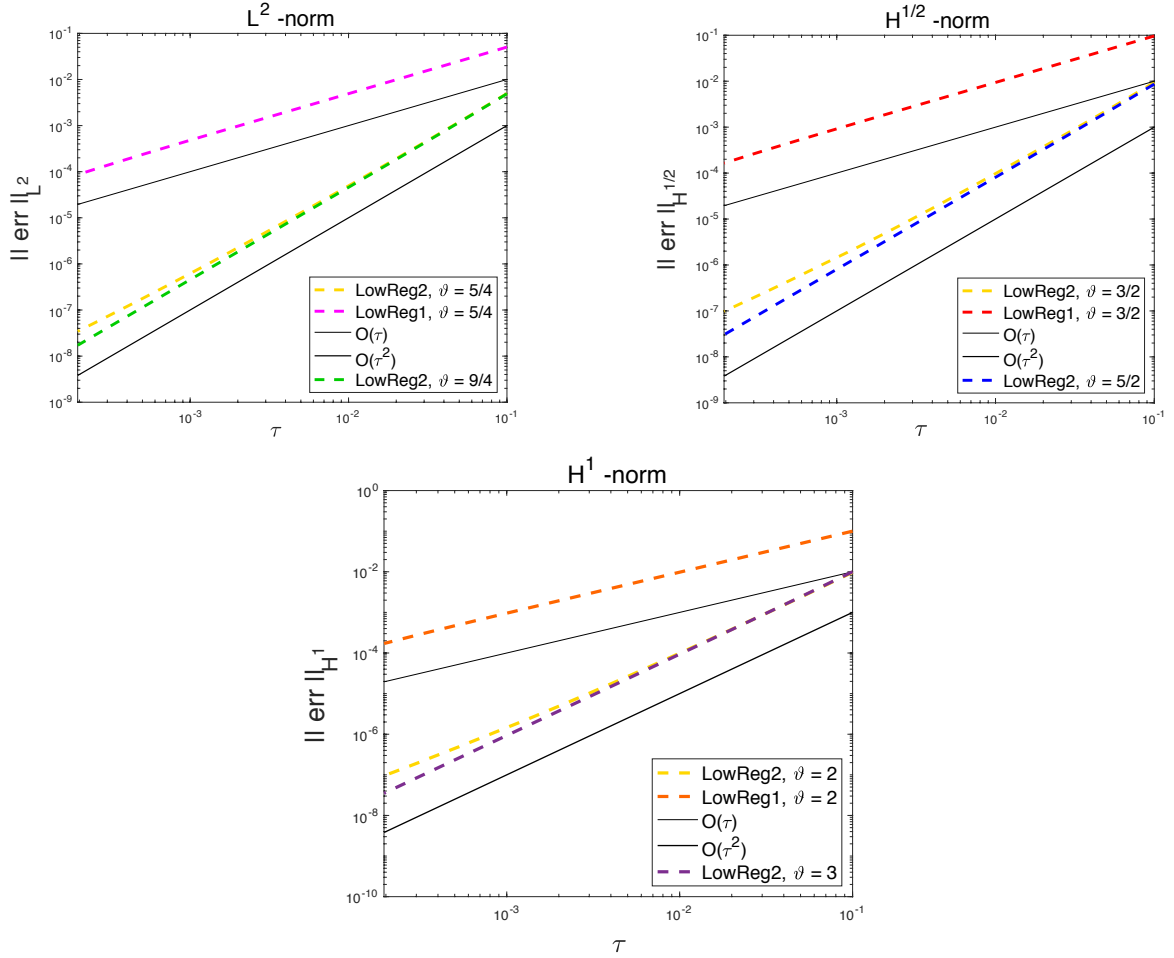


Figure 2.1 – Convergence plots for three different norms, taken from the article [AB23a]. The slopes of the continuous lines are one and two, respectively. Plot (a) : first and second order scheme with $\vartheta = 5/4$ (pink and yellow), and for the second-order scheme with $\vartheta = 9/4$ (green). Plot (b): first and second order scheme with $\vartheta = \frac{3}{2}$ (red and yellow), and for the second order scheme with $\vartheta = 5/2$ (blue). Plot (c): first and resp. second order schemes with $\vartheta = 2$ (orange and yellow) and second order with $\vartheta = 3$ (purple).

critical case $r = \frac{1}{2}$, we have $r_j = j + \frac{1}{2} + \epsilon$, $j = 1, 2$, where $\epsilon > 0$ can be taken arbitrarily small. Moreover, as expected, the yellow lines in Figure 2.1 show how the second order scheme exhibits order reduction for the less regular data and potential $u_0, V \in H^{r_1}$. Nevertheless, it successfully converges to second order for $u_0, V \in H^{r_2}$. We lastly note that the observed convergence is slightly better than predicted by Theorem 2.1.1 and 2.1.2 (see as well the work of [OS18]).

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Appendix

In this section we derive the bilinear H^r -estimates, for $r > 0$, as stated in Section 2.2. Namely we show the estimate (2.10) in both regimes $r > \frac{d}{2}$, and $0 < r \leq \frac{d}{2}$. We note that the case $r = 0$ of the L^2 -norm follows easily by the Sobolev embedding $H^\sigma \hookrightarrow L^\infty$, $\sigma > \frac{d}{2}$.

The notation and tools we use are based upon Littlewood-Paley Theory (see [BCD11, Chapter 2]). We will apply this machinery to our study on the torus \mathbb{T}^d . Given any tempered distribution u , the Littlewood-Paley theory provides the following decomposition,

$$u = \sum_{k \geq -1} \Delta_k u, \quad \mathcal{F}(\Delta_k u)(\xi) = \varphi_k(\xi) \hat{u}(\xi),$$

where $\varphi_k(\xi) = \varphi(\xi/2^k)$, for $k \geq 0$, $\varphi_{-1} = \chi$, and φ, χ satisfy the assertions in [BCD11, Proposition 2.10], namely they form a dyadic partition of unity. In the above and in the remainder of this section we use the fact that, as is the case when working on \mathbb{R}^d , one can make use of the Fourier transform on \mathbb{T}^d , where in the periodic case we have that $\xi \in \mathbb{Z}^d$.

Using the above Littlewood-Paley decomposition, we introduce Bony's decomposition in order to express the product of two tempered distributions uv as the following sum of three terms,

$$uv = T_u(v) + T_v(u) + R(u, v) \quad (2.69)$$

where $T_u(v) = \sum_j S_{j-1}u\Delta_j v$, $S_{j-1}u = \sum_{i \leq j-2} \Delta_i u$, and the remainder $R(u, v) = \sum_{|k-j| \leq 1} \Delta_k u \Delta_j v$.

In what follows we shall make use of the embedding $H^r \hookrightarrow B_{\infty, \infty}^{r-\frac{d}{2}}$, for non homogeneous Besov spaces, (see [BCD11, Proposition 2.71]).

We are now ready to demonstrate the estimate (2.10) in the regime $0 < r \leq \frac{d}{2}$. Let $\epsilon > 0$. First by [BCD11, Proposition 2.85] together with the embedding $H^{\frac{d}{2}} \hookrightarrow B_{\infty, \infty}^0$, we have the following estimate of the remainder,

$$\|R(u, v)\|_{H^r} \leq C_{r,d} \|v\|_{H^r} \|u\|_{H^{\frac{d}{2}}}, \quad r > 0.$$

Next, by using the first estimate of [BCD11, Theorem 2.82] together with the embedding $H^{\frac{d}{2}+\epsilon} \hookrightarrow L^\infty$ we have the following estimate on the paraproduct of v by u ,

$$\|T_u v\|_{H^r} \leq \|u\|_{H^{\frac{d}{2}+\epsilon}} \|v\|_{H^r}, \quad r > 0.$$

Using the second estimate of [BCD11, Theorem 2.82] we obtain that for any $0 < r \leq \frac{d}{2}$ the following estimate of the paraproduct of u by v holds,

$$\|T_v u\|_{H^r} \leq \begin{cases} \|u\|_{H^{\frac{d}{2}}} \|v\|_{H^r}, & \text{for } 0 < r < \frac{d}{2}, \\ \|u\|_{H^{\frac{d}{2}+\epsilon}} \|v\|_{H^{\frac{d}{2}}}, & \text{if } r = \frac{d}{2}, \end{cases}$$

where we used the embedding $H^r \hookrightarrow B_{\infty, \infty}^{r-\frac{d}{2}}$, and respectively $H^{\frac{d}{2}-\epsilon} \hookrightarrow B_{\infty, \infty}^{-\epsilon}$ in the case $r = \frac{d}{2}$. Therefore, when $0 < r \leq \frac{d}{2}$, by collecting the above bounds, together with the decomposition (2.69), we recover the estimate (2.10):

$$\|uv\|_{H^r} \leq C_{r,d} \|u\|_{H^{\frac{d}{2}+\epsilon}} \|v\|_{H^r}.$$

Finally, we show the estimate (2.10) in the regime $r > \frac{d}{2}$, with $\sigma = r$. By [BCD11, Corollary 2.86] we have,

$$\|uv\|_{H^r} \leq \frac{C^{r+1}}{r} (\|u\|_{L^\infty} \|v\|_{H^r} + \|u\|_{H^r} \|v\|_{L^\infty}), \quad r > 0.$$

Hence, given any $r > \frac{d}{2}$, using the embedding $H^r \hookrightarrow L^\infty$, we obtain the claimed estimate (2.10), with $\sigma = r$.

Chapter 3

Low regularity integrators via decorated trees

This chapter is based on the article [ABBS22b].

Abstract. We introduce a general framework of low regularity integrators which allows us to approximate the time dynamics of a large class of equations, including parabolic and hyperbolic problems, as well as dispersive equations, up to arbitrary high order on general domains. The structure of the local error of the new schemes is driven by nested commutators which in general require (much) lower regularity assumptions than classical methods do. Our main idea lies in embedding the central oscillations of the nonlinear PDE into the numerical discretisation. The latter is achieved by a novel decorated tree formalism inspired by singular SPDEs with Regularity Structures and allows us to control the nonlinear interactions in the system up to arbitrary high order on the infinite dimensional (continuous) as well as finite dimensional (discrete) level.

3.1 Introduction

We consider a general class of evolution equations under the form

$$\partial_t u_o - \mathcal{L}_o u_o = \sum_{l \in \mathfrak{L}_-} \Psi_o^l(\mathbf{u}_o^l) V_l(x), \quad (t, x) \in \mathbf{R} \times \Omega, \quad o \in \mathfrak{L}_+, \quad (3.1)$$

where $\mathfrak{L}_-, \mathfrak{L}_+$ are finite sets, $\Omega \subseteq \mathbf{R}^d$, $\mathbf{u}_o^l = (u_i)_{i \in \mathfrak{L}_+^{o,l}}$ and $\mathfrak{L}_+^{o,l} \subset \mathfrak{L}_+$. For every $(o, l) \in \mathfrak{L}_+ \times \mathfrak{L}_-$, \mathcal{L}_o denotes a linear (possibly) unbounded operator, Ψ_o^l represents the nonlinearity and V_l the potential or noise. The precise assumptions on the operator \mathcal{L}_o , the nonlinearity Ψ_o^l and the potential V_l are stated in Section 3.1.1 below. We add initial conditions $u_o(0) = v_o$ and when $\partial\Omega \neq \emptyset$ suitable boundary conditions which will be encoded in the domain of the operator \mathcal{L}_o .

Evolution equations of type (3.1) are meanwhile extensively studied in numerical analysis literature and a large variety of discretisation techniques for their time resolution was proposed, reaching, e.g., from splitting methods over exponential integrators up to Runge–Kutta and Lawson type schemes [Fao12, HNW93, HLW10, HO10, HLO20, Hol10, LR04, MQ02, SSC18]. While such *classical* discretisation techniques provide a good approximation to smooth solutions, they often drastically break down at low regularity: Rough data and high oscillations in general cause severe loss of convergence which leads to huge computational costs hindering in many situations reliable approximations. Nonlinear partial differential equations (PDEs) at low regularity are at large an ongoing challenge in numerical analysis.

In this work we introduce a general framework of low regularity integrators which allows us to approximate the time dynamics of (3.1) up to arbitrary high order under lower regularity assumptions than classical methods, such as Runge–Kutta, splitting, exponential integrators or Lawson schemes, require. Our new framework greatly enhances the low regularity framework recently introduced in [BS22] which is restricted to dispersive equations with periodic boundary conditions and polynomial nonlinearities $u^\ell \bar{u}^m$. Within our new framework we in particular overcome periodic boundary conditions and cover a much larger class of equations, including for instance parabolic, and hyperbolic problems, as well as dispersive equations. Furthermore, our model (3.1) allows for noise or potentials and non polynomial nonlinearities.

In order to bypass the limitations of [BS22] we introduce novel *commutator structures*. Such commutators were previously used in [RS21] for the derivation of first- and second-order low regularity integrators for a simplified version of (3.1) (in particular without potential, i.e., $V_l \equiv 1$). At low order the central oscillations in (3.1) can quite easily be computed and their dominant parts can be extracted “by hand” (see [RS21]). This is however no longer the case at higher order: The control of the underlying oscillations of (3.1) up to arbitrary high order involves a scale of nested, iterated oscillatory integrals depending on the nonlinear interaction between the leading differential operator \mathcal{L}_o and the nonlinearity $\sum_{l \in \mathfrak{L}_-} \Psi_o^l(\mathbf{u}_o^l) V_l(x)$ which is in particular challenging on the finite dimensional (discrete) level.

In order to overcome this, our key idea lies in developing a new class of decorated trees. This formalism is crucial as it allows us to encode the oscillatory systems of iterated integrals on the continuous as well as on the discrete level. We control the local error at each order with suitable nested commutators. The decorated trees used in this work are inspired by [BS22]. We develop a new framework overcoming the limitations of the formalism developed in [BS22] which heavily relied on Fourier expansion techniques, periodic boundary conditions and polynomial nonlinearities. Our decorated trees are close in spirit to the ones used in singular SPDEs in [BCCH20] where decorations on the nodes encode the drivers/potentials of the equation (3.1). This work is the second example after [BS22] where Regularity Structures decorated trees introduced in [Hai14, BHZ19] appear in context of numerical analysis which stresses their robustness. Another key difference with [BS22] lies in the fact that our setting does not allow for a Hopf algebra to conduct the local error analysis. The latter seems limited to Fourier space and the control of the corresponding Fourier modes. The lack of a Hopf algebra in this work is, however, not surprising as we push forward low regularity integrators to the much more general setting (3.1). As we are no longer in the Fourier case, the resonance analysis has to be replaced by a new splitting on the operators directly in Physical space given in Definition 3.3.2. This new idea is crucial for implementing a low regularity scheme and allows to bypass the limitation of the Fourier analysis when one can only consider operators that are polynomial in the frequencies in Fourier space.

Our main result is the new general low regularity scheme presented in Definition 3.4.2 with its error structure given in Theorem 3.4.3. The approximation relies crucially on the formulae given in Definition 3.3.2. We will illustrate our framework on the concrete examples of the Gross–Pitaevskii and the Sine–Gordon equation in full detail in Section 3.5. In the next subsection, we illustrate the main ideas of our scheme on a parabolic equation.

3.1.1 Linearization and decorated trees

Before introducing our linearization techniques based on decorated trees, let us first specify the assumptions on the nonlinearity Ψ and on the leading operator \mathcal{L}_o appearing in (3.1).

Assumption 1 (nonlinearity Ψ) *In the following we assume that the nonlinearity $\Psi_o^l(\mathbf{u}_o^l)$ is tensorized under the form*

$$\Psi_o^l(\mathbf{u}_o^l) = \mathcal{B}_o^l \left(\prod_{i \in \mathfrak{L}_+^{l,o}} f_{o,i}^l(u_i) \right), \quad f_{o,i}^l : \mathbf{C} \rightarrow \mathbf{C}^J, \quad (3.2)$$

where $(\mathcal{B}_o^l)_{(o,l) \in \mathfrak{L}_+ \times \mathfrak{L}_-}$ is a family of (linear) operators and we use the notation $\prod_i X^{(i)} = \sum_{k \leq J} \prod_i X_k^{(i)}$ where $X^{(i)} \in \mathbf{C}^J$.

Assumption 2 (leading operator \mathcal{L}_o) *The linear operator \mathcal{L}_o shall be defined on a Hilbert space X of complex valued functions $u \in \mathbf{C}$ with norm denoted by $\|\cdot\|$ and domain $D(\mathcal{L}_o)$. To make sense of the exponential functions, we in addition assume that \mathcal{L}_o generates a strongly continuous semigroup $\{e^{t\mathcal{L}_o}\}_{t \geq 0}$ of contractions on X .*

We illustrate the main idea of our general scheme via a simple example that contains already some important challenges which could not be overcome in previous works [BS22, RS21]. Let us consider the abstract parabolic equation:

$$\partial_t u - \Delta u = f(u)V, \quad u_0 = v, \quad (t, x) \in \mathbf{R} \times \Omega \quad (3.3)$$

with $\Omega \subseteq \mathbf{R}^d$ sufficiently smooth. In the case of $\partial\Omega \neq \emptyset$ we assume suitable boundary conditions encoded in $D(\Delta)$ and shall denote by V a potential or noise.

The starting point of our new class of schemes is based on Duhamel’s formula for (3.3) which is given by

$$u(t) = e^{t\Delta} v + \int_0^t e^{(t-\xi)\Delta} f(u(\xi))V d\xi. \quad (3.4)$$

Classical methods are in general based on Taylor series expansions of $u(\xi)$ (the solution of (3.3) at time $t = \xi$) around the initial value $u_0 = v$ in the sense that for small ξ we have at first order that

$$u(\xi) = v + \mathcal{O}(\xi u'). \quad (3.5)$$

This classical Taylor series expansion, however, requires regularity in the solution since from the PDE (3.3) we have

$$\mathcal{O}(\xi u') = \mathcal{O}(\xi \Delta u).$$

Hence, the numerical scheme will only converge to order one for sufficiently smooth solutions

$$u \in D(\Delta).$$

The situation is even worse for higher order methods which are in general based on higher order Taylor series expansions of the solution

$$u(\xi) = v + \xi u'(0) + \frac{\xi^2}{2} u''(0) + \dots + \frac{\xi^r}{r!} u^{(r)}(0) + \mathcal{O}(\xi^{r+1} u^{(r+1)}). \quad (3.6)$$

By using the PDE (3.3) we have at leading order

$$\mathcal{O}(\xi^{r+1} u^{(r+1)}) = \mathcal{O}(\xi^{r+1} \Delta^{r+1} u).$$

Hence, it follows that at order $r + 1$ the necessary regularity assumptions on the solutions is increased to

$$u \in D(\Delta^{r+1}). \quad (3.7)$$

Remark 3.1.1 Note that (3.7) does not only require sufficiently smooth solutions (i.e., that the $\partial^{2(r+1)}$ th derivative is bounded), but also additional compatibility conditions on the boundary whenever $\partial\Omega \neq \emptyset$. For example, for a second order approximation, namely when $r = 1$, the classical Taylor expansion (3.6) requires

$$u \in D(\Delta^2) = \{f \in D(\Delta); \Delta f \in D(\Delta)\}.$$

In case of Ω a bounded smooth open set of \mathbf{R}^d equipped with homogeneous Dirichlet boundary conditions this means that

$$u \in D(\Delta^2) = \{f \in (H^2 \cap H_0^1)(\Omega); \Delta f \in (H^2 \cap H_0^1)(\Omega)\}. \quad (3.8)$$

Hence, zero trace of the solution u and Δu on the boundary is imposed.

In this manuscript we want to overcome these high regularity assumptions by developing a new class of schemes with improved local error structures. It is essential to note that if we want to develop such a class of (high order) methods under low(er) regularity assumptions

$$u \in Y \supset D(\Delta^{r+1})$$

we cannot base our new schemes on classical Taylor series expansions of type (3.6).

Our idea to overcome the regularity assumptions (3.7) lies in embedding the central oscillations of the PDE into the numerical discretisation, while only approximating the lower order terms. More precisely, iterating Duhamel's formula (see also [BS22, RS21]) we have thanks to (3.4) at time $t = \xi$ that

$$u(\xi) = e^{\xi\mathcal{L}} v + \mathcal{O}(\xi)$$

where the central oscillations are captured in the term

$$e^{\xi\mathcal{L}} v$$

and the remainder $\mathcal{O}(\xi)$ does not involve any derivatives on the solution. In detail one has for $u(\xi) = e^{\xi\Delta} v + A(\xi)$ that

$$f(u(\xi)) = \sum_{k \leq r} \frac{A(\xi)^k}{k!} f^{(k)}(e^{\xi\Delta} v) + \mathcal{O}(A(\xi)^{r+1}) \quad (3.9)$$

where we truncate the expansion at r which is associated to the order of the scheme one wants to achieve. The remainder $A(t)$ will corresponds in practice (after a suitable approximation) to a finite sum of iterated integrals only involving bounded operators.

Plugging (3.9) into (3.4), we obtain the following expansion of the exact solution

$$u(t) = e^{t\Delta} v + \sum_{k \leq r} \int_0^t e^{(t-\xi)\Delta} \frac{A(\xi)^k}{k!} f^{(k)}(e^{\xi\Delta} v) V d\xi + \mathcal{O}(t^{r+2}), \quad (3.10)$$

where the central oscillations are embedded in the interaction of

$$e^{(t-\xi)\Delta} \quad \text{and} \quad f^{(k)}(e^{\xi\Delta} v)$$

and the remainder $\mathcal{O}(t^{r+2})$ does, in contrast to classical approximation techniques (3.6), not involve any derivatives on the solution.

The main challenge lies in controlling the oscillatory integrals in (3.10)

$$\sum_{k \leq r} \int_0^t e^{(t-\xi)\Delta} \frac{A(\xi)^k}{k!} f^{(k)}(e^{\xi\Delta} v) V d\xi \quad (3.11)$$

on the discrete level. Note that a classical Taylor series expansion of the oscillations $e^{\xi\Delta}$ would again lead to the high regularity assumptions (3.7). Our key idea to overcome this lies in embedding the central oscillations in (3.11) explicitly into our numerical discretization. In order to do so, in a first step we have to linearise the terms $f^{(k)}(e^{\xi\Delta} v)$. This will allow us to filter out the dominant oscillations while controlling the approximation error by commutators $\mathcal{C}[\cdot, \cdot]$ with an improved error structure introduced as follows:

Definition 3.1.2 For a function $H(v_1, \dots, v_n)$, $n \geq 1$ and a linear operator \mathcal{L} we set

$$\mathcal{C}[H, \mathcal{L}](v_1, \dots, v_n) = -\mathcal{L}(H(v_1, \dots, v_n)) + \sum_{i=1}^n D_i H(v_1, \dots, v_n) \cdot \mathcal{L}v_i$$

where $D_i H$ stands for the partial differential of H with respect to the variable v_i . We define the iterated commutator $\mathcal{C}^k[H, \mathcal{L}]$ recursively by

$$\mathcal{C}^{k+1}[H, \mathcal{L}] = \mathcal{C}^k[\mathcal{C}[H, \mathcal{L}], \mathcal{L}], \quad \mathcal{C}^0[H, \mathcal{L}] = H.$$

Let us illustrate this definition with our example (3.3). With the above notation (and $\mathcal{L} = \Delta$) one has for sufficiently smooth f :

$$f(e^{\xi\Delta} v) = \sum_{\ell=0}^r \frac{\xi^\ell}{\ell!} e^{\xi\Delta} \mathcal{C}^\ell[f, \Delta](v) + \mathcal{O}(\xi^{r+1} \mathcal{C}^{r+1}[f, \Delta](v)). \quad (3.12)$$

This linearisation produces an error of the form

$$\mathcal{C}^{r+1}[f, \Delta](v)$$

which in general requires less regularity and less compatibility conditions on the boundary than does a classical Taylor-series expansion of the propagator $e^{\xi\Delta}$. Indeed, up to order r we have

$$e^{\xi\Delta} = \sum_{k \leq r} \frac{\xi^k}{k!} \Delta^k + \mathcal{O}(\xi^{r+1} \Delta^{r+1}), \quad (3.13)$$

whereby

$$D(\mathcal{C}^{r+1}[f, \Delta]) \supset D(\Delta^{k+1}).$$

Hence, the commutator expansion (3.12) requires less regularity assumptions and compatibility conditions than classical Taylor expansion of the the propagator $e^{\xi\Delta}$. We illustrate this through an example in the following two remarks. This observation also holds true in the general setting (3.1).

Remark 3.1.3 In general it holds that

$$D(\mathcal{C}[f, \mathcal{L}]) \supset D(\mathcal{L}).$$

Let us for instance recall the example given in [RS21, Sec. 2.1] where $\mathcal{L} = \Delta$ on the torus \mathbf{T}^d and $f(u) = u^2$. Then one has $D(\mathcal{L}) = H^2$ (the classical Sobolev space) and

$$\mathcal{C}[f, \mathcal{L}](v) = -\sum_{k=1}^d (\partial_k v)^2.$$

If we choose to measure the error in L^2 , in order to bound the above expression we need $(\partial_k v)^2 \in L^2$. This follows for $v \in H^{1+\frac{d}{4}}$ by using the injection $H^{1+\frac{d}{4}} \hookrightarrow L^4$. Hence we have $v \in H^{1+\frac{d}{4}} \subset D(\mathcal{C}[f, \mathcal{L}])$. For an analysis in H^s -norm with $s \geq 0$ we refer to [AB23a].

We note that the above also holds true when working on a bounded domain of \mathbf{R}^d , equipped with homogeneous Dirichlet boundary conditions. Indeed, the same argument as above holds with $D(\Delta) = (H^2 \cap H_0^1)(\Omega)$, and where $v \in (H^{1+\frac{d}{4}} \cap H_0^1)(\Omega) \subset D(\mathcal{C}[f, \Delta])$.

Remark 3.1.4 The commutator term $\mathcal{C}^{r+1}[f, \Delta](v)$ in general asks for less regularity and compatibility conditions at the boundary than the classical Taylor's expansion (3.13). Indeed, in case of homogeneous Dirichlet boundary conditions

for example when $r = 1$, the commutator term $\mathcal{C}^2[f, \Delta](v)$ involves derivatives of at most second order. Namely, formally we have $\mathcal{C}^2[f, \Delta](v) = O(\Delta v)$, which requires $v \in D(\Delta) = (H^2 \cap H_0^1)(\Omega)$. A. classical second-order Taylor's expansion on the other hand asks for $v \in D(\Delta^2)$, which does not only requires v to have zero trace on the boundary, but also its second derivatives (see also Remark 3.1.1).

Let us now turn back to presenting the main idea of our new schemes on the example (3.3): Plugging (3.12) into (3.10), we get

$$u(t) = e^{t\Delta}v + \sum_{k, \ell \leq r} \int_0^t e^{(t-\xi)\Delta} \frac{A(\xi)^k}{k!} \frac{\xi^\ell}{\ell!} \left(e^{\xi\Delta} \mathcal{C}^\ell[f^{(k)}, \Delta](v) \right) V d\xi + \mathcal{O}(t^{r+2} \mathcal{C}^{r+1}[f^{(k)}, \Delta](v)) \quad (3.14)$$

where the leading error term is driven by the commutator

$$\mathcal{O}(t^{r+2} \mathcal{C}^{r+1}[f^{(k)}, \Delta](v)).$$

In general, the latter is more important (i.e., worse in terms of regularity assumptions) than the ones introduced by the approximation of $A(t)$ (cf. (3.9)) which is a polynomial in the initial condition v involving only bounded operators. Also, one can mention that in general \mathcal{L}_o is more singular than the \mathcal{B}_o^l , where the (linear) operators \mathcal{B}_o^l are given by the structure of the nonlinearity (3.2).

From the approximation (3.14), we can collect iterated integrals for building an approximate solution $w^r(v, t)$ up to order r . For example, when $r = 2$, we get

$$\begin{aligned} w^2(v, t) &= e^{t\Delta}v + \int_0^t e^{(t-\xi)\Delta} \left(e^{\xi\Delta} f(v) \right) V d\xi \\ &+ \int_0^t \xi e^{(t-\xi)\Delta} \left(e^{\xi\Delta} \mathcal{C}[f, \Delta](v) \right) V d\xi \\ &+ \int_0^t e^{(t-\xi)\Delta} \left(\int_0^\xi e^{(\xi-\xi_1)\Delta} \left(e^{\xi_1\Delta} f(v) \right) V d\xi_1 \right) \left(e^{\xi\Delta} f^{(1)}(v) \right) V d\xi. \end{aligned} \quad (3.15)$$

Remark 3.1.5 The remaining challenge lies in embedding the central oscillations triggered by

$$\begin{aligned} &e^{(t-\xi)\Delta} \left(e^{\xi\Delta} f(v) \right) V, \quad e^{(t-\xi)\Delta} \left(e^{\xi\Delta} \mathcal{C}[f, \Delta](v) \right) V, \\ &e^{(t-\xi)\Delta} \left(\int_0^\xi e^{(\xi-\xi_1)\Delta} \left(e^{\xi_1\Delta} f(v) \right) V d\xi_1 \right) \left(e^{\xi\Delta} f^{(1)}(v) \right) V \end{aligned}$$

into the numerical discretisation.

For this purpose we will introduce a recursive map Π defined on a set of trees \mathcal{T} to encode these iterated integrals. The set \mathcal{T} will be decorated trees whose formalism has been introduced in [BHZ19] and has been extensively used in [BCCH20] for giving wellposedness results for a large class of Stochastic partial differential equations (SPDEs). After the recent work [BS22], it is the second time that one uses this formalism also in context of Numerical Analysis. The iterated integrals for w^2 are given by trees of size two (having at most two edges) \mathcal{T}^2 :

$$\mathcal{T}^2 = \left\{ \begin{array}{c} \circ \\ | \\ \circ \\ | \\ \circ \\ | \\ \circ \end{array} \right\}.$$

Brown edges encode integrals of the form $\int_0^t e^{(t-\xi)\Delta} \dots d\xi$, white nodes the nonlinearity $e^{\xi\Delta} f(v) V$ and the nodes marked with a cross correspond to $\xi \left(e^{\xi\Delta} \mathcal{C}[f, \Delta](v) \right) V$. Incoming edges to a grey dot induce derivatives on f which will allow us to encode the third term in (3.15).

Our decorated trees strongly differ from the ones introduced in [BS22]: The scheme introduced in [BS22] heavily relies on Fourier series expansion techniques and is therefore restricted to periodic boundary conditions. In particular, the tree structure in [BS22] is based on Fourier decorations. The latter allowed us to easily filter out the dominant frequency interactions in the system based on the underlying structure of resonances of the PDE. In order to handle the general setting (3.1), and in particular deal with non periodic boundary conditions and non polynomial nonlinearities, we can, however, not make use of the previously proposed resonance analysis. Instead, we have to introduce new tools based on the analysis of the operator interactions and an extensive use of the commutator based approximation (3.12). Let us

illustrate this analysis on the first iterated integral that we denote by $\left(\Pi \overset{\circ}{\mathbb{I}}\right)(t)$. It takes the following form

$$\begin{aligned} \left(\Pi \overset{\circ}{\mathbb{I}}\right)(t) &= \int_0^t e^{(t-\xi)\Delta} \prod_{i=1}^2 e^{\xi \mathcal{L}_i} u_i d\xi, \\ \mathcal{L}_1 &= \Delta, \quad u_1 = f(v), \quad \mathcal{L}_2 = 0, \quad u_2 = V. \end{aligned}$$

The first step is to distribute $e^{(t-\xi)\Delta}$ on the product $\prod_{i=1}^2 e^{\xi \mathcal{L}_i} u_i$:

$$\begin{aligned} e^{(t-\xi)\Delta} \left(\prod_{i=1}^2 e^{\xi \mathcal{L}_i} u_i \right) &= \prod_{i=1}^2 e^{\xi \mathcal{L}_i + (t-\xi)\Delta} u_i \\ &+ \sum_{1 \leq k \leq r} \frac{(t-\xi)^k}{k!} \mathcal{C}^k[(e^{t\Delta} \mathcal{M}_{\{1\}})(e^{(t-\xi)\Delta} \mathcal{M}_{\{2\}}), \Delta](u_1, u_2) \\ &+ \mathcal{O}(t^{r+1} \mathcal{C}^{r+1}[\mathcal{M}_{\{1,2\}}, \Delta](u_1, u_2)) \end{aligned} \quad (3.16)$$

where we have used the following notations: Let $(u_i)_{i \in I}$ and $(v_j)_{j \in J}$ be two finite sets of functions and \mathcal{L}_1 and \mathcal{L}_2 two linear operators. Then we set

$$(\mathcal{L}_1 \mathcal{M}_I \mathcal{L}_2 \mathcal{M}_J)(u_{i \in I}, v_{j \in J}) := \mathcal{L}_1 \left(\prod_{i \in I} u_i \right) \mathcal{L}_2 \left(\prod_{j \in J} v_j \right)$$

and

$$\mathcal{C}[\mathcal{M}_I, \mathcal{L}_1](u_{i \in I}) := -\mathcal{L}_1 \mathcal{M}_I(u_{i \in I}) + \sum_{j \in I} \mathcal{M}_I(\dots, \mathcal{L}_1 u_j, \dots).$$

Remark 3.1.6 We can notice that the term $e^{-\xi\Delta}$ does, however, not make sense (recall that $\xi \geq 0$). In the dispersive setting of [BS22], one did not have such an issue (as for instance $e^{i\xi\Delta}$ is well defined for all $\xi \in \mathbf{R}$) and hence one could perform the resonance analysis only on the terms depending on ξ . In our general setting (3.1) we have to be more careful and take the oscillations of the full operator $e^{(t-\xi)\Delta}$ into account.

The second step is to identify the dominant part in the operators $\mathcal{L}_i - \Delta$ in (3.16). For this purpose we set $\mathcal{A}_i = \mathcal{L}_i - \Delta$ and introduce the splitting

$$\mathcal{A}_i = a_i \mathcal{L}_{\text{dom}} + \mathcal{A}_{\text{low}}^i, \quad D(\mathcal{L}_{\text{dom}}) \subset D(\mathcal{A}_{\text{low}}^i)$$

where $a_i \in \{0, 1\}$. The purpose of this splitting lies in the fact that in the construction of our schemes we will separate the dominant from the lower order oscillations and only embed the dominant parts exactly into our numerical discretization, while Taylor expanding the lower order parts. Note that in the above example one for instance has that

$$\mathcal{A}_1 = 0, \quad \mathcal{A}_2 = -\Delta,$$

and hence, $a_1 = 0$, $a_2 = 1$, $\mathcal{A}_{\text{low}}^i = 0$ for $i \in \{1, 2\}$ and $\mathcal{L}_{\text{dom}} = -\Delta$. In this simple case one does not need any further approximation and one can write the following approximation at order r :

$$\left(\Pi^r \overset{\circ}{\mathbb{I}}\right)(t) = \sum_{0 \leq k \leq r} \int_0^t \frac{(t-\xi)^k}{k!} \mathcal{C}^k[(e^{t\Delta} \mathcal{M}_{\{1\}})(e^{(t-\xi)\Delta} \mathcal{M}_{\{2\}}), \Delta](u_1, u_2) d\xi.$$

Remark 3.1.7 In most applications, one does not have to go through the second step of the approximation like the example shown above. The second step is needed for linear combination of operators like $\partial_x^2 + \partial_x$. One may have to approximate the following iterated integral (with notation $\Delta = \partial_x^2$):

$$\int_0^t e^{(t-\xi)\Delta} \left(e^{\xi(\Delta + \partial_x)} v_2 \right) V d\xi.$$

This integral is coming from a system of the form:

$$\partial_t u_1 - \Delta u_1 = u_2 V, \quad u_1(0) = v_1, \quad (3.17)$$

$$\partial_t u_2 - \Delta u_2 - \partial_x u_2 = 0, \quad u_2(0) = v_2.$$

Then, from (3.16), we get

$$\sum_{1 \leq k \leq r} \frac{(t-\xi)^k}{k!} \mathcal{C}^k [(e^{t\Delta + \xi \partial_x} \mathcal{M}_{\{1\}})(e^{(t-\xi)\Delta} \mathcal{M}_{\{2\}}), \Delta](v_2, V).$$

Now, $\mathcal{A}_{\text{low}}^1 = \partial_x$ and one has to Taylor-expand the term $e^{\xi \partial_x}$. This leads to the following approximation:

$$\begin{aligned} \int_0^t e^{(t-\xi)\Delta} (e^{\xi(\Delta + \partial_x)} v_2) V d\xi &= \int_0^t \sum_{0 \leq k+\ell \leq r} \frac{(t-\xi)^k}{k!} \frac{\xi^\ell}{\ell!} \\ &\quad \mathcal{C}^k [(e^{t\Delta} \mathcal{M}_{\{1\}})(e^{(t-\xi)\Delta} \mathcal{M}_{\{2\}}), \Delta](\partial_x^\ell v_2, V) d\xi \\ &\quad + \sum_{k+\ell=r+1} \mathcal{O}(t^{r+2} \mathcal{C}^k[\mathcal{M}_{\{1,2\}}, \Delta](\partial_x^\ell v_2, V)). \end{aligned}$$

In the next section, we will present our main strategy in the general setting (3.1).

3.1.2 Main strategy of the general numerical scheme

Duhamel's formulation of (3.1) is given by

$$u_o(\tau) = e^{\tau \mathcal{L}_o} v_o + \int_0^\tau e^{(\tau-\xi)\mathcal{L}_o} \sum_{l \in \mathfrak{L}_-} \Psi_l(\mathbf{u}_o^l) V_l d\xi. \quad (3.18)$$

By iterating this formulation together with (3.12) and (3.9), we get iterated integrals that can be represented via decorated trees. Let $r+1$ be the order of the scheme, we first truncate this expansion and get the following approximation of the solution:

$$w_o^r(\hat{\mathbf{v}}, \tau) = e^{\tau \mathcal{L}_o} v_o + \sum_{T \in \mathcal{V}^r} (\Pi T)(\hat{\mathbf{v}}, \tau) \quad (3.19)$$

where $\hat{\mathbf{v}} = (\mathbf{v}, \mathbf{V})$, $\mathbf{v} = (v_o)_{o \in \mathfrak{L}_+}$, $\mathbf{V} = (V_l)_{l \in \mathfrak{L}_-}$, \mathcal{V}^r is a finite set of decorated trees, and $(\Pi T)(\hat{\mathbf{v}}, \tau)$ represents the iterated integral associated to T . The exponent r in \mathcal{V}^r means that we consider only trees of size r which are the trees producing an iterated integral with r integrals. Proposition 3.4.1 shows that w_o^r solves (3.18) with an error involving $\mathcal{C}^{r+1}[f, \mathcal{L}_o]$ with f a function coming from the coefficients Ψ_o . The main improvement lies in the error structure: The error $\mathcal{C}^{r+1}[f, \mathcal{L}_o]$ is in general better than \mathcal{L}_o^r in the sense of requiring lower regularity assumptions on the solution.

The main difficulty boils down to developing for every $T \in \mathcal{V}^r$ a suitable approximation to the iterated integrals $(\Pi T)(\hat{\mathbf{v}}, \tau)$ with the aim of minimising the local error structure (in the sense of regularity), see also Remark 3.1.5. In order to achieve this, the key idea lies in commutator based approximations (3.12) which replace the resonance analysis given in [BS22]. The approximation of (ΠT) is given by a new map on decorated trees denoted by $\Pi_A^r T$ where $r+1$ is the order of the scheme and A is a domain corresponding to the a priori assumed regularity of $\hat{\mathbf{v}}$. Our general scheme takes the form

$$w_{o,A}^r(\hat{\mathbf{v}}, \tau) = e^{\tau \mathcal{L}_o} v_o + \sum_{T \in \mathcal{V}^r} (\Pi_A^r T)(\hat{\mathbf{v}}, \tau) \quad (3.20)$$

where the map $\Pi_A^r T$ is a low regularity approximation of order r of the map ΠT in (3.19) in the sense that

$$(\Pi T - \Pi_A^r T)(\hat{\mathbf{v}}, \tau) = \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T, \hat{\mathbf{v}}, A)). \quad (3.21)$$

Here $\mathcal{L}_{\text{low}}^r(T, \hat{\mathbf{v}}, A)$ involves nested commutators that require in general less regularity than powers of the full operator \mathcal{L}_o^r (see also Remark 3.1.3). The scheme (3.20) and the local error approximations (3.21) are the main results of this work (see Theorem 3.4.3). The approximation $\Pi_A^r T$ is constructed from a character Π_A defined on the vector space \mathcal{H} spanned by decorated forests taking values in a space \mathcal{C} that will depend on the operators \mathcal{L}_o and $\hat{\mathbf{v}}$. We add a decoration r at the root with the meaning that we will consider an approximation of order r . This is performed by the symbol \mathcal{D}^r that gives $\Pi_A \mathcal{D}^r(T) = \Pi_A^r T$.

As in [BS22], we define the map Π_A recursively from an operator \mathcal{K} . This operator computes a suitable approximation (matching the regularity of the solution) of the integrals introduced by the iteration of Duhamel's formula. Here the main difference is that we perform the analysis directly on the operator without going into Fourier space. We single out the dominant parts of the operators we are dealing with. These dominant parts are integrated exactly and only the lower order terms are approximated which allows for an improved local error structure compared to classical approaches.

For the local error analysis, a structure of Hopf algebra and comodule was used in [BS22] for singling out oscillations. It was based on a variant of the Butcher-Connes-Kreimer coproduct [But72, CK99, CK00] inspired by [BHZ19]. This structure can be seen as a deformation of the Butcher-Connes-Kreimer coproduct (see [BM23]). The central object used as in Quantum Field Theory for the local error analysis in [BS22] was a Birkhoff factorisation similar to the one presenting in [BHZ19] for recentering iterated integrals. This is put into perspective in the work [BEF20]. The context of commutators is much more involved than the one in Fourier space. We therefore do not use such a construction but rather the recursive formulae for computing the local error. It is given in Definition 3.3.8. Via Proposition 3.3.7, we illustrate what are the dominant operators involved in the computation of the local error.

3.1.3 Outline of the paper

Let us give a short review of the content of this paper. In Section 3.2, we introduce the general algebraic framework by first defining a suitable vector space of decorated trees $\hat{\mathcal{T}}$ and decorated forests $\hat{\mathcal{H}}$. Next, we set how to compute the dominant part of a set of operators (see Definition 3.2.1). We define then the dominant operators associated to a decorated forest (see Definition 3.2.3). Then, we introduced new spaces of decorated trees \mathcal{T} that we call approximated decorated trees. They carry an extra decoration r at the root and they represent approximation at order r of the corresponding iterated integrals. We also introduced new decorated forests based on the same construction.

In Section 3.3, we construct the approximation of the iterated integrals given by the character $\Pi : \hat{\mathcal{H}} \rightarrow \mathcal{C}$ (see (3.38)) through the character $\Pi_A : \mathcal{H} \rightarrow \mathcal{C}$ (see (3.42)) where A is a domain that is the regularity of $\hat{\mathbf{v}}$. This is the regularity assumed a priori before writing the scheme. The approximation Π_A relies on a recursive construction where the operator \mathcal{K} given in Definition 3.3.2 is heavily used. The local error analysis which is the error estimate on the difference between Π and its approximation Π_A is given in Theorem 3.3.9. It is built upon a recursive definition (see Definition 3.3.8) involving Taylor remainders of Π_A with commutators. They are given in Lemma 3.3.6. Proposition 3.3.7 gives the structures of the dominant operators appearing in the local error analysis. In Section 3.4, we introduce truncated series of decorated trees that solves up to order r equation 3.1 (see Proposition 3.4.1). Then, from this series built upon the character Π , one can write the general scheme (see Definition 3.5.7) which boils down to replace Π by its approximation Π_A . In the end, we compute its local error structure (see Theorem 3.4.3) based on the local error between Π and Π_A for each decorated tree that appears in the expansion of the scheme.

In Section 3.5, we illustrate the general framework on various applications. The main example is the Gross-Pitaevskii (GP) equation that includes both a potential and a rough initial data. With our general framework we derive a first and second order scheme for GP and carry out precisely its local error analysis. We also discuss adapted filter operators for the stability of the low regularity scheme in Section 3.5.2. The last example of this section is the Klein and Sine-Gordon equations which illustrated our framework for non-polynomial nonlinearities.

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3.2 Decorated trees

In this section, we introduce the formalism of decorated trees that is used for describing the iterated integrals stemming from the iteration of the Duhamel's formula (3.18) of our main equation (3.1). Decorations on the nodes will encode monomials ξ^k and potentials V_l that appear in the equation whereas decorations on the edges encode the various integrals in time. The two spaces of importance are $\hat{\mathcal{T}}$ (resp. $\hat{\mathcal{H}}$) space of decorated trees (resp. forests). They correspond to iterated integrals without approximations. We define on these combinatorial objects the dominant operators that are used for the discretisation (see Definition 3.2.3). In the end, we consider the spaces \mathcal{T} and \mathcal{H} obtained by adding decorations at the root. This decoration gives the order at which we want to approximate these iterated integrals.

3.2.1 Definitions and dominant operators

We assume a finite set \mathcal{L} which has the following splitting $\mathcal{L} = \mathcal{L}_+ \sqcup \mathcal{L}_-$. We consider a family of differential operators $(\mathcal{L}_o)_{o \in \mathcal{L}_+}$ indexed by \mathcal{L}_+ and a family of potentials $(V_l)_{l \in \mathcal{L}_-}$ indexed by \mathcal{L}_- . We suppose given $(\mathcal{L}_+^{o,l})_{(o,l) \in \mathcal{L}_+ \times \mathcal{L}_-}$ a collection of subsets of \mathcal{L}_+ . We define the set of decorated trees $\hat{\mathcal{T}}$ as elements of the form $T_c^{n,f} = (T, \mathbf{n}, \mathbf{f}, \mathbf{e})$ where

— T is a non-planar rooted tree with root ϱ_T , node set N_T and edge set E_T . We denote the leaves of T by L_T .

- the map $\mathfrak{e} : E_T \rightarrow \mathfrak{L}_+$ are edge decorations. An edge decorated by $o \in \mathfrak{L}_+$ will encode an integral of the form $\int_0^t e^{(t-s)\mathcal{L}_o} \dots ds$.
- the map $\mathfrak{n} : N_T \rightarrow \mathbf{N}$ are node decorations. They correspond to monomials of the form ξ^k , $k \in \mathbf{N}$ that appear in iterated integrals.
- the map $\mathfrak{f} : N_T \rightarrow \mathfrak{L}_-$ are node decorations encoding the various potentials V_i .

When the node decoration \mathfrak{n} is omitted, we will denote the decorated trees as $T_\mathfrak{e}^\mathfrak{f}$. This set of decorated trees is denoted by $\hat{\mathcal{T}}_0$. We say that $\bar{T}_\mathfrak{e}^\mathfrak{f}$ is a decorated subtree of $T_\mathfrak{e}^\mathfrak{f} \in \hat{\mathcal{T}}_0$ if \bar{T} is a subtree of T and the restriction of the decorations \mathfrak{e} and \mathfrak{f} of T to \bar{T} are given by $\bar{\mathfrak{e}}$ and $\bar{\mathfrak{f}}$. We denote by $\hat{\mathcal{P}}$ the set of planted trees $T_\mathfrak{e}^{\mathfrak{n}, \mathfrak{f}}$ that are decorated trees with only one edge connected to the root and with no decorations at the root. Similarly when the node decoration \mathfrak{n} is omitted we denote this set $\hat{\mathcal{P}}_0$. We denote by \hat{H} (and resp. \hat{H}_0) the (unordered) forests composed of trees in $\hat{\mathcal{P}}$ (and resp. $\hat{\mathcal{P}}_0$) (including the empty forest denoted by $\mathbf{1}$). Their linear spans are denoted by $\hat{\mathcal{H}}$ (and resp. $\hat{\mathcal{H}}_0$).

In order to represent these decorated trees, we introduce a symbolic notation. An edge decorated by $o \in \mathfrak{L}_+$ is denoted by \mathcal{I}_o . The symbol $\mathcal{I}_o(\cdot) : \hat{\mathcal{T}} \rightarrow \hat{\mathcal{H}}$ is viewed as the operation that connects the root of a decorated tree to a new root with no decorations via an edge decorated by o . Any decorated tree T admits the following decomposition:

$$T = \lambda_l^\ell \prod_{i=1}^m \mathcal{I}_{o_i}(T_i) \quad (3.22)$$

where the T_i are decorated trees, λ_l^ℓ corresponds to the decorations at the root with $\ell \in \mathbf{N}$ and $l \in \mathfrak{L}_-$. The product in (3.22) is viewed as the forest product. This decomposition means that every decorated tree can be identified with a forest $\prod_{i=1}^m \mathcal{I}_{o_i}(T_i)$ and a decoration λ_l^ℓ . When $\ell = 0$, we will use the shorthand notation: $\lambda_l^0 = \lambda_l$. Below, we provide an example of such decorated trees:

$$\lambda_{l_0}^{\ell_0} \mathcal{I}_{o_1}(\lambda_{l_1}^{\ell_1}) \mathcal{I}_{o_2}(\lambda_{l_2}^{\ell_2}) \mathcal{I}_{o_3}(\lambda_{l_3}^{\ell_3}) = \quad (3.23)$$

Iterated integrals will be associated to these decorated trees. In order to approximate them numerically we will have to resolve the underlying oscillations by extracting the dominant parts of the leading operators. In the next definition, we introduce these dominant parts.

Definition 3.2.1 Let \mathcal{A}_i , $i \in \{1, \dots, m\}$ be a finite set of operators with domains $D(\mathcal{A}_i)$ in the sense that $\mathcal{A}_i : D(\mathcal{A}_i) \subseteq X \rightarrow X$. We define $\mathcal{P}_{\text{dom}}(\{\mathcal{A}_1, \dots, \mathcal{A}_m\})$ as follows: We first consider $I \subset \{1, \dots, m\}$ such that \mathcal{A}_i , $i \in I$ are of smaller domain in the sense that:

$$D(\mathcal{A}_i) = D(\mathcal{A}_j), \quad i, j \in I, \quad D(\mathcal{A}_i) \subsetneq D(\mathcal{A}_\ell), \quad \ell \in \{1, \dots, m\} \setminus I, \quad i \in I.$$

If there exists an operator \mathcal{L}_{dom} such that for every $i \in I$

$$\mathcal{A}_i = \mathcal{L}_{\text{dom}} + \mathcal{A}_{\text{low}}^i. \quad (3.24)$$

where \mathcal{L}_{dom} satisfies $D(\mathcal{L}_{\text{dom}}) \subsetneq D(\mathcal{A}_{\text{low}}^i)$, then we set

$$\mathcal{P}_{\text{dom}}(\{\mathcal{A}_1, \dots, \mathcal{A}_m\}) = \mathcal{L}_{\text{dom}}.$$

Otherwise, it is equal to 0.

Remark 3.2.2 The identity (3.24) has to be understood as a decomposition between lower and upper part of the operators \mathcal{A}_i . What is important in order to have a non-zero dominant part is to have a factorisation with some operator \mathcal{L}_{dom} . It is similar to the approach in Fourier space presented in [BS22, Def. 2.2] when one was looking at the form of the higher monomials of polynomials in the frequencies.

Example 6 We illustrate the previous definition with $\{0, \mathcal{L}\}$, where \mathcal{L} has the domain $D(\mathcal{L}) \neq X$. Then

$$\mathcal{P}_{\text{dom}}(\{0, \mathcal{L}\}) = \mathcal{L}$$

and for $\{0, -\mathcal{L}, \mathcal{L}\}$, one has

$$\mathcal{P}_{\text{dom}}(\{0, -\mathcal{L}, \mathcal{L}\}) = 0.$$

The latter follows as $D(-\mathcal{L}) = D(\mathcal{L})$ and the coefficients in front of \mathcal{L} are different (1 and -1).

Given a decorated tree, we want to compute its dominant part and lower part using the map \mathcal{P}_{dom} . We suppose given a space of operators \mathcal{O}_{\checkmark} in X and we denote by \mathcal{OS} the collection of finite sets of operators belonging to \mathcal{O}_{\checkmark} . Given two sets \mathcal{A}_1 and \mathcal{A}_2 , we denote their union by $\mathcal{A}_1 \cup \mathcal{A}_2$. Given a finite set of operators \mathcal{A} and an operator \mathcal{L} , we define $\mathcal{L} \oplus \mathcal{A}$ as the set where \mathcal{L} is added to each component of \mathcal{A} :

$$\mathcal{L} \oplus \mathcal{A} = \cup_{\mathcal{L}_o \in \mathcal{A}} \{\mathcal{L} + \mathcal{L}_o\}.$$

The term $\mathcal{A} \ominus \mathcal{L}$ is computed as follows for each component \mathcal{L}_o of \mathcal{A} . If the dominant part of \mathcal{L}_o is equal to \mathcal{L} , in the sense that one has the following decomposition:

$$\mathcal{L}_o = \mathcal{L} + \bar{\mathcal{L}} \quad (3.25)$$

with $D(\mathcal{L}) \subsetneq D(\bar{\mathcal{L}})$, then we replace \mathcal{L}_o by $\bar{\mathcal{L}}$. Otherwise, we keep \mathcal{L}_o . We define $\max(\mathcal{L}, \mathcal{A})$ as the operation that replaces each element \mathcal{L}_o satisfying (3.25) by \mathcal{L} otherwise we replace it by 0. Equipped with these notations, we are able to state the main definition for computing the dominant part associated to a decorated tree:

Definition 3.2.3 We recursively define $\mathcal{R}_{\text{dom}}^o : \hat{\mathcal{T}}_0 \rightarrow \mathcal{OS}$, $\mathcal{R}_{\text{dom}} : \hat{\mathcal{P}}_0 \rightarrow \mathcal{OS}$, $\mathcal{R}_{\text{low}} : \hat{\mathcal{P}}_0 \rightarrow \mathcal{OS}$ and $\mathcal{L}_{\text{dom}} : \hat{\mathcal{P}}_0 \rightarrow \mathcal{O}_{\checkmark}$ as:

$$\begin{aligned} \mathcal{R}_{\text{dom}}^o(\lambda_i \prod_i \mathcal{I}_{o_i}(T_i)) &= \{\mathcal{L}_{\bar{o}}, \bar{o} \in \mathfrak{L}_+^{o, \dagger}\} \cup \bigcup_i \mathcal{R}_{\text{dom}}(\mathcal{I}_{o_i}(T_i)), \\ \mathcal{L}_{\text{dom}}(\mathcal{I}_o(T)) &= \mathcal{P}_{\text{dom}}(-\mathcal{L}_o \oplus \mathcal{R}_{\text{dom}}^o(T)), \\ \mathcal{R}_{\text{dom}}(\mathcal{I}_o(T)) &= \mathcal{L}_o \oplus \max(\mathcal{L}_{\text{dom}}, -\mathcal{L}_o \oplus \mathcal{R}_{\text{dom}}^o(T)), \\ \mathcal{R}_{\text{low}}(\mathcal{I}_o(T)) &= (\text{id} \ominus \mathcal{P}_{\text{dom}})(-\mathcal{L}_o \oplus \mathcal{R}_{\text{dom}}^o(T)). \end{aligned}$$

We extend these maps to $\hat{\mathcal{T}}$ and $\hat{\mathcal{P}}$ by ignoring the node decorations \mathbf{n} .

Example 7 We illustrate the previous abstract definitions on some trees stemming from the cubic nonlinear Schrödinger equation

$$i\partial_t u + \Delta u = |u|^2 u, \quad u_0 = v \quad (3.26)$$

set on \mathbf{R}^d , $1 \leq d \leq 3$. For the equation (3.26), we have two variables which are u and \bar{u} . Thus, we rewrite (3.26) in the following form:

$$\begin{aligned} \partial_t u_o - \mathcal{L}_o u_o &= -i(u_o)^2 u_{\bar{o}}, \quad u_o(0) = v_o \\ \partial_t u_{\bar{o}} - \mathcal{L}_{\bar{o}} u_{\bar{o}} &= i(u_{\bar{o}})^2 u_o, \quad u_{\bar{o}}(0) = v_{\bar{o}} \end{aligned} \quad (3.27)$$

where one has $\mathcal{L}_o = i\Delta$, $\mathfrak{L}_+ = \{o, \bar{o}\}$, $\mathfrak{L}_- = \{0\}$, $\mathfrak{L}_+^{o,0} = \mathfrak{L}_+^{\bar{o},0} = \{o, \bar{o}\}$ with $V_0 = 1$, $\mathcal{B}_+^o = \mathcal{B}_+^{\bar{o}} = \text{id}$, $\mathcal{L}_o = \mathcal{L}$, $\mathcal{L}_{\bar{o}} = -\mathcal{L}$ and $X = L^2(\mathbf{R}^d)$, $D(\mathcal{L}) = H^2$, $u_o = u$, $u_{\bar{o}} = \bar{u}$, $v_o = v$, $v_{\bar{o}} = \bar{v}$. The nonlinearities are given by: $f_{o,o}^0(u) = -iu^2$, $f_{o,\bar{o}}^0(\bar{u}) = \bar{u}$, $f_{\bar{o},\bar{o}}^0(\bar{u}) = +i\bar{u}^2$ and $f_{\bar{o},o}^0(u) = u$. Let us recall the meaning of the subscripts in $f_{o,\bar{o}}^0$: The 0 corresponds to the driver V_0 , \bar{o} that it appears in the equation for \bar{u} and the last subscript says that $f_{o,\bar{o}}^0$ depends only on the variable u . Next we consider the following decorated tree

$$T = \mathcal{I}_o(\lambda_0) = \text{!} \quad (3.28)$$

which encodes the iterated integral:

$$-i \int_0^t e^{(t-s)\mathcal{L}} \left(\left(e^{s\mathcal{L}} v^2 \right) \left(e^{-s\mathcal{L}} \bar{v} \right) \right) ds. \quad (3.29)$$

The brown edge stands for the integral in time $\int_0^t e^{(t-s)\mathcal{L}} \dots ds$. The white dot associated to the potential V_0 encodes the product $-i(e^{s\mathcal{L}} v^2)(e^{-s\mathcal{L}} \bar{v})$. Indeed, it is connected via an edge associated to \mathcal{L} , so we know that we have to consider the nonlinearity associated to V_0 in the equation for u . One gets from the definition of $\mathfrak{L}_+^{o,0}$

$$\mathcal{R}_{\text{dom}}^o(o) = \{-\mathcal{L}, \mathcal{L}\}.$$

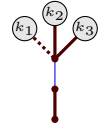
Then applying the previous definitions (see Definition 3.2.3), one gets

$$\begin{aligned} -\mathcal{L} \oplus \mathcal{R}_{\text{dom}}^o(o) &= \{-2\mathcal{L}, 0\}, \quad \mathcal{L}_{\text{dom}}(T) = \mathcal{P}_{\text{dom}}(\{-2\mathcal{L}, 0\}) = -2\mathcal{L}, \\ \mathcal{R}_{\text{dom}}(T) &= \mathcal{L} \oplus \max(\mathcal{L}_{\text{dom}}, -\mathcal{L} \oplus \{-\mathcal{L}, \mathcal{L}\}) = \{-\mathcal{L}, \mathcal{L}\} \end{aligned}$$

$$\mathcal{R}_{\text{low}}(T) = (\text{id} \ominus \mathcal{P}_{\text{dom}})(\{-2\mathcal{L}, 0\}) = \{-2\mathcal{L}, 0\} \ominus -2\mathcal{L} = \{0\}.$$


Remark 3.2.4 One can notice that some of the notations that we have introduced are similar to the one used in [BS22] which took a direct inspiration from the algebraic structures developed for singular SPDEs in [BHZ19, BCCH20]. Our decorations are however different to [BS22], because we focus on a more general set up no longer restricted to periodic dispersive equations:

- The conjugate operator was encoded in [BS22] with edge decorations in $\{-1, 1\}$ which allows the computation of the frequency interactions. Now, we have a larger set of operators by having a bigger set \mathfrak{L}_+ with elements such as \bar{o} like in the NLS example. One has $\mathcal{L}_{\bar{o}} = \bar{\mathcal{L}} = \mathcal{L}_{(o, -1)}$ where the last identity corresponds to the old notation coming from [BS22].
- Another change on the edge decorations is that in [BS22] certain edges correspond to some integrals in time others not. This excludes the parabolic case. If we rewrite an integral of the form $\int_0^t e^{(t-s)\mathcal{L}} \dots ds$ into $e^{t\mathcal{L}} \int_0^t e^{-s\mathcal{L}} \dots ds$ then it does not make sense when $\mathcal{L} = \Delta$. We recall one decorated tree coming from [BS22]:



$$\equiv -ie^{-itk^2} \int_0^t e^{isk^2} \left(e^{isk_1^2} e^{-isk_2^2} e^{-isk_3^2} \right) ds, \quad (3.30)$$

where $k = -k_1 + k_2 + k_3$, the leaves are decorated by the frequencies k_1, k_2, k_3 and the inner nodes are decorated by k . The blue edge encodes an integral in time $-i \int_0^t e^{isk^2} \dots ds$, the brown edges are used for a factor e^{-isk^2} and the dashed brown edges are for e^{isk^2} . If we consider the same integral not in Fourier mode, one can rewrite it as



$$\equiv -i \int_0^t e^{(t-s)\mathcal{L}} \left(\left(e^{s\mathcal{L}} v \right)^2 \left(e^{-s\mathcal{L}} \bar{v} \right) \right) ds \quad (3.31)$$

where $\mathcal{L} = i\Delta$, the blue dot corresponds to \bar{v} and the blue edge now encodes an integral of the form $\int_0^t e^{(t-s)\mathcal{L}} \dots ds$. In (3.31), we have to incorporate the initial data v and \bar{v} in the definition while they are implicit when the integral is written in Fourier space in (3.30) (one has just to multiply the integral with $\tilde{v}_{k_1} \tilde{v}_{k_2} \tilde{v}_{k_3}$). In fact, the coding given by (3.31) is sufficient for cubic NLS, but not for the general case we have in mind that contains potentials and non-polynomial nonlinearities.

- We add new decorations at the nodes stemming from the drivers V_l of (3.1). The initial conditions are associated to the drivers and the equations we are using via the sets $\mathfrak{L}_+^{o,1}$. Let us take for example a nonlinearity of the form

$$f(u)g(\bar{u})V_l.$$

Then, after inserting the approximation $u(s) = e^{s\mathcal{L}}v + A(s)$, one gets thanks to (3.12)

$$\left(e^{s\mathcal{L}} f(v) \right) \left(e^{s\bar{\mathcal{L}}} g(\bar{v}) \right) V_0 \equiv o = \lambda_0. \quad (3.32)$$

Next if we integrate by $\int_0^t e^{(t-s)\mathcal{L}} \dots ds$ encoded by a brown edge, we obtain the following integral when $f(u) = u^2$ and $g(\bar{u}) = \bar{u}$:

$$\mathcal{I}_o(\lambda_0) = \int_0^t \equiv -i \int_0^t e^{i(\tau-s)\Delta} \left(\left(e^{is\Delta} v^2 \right) \left(e^{-is\Delta} \bar{v} \right) \right) ds \quad (3.33)$$

The main difference between (3.31) and (3.33) is $(e^{is\Delta}v)^2$ which is replaced by $e^{is\Delta}v^2$. We are dealing in (3.33) with integrals that contain less factors of the form $e^{is\Delta}v$.

Example 8 As a second example, let us consider the Gross–Pitaevskii equation. The main difference with the cubic NLS equation (3.26) is the adjunction of a potential V . The equation takes the form:

$$i\partial_t u + \Delta u = |u|^2 u + uV, \quad u_0 = v \quad (3.34)$$

set on \mathbf{R}^d , $d \leq 3$. Now, one has $\mathfrak{L}_- = \{0, 1\}$, $\mathfrak{L}_+^{o,1} = \{o\}$, $\mathfrak{L}_+^{\bar{o},1} = \{\bar{o}\}$ with $V_1 = V$. The other sets remain the same, and are defined in Example 7. The new nonlinearities coming from the added potential term are given by: $f_{o,o}^1(u) = -iu$ and $f_{\bar{o},\bar{o}}^1(\bar{u}) = i\bar{u}$. Hence, together with the nonlinearities defined in (3.26), we indeed recover the nonlinear terms of (3.34)

from the general form (3.1) :

$$\begin{aligned} \sum_{l \in \mathcal{L}_-} \Psi_o^l(\mathbf{u}_o^l) V_l(x) &= \Psi_o^0(\mathbf{u}_o^0) V_0(x) + \Psi_o^1(\mathbf{u}_o^1) V_1(x) \\ &= f_{o,o}^0(u_o) f_{o,\bar{o}}^0(u_{\bar{o}}) + f_{o,o}^1(u_o) V \\ &= -i(u_o)^2 u_{\bar{o}} - i u_o V, \end{aligned}$$

where we recall that we set $\mathcal{B}_o^1 = \mathcal{B}_{\bar{o}}^1 = \text{id}$. We rewrite equation (3.34) into

$$\begin{aligned} \partial_t u_o - \mathcal{L}_o u_o &= -i(u_o)^2 u_{\bar{o}} - i u_o V, & u_o(0) &= v_o \\ \partial_t u_{\bar{o}} - \mathcal{L}_{\bar{o}} u_{\bar{o}} &= i(u_{\bar{o}})^2 u_o + i u_{\bar{o}} V, & u_{\bar{o}}(0) &= v_{\bar{o}} \end{aligned} \quad (3.35)$$

where for simplicity we have assumed a real potential $\bar{V} = V$. The central iterated integrals up to second order then take the form

$$\begin{aligned} \mathcal{I}_o(\lambda_1) &= \text{blue dot} \equiv -i \int_0^t e^{(t-s)\mathcal{L}} \left(\left(e^{s\mathcal{L}} v \right) V \right) ds \\ \mathcal{I}_{\bar{o}}(\lambda_1) &= \text{blue dot} \equiv i \int_0^t e^{(s-t)\mathcal{L}} \left(\left(e^{-s\mathcal{L}} \bar{v} \right) V \right) ds \\ \mathcal{I}_o(\lambda_0 \mathcal{I}_o(\lambda_1)) &= \text{blue dot} \\ &\equiv - \int_0^t e^{(t-s)\mathcal{L}} \left(\left(\int_0^s e^{(s-r)\mathcal{L}} \left(\left(e^{r\mathcal{L}} v \right) V \right) dr \right) \left(e^{s\mathcal{L}} v \right) \left(e^{-s\mathcal{L}} \bar{v} \right) \right) ds, \\ \mathcal{I}_o(\lambda_0 \mathcal{I}_{\bar{o}}(\lambda_1)) &= \text{blue dot} \\ &\equiv \int_0^t e^{(t-s)\mathcal{L}} \left(\left(\int_0^s e^{(r-s)\mathcal{L}} \left(\left(e^{-r\mathcal{L}} \bar{v} \right) V \right) dr \right) \left(e^{s\mathcal{L}} v^2 \right) \right) ds, \end{aligned}$$

where we have used a blue dot for encoding the potential V . A full list of these trees is given in the Section 3.5.1.

3.2.2 Approximated decorated trees

We denote by \mathcal{T} the set of decorated trees $T_{\mathfrak{e},r}^{\mathfrak{n},\mathfrak{f}} = (T, \mathfrak{n}, \mathfrak{f}, \mathfrak{e}, r)$ where

- $T_{\mathfrak{e}}^{\mathfrak{n},\mathfrak{f}} \in \hat{\mathcal{T}}$.
- The decoration of the root is given by $r \in \mathbf{Z}$, $r \geq -1$ such that

$$r + 1 \geq \text{deg}(T_{\mathfrak{e}}^{\mathfrak{n},\mathfrak{f}}) \quad (3.36)$$

where deg is defined recursively by

$$\text{deg}(\mathbf{1}) = 0, \quad \text{deg}(\lambda_{\mathfrak{e}}^{\ell} \prod_{i=1}^m \mathcal{I}_{o_i}(T_i)) = \ell + 1 + \max(\text{deg}(T_1), \dots, \text{deg}(T_m)).$$

We call \mathcal{T} approximated decorated trees following the terminology introduced in [BS22]. Indeed, the decoration r at the root means that we consider an approximation at order r of the iterated integrals associated to the same trees without this decoration. The quantity $\text{deg}(T_{\mathfrak{e}}^{\mathfrak{n}})$ is the maximum number of edges and node decorations \mathfrak{n} lying on the same path from one leaf to the root.

We denote by \mathcal{P} the planted trees satisfying the same condition as \mathcal{T} . The forests formed of these trees are given by H and their linear span by \mathcal{H} . They are of the form $\mathcal{I}_o^r(T)$. The map $\mathcal{I}_o^r(\cdot) : \hat{\mathcal{T}} \rightarrow \mathcal{H}$ is defined as the same as for $\mathcal{I}_o(\cdot)$ except now that the root is decorated by r and it could be zero if the inequality (3.36) is not satisfied. It can be naturally extended into a map from \mathcal{T} into \mathcal{H} by removing the r decoration at the root of the tree that is grafted onto a new root. We define the map $\mathcal{D}_r : \hat{\mathcal{P}} \rightarrow \mathcal{H}$ which adds the decoration r and performs the projection along the identity (3.36). It is given by

$$\mathcal{D}_r(\mathbf{1}) = \mathbf{1}_{\{0 \leq r+1\}}, \quad \mathcal{D}_r(\mathcal{I}_o(T)) = \mathcal{I}_o^r(T) \quad (3.37)$$

We extend this map to \mathcal{T} by:

$$\mathcal{D}_r(\lambda_i^\ell \prod_{i=1}^m \mathcal{I}_{o_i}(T_i)) = \lambda_i^\ell \prod_{i=1}^m \mathcal{I}_{o_i}^{r-\ell}(T_i)$$

where the term on the right hand-side is identified with $\lambda_i^\ell \prod_{i=1}^m \mathcal{I}_{o_i}(T_i)$ where the decoration r is added to its root with the projection given by (3.36).

3.3 Approximations of iterated integrals

In this section, we introduce the iterated integrals associated to decorated trees via a character $\Pi : \hat{\mathcal{H}} \rightarrow \mathcal{C}$, a multiplicative map for the forest product. We approximate this map via a new character $\Pi_A : \mathcal{H} \rightarrow \mathcal{C}$ defined on approximated decorated forests with A a domain to which $\hat{\mathbf{v}}$ belongs to. The crucial part of the recursive definition of Π_A is given by an operator \mathcal{K} that filter out the dominant part of the operators. It expands only the lower order parts into a Taylor series expansion while integrating exactly the dominant part (see Definition 3.3.2). The definition of these operators is similar to the one in Fourier given in [BS22]. Then, in the second part of this section, we conduct the local error analysis by comparing Π with Π_A with the main result given in Theorem 3.3.9. The main argument for establishing this bound is a recursive definition (see Definition 3.3.8) which involves several Taylor remainders (see Lemma 3.3.6). These remainders are stemming from the various approximations performed by the map \mathcal{K} . Such a description is analogue to the Fourier case that can provide a further expansion of the local error analysis via a Birkhoff factorisation involving a Butcher-Connes-Kreimer coproduct. We do not have such a characterisation for our scheme. However in Proposition 3.3.7 we are able to show how dominant operators are involved in the local error analysis. This was previously observed in the Fourier case.

3.3.1 Characters on decorated forests

We first introduce the linear space \mathcal{C} in which the iterated integrals associated to Duhamel's formula (3.18) live. Any element $f \in \mathcal{C}$ is such that for every $\tau \in \mathbf{R}_+$, one has that $f(\cdot, \tau)$ is an operator on $\hat{\mathbf{v}}$. We define a character Π on $\hat{\mathcal{H}}$ taking values in \mathcal{C} . It is given for $T \in \hat{\mathcal{T}}$ and $F_1, F_2 \in \hat{\mathcal{H}}$ by

$$\begin{aligned} (\Pi \mathcal{I}_o(T))(\hat{\mathbf{v}}, \tau) &= \int_0^\tau e^{(\tau-\xi)\mathcal{L}_o}(\tilde{\Pi}_o T)(\hat{\mathbf{v}}, \xi) d\xi, \\ (\Pi F_1 F_2)(\hat{\mathbf{v}}, \xi) &= (\Pi F_1)(\hat{\mathbf{v}}, \xi) (\Pi F_2)(\hat{\mathbf{v}}, \xi) \end{aligned} \quad (3.38)$$

where $F_1 F_2$ is the forest product and $\tilde{\Pi}_o$ is given on a decorated tree $T = \lambda_i^k \prod_{i=1}^n \mathcal{I}_{o_i}(T_i)$ by

$$\left(\tilde{\Pi}_o \lambda_i^k \prod_{i=1}^n \mathcal{I}_{o_i}(T_i) \right) (\hat{\mathbf{v}}, \xi) = \mathcal{B}_o^! \left(\frac{\Upsilon_{\text{root}}^{\Psi_o}[T]}{S_{\text{root}}(T)} V_i \xi^k \Pi \left(\prod_{i=1}^n \mathcal{I}_{o_i}(T_i) \right) \right) (\hat{\mathbf{v}}, \xi) \quad (3.39)$$

where $S_{\text{root}}(T)$ is the symmetry factor associated to the root of the decorated tree T and the (linear) operators $\mathcal{B}_o^!$ are given by the structure of the nonlinearity (3.2). The symmetry factor is defined by setting $S_{\text{root}}(\mathbf{1}) = 1$ and

$$S_{\text{root}} \left(\lambda_i^k \prod_{i,j} (\mathcal{I}_{o_i}(T_{i,j}))^{\beta_{i,j}} \right) = k! \prod_{i,j} \beta_{i,j}! \quad (3.40)$$

with $T_{i,j} \neq T_{i,\ell}$ for $j \neq \ell$. The coefficient $\Upsilon_{\text{root}}^{\Psi_o}[T]$ in (3.38) is given by

$$\Upsilon_{\text{root}}^{\Psi_o}[T](\mathbf{v}, \xi) = (\partial_k D_{o_1} \cdots D_{o_n} \hat{\Psi}_o^!)(\mathbf{v}, \xi) \quad (3.41)$$

where for $\Psi_o^!(\mathbf{u}_o) = \mathcal{B}_o^! \left(\prod_{i \in \mathcal{O}_+^{1,o}} f_{o,i}^!(u_i) \right)$ we have

$$\hat{\Psi}_o^!(\mathbf{v}, \xi) = \prod_{i \in \mathcal{O}_+^{1,o}} e^{\xi \mathcal{L}_i} f_{o,i}^!(v_i).$$

The various derivatives ∂, D_o follow the Leibniz rule and are given by:

$$D_{o_i} \mathcal{C}^\ell \left[D_{o_i}^k f_{o,o_i}^!, \mathcal{L}_{o_i} \right] = \mathcal{C}^\ell \left[D_{o_i}^{k+1} f_{o,o_i}^!, \mathcal{L}_{o_i} \right],$$

$$\partial \mathcal{C}^\ell \left[D_{o_i}^k f_{o_i}^l, \mathcal{L}_{o_i} \right] = \mathcal{C}^{\ell+1} \left[D_{o_i}^k f_{o_i}^l, \mathcal{L}_{o_i} \right],$$

where D_{o_i} stands for the derivative with respect to v_{o_i} . One has $D_{o_i} f(v_{o_j}) = 0$ for $o_i \neq o_j$ and by convention we set $D_{o_i}(e^{\xi \mathcal{L}_{o_i} v_{o_i}}) = 1$. The derivative ∂_o adds a commutator depending on \mathcal{L}_{o_i} to $f_{o_i}^l$.

Remark 3.3.1 The subscript o in $\tilde{\Pi}_o$ is needed in the definition for identifying which nonlinearity has to be used in the coefficient $\Upsilon_{\text{root}}^{\Psi_o}[T]$. This is also a crucial difference with [BS22] where the coefficients $\Upsilon_{\text{root}}^{\Psi_o}[T]$ are detached from the definition of the iterated integral. This is possible due to the fact that one only works in Fourier space in [BS22]. We have used the subscript root to stress that $\Upsilon_{\text{root}}^{\Psi_o}[T]$ computes a coefficient of T taking into account only its edges connected to its root. This is in contrast with the classical elementary differential for B-series where all the nodes of the tree are considered for computing it. In fact, the rest of the coefficient is computed recursively via an iteration of Π in (3.39).

Example 9 We continue Example 8 on the Gross-Pitaevskii equation and illustrate the definition of $\Pi, \tilde{\Pi}_o$. One has

$$\begin{aligned} (\tilde{\Pi}_o \lambda_0)(\hat{\mathbf{v}}, \xi) &= (-ie^{\xi \mathcal{L} v^2})(e^{-\xi \mathcal{L} \bar{v}}), & (\tilde{\Pi}_o \lambda_0)(\hat{\mathbf{v}}, \xi) &= (ie^{-\xi \mathcal{L} \bar{v}^2})(e^{\xi \mathcal{L} v}), \\ (\tilde{\Pi}_o \lambda_1)(\hat{\mathbf{v}}, \xi) &= (-ie^{\xi \mathcal{L} v})V, & (\tilde{\Pi}_o \lambda_1)(\hat{\mathbf{v}}, \xi) &= (ie^{-\xi \mathcal{L} \bar{v}})V, \end{aligned}$$

since

$$\begin{aligned} S_{\text{root}}(\lambda_0) &= S_{\text{root}}(\lambda_1) = 1, & V_0 &= 1, & V_1 &= V, & \mathcal{B}_o^0 &= \mathcal{B}_o^1 = \text{id}, \\ \Upsilon_{\text{root}}^{\Psi_o}[\lambda_0](\mathbf{v}, \xi) &= (-ie^{\xi \mathcal{L} v^2})(e^{-\xi \mathcal{L} \bar{v}}), & \Upsilon_{\text{root}}^{\Psi_{\bar{o}}}[\lambda_0](\mathbf{v}, \xi) &= (ie^{-\xi \mathcal{L} \bar{v}^2})(e^{\xi \mathcal{L} v}), \\ \Upsilon_{\text{root}}^{\Psi_o}[\lambda_1](\mathbf{v}, \xi) &= -ie^{\xi \mathcal{L} v}, & \Upsilon_{\text{root}}^{\Psi_{\bar{o}}}[\lambda_1](\mathbf{v}, \xi) &= ie^{-\xi \mathcal{L} \bar{v}}. \end{aligned}$$

Hence,

$$\begin{aligned} (\Pi \mathcal{I}_o(\lambda_0))(\hat{\mathbf{v}}, \tau) &= \int_0^\tau e^{(\tau-\xi)\mathcal{L}_o} (\tilde{\Pi}_o \lambda_0)(\hat{\mathbf{v}}, \xi) d\xi \\ &= -i \int_0^\tau e^{(\tau-\xi)\mathcal{L}_o} (e^{\xi \mathcal{L} v^2})(e^{-\xi \mathcal{L} \bar{v}}) d\xi. \end{aligned}$$

Then again, using the definition of the characters Π , and $\tilde{\Pi}_o$ in (3.38), we obtain

$$\begin{aligned} (\tilde{\Pi}_o \lambda_0^1)(\hat{\mathbf{v}}, \xi) &= \frac{\Upsilon_{\text{root}}^{\Psi_o}[\lambda_0^1]}{S_{\text{root}}(\lambda_0^1)}(\mathbf{v}, \xi) V_0 \xi \\ &= -i\xi (e^{\xi \mathcal{L} \mathcal{C}[u^2, \mathcal{L}]}(v))(e^{-\xi \mathcal{L} \bar{v}}), \end{aligned}$$

since,

$$\begin{aligned} \Upsilon_{\text{root}}^{\Psi_o}[\lambda_0^1](\mathbf{v}, \xi) &= (\partial_1 \hat{\Psi}_o^0)(\mathbf{v}, \xi) \\ &= \partial_1 [(e^{\xi \mathcal{L} f_{o,o}^0}(v_o))(e^{-\xi \mathcal{L} f_{o,\bar{o}}^0}(v_{\bar{o}}))] \\ &= -i (e^{\xi \mathcal{L} \mathcal{C}[u^2, \mathcal{L}]}(v))(e^{-\xi \mathcal{L} \bar{v}}) \end{aligned}$$

and $S_{\text{root}}(\lambda_0^1) = 1$.

Let A be a given domain of regularity of $\hat{\mathbf{v}}$ that corresponds to the regularity we assume a priori on the initial data and the potentials. We introduce an approximation of Π via a new character Π_A defined on \mathcal{H} , by:

$$\begin{aligned} (\Pi_A \mathcal{I}_o^r(T))(\hat{\mathbf{v}}, \xi) &= \mathcal{K}_{o,A}^r((\tilde{\Pi}_{o,A} \mathcal{D}_{r-1}(T))(\hat{\mathbf{v}}, \cdot))(\xi) \\ \left(\tilde{\Pi}_{o,A} \lambda_1^k \prod_{i=1}^n \mathcal{I}_{o_i}^r(T_i) \right) (\hat{\mathbf{v}}, \xi) &= \mathcal{B}_o^l \left(\frac{\Upsilon_{\text{root}}^{\Psi_o}[T]}{S_{\text{root}}(T)} V_1 \xi^k \prod_{i=1}^n (\Pi_A \mathcal{I}_{o_i}^r(T_i)) \right) (\hat{\mathbf{v}}, \xi) \end{aligned} \quad (3.42)$$

where $T = \lambda_1^k \prod_{i=1}^n \mathcal{I}_{o_i}^r(T_i)$ and the operator $\mathcal{K}_{o,A}^r$ is given in Definition 3.3.2. As one can notice the approximation follows the recursive definition of Π and $\tilde{\Pi}_o$. The main difference occurs when one replaces the integral in time given in (3.38) by

the operator $\mathcal{K}_{o,A}^r$. This operator is used to give an approximation of order $r + 1$ to the following integral:

$$\int_0^t e^{(t-s)\mathcal{L}_o} \mathcal{B} \left(s^\ell \prod_{i=1}^m e^{s\mathcal{L}_i} u_i \right) ds \quad (3.43)$$

where \mathcal{B} , \mathcal{L}_i are some operators and the u_i depend on $\hat{\mathbf{v}}$. The approximation should take into account the various interactions between the operators \mathcal{L}_o and \mathcal{L}_i . In the sequel, we will use the following shorthand notations:

$$\Pi_A^r = \Pi_A \mathcal{D}_r, \quad \tilde{\Pi}_{o,A}^r = \tilde{\Pi}_{o,A} \mathcal{D}_r$$

where now Π_A^r and $\tilde{\Pi}_{o,A}^r$ are defined on $\hat{\mathcal{H}}$ and $\hat{\mathcal{P}}$.

Definition 3.3.2 Let us consider a function F of the form

$$F(\hat{\mathbf{v}}, \xi) = \xi^\ell \mathcal{B} \left(\prod_{i \in J} e^{\xi \mathcal{L}_i} u_i(\hat{\mathbf{v}}) \right)$$

where \mathcal{B} is a linear operator, the operators \mathcal{L}_i satisfy Assumption (2), and J is a finite set. We suppose that the u_i are smooth functions of $\hat{\mathbf{v}}$, and we assume a given domain A for which we have $\hat{\mathbf{v}} \in A$. Let $r > 0$, $o \in \mathfrak{L}_+$ and the operator \mathcal{L}_o associated to the decoration o . We assume that \mathcal{B} commutes with \mathcal{L}_o . Given $(k_i)_{i \in J}$ with $k_i \in \mathbf{N}$, we define

$$G_{n,(k_i)_{i \in J}} : \hat{\mathbf{v}} \rightarrow \mathcal{L}_o^n \mathcal{B} \left(\prod_{i \in J} \mathcal{L}_i^{k_i} u_i(\hat{\mathbf{v}}) \right).$$

Note that the domain of G depends on the space X and its associated norm. Now we distinguish two cases:

— If $A \subseteq D(G_{n,(k_i)_{i \in J}})$ for all $(k_i)_{i \in J}$ and n be such that, $\sum_i k_i + n \leq r - \ell + 1$ we can carry out a Taylor-series expansion of all the operators and set:

$$\begin{aligned} & \mathcal{K}_{o,A}^r(F(\hat{\mathbf{v}}, \cdot))(\tau) \\ &= \sum_{\sum_i k_i + n \leq r - \ell} \int_0^\tau \frac{(\tau - \xi)^n \xi^{\sum_{i \in J} k_i + \ell}}{n! \prod_{i \in J} k_i!} \mathcal{L}_o^n \mathcal{B} \left(\prod_{i \in J} \mathcal{L}_i^{k_i} u_i(\hat{\mathbf{v}}) \right) d\xi. \end{aligned} \quad (3.44)$$

— Otherwise, we set

$$\mathcal{A}_i = \mathcal{L}_i - \mathcal{L}_o, \quad \mathcal{L}_{\text{dom}} = \mathcal{P}_{\text{dom}}(\{\mathcal{A}_1, \dots, \mathcal{A}_m\}).$$

Then, if $\mathcal{L}_{\text{dom}} \neq 0$, let $I \subset J$ such that for every $i \in I$, one has

$$\mathcal{A}_i = \mathcal{L}_{\text{dom}} + \mathcal{A}_{\text{low}}^i, \quad D(\mathcal{L}_{\text{dom}}) \subset D(\mathcal{A}_{\text{low}}^i),$$

and for $i \in J \setminus I$

$$\mathcal{A}_i = \mathcal{A}_{\text{low}}^i, \quad D(\mathcal{L}_{\text{dom}}) \subset D(\mathcal{A}_i).$$

One can rewrite F as

$$F(\cdot, \xi) = \xi^\ell \mathcal{B} \left(\left(\prod_{i \in I} e^{\xi(\mathcal{L}_o + \mathcal{L}_{\text{dom}} + \mathcal{A}_{\text{low}}^i)} u_i \right) \left(\prod_{i \in J \setminus I} e^{\xi(\mathcal{L}_o + \mathcal{A}_{\text{low}}^i)} u_i \right) \right). \quad (3.45)$$

We assume that the operators that appear in (3.45) commute and generate a continuous semigroup. If this is not the case, one needs to apply the approximation (3.44). We have to distinguish two cases:

(i) If $\mathcal{L}_{\text{dom}} \neq 0$ then

$$\begin{aligned} & \mathcal{K}_{o,A}^r(F)(\tau) = \int_0^\tau \sum_{q \leq r - \ell} \sum_{q = n + m + p + \sum_{i \in J} k_i} \frac{(\tau - \xi)^m \xi^{\ell + \sum_{i \in J} k_i}}{p! m! n! \prod_{i \in J} k_i!} \\ & \mathcal{B} \left(\mathcal{C}^m \left[\left(e^{\tau \mathcal{L}_o} \mathcal{C}^n [\mathcal{M}_{J \setminus I}, \tau \mathcal{L}_o] \right) \left(e^{\xi \mathcal{L}_{\text{dom}} + \tau \mathcal{L}_o} \mathcal{C}^p [\mathcal{M}_I, \xi \mathcal{L}_{\text{dom}} + \tau \mathcal{L}_o] \right), \mathcal{L}_o \right] \right. \\ & \left. \left((\mathcal{A}_{\text{low}}^i)^{k_i} u_i \right)_{i \in J} \right) d\xi. \end{aligned} \quad (3.46)$$

(ii) If $\mathcal{L}_{\text{dom}} = 0$ then

$$\begin{aligned} \mathcal{K}_{o,A}^r(F)(\tau) &= \int_0^\tau \sum_{q \leq r-\ell} \sum_{q=n+m+\sum_{i \in J} k_i} \frac{(\tau - \xi)^m \xi^{\sum_{i \in J} k_i}}{m! n! \prod_{i \in J} k_i!} \\ &\mathcal{B}\left(\mathcal{C}^m\left[\left(e^{\tau \mathcal{L}_o} \mathcal{C}^m[\mathcal{M}_J, \tau \mathcal{L}_o]\right), \mathcal{L}_o\right]\left(\left(\mathcal{A}_i\right)^{k_i} u_i\right)_{i \in J}\right) d\xi. \end{aligned} \quad (3.47)$$

Remark 3.3.3 In general, one has to face more complicated products to approximate. They are of the form:

$$F(\hat{\mathbf{v}}, \xi) = \xi^\ell \mathcal{B}\left(\prod_{i \in K} \mathcal{B}_i\left(\prod_{j \in J_i} e^{\xi \mathcal{L}_j} u_{i,j}(\hat{\mathbf{v}})\right)\right)$$

Such a product will not appear in the Gross-Pitaevski equation neither for the first order of Sine-Gordon. In that case, one can perform the same analysis computing dominant and lower parts. To be in the cases (i) and (ii), there must exist some $I \subset K$ such that one has to get the following factorisation:

$$\begin{aligned} F(\hat{\mathbf{v}}, \xi) &= \xi^\ell \mathcal{B}\left(\prod_{i \in I} \mathcal{B}_i\left(\prod_{j \in J_i} e^{\xi(\mathcal{L}_o + \mathcal{L}_{\text{dom}} + \mathcal{A}_{\text{low}}^j)} u_{i,j}\right)\right) \\ &\left(\prod_{i \in K \setminus I} \mathcal{B}_i\left(\prod_{j \in J_i} e^{\xi(\mathcal{L}_o + \mathcal{A}_{\text{low}}^j)} u_{i,j}\right)\right) \end{aligned}$$

Then, one has just to replace the products \mathcal{M} by new ones taking into account the operators \mathcal{B}_i :

$$\prod_{i \in I} \mathcal{B}_i(\mathcal{M}_{J_i}), \quad \prod_{i \in K \setminus I} \mathcal{B}_i(\mathcal{M}_{J_i})$$

instead of \mathcal{M}_I and $\mathcal{M}_{K \setminus I}$. If F happens not to have this form one performs the full Taylor expansion as in (3.44).

Remark 3.3.4 The $\{k_i\}_{i \in J}$ appear after having Taylor expanded the lower order parts of the operators. Let us mention that this step is necessary in a coupled system with two differential operators \mathcal{L}_1 and \mathcal{L}_2 that differ from a lower differential operator see equation (3.17).

Remark 3.3.5 The previous approximation is optimized according to an a priori given domain A . For solutions and potentials regular enough, for example when the following inclusions hold: $A \subset D(\mathcal{L}_i)$ or/and $A \subset D(\mathcal{L}_{\text{dom}})$, then in these cases, one can perform Taylor expansions (see (3.44)) in order to simplify the scheme. This approach is deeply used in Section 3.5.1 for the construction of the second order low-regularity scheme for Gross-Pitaevskii, and in Sections 3.5.1 and 3.5.3 to construct a simplified first-order scheme for the Gross-Pitaevskii and Sine-Gordon equation when we assume more regularity on the solution and/or potential. Moreover, given that the boundary conditions are encoded in the domain of the operator \mathcal{L}_o and \mathcal{L}_{dom} , we also define the domain A with the prescribed boundary conditions.

Example 10 We illustrate Definition 3.3.2 on a tree coming from the NLS equation with $A = (H^2(\Omega))^2$, $\hat{\mathbf{v}} = (v, \bar{v})$, where for simplicity we assume that $\Omega = \mathbf{R}^d$.

$$\begin{aligned} (\Pi_A \mathcal{I}_o^r(\lambda_0))(\hat{\mathbf{v}}, \xi) &= \mathcal{K}_{o,A}^r((\tilde{\Pi}_{o,A} \mathcal{D}_{r-1}(\lambda_0))(\hat{\mathbf{v}}, \cdot))(\xi) \\ (\tilde{\Pi}_{o,A} \mathcal{D}_{r-1}(\lambda_0))(\hat{\mathbf{v}}, \xi) &= \left(-ie^{\xi \mathcal{L}} v^2\right) \left(e^{-\xi \mathcal{L}} \bar{v}\right). \end{aligned}$$

Then using the notations in Definition 3.3.2, one gets

$$\begin{aligned} F(\hat{\mathbf{v}}, \xi) &= \prod_{i \in \{1,2\}} e^{\xi \mathcal{L}_i} u_i(\hat{\mathbf{v}}), \quad u_1(\hat{\mathbf{v}}) = -iv^2, \quad u_2(\hat{\mathbf{v}}) = \bar{v}, \\ &\mathcal{L}_1 = \mathcal{L}, \quad \mathcal{L}_2 = -\mathcal{L}. \end{aligned}$$

We can now compute the operator interactions as follows

$$\begin{aligned} \mathcal{A}_1 &= \mathcal{L}_1 - \mathcal{L} = 0, \quad \mathcal{A}_2 = \mathcal{L}_2 - \mathcal{L} = -2\mathcal{L} \\ \mathcal{L}_{\text{dom}} &= \mathcal{P}_{\text{dom}}(\{\mathcal{A}_1, \mathcal{A}_2\}) = \mathcal{P}_{\text{dom}}(\{0, -2\mathcal{L}\}) = -2\mathcal{L}, \quad \mathcal{A}_{\text{low}}^1 = \mathcal{A}_{\text{low}}^2 = 0. \end{aligned}$$

We have $\mathcal{L}_{\text{dom}} = -2\mathcal{L} \neq 0$, therefore we apply the first point (i) of Definition 3.3.2:

$$\begin{aligned} \mathcal{K}_{o,A}^r(F)(\tau) &= \int_0^\tau \sum_{q \leq r-\ell} \sum_{q=n+m+p} \frac{(\tau-\xi)^m}{p!m!n! \prod_{i \in J} k_i!} \\ &\mathcal{C}^m \left[\left(e^{\tau \mathcal{L}_o} \mathcal{C}^n [\mathcal{M}_{J \setminus I}, \tau \mathcal{L}_o] \right) \left(e^{\xi \mathcal{L}_{\text{dom}} + \tau \mathcal{L}_o} \mathcal{C}^p [\mathcal{M}_I, \xi \mathcal{L}_{\text{dom}} + \tau \mathcal{L}_o] \right), \mathcal{L}_o \right] \\ &((u_i)_{i \in J}) d\xi. \end{aligned}$$

We have $I = \{2\}$ and $J = \{1, 2\}$, therefore for every $n, p \neq 0$

$$\mathcal{C}^n [\mathcal{M}_{J \setminus I}, \tau \mathcal{L}_o] = \mathcal{C}^p [\mathcal{M}_I, \xi \mathcal{L}_{\text{dom}} + \tau \mathcal{L}_o] = 0.$$

Hence, from the above computations and by considering the case where $r = 1$ (i.e., a second order scheme) we obtain the following,

$$\begin{aligned} \mathcal{K}_{o,A}^1(F)(\tau) &= B + C \\ B &= \int_0^\tau (\tau - \xi) \mathcal{C} \left[\left(e^{\tau \mathcal{L}_o} \mathcal{M}_{\{1\}} \right) \left(e^{\xi \mathcal{L}_{\text{dom}} + \tau \mathcal{L}_o} \mathcal{M}_{\{2\}} \right), \mathcal{L}_o \right] (u_1, u_2) d\xi \\ C &= \int_0^\tau \left(e^{\tau \mathcal{L}_o} u_1 \right) \left(e^{\xi \mathcal{L}_{\text{dom}} + \tau \mathcal{L}_o} u_2 \right) d\xi. \end{aligned}$$

In the end, one has

$$\begin{aligned} (\Pi_A \mathcal{I}_o^1(\lambda_0))(\hat{\mathbf{v}}, \tau) &= -i \int_0^\tau \left(e^{\tau \mathcal{L}} v^2 \right) \left(e^{(\tau-2\xi) \mathcal{L}} \bar{v} \right) d\xi \\ &+ \int_0^\tau (\tau - \xi) \mathcal{C} \left[\left(e^{\tau \mathcal{L}} \mathcal{M}_{\{1\}} \right) \left(e^{(\tau-2\xi) \mathcal{L}} \mathcal{M}_{\{2\}} \right), \mathcal{L} \right] (-iv^2, \bar{v}) d\xi. \end{aligned}$$

3.3.2 Local error analysis for approximated iterated integrals

Before comparing the character Π with Π_A , one has to understand the error introduced by the approximation operator \mathcal{K} . This depends on the various cases in Definition 3.3.2.

Lemma 3.3.6 *We keep the notations of Definition 3.3.2. We suppose that $r \geq \ell$ then one has*

$$\int_0^\tau e^{(\tau-\xi) \mathcal{L}_o} F(\hat{\mathbf{v}}, \xi) d\xi - \mathcal{K}_{o,A}^r(F(\hat{\mathbf{v}}, \cdot))(\tau) = \mathcal{O}(\tau^{r+2}) R_{o,A}^r(F)(\hat{\mathbf{v}}, \cdot)(\tau) \quad (3.48)$$

where $R_{o,A}^r(F)$ takes the following values:

(i) *If we are using the approximation (3.44), we get the following error:*

$$R_{o,A}^r(F) = \sum_{\sum_i k_i + n = r - \ell + 1} \mathcal{L}_o^n \mathcal{B} \left(\prod_{i \in J} \mathcal{L}_i^{k_i} u_i \right).$$

(ii) *If $\mathcal{L}_{\text{dom}} \neq 0$ then*

$$\begin{aligned} R_{o,A}^r(F) &= \sum_{\sum_{i \in J} k_i + m + n + p = r - \ell + 1} \mathcal{B} \left(\mathcal{C}^m \left[\left(\mathcal{C}^n [\mathcal{M}_{J \setminus I}, \mathcal{L}_o] \right) \right. \right. \\ &\left. \left. \left(\mathcal{C}^p [\mathcal{M}_I, \mathcal{L}_{\text{dom}} + \mathcal{L}_o] \right), \mathcal{L}_o \right] \left((\mathcal{A}_{i_{\text{low}}}^i)^{k_i} u_i \right)_{i \in J} \right). \end{aligned}$$

(iii) *If $\mathcal{L}_{\text{dom}} = 0$ then*

$$R_{o,A}^r(F) = \sum_{\sum_{i \in J} k_i + m + n + p = r - \ell + 1} \mathcal{B} \left(\mathcal{C}^m \left[\mathcal{C}^n [\mathcal{M}_J, \mathcal{L}_o], \mathcal{L}_o \right] \left((\mathcal{A}_i)^{k_i} u_i \right)_{i \in J} \right).$$

Proof. The proof reduces to applying several times Taylor expansions and using identity (3.12). \square

Example 11 We want to compute the second order error term for the tree $\mathcal{I}_o(\lambda_0)$ illustrating point (ii) of Lemma 3.3.6. From Example 10, we are in the case where $D(\mathcal{L}_{\text{dom}}) = D(\mathcal{L}_o)$ and we have

$$R_{o,A}^1(\tilde{\Pi}_{o,A}\lambda_0)(\hat{\mathbf{v}}) = \sum_{m+n+p=2} \mathcal{C}^m[(\mathcal{C}^n[\mathcal{M}_{J \setminus I}, \mathcal{L}_o]) \\ (\mathcal{C}^p[\mathcal{M}_I, \mathcal{L}_{\text{dom}} + \mathcal{L}_o]), \mathcal{L}_o](-iv^2, \bar{v})$$

where $I = \{2\}$ and $J = \{1, 2\}$ and where the only non-zero term in the above is when $(m, n, p) = (2, 0, 0)$. Hence, we have,

$$R_{o,A}^1(\tilde{\Pi}_{o,A}\lambda_0)(\hat{\mathbf{v}}) = \mathcal{C}^2[\mathcal{M}_{\{1,2\}}, \mathcal{L}_o](-iv^2, \bar{v}).$$

The next proposition follows the steps of [BS22, Prop. 3.9]. It singles out the dominant parts of the oscillations and shows that approximated iterated integrals are connected with Definition 3.2.3. This decomposition was also connected to the Birkoff factorisation given in [BS22]. It provides information about the dominant operators that will be involved in the local error analysis. In the next proposition, we assume that $\mathcal{B}_o^! = \text{id}$. In the general case, one can write a similar statement using Remark 3.3.3.

Proposition 3.3.7 *For every tree $\mathcal{I}_o(T) \in \mathcal{H}$, one has the following decomposition:*

$$(\Pi_A \mathcal{I}_o^r(T))(\hat{\mathbf{v}}, \xi) = \sum_{\bar{T} \subset \mathcal{I}_o(T)} \prod_{\mathcal{L} \in \mathcal{R}_{\text{dom}}(\bar{T})} \left(e^{i\xi \mathcal{L}} B^r(T, \bar{T}, \mathcal{L})(\hat{\mathbf{v}}, \xi) \right) \\ + \left(e^{i\xi \mathcal{L}_o} B^r(T, \mathbf{1}, \mathcal{L}_o)(\hat{\mathbf{v}}, \xi) \right) \left(e^{i\xi \mathcal{L}_o} C^r(T, \mathbf{1}, \mathcal{L}_o)(\hat{\mathbf{v}}, \xi) \right) \quad (3.49)$$

where the sum is over all subtrees $\bar{T} \neq \mathbf{1}$ that have at least one edge and that contain the root of $\mathcal{I}_o(T)$. The $B^r(T, \bar{T}, \mathcal{L})(\hat{\mathbf{v}}, \xi)$, $B^r(T, \mathbf{1}, \mathcal{L}_o)(\hat{\mathbf{v}}, \xi)$ and $C^r(T, \mathbf{1}, \mathcal{L}_o)(\hat{\mathbf{v}}, \xi)$ are polynomials in ξ and the $\mathcal{R}_{\text{dom}}(\bar{T})$ are given in Definition 3.2.3.

Proof. We proceed by induction on the size of T and we suppose that $T = \lambda_1^\ell \prod_i \mathcal{I}_{o_i}(T_i)$ where one can apply the induction hypothesis on each $\mathcal{I}_{o_i}(T_i)$. One has from (3.42)

$$(\Pi_A \mathcal{I}_o^r(T))(\hat{\mathbf{v}}, \xi) = \mathcal{K}_{o,A}^r \left(\tilde{\Pi}_{o,A}(\mathcal{D}_{(r-1)}(T))(\hat{\mathbf{v}}, \cdot) \right)(\xi)$$

and

$$\tilde{\Pi}_{o,A}(\mathcal{D}_{(r-1)}(T))(\hat{\mathbf{v}}, \xi) = \frac{\Upsilon_{\text{root}}^{\Psi_o}[T]}{S_{\text{root}}(T)}(\mathbf{v}, \xi) V_1 \xi^\ell \prod_i \left(\Pi_A \mathcal{I}_{o_i}^{(r-1-\ell)}(T_i) \right)(\hat{\mathbf{v}}, \xi).$$

By applying the induction hypothesis on the $\mathcal{I}_{o_i}(T_i)$, one has the following decomposition

$$\tilde{\Pi}_{o,A}(\mathcal{D}_{(r-1)}(T))(\hat{\mathbf{v}}, \xi) = \frac{\Upsilon_{\text{root}}^{\Psi_o}[T]}{S_{\text{root}}(T)}(\mathbf{v}, \xi) V_1 \prod_i \sum_{\bar{T}_i \subset \mathcal{I}_{o_i}(T_i)} \\ \prod_{\mathcal{L} \in \mathcal{R}_{\text{dom}}(\bar{T}_i)} \left(e^{i\xi \mathcal{L}} B^{r-1-\ell}(T_i, \bar{T}_i, \mathcal{L})(\hat{\mathbf{v}}, \xi) \right) \\ + \left(e^{i\xi \mathcal{L}_{o_i}} B^r(T_i, \mathbf{1}, \mathcal{L}_{o_i})(\hat{\mathbf{v}}, \xi) \right) \left(e^{i\xi \mathcal{L}_{o_i}} C^r(T_i, \mathbf{1}, \mathcal{L}_{o_i})(\hat{\mathbf{v}}, \xi) \right)$$

where the $B^r(T_i, \bar{T}_i, \mathcal{L})(\hat{\mathbf{v}}, \xi)$, $B^r(T_i, \mathbf{1}, \mathcal{L}_{o_i})(\hat{\mathbf{v}}, \xi)$ and $C^r(T_i, \mathbf{1}, \mathcal{L}_{o_i})(\hat{\mathbf{v}}, \xi)$ are polynomials in ξ . As a consequence of Definition 3.3.2, the map $\mathcal{K}_{o,A}^r$ applied to the term coming from a subforest $\bar{T} = \lambda_1^\ell \prod_i \bar{T}_i$, integrates exactly in the end a term of the form

$$\int_0^\xi \left(e^{\xi \mathcal{L}_o} P(\hat{\mathbf{v}}, s) \right) \left(e^{s \mathcal{L}_{\text{dom}}(\mathcal{I}_o(\bar{T})) + \xi \mathcal{L}_o} Q(\hat{\mathbf{v}}, s) \right) ds$$

where $P(\hat{\mathbf{v}}, s)$ and $Q(\hat{\mathbf{v}}, s)$ are polynomials in s . Then, by computing this integral, we obtain two terms of the form

$$\left(e^{s \mathcal{L}_o} P_1(\hat{\mathbf{v}}, s) \right) \left(e^{is \mathcal{L}_{\text{dom}}(\mathcal{I}_o(\bar{T}))} Q_1(\hat{\mathbf{v}}, s) \right), \quad \left(e^{s \mathcal{L}_o} P_2(\hat{\mathbf{v}}, s) \right) \left(e^{s \mathcal{L}_o} Q_2(\hat{\mathbf{v}}, s) \right)$$

where P_1, Q_1 and P_2 are also polynomials in s . The first term corresponds to the subtree $\mathcal{I}_o(\bar{T})$ and the second term corresponds to $\mathbf{1}$. Therefore, the structure of (3.49) is preserved. \square

The next definition computes the local error using the recursive construction of the decorated trees. It follows the same structure as in [BS22], the main difference being that now $\Upsilon_{\text{root}}^{\Psi_o}$ has to be added to this definition.

Definition 3.3.8 Let $r \in \mathbf{Z}$ and a domain A of $\hat{\mathbf{v}}$. We recursively define $\mathcal{L}_{\text{low}}^r(\cdot, \hat{\mathbf{v}}, A)$ and $\mathcal{L}_{\text{low}}^{r,o}(\cdot, \hat{\mathbf{v}}, A)$, $o \in \mathfrak{L}_+$ as

$$\mathcal{L}_{\text{low}}^r(T, \hat{\mathbf{v}}, A) = 1, \quad r < 0, \quad \mathcal{L}_{\text{low}}^r(\mathbf{1}, \hat{\mathbf{v}}, A) = 1.$$

Else for $T = \lambda_1^\ell \prod_i \mathcal{I}_{a_i}(T_i)$, one has

$$\begin{aligned} \mathcal{L}_{\text{low}}^{r,o}(\lambda_1^\ell \prod_i \mathcal{I}_{a_i}(T_i), \hat{\mathbf{v}}, A) = & \quad (3.50) \\ \mathcal{B}_o^! \left(\frac{\Upsilon_{\text{root}}^{\Psi_o}[T]}{S_{\text{root}}(T)}(\mathbf{v}, 0) V_1 \left(\sum_i \mathcal{L}_{\text{low}}^{r-\ell}(\mathcal{I}_{a_i}(T_i), \hat{\mathbf{v}}, A) \right) \right). \end{aligned}$$

And

$$\mathcal{L}_{\text{low}}^r(\mathcal{I}_o(T), \hat{\mathbf{v}}, A) = \mathcal{L}_{\text{low}}^{r-1,o}(T, \hat{\mathbf{v}}, A) + R_{o,A}^r \left(\left(\tilde{\Pi}_{o,A}^{r-1} T \right) (\hat{\mathbf{v}}, \cdot) \right), \quad (3.51)$$

where $R_{o,A}^r$ is defined in Lemma 3.3.6

Example 12 We continue Example 11. For the decorated tree $T = \mathcal{I}_o(\lambda_0)$, one obtains:

$$\begin{aligned} \mathcal{L}_{\text{low}}^1(T, \hat{\mathbf{v}}, A) &= \mathcal{L}_{\text{low}}^0(\lambda_0, \hat{\mathbf{v}}, A) + R_{o,A}^1 \left(\left(\tilde{\Pi}_{o,A}^0 T \right) (\hat{\mathbf{v}}, \cdot) \right) \\ &= -iv^2\bar{v} + \mathcal{C}^2[\mathcal{M}_{\{1,2\}}, \mathcal{L}_o](-iv^2, \bar{v}). \end{aligned}$$

One notices that the first term asks less regularity on v in comparison to the second.

The next theorem shows that the characters Π_A and $\tilde{\Pi}_{o,A}$ are good approximations of Π and $\tilde{\Pi}_o$ with a local error given by Definition 3.3.8. We follow the same steps as in the proof of [BS22, Thm 3.17].

Theorem 3.3.9 For $T = \lambda_1^\ell \prod_i \mathcal{I}_{a_i}(T_i)$ one has,

$$\left(\tilde{\Pi}_o T - \tilde{\Pi}_{o,A} \mathcal{D}_r(T) \right) (\hat{\mathbf{v}}, \tau) = \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^{r,o}(T, \hat{\mathbf{v}}, A)) \quad (3.52)$$

and for $T = \mathcal{I}_o(\bar{T})$, one gets

$$\left(\Pi T - \Pi_A \mathcal{D}_r(T) \right) (\hat{\mathbf{v}}, \tau) = \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T, \hat{\mathbf{v}}, A)). \quad (3.53)$$

Proof. We proceed by induction by using the recursive definition (3.42) of Π_A and $\tilde{\Pi}_{o,A}$. First, one gets

$$\left(\Pi - \Pi_A \right) (\mathbf{1}) (\hat{\mathbf{v}}, \tau) = 0 = \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(\mathbf{1}, \hat{\mathbf{v}}, A)).$$

Then for $T = \lambda_1^\ell \prod_i \mathcal{I}_{a_i}(T_i)$ and every $o \in \mathfrak{L}_+$, one has

$$\begin{aligned} \left(\tilde{\Pi}_o - \tilde{\Pi}_{o,A}^r \right) (T) (\hat{\mathbf{v}}, \tau) &= \tau^\ell \mathcal{B}_o^! \left(\frac{\Upsilon_{\text{root}}^{\Psi_o}[T]}{S_{\text{root}}(T)}(\mathbf{v}, \tau) V_1 \sum_i \left(\Pi - \Pi_A^{r-\ell} \right) (\mathcal{I}_{a_i}(T_i)) (\hat{\mathbf{v}}, \tau) \right. \\ &\quad \left. \prod_{j \neq i} \left(\Pi_A^{r-\ell} + \Pi \right) (\mathcal{I}_{a_j}(T_j)) (\hat{\mathbf{v}}, \tau) \right). \end{aligned}$$

Then by applying the induction hypothesis (3.53) to each $\mathcal{I}_{a_i}(T_i)$, one gets

$$\begin{aligned} \left(\tilde{\Pi}_o - \tilde{\Pi}_{o,A}^r \right) (T) (\hat{\mathbf{v}}, \tau) &= \mathcal{O} \left(\tau^{r+2} \mathcal{B}_o^! \left(\frac{\Upsilon_{\text{root}}^{\Psi_o}[T]}{S_{\text{root}}(T)}(\mathbf{v}, 0) V_1 \sum_i \mathcal{L}_{\text{low}}^{r-\ell}(\mathcal{I}_{a_i}(T_i), \hat{\mathbf{v}}, A) \right) \right) \\ &= \mathcal{O} \left(\tau^{r+2} \mathcal{L}_{\text{low}}^r(\lambda_1^\ell \prod_i \mathcal{I}_{a_i}(T_i), \hat{\mathbf{v}}, A) \right). \end{aligned}$$

For $T = \mathcal{I}_o(\bar{T})$, one has

$$\begin{aligned} (\Pi - \Pi_A^r)(T)(\hat{\mathbf{v}}, \tau) &= \int_0^\tau e^{\xi \mathcal{L}_o} (\tilde{\Pi}_o - \tilde{\Pi}_{o,A}^{r-1})(\bar{T})(\hat{\mathbf{v}}, \xi) d\xi \\ &+ \int_0^\tau e^{\xi \mathcal{L}_o} (\tilde{\Pi}_{o,A}^{r-1} \bar{T})(\hat{\mathbf{v}}, \xi) d\xi - \mathcal{K}_o^r((\tilde{\Pi}_{o,A}^{r-1} T)(\hat{\mathbf{v}}, \cdot))(\tau) \\ &= \int_0^\tau \mathcal{O}(\xi^{r+1} \mathcal{L}_{\text{low}}^{r-1,o}(\bar{T}, \hat{\mathbf{v}}, A)) d\xi + \mathcal{O}(\tau^{r+2} R_{o,A}^r((\tilde{\Pi}_{o,A}^{r-1} \bar{T})(\hat{\mathbf{v}}, \cdot))) \\ &= \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T, \hat{\mathbf{v}}, A)). \end{aligned}$$

where the term $R_{o,A}^r((\tilde{\Pi}_{o,A}^{r-1} \bar{T})(\hat{\mathbf{v}}, \cdot))$ is obtained by applying Lemma 3.3.6. \square

3.4 Low regularity numerical scheme

The writing of our low regularity numerical scheme follows two steps. The first one is to write a truncated decorated trees series that will solve the Duhamel's formula up to order r (see Proposition 3.4.1). This series is formed of iterated integrals produced by the character Π . Then, one replaces Π by Π_A to get the scheme. Such steps were already used in [BS22]. Let us mention that the first step is more involved here due to the fact that we work with a more general setting.

3.4.1 Exact solution up to order r

Recall the mild solution of (3.1) given by Duhamel's formula

$$u_o(t) = e^{t \mathcal{L}_o} v_o + \sum_{l \in \mathfrak{L}_-} \int_0^t e^{(t-\xi) \mathcal{L}_o} \Psi_o^l(\mathbf{u}_o^l) V_l d\xi, \quad (3.54)$$

where the nonlinearity $\Psi_o^l(\mathbf{u}_o^l)$ is given by

$$\Psi_o^l(\mathbf{u}_o^l) = \mathcal{B}_o^l \left(\prod_{i \in \mathfrak{L}_+^{l,o}} f_{o,i}^l(u_i) \right).$$

In the following we want to construct a scheme with a local error of order

$$\mathcal{O}(\tau^{r+2}).$$

Therefore, before describing our numerical scheme, we need to remove the trees which are already of size $\mathcal{O}(\tau^{r+2})$. Indeed, a simple recursion shows that one has for every tree $\mathcal{I}_o(T)$

$$(\Pi \mathcal{I}_o(T))(\hat{\mathbf{v}}, \tau) = \mathcal{O}(p(T, \hat{\mathbf{v}}) \tau^{n_+(T)}) \quad (3.55)$$

where $p(T, \hat{\mathbf{v}})$ is a polynomial in the variables $\hat{\mathbf{v}}$ that does not contain any operators $(\mathcal{L}_o)_{o \in \mathfrak{L}_+}$ and at most $|N_T|$ operators \mathcal{B} . The map n_+ is defined on $T_{\mathfrak{L}_+}^{n,f}$ as

$$n_+(T_{\mathfrak{L}_+}^{n,f}) = \sum_{v \in N_T} \mathbf{n}(v) + |E_T|$$

which corresponds to the number of integrations in time and polynomial decorations. We define the space of decorated trees $\mathcal{T}_o^r \subset \mathcal{T}_o$ as

$$\mathcal{T}_o^r = \{\mathcal{I}_o(T), T \in \mathcal{T}^r\}, \quad \mathcal{T}^r = \{T \in \mathcal{T}, n_+(T) \leq r, (\Pi \mathcal{I}_o(T)) \neq 0\}.$$

The condition $(\Pi \mathcal{I}_o(T)) \neq 0$ guarantees that we consider only trees which have been generated by iterations of Duhamel's formula 3.54. In the following we consider

$$w_o^r(\hat{\mathbf{v}}, \tau) = e^{\tau \mathcal{L}_o} v_o + \sum_{T \in \mathcal{T}^r} (\Pi \mathcal{I}_o(T))(\hat{\mathbf{v}}, \tau) \quad (3.56)$$

which solves (3.54) up to order $r+1$ in the following sense:

Proposition 3.4.1 *One has that*

$$w_{\bar{o}}^r(\hat{\mathbf{v}}, t) = e^{\tau \mathcal{L}_{\bar{o}}} v_{\bar{o}} + \sum_{l \in \mathfrak{L}_-} \int_0^\tau e^{(\tau-\xi) \mathcal{L}_{\bar{o}}} \Psi_{\bar{o}}^l(\mathbf{w}_{\bar{o}}^{l,r})(\hat{\mathbf{v}}, \xi) V_l d\xi + \mathcal{O}(\tau^{r+2})$$

where $\mathbf{w}_{\bar{o}}^{l,r}$ denotes the term $(w_{\bar{o}}^r)_{\bar{o} \in \mathfrak{L}_+^{l,o}}$ and the remainder $\mathcal{O}(\tau^{r+2})$ involves commutators under the form:

$$\mathcal{C}^r[f, \mathcal{L}_{\bar{o}}]$$

(however, not full powers of $\mathcal{L}_{\bar{o}}^r$) with f a function coming from the coefficients $\Psi_{\bar{o}}$.

Proof. Let B be given by

$$\begin{aligned} B &= e^{\tau \mathcal{L}_{\bar{o}}} v_{\bar{o}} + \sum_{l \in \mathfrak{L}_-} \int_0^\tau e^{(\tau-\xi) \mathcal{L}_{\bar{o}}} \Psi_{\bar{o}}^l(\mathbf{w}_{\bar{o}}^{l,r})(\hat{\mathbf{v}}, \xi) V_l d\xi \\ &= e^{\tau \mathcal{L}_{\bar{o}}} v_{\bar{o}} + \sum_{l \in \mathfrak{L}_-} \int_0^\tau e^{(\tau-\xi) \mathcal{L}_{\bar{o}}} \mathcal{B}_{\bar{o}}^l \left(\prod_{\bar{o} \in \mathfrak{L}_+^{l,o}} f_{\bar{o}, \bar{o}}^l(w_{\bar{o}}^r(\hat{\mathbf{v}}, \xi)) \right) V_l d\xi. \end{aligned}$$

Then, we have

$$w_{\bar{o}}^r(\hat{\mathbf{v}}, \xi) = e^{\xi \mathcal{L}_{\bar{o}}} v_{\bar{o}} + R_{r,o}(\hat{\mathbf{v}}, \xi), \quad R_{r,o}(\hat{\mathbf{v}}, \xi) = \sum_{T \in \mathcal{T}^r} (\Pi \mathcal{L}_o(T))(\hat{\mathbf{v}}, \xi).$$

By performing Taylor expansions around the point $e^{\xi \mathcal{L}_{\bar{o}}} v_{\bar{o}}$, one gets:

$$\begin{aligned} B &= e^{\tau \mathcal{L}_{\bar{o}}} v_{\bar{o}} + \sum_{l \in \mathfrak{L}_-} \int_0^\tau e^{(\tau-\xi) \mathcal{L}_{\bar{o}}} \mathcal{B}_{\bar{o}}^l \sum_{\sum_{\bar{o}} k_{\bar{o}} \leq r} \frac{1}{\prod_{\bar{o}} k_{\bar{o}}!} \\ &\quad \prod_{\bar{o} \in \mathfrak{L}_+^{l,o}} R_{r,\bar{o}}^{k_{\bar{o}}}(\hat{\mathbf{v}}, \xi) f_{\bar{o}, \bar{o}}^{l, (k_{\bar{o}})}(e^{\xi \mathcal{L}_{\bar{o}}} v_{\bar{o}}) V_l d\xi + \mathcal{O}(\tau^{r+2}) \end{aligned}$$

where the sum $\sum_{\bar{o}}$ and the product $\prod_{\bar{o}}$ run over $\bar{o} \in \mathfrak{L}_+^{l,o}$. The error $\mathcal{O}(\tau^{r+2})$ depends on the derivatives of $f_{\bar{o}, \bar{o}}^{l, (k_{\bar{o}})}$ and on a polynomial in $\hat{\mathbf{v}}$ using the bound (3.55). The next step of the approximation is to pull out the term $e^{\xi \mathcal{L}_{\bar{o}}} v_{\bar{o}}$:

$$\begin{aligned} f_{\bar{o}, \bar{o}}^{l, (k_{\bar{o}})}(e^{\xi \mathcal{L}_{\bar{o}}} v_{\bar{o}}) &= e^{\xi \mathcal{L}_{\bar{o}}} f(v_{\bar{o}}) + \sum_{\ell_{\bar{o}}=1}^{\xi \ell_{\bar{o}}} \frac{\xi^{\ell_{\bar{o}}}}{\ell_{\bar{o}}!} e^{\xi \mathcal{L}_{\bar{o}}} \mathcal{C}^{\ell_{\bar{o}}} [f_{\bar{o}, \bar{o}}^{l, (k_{\bar{o}})}, \mathcal{L}_{\bar{o}}](v_{\bar{o}}) \\ &\quad + \mathcal{O}(\xi^{r+1} \mathcal{C}^{r+1} [f_{\bar{o}, \bar{o}}^{l, (k_{\bar{o}})}, \mathcal{L}_{\bar{o}}](v_{\bar{o}})). \end{aligned}$$

The remainder coming from this approximation is the leading error. It involves $\mathcal{L}_{\bar{o}}$ with an iterated commutator. For the next computations, we will omit this error and write all the identities up to some terms which are neglectable in comparison to this error. Inserting the previous expansion into A and neglecting the terms which are of order bigger than $\mathcal{O}(\tau^{r+2})$, we get:

$$\begin{aligned} B &= e^{\tau \mathcal{L}_{\bar{o}}} v_{\bar{o}} + \sum_{l \in \mathfrak{L}_-} \int_0^\tau e^{(\tau-\xi) \mathcal{L}_{\bar{o}}} \sum_{\sum_{\bar{o}} \ell_{\bar{o}} + \sum_{\bar{o}, i} n_+(T_{\bar{o}, i}) \leq r} \frac{\xi^{\sum_{\bar{o}} \ell_{\bar{o}}}}{\prod_{\bar{o}} k_{\bar{o}}! \ell_{\bar{o}}!} \\ &\quad \mathcal{B}_{\bar{o}}^l \left(\prod_{\bar{o} \in \mathfrak{L}_+^{l,o}} \prod_{i=1}^{k_{\bar{o}}} (\Pi \mathcal{L}_{\bar{o}}(T_{\bar{o}, i}))(\hat{\mathbf{v}}, \xi) \left(e^{\xi \mathcal{L}_{\bar{o}}} \mathcal{C}^{\ell_{\bar{o}}} [f_{\bar{o}, \bar{o}}^{l, (k_{\bar{o}})}, \mathcal{L}_{\bar{o}}](v_{\bar{o}}) \right) V_l \right) d\xi \end{aligned}$$

where the $T_{\bar{o}, i}$ are decorated trees and $\sum_{\bar{o}, i} n_+(T_{\bar{o}, i})$ is a shorthand notation for

$$\sum_{\bar{o} \in \mathfrak{L}_+^{l,o}} \sum_{k_{\bar{o}}} \sum_{i=1}^{k_{\bar{o}}} n_+(T_{\bar{o}, i}).$$

Then, if we fix the product $\prod_{i=1}^{k_{\bar{o}}} \mathcal{I}_{\bar{o}}(T_{\bar{o},i})$, one has:

$$\prod_{i=1}^{k_{\bar{o}}} \mathcal{I}_{\bar{o}}(T_{\bar{o},i}) = \prod_i \mathcal{I}_{\bar{o}}(\tilde{T}_{\bar{o},i})^{k_{\bar{o},i}}$$

where the $\tilde{T}_{\bar{o},i}$ are distincts and $\sum_i k_{\bar{o},i} = k_{\bar{o}}$. This term appears in B with the following combinatorial coefficient:

$$\frac{k_{\bar{o}}!}{\prod_i k_{\bar{o},i}!}.$$

Let us notice

$$S_{\text{root}} \left(\lambda_{\bar{o}}^k \prod_{\bar{o},i} \mathcal{I}_{\bar{o}}(\tilde{T}_{\bar{o},i})^{k_{\bar{o},i}} \right) = k! \prod_{\bar{o},i} k_{\bar{o},i}!$$

and

$$\sum_{\bar{o}} \prod_{\ell_{\bar{o}}=\ell} \prod_{\bar{o} \in \mathfrak{L}_+^{\ell_{\bar{o}}}} \frac{1}{\ell_{\bar{o}}!} \left(e^{\xi \mathcal{L}_{\bar{o}}} \mathcal{C}^{\ell_{\bar{o}}} [f_{\bar{o},\bar{o}}^{\ell_{\bar{o}}}, \mathcal{L}_{\bar{o}}](v_{\bar{o}}) \right) = \frac{\partial_{\ell}}{\ell!} \prod_{\bar{o} \in \mathfrak{L}_+^{\ell}} \left(e^{\xi \mathcal{L}_{\bar{o}}} f_{\bar{o},\bar{o}}^{\ell_{\bar{o}}} (v_{\bar{o}}) \right).$$

In this identity, we exploit the Leibniz rule for the derivative ∂ . It can be understood as a variant of Faa di Bruno formula see [BCCH20, Lem. A.1]. We can rewrite B into

$$\begin{aligned} B &= e^{\tau \mathcal{L}_o} v_o + \sum_{l \in \mathfrak{L}_-} \int_0^{\tau} e^{(\tau-\xi) \mathcal{L}_o} \mathcal{B}_o^l \left(\sum_{\ell + \sum_{\bar{o},i} n_+(\tilde{T}_{\bar{o},i}) \leq r} \frac{\xi^{\ell}}{\ell!} \partial_{\ell} \right. \\ &\quad \left. \prod_{\bar{o} \in \mathfrak{L}_+^{\ell}} \prod_i \frac{1}{k_{\bar{o},i}!} \left(\prod \mathcal{I}_{\bar{o}}(\tilde{T}_{\bar{o},i})^{k_{\bar{o},i}} \right) (\hat{\mathbf{v}}, \xi) \left(e^{\xi \mathcal{L}_{\bar{o}}} f_{\bar{o},\bar{o}}^{\ell_{\bar{o}}} (v_{\bar{o}}) \right) V_l \right) d\xi \\ &= e^{\tau \mathcal{L}_o} v_o + \sum_{l \in \mathfrak{L}_-} \int_0^{\tau} e^{(\tau-\xi) \mathcal{L}_o} \mathcal{B}_o^l \left(\sum_{\ell + \sum_{\bar{o},i} n_+(\tilde{T}_{\bar{o},i}) \leq r} \frac{\xi^{\ell}}{S_{\text{root}} \left(\lambda_{\bar{o}}^{\ell} \prod_{\bar{o},i} \mathcal{I}_{\bar{o}}(\tilde{T}_{\bar{o},i})^{k_{\bar{o},i}} \right)} \right. \\ &\quad \left. \prod_{\bar{o} \in \mathfrak{L}_+^{\ell}} \prod_i \left(\prod \mathcal{I}_{\bar{o}}(\tilde{T}_{\bar{o},i})^{k_{\bar{o},i}} \right) (\hat{\mathbf{v}}, \xi) \Upsilon_{\text{root}}^{\Psi_o} \left(\lambda_{\bar{o}}^{\ell} \prod_{\bar{o},i} \mathcal{I}_{\bar{o}}(\tilde{T}_{\bar{o},i})^{k_{\bar{o},i}} \right) (\mathbf{v}, \xi) V_l \right) d\xi. \end{aligned}$$

Then,

$$\begin{aligned} B &= e^{\tau \mathcal{L}_o} v_o + \sum_{l \in \mathfrak{L}_-} \int_0^{\tau} e^{(\tau-\xi) \mathcal{L}_o} \sum_{\ell + \sum_{\bar{o},i} n_+(\tilde{T}_{\bar{o},i}) \leq r} \left(\prod_{\bar{o},i} \lambda_{\bar{o}}^{\ell} \prod \mathcal{I}_{\bar{o}}(\tilde{T}_{\bar{o},i})^{k_{\bar{o},i}} \right) (\hat{\mathbf{v}}, \xi) d\xi \\ &= e^{\tau \mathcal{L}_o} v_o + \sum_{T \in \mathcal{T}^r} \int_0^{\tau} e^{(\tau-\xi) \mathcal{L}_o} \left(\tilde{\Pi}_o T \right) (\hat{\mathbf{v}}, \xi) d\xi \\ &= e^{\tau \mathcal{L}_o} v_o + \sum_{T \in \mathcal{T}^r} \left(\prod \mathcal{I}_o(T) \right) (\hat{\mathbf{v}}, \tau) = w_o^r(\hat{\mathbf{v}}, \tau) \end{aligned}$$

which concludes the proof. \square

3.4.2 Numerical scheme and local error analysis

Now, we are able to describe the general numerical scheme:

Definition 3.4.2 (The general numerical scheme) For fixed $r \in \mathbf{N}$ and a domain A , we define the general numerical scheme as:

$$u_{o,A}^r(\hat{\mathbf{v}}, \tau) = e^{\tau \mathcal{L}_o} v_o + \sum_{T \in \mathcal{T}^{r+1}} \Pi_A^r(\mathcal{I}_o(T))(\hat{\mathbf{v}}, \tau). \quad (3.57)$$

The numerical scheme (3.57) approximates the exact solution locally up to order $r + 2$. More precisely, the following theorem holds.

Theorem 3.4.3 (Local error) *The numerical scheme (3.57) with initial value $v_o = u_o(0)$ approximates the exact solution u_o up to a local error of type*

$$u_{o,A}^r(\hat{\mathbf{v}}, \tau) - u_o(\hat{\mathbf{v}}, \tau) = \sum_{T \in \mathcal{T}^{r+1}} \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(\mathcal{I}_o(T), \hat{\mathbf{v}}, A))$$

where the operator $\mathcal{L}_{\text{low}}^r(\mathcal{I}_o(T), \hat{\mathbf{v}}, A)$, given in Definition 3.3.8, embeds the necessary regularity of the solution.

Proof. We recall that the exact solution u_o up to order r is given by

$$w_o^r(\hat{\mathbf{v}}, \tau) = e^{\tau \mathcal{L}_o} v_o + \sum_{T \in \mathcal{T}^r} (\Pi \mathcal{L}_o(T))(\hat{\mathbf{v}}, \tau)$$

which satisfies from Proposition 3.4.1

$$u_o(\tau) - w_o^r(\tau) = \mathcal{O}(\tau^{r+2} p(\hat{\mathbf{v}}, (\mathcal{L}_o)_{o \in \mathfrak{L}_+})) \quad (3.58)$$

for some polynomial p such that every \mathcal{L}_o appear under the form $\mathcal{C}^{r+1}[f, \mathcal{L}_o]$. Thanks to Theorem 3.3.9 we furthermore obtain that

$$\begin{aligned} u_{o,A}^r(\hat{\mathbf{v}}, \tau) - w_o^r(\hat{\mathbf{v}}, \tau) &= \sum_{T \in \mathcal{T}^r} (\Pi - \Pi_A^r)(\mathcal{I}_o(T))(\hat{\mathbf{v}}, \tau) \\ &= \sum_{T \in \mathcal{T}^r} \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(\mathcal{I}_o(T), \hat{\mathbf{v}}, A)). \end{aligned} \quad (3.59)$$

Next we write

$$u_{o,A}^r(\hat{\mathbf{v}}, \tau) - u_o(\hat{\mathbf{v}}, \tau) = u_{o,A}^r(\hat{\mathbf{v}}, \tau) - w_o^r(\hat{\mathbf{v}}, \tau) + w_o^r(\hat{\mathbf{v}}, \tau) - u_o(\hat{\mathbf{v}}, \tau)$$

where by the definition of $\mathcal{L}_{\text{low}}^r(T, \hat{\mathbf{v}}, A)$ we easily see that the approximation error (3.59) is dominant compared to (3.58). Indeed, we will have also commutators of the form $\mathcal{C}^{r+1}[f, \mathcal{L}_o]$ and $\mathcal{C}^{r+1}[f, \mathcal{L}_{\text{dom}}]$ due to Proposition 3.3.7. The extra regularity needed is coming from the Taylor expansion of the lower part in Definition 3.3.2. \square

Remark 3.4.4 Theorem 3.4.3 provides a local error estimate (order of consistency) for the low regularity schemes (3.57). With the aid of stability one can easily obtain a global error estimate with the aid of Lady Windamere's fan argument [HLW10]. However, the necessary stability estimates in general rely on the algebraic structure of the underlying space.

In case of parabolic problems the parabolic smoothing property can be used to obtain global error estimates in low regularity spaces. With the aid of semi group theory the regularity assumptions on the solution may be even pushed down further thanks to the point wise smoothing properties. The situation of dispersive PDEs is more involved. In the stability analysis in Sobolev spaces H^r one classically exploits bilinear estimates of type

$$\|vw\|_r \leq c_{r,d} \|v\|_r \|w\|_r.$$

The latter only hold for $r > d/2$ and thus restricts the analysis to sufficiently smooth Sobolev spaces H^r with $r > d/2$. To obtain (sharp) L^2 global error estimates one needs to exploit discrete Strichartz estimates and discrete Bourgain spaces in the periodic setting, see, e.g., [IZ09, ORS21, ORS22b]. The main difficulty thereby lies in the fact that their continuous counterparts are not point wise in time.

A general global error analysis in the general setting presented is out of the scope of this paper. Nevertheless, in the case of the Gross-Pitaevskii equation first and second order convergence is obtained in [AB23a].

3.5 Examples

In this section we illustrate our general framework (see Definition 3.57) and its local error analysis (see Theorem 3.4.3) on two examples: The Gross-Pitaevskii equation (see Section 3.5.1) and the Sine-Gordon equation (see Section 3.5.3).

3.5.1 The Gross–Pitaevskii equation

As a first example let us consider the Gross–Pitaevskii (GP) equation

$$i\partial_t u(t, x) + \Delta u(t, x) = V(x)u(t, x) + |u(t, x)|^2 u(t, x) \quad (t, x) \in \mathbf{R} \times \Omega \quad (3.60)$$

on a sufficiently smooth domain $\Omega \subset \mathbf{R}^d$ in dimension $d \leq 3$, and an initial condition

$$u|_{t=0} = u_0. \quad (3.61)$$

We prescribe homogeneous Dirichlet boundary conditions,

$$u(t, \cdot)|_{\partial\Omega} = 0, \quad V(\cdot)|_{\partial\Omega} = 0,$$

where Ω is a smooth open set with compact boundary. We define the operator $\mathcal{L} = i\Delta$ on the Hilbert space $L^2(\Omega)$. Its domain is given by

$$D(\Delta) = D(\mathcal{L}) = (H^2 \cap H_0^1)(\Omega) \quad (3.62)$$

where $H^2(\Omega), H_0^1(\Omega)$ denote the classical Sobolev spaces.

One setting of the Gross-Pitaevskii equation is to describe the dynamics of Bose-Einstein condensates in a potential trap. In many physically relevant situations the potential is rough or disordered ([HP17], [NBP13], [WWW⁺98]) which motivates the study of the low-regularity framework.

First order low regularity integrator for Gross–Pitaevskii

Corollary 3.5.1 *At first order our general low regularity scheme (3.57) for the Gross–Pitaevskii equation (3.60) takes the form*

$$\begin{aligned} u^{n+1} = \Phi_{GP}^\tau(u^n) = e^{i\tau\Delta} u^n - i\tau \Big[& (e^{i\tau\Delta} u^n)(e^{i\tau\Delta} \varphi_1(-i\tau\Delta)V) \\ & + (e^{i\tau\Delta} (u^n)^2)(e^{i\tau\Delta} \varphi_1(-2i\tau\Delta)\bar{u}^n) \Big] \end{aligned} \quad (3.63)$$

where the filter function φ_1 is defined as $\varphi_1(\sigma) = \frac{e^\sigma - 1}{\sigma}$. The scheme (3.63) is locally of order $\mathcal{O}(\tau^2 |\nabla|(u + V))$.

In case of more regular solutions and potential the above low regularity scheme can be simplified to

$$u^{n+1} = e^{i\tau\Delta} u^n - i\tau(u^n V + (u^n)^2 \bar{u}^n), \quad (3.64)$$

which is locally of order $\mathcal{O}(\tau^2 \Delta(u + V))$.

Proof. We choose $r = 0$ in Definition 3.4.2 in order to obtain a local error of order one. We recall from Example 8 that for the Gross-Pitaevskii equation we have that $\mathcal{L}_o = i\Delta$, $V_0 = 1$, $V_1 = V$, $\mathfrak{L}_+ = \{o, \bar{o}\}$, $u_o = u$, $u_{\bar{o}} = \bar{u}$, $v_o = 1$ and $v_{\bar{o}} = \bar{v}$. From equation (3.57) it then follows that the first-order scheme is of the form,

$$u_{o,A}^0(\hat{\mathbf{v}}, \tau) = e^{i\tau\Delta} v + \sum_{T \in \mathcal{T}^1} \Pi_A^0(\mathcal{I}_o(T))(\hat{\mathbf{v}}, \tau), \quad (3.65)$$

where $\hat{\mathbf{v}} = (v, \bar{v}, V)$ and where on has

$$\mathcal{T}^1 = \{T_0, T_1\}, \quad T_0 = \lambda_0 = \circ, \quad T_1 = \lambda_1 = \bullet.$$

We recall from (3.28) that

$$\mathcal{I}_o(\lambda_0) = \mathfrak{I}^\circ$$

encodes the iterated integral

$$(\Pi_{\mathcal{I}_o}(\lambda_0))(\hat{\mathbf{v}}, \tau) = -i \int_0^\tau e^{i(\tau-s)\Delta} \left(\left(e^{is\Delta} v^2 \right) \left(e^{-is\Delta} \bar{v} \right) \right) ds \quad (3.66)$$

and that

$$\mathcal{I}_o(\lambda_1) = \mathfrak{I}^\bullet$$

encodes the iterated integral

$$(\Pi \mathcal{I}_o(\lambda_0))(\hat{\mathbf{v}}, \tau) = -i \int_0^\tau e^{i(\tau-s)\Delta} \left((e^{is\Delta} v) V \right) ds. \quad (3.67)$$

In order to compute the approximation (3.65), we refer to equation (3.42) where the approximated character Π_A^r is defined. We have, for $i = 0, 1$, that

$$\begin{aligned} (\Pi_A^0 \mathcal{I}_o(\lambda_i))(\hat{\mathbf{v}}, \tau) &= \mathcal{K}_{o,A}^0(\tilde{\Pi}_{o,A} \mathcal{D}_{-1}(\lambda_i)(\hat{\mathbf{v}}, \cdot))(\tau) \\ &= \mathcal{K}_{o,A}^0 \left(\frac{\Upsilon_{\text{root}}^{\Psi_o}[\lambda_i]}{S_{\text{root}}(\lambda_i)}(\hat{\mathbf{v}}, \cdot) V_i \right)(\tau) \end{aligned}$$

where to obtain the second line we used the definition 3.37 of \mathcal{D}_{-1} , namely that $\mathcal{D}_{-1}(\lambda_i) = \lambda_i$. By recalling the computations made in Example 9 one has,

$$\begin{aligned} S_{\text{root}}(\lambda_0) &= S_{\text{root}}(\lambda_1) = 1, \\ \Upsilon_{\text{root}}^{\Psi_o}[\lambda_0](\mathbf{v}, \xi) &= \left(-ie^{i\xi\Delta} v^2 \right) \left(e^{-i\xi\Delta} \bar{v} \right), \quad \Upsilon_{\text{root}}^{\Psi_o}[\lambda_1](\mathbf{v}, \xi) = -ie^{i\xi\Delta} v, \end{aligned}$$

where $\mathbf{v} = (v, \bar{v})$ and we recall that we set $\mathcal{B}_o^l = \text{id}$ for $(o, l) \in \mathfrak{L}_+ \times \mathfrak{L}_-$ when studying the equation (3.60). Hence, by collecting the above computations one has,

$$\begin{aligned} \Pi_A^0(\mathcal{I}_o(\lambda_0))(\hat{\mathbf{v}}, \tau) &= \mathcal{K}_{o,A}^0(F^1(\hat{\mathbf{v}}, \cdot))(\tau), \\ \Pi_A^0(\mathcal{I}_o(\lambda_1))(\hat{\mathbf{v}}, \tau) &= \mathcal{K}_{o,A}^0(F^2(\hat{\mathbf{v}}, \cdot))(\tau) \end{aligned} \quad (3.68)$$

where

$$F^1(\hat{\mathbf{v}}, \xi) := -i(e^{i\xi\Delta} v^2)(e^{-i\xi\Delta} \bar{v}) \quad (3.69)$$

and

$$F^2(\hat{\mathbf{v}}, \xi) := -i(e^{i\xi\Delta} v) V. \quad (3.70)$$

We are left to apply Definition 3.3.2 of the operator $\mathcal{K}_{o,A}^0$ on (3.69) and (3.70) which will yield a first-order approximation of the integrals (3.66) and (3.67). The approximation of these integrals, and hence the structure of the scheme, will depend on the regularity assumptions on the initial data v and the potential V . We first show the construction of the first order scheme (3.63), which requires H^1 -regularity on v and V . Hence, by taking into account the boundary conditions, we fix $A = H_0^1(\Omega)^3$ and construct a first order scheme for $(v, \bar{v}, V) \in A$ (see also Remark 3.3.5 for further details on the choice of A).

The case of $A = (H_0^1(\Omega))^3$:

We first note that given our regularity assumptions we have that $v, V \notin D(\mathcal{L}_o) = H^2(\Omega) \cap H_0^1(\Omega)$. Hence, our approximation cannot consist of merely applying Taylor-expansions (3.44) of all the operators, since it would require H^2 regularity on the initial data and on the potential. Indeed, given that $r, \ell = 0$ we have that

$$\cup_{n+\sum_{i \in J} k_i \leq 1} D(G_{n, (k_i)_{i \in J}}) \subseteq (H^2(\Omega))^3$$

which implies that we do not have that $A \subseteq D(G_{n, (k_i)_{i \in J}})$, for all $n + \sum_{i \in J} k_i \leq 1$. In order to make an approximation of order one of the integrals (3.68) while only requiring $H^1(\Omega)$ regularity on the initial data and potential we will apply the first point (i) of Definition 3.3.2.

We start by dealing with F^1 , namely the first order approximation of the integral (3.66).

1. Computation of $\Pi_A^0(\mathcal{I}_o(\lambda_0))(\hat{\mathbf{v}}, \tau)$. Using the notations in Definition 3.3.2 we compute the operator interactions, as is done in example 10 to obtain the following,

$$\mathcal{L}_1 = i\Delta, \quad \mathcal{L}_2 = -\mathcal{L}_1, \quad J = \{1, 2\}, \quad \text{and hence, } \mathcal{A}_1 = 0, \quad \mathcal{A}_\epsilon = -2i\Delta.$$

This implies that

$$\mathcal{L}_{\text{dom}} = \mathcal{A}_\epsilon = -2i\Delta, \quad I = \{2\},$$

and that

$$\mathcal{A}_{\text{low}}^1 = \mathcal{A}_1 = 0, \quad \mathcal{A}_{\text{low}}^2 = \mathcal{A}_2 - \mathcal{L}_{\text{dom}} = 0.$$

We note that following (3.45) we indeed recover the same initial expression (3.79) of F^1 :

$$F^1(\hat{\mathbf{v}}, \xi) = (e^{-i\xi\Delta} u_2^a)(e^{i\xi\Delta} u_1^a), \quad u_1^a = -iv^2, \quad u_2^a = \bar{v}.$$

We are now ready to compute $\mathcal{K}_{o,A}^0(F^1)$ using equation (3.46). Given the form of F^1 , and the order of the scheme we enter the case where $l = 0$ and $r = 0$ respectively. This implies that $q = 0 = n = m = p$. Hence, $\mathcal{K}_{o,A}^0(F^1)$ takes the following simple form,

$$\begin{aligned} \mathcal{K}_{o,A}^0(F^1(\hat{\mathbf{v}}, \cdot))(\tau) &= \int_0^\tau (e^{i\tau\Delta} \mathcal{M}_{\{1\}})(e^{-2i\xi\Delta+i\tau\Delta} \mathcal{M}_{\{2\}})(-iv^2, \bar{v}) d\xi \\ &= -i \int_0^\tau (e^{i\tau\Delta} v^2)(e^{-2i\xi\Delta+i\tau\Delta} \bar{v}) d\xi. \end{aligned} \quad (3.71)$$

By integrating exactly the above expression using the φ_1 function, and by (3.68) we have hence shown that,

$$\Pi_A^0(\mathcal{I}_o(\lambda_0))(\hat{\mathbf{v}}, \tau) = -i\tau(e^{i\tau\Delta} v^2)(e^{i\tau\Delta} \varphi_1(-2i\tau\Delta)\bar{v}). \quad (3.72)$$

2. Computation of $\Pi_A^0(\mathcal{I}_o(\lambda_1))(\hat{\mathbf{v}}, \tau)$. Similarly, we apply definition 3.3.2 to compute $\mathcal{K}_{o,A}^0(F^2)$. Given the expression (3.70) of F^2 , one has

$$\begin{aligned} \mathcal{L}_1 &= i\Delta, \quad \mathcal{L}_2 = 0, \quad J = \{1, 2\}, \quad u_1^b = -iv, \quad u_2^b = V, \quad \text{and hence,} \\ \mathcal{A}_1 &= 0, \quad \mathcal{A}_\infty = -i\Delta. \end{aligned}$$

This implies that

$$\mathcal{L}_{\text{dom}} = \mathcal{A}_\infty = -i\Delta, \quad I = \{2\},$$

and that

$$\mathcal{A}_{\text{low}}^1 = \mathcal{A}_1 = 0, \quad \mathcal{A}_{\text{low}}^2 = \mathcal{A}_2 - \mathcal{L}_{\text{dom}} = 0.$$

Then, again by equation (3.46) we have

$$\begin{aligned} \mathcal{K}_{o,A}^0(F^2)(\tau) &= \int_0^\tau (e^{i\tau\Delta} \mathcal{M}_{\{1\}})(e^{i(\tau-\xi)\Delta} \mathcal{M}_{\{2\}})(-iv, V) d\xi \\ &= -i \int_0^\tau (e^{i\tau\Delta} v)(e^{i(\tau-\xi)\Delta} V) d\xi \\ &= -i\tau(e^{i\tau\Delta} v)(e^{i\tau\Delta} \varphi_1(-i\tau\Delta)V). \end{aligned}$$

Hence, we have

$$\Pi_A^0(\mathcal{I}_o(\lambda_1))(\hat{\mathbf{v}}, \tau) = -i\tau(e^{i\tau\Delta} v)(e^{i\tau\Delta} \varphi_1(-i\tau\Delta)V).$$

Plugging the above computation into (3.65) yields the first order scheme (3.63).

The case of $A = (H^2 \cap H_0^1)(\Omega)^3$:

Given that $A = D(\mathcal{L}_o)^3$, we apply the Taylor expansion (3.44) with $r = \ell = 0$, to obtain:

$$\begin{aligned} \mathcal{K}_{o,A}^0\left((\Upsilon_{\text{root}}^{\Psi_o}[\lambda_0] + \Upsilon_{\text{root}}^{\Psi_o}[\lambda_1])(\mathbf{v}, \cdot)\right)(\tau) &= \int_0^\tau \Pi_{i \in \{1,2\}} u_i^a d\xi + \int_0^\tau \Pi_{i \in \{1,2\}} u_i^b d\xi \\ &= -i\tau(v^2 v + vV), \end{aligned}$$

which thanks to (3.65) yields the first order scheme (3.64).

Local error analysis. Using the recursive formula in Definition 3.3.8, one gets for $T \in \{\lambda_0, \lambda_1\}$

$$\mathcal{L}_{\text{low}}^0(\mathcal{I}_o(T), \hat{\mathbf{v}}, A) = \mathcal{L}_{\text{low}}^{-1,o}(T, \hat{\mathbf{v}}, A) + R_{o,A}^0((\Pi_A \mathcal{I}_o^0(T))(\hat{\mathbf{v}}, \cdot)).$$

Then by (3.50), we get for $l \in \{0, 1\}$

$$\mathcal{L}_{\text{low}}^{-1,o}(\lambda_l, \hat{\mathbf{v}}, A) = \frac{\Upsilon_{\text{root}}^{\Psi_o}[T]}{S_{\text{root}}(\lambda_l)}(\mathbf{v}, 0)V_l$$

which gives

$$\mathcal{L}_{\text{low}}^{-1,o}(\lambda_1, \hat{\mathbf{v}}, A) = -ivV, \quad \mathcal{L}_{\text{low}}^{-1,o}(\lambda_0, \hat{\mathbf{v}}, A) = -iv^2\bar{v}.$$

It remains to compute $R_{o,A}^0((\Pi_A T))$ whose value will depend on A . We start with the case $A = (H_0^1(\Omega))^3$. From our previous computations for the scheme, one has to apply (ii) from Lemma 3.3.6 that gives using notations of the proof of Corollary 3.5.1

$$R_{o,A}^r((\tilde{\Pi}_{o,A}\lambda_0)(\hat{\mathbf{v}}, \cdot)) = \sum_{\sum_{i \in J} k_i + m + n + p = r - \ell + 1} \mathcal{C}^m[(\mathcal{C}^n[\mathcal{M}_{J \setminus I}, \mathcal{L}_o]) \\ (\mathcal{C}^p[\mathcal{M}_I, \mathcal{L}_{\text{dom}} + \mathcal{L}_o], \mathcal{L}_o)((\mathcal{A}_{\text{low}}^i)^{k_i} u_i^a)_{i \in J}).$$

Here, $r = \ell = k_i = 0$, so it remains $m + n + p = 1$. As I and $J \setminus I$ are singleton, there is only one non zero value given by $m = 1$. In the end, one obtains

$$R_{o,A}^0((\tilde{\Pi}_{o,A}\lambda_0)(\hat{\mathbf{v}}, \cdot)) = \mathcal{C}[\mathcal{M}_{\{1,2\}}, i\Delta](-iv^2, \bar{v}).$$

With a similar computation, one gets

$$R_{o,A}^0((\tilde{\Pi}_{o,A}\lambda_1)(\hat{\mathbf{v}}, \cdot)) = \mathcal{C}[\mathcal{M}_{\{1,2\}}, i\Delta](-iv, V).$$

In both cases, one sees that these terms ask first order derivatives on v and V . Indeed using Definition 3.1.2 of the commutator we have,

$$\mathcal{C}[\mathcal{M}_{\{1,2\}}, i\Delta](w, z) = -2i\nabla w \cdot \nabla z. \quad (3.73)$$

Next, for $A = (H^2 \cap H_0^1)(\Omega)^3$, one has to use (i) from Lemma 3.3.6, namely

$$R_{o,A}^r((\tilde{\Pi}_{o,A}\lambda_0)(\hat{\mathbf{v}}, \cdot)) = \sum_{\sum_i k_i + n = r - \ell + 1} \mathcal{L}_o^n \left(\prod_{i \in J} \mathcal{L}_i^{k_i} u_i^a \right)$$

Here, $r = \ell = 0$, there for one obtains three terms:

$$R_{o,A}^0((\tilde{\Pi}_{o,A}\lambda_0)(\hat{\mathbf{v}}, \cdot)) = \Delta(v^2\bar{v}) + \Delta(v^2)\bar{v} - v^2\Delta\bar{v}$$

A similar computation shows

$$R_{o,A}^0((\tilde{\Pi}_{o,A}\lambda_1)(\hat{\mathbf{v}}, \cdot)) = \Delta(vV) + \Delta(v)V + v\Delta V$$

which allows us to conclude. \square

Remark 3.5.2 (Error improvement) Classical approximation techniques, such as splitting or exponential integrator methods (see, e.g., [CG12, JL00, Lub08]) introduce a local error structure of type $\mathcal{O}(\Delta u(t), \Delta V)$ and hence requires the solution and potential $(u(t), V) \in D(\Delta)^2 = (H^2 \cap H_0^1)(\Omega)^2$ (see also (3.62)). The scheme (3.64) together with its local error coincides with a first order scheme obtained via exponential integrator methods. The local error of the low regularity GP integrator (3.63) on the other hand only requires the boundedness of first instead of second order spatial derivatives of the potential V and solution u . The first-order scheme (3.63) coincides with the first order scheme obtained in [AB23a], where the author proves first order convergence in H^s -norm while asking for low-regularity assumptions on the solution.

Second order Duhamel integrator for Gross–Pitaevskii

We first recall from equation (3.15) in our first example, that by following the Taylor expansion (3.9) and linearization (3.12) steps, we seek to provide a second order low-regularity approximation to the following iterated integrals:

$$w^2(\mathbf{v}, \tau) = e^{i\tau\Delta}v - i \int_0^\tau e^{i(\tau-\xi)\Delta} \left((e^{i\xi\Delta}v^2)(e^{-i\xi\Delta}\bar{v}) + (e^{i\xi\Delta}v)V \right) d\xi \quad (3.74) \\ - i \int_0^\tau \xi e^{i(\tau-\xi)\Delta} \left((e^{i\xi\Delta}\mathcal{C}[u^2, i\Delta](v))(e^{-i\xi\Delta}\bar{v}) \right) d\xi \\ - \int_0^\tau e^{i(\tau-\xi)\Delta} \left(\left(\int_0^\xi e^{i(\xi-\xi_1)\Delta} \left((e^{i\xi_1\Delta}v^2)(e^{-i\xi_1\Delta}\bar{v}) \right) \right. \right. \\ \left. \left. + (e^{i\xi_1\Delta}v)V \right) d\xi_1 \right) (2(e^{i\xi\Delta}v)(e^{-i\xi\Delta}\bar{v}) + V) d\xi$$

$$+ \int_0^\tau e^{i(\tau-\xi)\Delta} \left(\left(\int_0^\xi e^{-i(\xi-\xi_1)\Delta} \left((e^{-i\xi_1\Delta} \bar{v}^2) (e^{i\xi_1\Delta} v) \right. \right. \right. \\ \left. \left. \left. + (e^{-i\xi_1\Delta} \bar{v}) \bar{V} \right) d\xi_1 \right) (e^{i\xi\Delta} v^2) \right) d\xi.$$

Corollary 3.5.3 *At second order our general low regularity scheme (3.57) for the Gross-Pitaevskii equation (3.60) takes the form,*

$$\begin{aligned} u^{n+1} &= e^{i\tau\Delta} u^n - i\tau \left((e^{i\tau\Delta} (u^n)^2) (e^{i\tau\Delta} \varphi_1(-2i\tau\Delta) \bar{u}^n) \right. \\ &\quad \left. + (e^{i\tau\Delta} u^n) (e^{i\tau\Delta} \varphi_1(-i\tau\Delta) V) \right) \\ &\quad - i\tau^2 \mathcal{C}[(e^{i\tau\Delta} \mathcal{M}_{\{1\}}) (e^{i\tau\Delta} (\varphi_1(-2i\tau\Delta) - \varphi_2(-2i\tau\Delta)) \mathcal{M}_{\{2\}}), i\Delta] ((u^n)^2, \bar{u}^n) \\ &\quad - i\tau^2 \mathcal{C}[(e^{i\tau\Delta} \mathcal{M}_{\{1\}}) (e^{i\tau\Delta} (\varphi_1(-i\tau\Delta) - \varphi_2(-i\tau\Delta)) \mathcal{M}_{\{2\}}), i\Delta] (u^n, V) \\ &\quad - i\tau^2 \left(e^{i\tau\Delta} \mathcal{C}[u^2, i\Delta] (u^n) \right) \left(e^{i\tau\Delta} \varphi_2(-2i\tau\Delta) \bar{u}^n \right) \\ &\quad - \frac{\tau^2}{2} (u^n |u^n|^4 + 3u^n |u^n|^2 V - |u^n|^2 u^n \bar{V} + u^n V^2) \\ &= \Phi_{GP2}^\tau(u^n), \end{aligned} \tag{3.75}$$

where the filter function φ_2 is defined as $\varphi_2(\sigma) = \frac{e^\sigma - \varphi_1(\sigma)}{\sigma}$. The scheme (3.75) is locally of order $\mathcal{O}(\tau^3 \Delta(u+V))$.

Remark 3.5.4 In case of more regular solution and potential the second order scheme (3.75) can be simplified, recovering for sufficiently smooth solutions and potential $(u(t), V) \in D(\Delta^2)^2$ classical schemes (see also Remark 3.5.5 below).

Proof. We choose $r = 1$ in Definition 3.4.2 in order to obtain a local error of order two. From equation (3.57) it then follows that the second-order scheme is of the form,

$$u^1(\hat{\mathbf{v}}, \tau) = e^{i\tau\Delta} v + \sum_{T \in \mathcal{T}^2} \Pi_A^1(\mathcal{I}_o(T))(\hat{\mathbf{v}}, \tau), \tag{3.76}$$

where $\hat{\mathbf{v}} = (\mathbf{v}, \mathbf{V})$ and where are interested in the decorated trees $\mathcal{I}_o(T)$ where T belongs to \mathcal{T}^2 defined by,

$$\begin{aligned} \mathcal{T}^2 &= \{T_0, \dots, T_8\}, \quad T_0 = \lambda_0 = \circ, \quad T_1 = \lambda_1 = \bullet, \quad T_2 = \lambda_0^1 = \circ \otimes, \\ T_3 &= \lambda_0 \mathcal{I}_o(\lambda_0) = \begin{array}{c} \circ \\ | \\ \circ \end{array}, \quad T_4 = \lambda_0 \mathcal{I}_o(\lambda_1) = \begin{array}{c} \bullet \\ | \\ \circ \end{array}, \quad T_5 = \lambda_1 \mathcal{I}_o(\lambda_0) = \begin{array}{c} \circ \\ | \\ \bullet \end{array}, \\ T_6 &= \lambda_1 \mathcal{I}_o(\lambda_1) = \begin{array}{c} \bullet \\ | \\ \bullet \end{array}, \quad T_7 = \lambda_0 \mathcal{I}_{\bar{o}}(\lambda_0) = \begin{array}{c} \circ \\ | \\ \circ \\ | \\ \circ \end{array}, \quad T_8 = \lambda_0 \mathcal{I}_{\bar{o}}(\lambda_1) = \begin{array}{c} \bullet \\ | \\ \circ \\ | \\ \circ \end{array}. \end{aligned}$$

As stated previously, the approximation of the above integrals, and hence the structure of the scheme, will depend on the regularity assumptions of the initial data v and the potential V . Here, we show the construction of a second order scheme which requires H^2 -regularity on v and V . Hence, by taking into account the boundary conditions, we fix $A = (H^2(\Omega) \cap H_0^1(\Omega))^3$ and construct a second order scheme for $(v, \bar{v}, V) \in A$.

1. Computation of $\Pi_A^1(\mathcal{I}_o(\lambda_0))(\hat{\mathbf{v}}, \tau)$.

We recall that $\mathcal{I}_o(\lambda_0)$ encodes the first integral (3.66). Next, we make the following remark; given our regularity assumptions $(v, \bar{v}, V) \in A$, we have that $v, V \notin D(\mathcal{L}_o^2) \subset H^4(\Omega)$. Hence, our approximation cannot consist of merely applying Taylor-expansions (3.44) of all the operators, since it would require H^4 regularity on the initial data and on the potential, together with the according boundary conditions. Indeed, given that $r = 1$ and $\ell = 0$ we have that

$$\cup_{n+\sum_{i \in J} k_i \leq 2} D(G_{n, (k_i)_{i \in J}}) \subseteq (H^4(\Omega))^3$$

which implies that we do not have that $A \subseteq D(G_{n, (k_i)_{i \in J}})$, for all $n + \sum_{i \in J} k_i \leq 2$. In order to make an approximation of order two of the integrals (3.68) while only requiring $H^2(\Omega)$ regularity on the initial data we will apply the first point (i) of Definition 3.3.2, as done in Example 10. Indeed, following the results established in Example 10 we have:

$$\begin{aligned} (\Pi_A \mathcal{I}_o^1(\lambda_0))(\hat{\mathbf{v}}, \xi) &= -i \int_0^\tau \left(e^{i\tau\Delta} v^2 \right) \left(e^{i(\tau-2\xi)\Delta} \bar{v} \right) d\xi \\ &\quad + \int_0^\tau (\tau - \xi) \mathcal{C}[(e^{i\tau\Delta} \mathcal{M}_{\{1\}}) (e^{i(\tau-2\xi)\Delta} \mathcal{M}_{\{2\}}), i\Delta] (-iv^2, \bar{v}) d\xi \\ &= -i[\tau(e^{i\tau\Delta} v^2) (e^{i\tau\Delta} \varphi_1(-2i\tau\Delta) \bar{v}) \end{aligned}$$

$$+ \tau^2 \mathcal{C}[(e^{i\tau\Delta} \mathcal{M}_{\{1\}})(e^{i\tau\Delta} (\varphi_1(-2i\tau\Delta) - \varphi_2(-2i\tau\Delta)) \mathcal{M}_{\{2\}}), i\Delta](v^2, \bar{v})]$$

2. Computation of $\Pi_A^1(\mathcal{I}_o(\lambda_1))(\hat{\mathbf{v}}, \tau)$.

We recall that $\mathcal{I}_o(\lambda_1)$ encodes the second integral (3.67). Using the same arguments as in the above together with the computations of $\Pi_A^0(\mathcal{I}_o(\lambda_1))(\hat{\mathbf{v}}, \tau)$ made in the proof of Corollary 3.5.1, it follows that,

$$\begin{aligned} (\Pi_A \mathcal{I}_o^1(\lambda_1))(\hat{\mathbf{v}}, \xi) &= -i \left(\tau (e^{i\tau\Delta} v) (e^{i\tau\Delta} \varphi_1(-i\tau\Delta) V) \right. \\ &\quad \left. + \tau^2 \mathcal{C}[(e^{i\tau\Delta} \mathcal{M}_{\{1\}})(e^{i\tau\Delta} (\varphi_1(-i\tau\Delta) - \varphi_2(-i\tau\Delta)) \mathcal{M}_{\{2\}}), i\Delta](v, V) \right). \end{aligned}$$

3. Computation of $\Pi_A^1(\mathcal{I}_o(\lambda_0^1))(\hat{\mathbf{v}}, \tau)$.

We have that

$$\mathcal{I}_o(\lambda_0^1) = \begin{array}{c} \circ \\ | \\ \circ \end{array}$$

encodes the iterated integral

$$-i \int_0^\tau \xi e^{i(\tau-\xi)\Delta} \left((e^{i\xi\Delta} \mathcal{C}[u^2, i\Delta](v)) (e^{-i\xi\Delta} \bar{v}) \right) d\xi$$

Using the computation made in example (9) we have,

$$\begin{aligned} (\Pi_A^1 \mathcal{I}_o(\lambda_0^1))(\hat{\mathbf{v}}, \tau) &= \mathcal{K}_{o,A}^1((\tilde{\Pi}_{o,A} \mathcal{D}_0(\lambda_0^1))(\hat{\mathbf{v}}, \cdot))(\tau) \\ &= \mathcal{K}_{o,A}^1 \left(\frac{\Upsilon_{\text{root}}^{\Psi_o}[\lambda_0^1]}{S_{\text{root}}(\lambda_0^1)}(\mathbf{v}, \xi) V_0 \xi \right) (\tau) \\ &= \mathcal{K}_{o,A}^1 \left(\xi \left(e^{\xi\mathcal{L}} \mathcal{C}[u^2, \Delta](v) \right) \left(e^{-\xi\mathcal{L}} \bar{v} \right) \right) (\tau). \end{aligned}$$

To apply Definition 3.3.2 we let $u_1 = \mathcal{C}[u^2, \Delta](v)$, and $u_2 = \bar{v}$. The operator interactions are the same as those computed previously. We are in the case where $r = 1 = \ell$, hence $q = 0 = m = n = p$. From Definition 3.3.2 part i., it then follows that,

$$\begin{aligned} (\Pi_A^0 \mathcal{I}_o(\lambda_0^1))(\hat{\mathbf{v}}, \tau) &= \int_0^\tau \xi [(e^{i\tau\Delta} \mathcal{M}_{\{1\}})(e^{-2i\xi\Delta+i\tau\Delta} \mathcal{M}_{\{2\}})](u_1, u_2) d\xi \\ &= -i\tau^2 \left(e^{i\tau\Delta} \mathcal{C}[u^2, i\Delta](v) \right) \left(e^{i\tau\Delta} \varphi_2(-2i\tau\Delta) \bar{v} \right) \end{aligned}$$

4. Computation of $\Pi_A^1(\mathcal{I}_o(T_3))(\hat{\mathbf{v}}, \tau)$.

We have that

$$\mathcal{I}_o(T_3) = \begin{array}{c} \circ \\ | \\ \circ \\ | \\ \circ \end{array}$$

encodes the iterated integral

$$- \int_0^\tau e^{i(\tau-\xi)\Delta} \left(\left(\int_0^\xi e^{i(\xi-\xi_1)\Delta} \left((e^{i\xi_1\Delta} v^2) (e^{-i\xi_1\Delta} \bar{v}) \right) d\xi_1 \right) 2(e^{i\xi\Delta} v) (e^{-i\xi\Delta} \bar{v}) \right) d\xi,$$

By definition of the projection operator \mathcal{D}_r and (3.3.2) we have,

$$\begin{aligned} \Pi_A^1(\mathcal{I}_o(T_3))(\hat{\mathbf{v}}, \tau) &= \mathcal{K}_{o,A}^1(\tilde{\Pi}_{o,A} \mathcal{D}_0(\lambda_0 \mathcal{I}_o(\lambda_0))(\hat{\mathbf{v}}, \cdot))(\tau) \\ &= \mathcal{K}_{o,A}^1(\tilde{\Pi}_{o,A}(\lambda_0 \mathcal{I}_o^0(\lambda_0)))(\hat{\mathbf{v}}, \tau) \\ &= \mathcal{K}_{o,A}^1 \left(\frac{\Upsilon_{\text{root}}^{\Psi_o}[T_3]}{S_{\text{root}}(T_3)}(\mathbf{v}, \xi) V_0 (\Pi_A \mathcal{I}_o^0(\lambda_0))(\hat{\mathbf{v}}, \xi) \right) (\tau) \end{aligned} \tag{3.77}$$

where $V_0 = 1$. Hence, in order to compute the above approximation we are left to compute $S_{\text{root}}(T_3)$, $\Upsilon_{\text{root}}^{\Psi_o}[T_3]$, and $(\Pi_A \mathcal{I}_o^0(\lambda_0))(\hat{\mathbf{v}}, \xi)$. First, by definition (3.40) of $S_{\text{root}}(T_3)$ we have that $i = 1 = j$ and $\beta_{1,1} = 1$, where $o_1 = o$. Hence, we

have that $S_{\text{root}}(T_3) = 1$. Second, by definition (3.41) of $\Upsilon_{\text{root}}^{\Psi_o}[T]$ we have that,

$$\begin{aligned}\Upsilon_{\text{root}}^{\Psi_o}[T_3](\mathbf{v}, \xi) &= (D_o \hat{\Psi}_o^0)(\mathbf{v}, \xi) \\ &= D_o \left((e^{i\xi\Delta}(-iv_o^2))(e^{-i\xi\Delta}v_{\bar{o}}) \right) \\ &= -2i(e^{i\xi\Delta}v)(e^{-i\xi\Delta}\bar{v})\end{aligned}$$

since $v_o = v$, and $v_{\bar{o}} = \bar{v}$. Finally, following the computations made at the beginning of example 10 we have,

$$(\Pi_A \mathcal{I}_o^0(\lambda_0))(\hat{\mathbf{v}}, \xi) = \mathcal{K}_{o,A}^0(F(\hat{\mathbf{v}}, \cdot))(\xi)$$

where

$$F(\mathbf{v}, \xi) = \prod_{i \in \{1,2\}} e^{\xi \mathcal{L}_i u_i}, \quad u_1 = -iv^2, \quad u_2 = \bar{v}, \quad \mathcal{L}_1 = i\Delta, \quad \mathcal{L}_2 = -i\Delta$$

In our current setting we have that $r = 0 = \ell$ and hence $D(\mathcal{L}_o^{r-\ell+1}) = D(\Delta)$. Given the regularity assumptions on v , namely that $v \in H^2 \cap H_0^1$, it follows that $v \in D(\Delta)$. Following (3.44) we can then Taylor expand all the operators appearing in the integral which yields the following approximation,

$$(\Pi_A \mathcal{I}_o^0(\lambda_0))(\hat{\mathbf{v}}, \xi) = \mathcal{K}_{o,A}^0(F(\hat{\mathbf{v}}, \cdot))(\xi) = \int_0^\xi \prod_{i \in \{1,2\}} u_i d\xi = -i\xi v^2 \bar{v}.$$

Hence, plugging the above computations in (3.77) yields,

$$\begin{aligned}\Pi_A^1(\mathcal{I}_o(T_3))(\mathbf{v}, \tau) &= -2\mathcal{K}_{o,A}^1 \left(\xi (e^{i\xi\Delta}v)(e^{-i\xi\Delta}\bar{v})v^2\bar{v} \right)(\tau) \\ &= -2\mathcal{K}_{o,A}^1 \left(\tilde{F}(\hat{\mathbf{v}}, \xi) \right)(\tau)\end{aligned}\tag{3.78}$$

where

$$\begin{aligned}\tilde{F}(\hat{\mathbf{v}}, \xi) &= \xi^\ell \prod_{i \in \{1,2,3\}} e^{\xi \mathcal{L}_i u_i}, \quad \mathcal{L}_1 = i\Delta, \quad \mathcal{L}_2 = -i\Delta, \quad \mathcal{L}_3 = 0, \\ &u_1 = v \quad u_2 = \bar{v}, \quad u_3 = v^2\bar{v} \text{ and } \ell = 1.\end{aligned}\tag{3.79}$$

In our current setting we have that $r = 1 = \ell$ and hence $D(\mathcal{L}_o^{r-\ell+1}) = D(\Delta)$. Given that $v \in D(\Delta)$, by following (3.44) we can once again Taylor expand the remaining operators inside the integral which yields the following approximation,

$$\mathcal{K}_{o,A}^1 \left(\tilde{F}(\hat{\mathbf{v}}, \xi) \right)(\tau) = \int_0^\tau \xi \prod_{i \in \{1,2,3\}} u_i d\xi = \frac{\tau^2}{2} v |v|^4,$$

by definition of the $(u_i)_{i=1,\dots,4}$. Hence, from (3.78) it follows that,

$$\Pi_A^1(\mathcal{I}_o(T_3))(\hat{\mathbf{v}}, \tau) = -\tau^2 v |v|^4.$$

5. Computation of $\Pi_A^1(\mathcal{I}_o(T_4))(\hat{\mathbf{v}}, \tau)$, $\Pi_A^1(\mathcal{I}_o(T_5))(\hat{\mathbf{v}}, \tau)$, and $\Pi_A^1(\mathcal{I}_o(T_6))(\hat{\mathbf{v}}, \tau)$. We have that

$$\mathcal{I}_o(T_4) = \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array}, \quad \mathcal{I}_o(T_5) = \begin{array}{c} \circ \\ | \\ \bullet \\ | \\ \bullet \end{array}, \quad \mathcal{I}_o(T_6) = \begin{array}{c} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array}.$$

respectively encode

$$\begin{aligned}& - \int_0^\tau e^{i(\tau-\xi)\Delta} \left(\left(\int_0^\xi e^{i(\xi-\xi_1)\Delta} \left((e^{i\xi_1\Delta}v) \right) d\xi_1 \right) 2(e^{i\xi\Delta}v)(e^{-i\xi\Delta}\bar{v}) \right) d\xi, \\ & - \int_0^\tau e^{i(\tau-\xi)\Delta} \left(\left(\int_0^\xi e^{i(\xi-\xi_1)\Delta} \left((e^{i\xi_1\Delta}v^2)(e^{-i\xi_1\Delta}\bar{v}) \right) d\xi_1 \right) V \right) d\xi,\end{aligned}$$

$$- \int_0^\tau e^{i(\tau-\xi)\Delta} \left(\left(\int_0^\xi e^{i(\xi-\xi_1)\Delta} \left((e^{i\xi_1\Delta} v) V \right) d\xi_1 \right) V \right) d\xi,$$

namely the remaining integrals in the third line of (3.74). These computation follow exactly the same lines as for the computation of $\Pi_A^1(\mathcal{I}_o(T_3))$. Namely, given our regularity assumptions we can apply the Taylor based expansion (3.44), to obtain,

$$\begin{aligned} (\Pi_A^1(\mathcal{I}_o(T_4)) + \Pi_A^1(\mathcal{I}_o(T_5)))(\hat{\mathbf{v}}, \tau) &= -2 \int_0^\tau \xi \prod_{i \in \{1,2,3,4\}} u_i^a d\xi - \int_0^\tau \xi \prod_{i \in \{1,2,3\}} u_i^b \\ &= -\tau^2 |v|^2 v V + -\frac{\tau^2}{2} V v^2 \bar{v}, \\ &= -\frac{3\tau^2}{2} |v|^2 v V, \end{aligned}$$

and

$$\Pi_A^1(\mathcal{I}_o(T_6))(\hat{\mathbf{v}}, \tau) = - \int_0^\tau \xi \prod_{i \in \{1,2,3\}} u_i^c = -\frac{\tau^2}{2} V^2 v,$$

where $(u_1^a, u_2^a, u_3^a, u_4^a) = (v, V, v, \bar{v})$, $(u_1^b, u_2^b, u_3^b) = (V, v^2, \bar{v})$, and $(u_1^c, u_2^c, u_3^c) = (V, v, V)$.

6. Computation of $\Pi_A^1(\mathcal{I}_o(T_7))(\hat{\mathbf{v}}, \tau)$.

We have that,

$$\mathcal{I}_o(T_7) = \begin{array}{c} \circ \\ \vdots \\ \circ \\ \mathbf{I} \end{array}$$

encodes the iterated integral

$$\int_0^\tau e^{i(\tau-\xi)\Delta} \left(\left(\int_0^\xi e^{-i(\xi-\xi_1)\Delta} \left((e^{-i\xi_1\Delta} \bar{v}^2) (e^{i\xi_1\Delta} v) \right) d\xi_1 \right) (e^{i\xi\Delta} v^2) \right) d\xi.$$

Similar to the computations done in (3.77) it follows that,

$$\begin{aligned} (\Pi_A^1 \mathcal{I}_o(T_7))(\hat{\mathbf{v}}, \tau) &= \mathcal{K}_{o,A}^1(\tilde{\Pi}_{o,A} \mathcal{D}_0(\lambda_0 \mathcal{I}_{\bar{o}}(\lambda_0)))(\hat{\mathbf{v}}, \cdot)(\tau) \\ &= \mathcal{K}_{o,A}^1(\tilde{\Pi}_{o,A}(\lambda_0 \mathcal{I}_{\bar{o}}^0(\lambda_0)))(\hat{\mathbf{v}}, \cdot)(\tau) \\ &= \mathcal{K}_{o,A}^1 \left(\frac{\Upsilon_{\text{root}}^{\Psi_o}[T_7]}{S_{\text{root}}(T_7)}(\mathbf{v}, \cdot) (\Pi_A \mathcal{I}_{\bar{o}}^0(\lambda_0))(\hat{\mathbf{v}}, \cdot) \right) (\tau). \end{aligned} \tag{3.80}$$

We are left to calculate $\Upsilon_{\text{root}}^{\Psi_o}[T_7]$, $S_{\text{root}}(T_7)$, and $(\Pi_A \mathcal{I}_{\bar{o}}^0(\lambda_0))(\hat{\mathbf{v}}, \xi)$. First, by definition (3.40) of $S_{\text{root}}(T_7)$ we have that $i = 1 = j$ and $\beta_{1,1} = 1$, where $o_1 = \bar{o}$. Hence, we have that $S_{\text{root}}(T_7) = 1$. Secondly, by definition (3.41) of $\Upsilon_{\text{root}}^{\Psi_o}[T]$ we have that,

$$\begin{aligned} \Upsilon_{\text{root}}^{\Psi_o}[T_7] &= (D_{\bar{o}} \hat{\Psi}_o^0)(\mathbf{v}, \xi) \\ &= -i D_{\bar{o}} \left((e^{i\xi\Delta} (v_o^2)) (e^{-i\xi\Delta} v_{\bar{o}}) \right) \\ &= -i (e^{i\xi\Delta} v^2) \end{aligned}$$

since $v_o = v$, and $v_{\bar{o}} = \bar{v}$. Thirdly, by following definition (3.3.2) we have,

$$(\Pi_A \mathcal{I}_{\bar{o}}^0(\lambda_0))(\hat{\mathbf{v}}, \xi) = \mathcal{K}_{\bar{o},A}^0((\tilde{\Pi}_{\bar{o},A} \lambda_0)(\hat{\mathbf{v}}, \cdot))(\xi) = \mathcal{K}_{\bar{o},A}^0 \left(\frac{\Upsilon_{\text{root}}^{\Psi_{\bar{o}}}[\lambda_0]}{S_{\text{root}}(\lambda_0)}(\hat{\mathbf{v}}, \cdot) \right) (\xi)$$

where by equation (3.40) we have that $S_{\text{root}}(\lambda_0) = 1$ and by equation (3.41) it follows that,

$$\begin{aligned} \Upsilon_{\text{root}}^{\Psi_{\bar{o}}}[\lambda_0](\mathbf{v}, \zeta) &= \prod_{\iota \in \mathfrak{S}_+^{0,\bar{o}}} e^{\zeta \mathcal{L}_\iota} f_{\bar{o},\iota}^0(v_\iota) = (e^{i\zeta\Delta} f_{\bar{o},o}^0(v)) (e^{-i\zeta\Delta} f_{\bar{o},\bar{o}}^0(\bar{v})) \\ &= (e^{i\zeta\Delta} v) (e^{-i\zeta\Delta} (i\bar{v}^2)). \end{aligned}$$

Collecting the above computations, we have,

$$(\Pi_A \mathcal{I}_{\bar{o}}^0(\lambda_0))(\hat{\mathbf{v}}, \xi) = \mathcal{K}_{\bar{o}, A}^0(F(\hat{\mathbf{v}}, \cdot))(\xi)$$

where

$$F(\hat{\mathbf{v}}, \xi) = \prod_{i \in \{1, 2\}} e^{\xi \mathcal{L}_i} u_i, \quad u_1 = v, \quad u_2 = i\bar{v}^2, \quad \mathcal{L}_1 = i\Delta, \quad \mathcal{L}_2 = -i\Delta,$$

and where we consider the operator $\mathcal{L}_{\bar{o}} = -i\Delta$ associated to the decoration $\bar{o} \in \mathfrak{L}_+$. Given that $v \in D(\Delta)$, by following (3.44) we can once again Taylor expand the operators inside the integral which yields the following approximation,

$$(\Pi_A \mathcal{I}_{\bar{o}}^0(\lambda_0))(\hat{\mathbf{v}}, \xi) = \mathcal{K}_{\bar{o}, A}^0(F(\hat{\mathbf{v}}, \cdot))(\xi) = \int_0^\xi \prod_{i \in \{1, 2\}} u_i d\xi = i\xi v \bar{v}^2.$$

Hence, by collecting the above computations it follows from (3.80) that,

$$(\Pi_A^1 \mathcal{I}_o(T_7))(\hat{\mathbf{v}}, \tau) = \mathcal{K}_{o, A}^1\left(\xi(e^{i\xi\Delta} v^2) v \bar{v}^2\right)(\tau) = \mathcal{K}_{o, A}^1\left(\tilde{F}(\hat{\mathbf{v}}, \cdot)\right)(\tau),$$

where

$$\begin{aligned} \tilde{F}(\hat{\mathbf{v}}, \xi) &= \xi^\ell \prod_{i \in \{1, 2, 3\}} e^{\xi \mathcal{L}_i} u_i, & \mathcal{L}_1 &= i\Delta, \quad \mathcal{L}_2 = \mathcal{L}_3 = 0, \\ & & u_1 &= v^2, \quad u_2 = v, \quad u_3 = \bar{v}^2 \text{ and } \ell = 1. \end{aligned}$$

Given that $v \in D(\Delta)$, by following (3.44) we can once again Taylor expand the remaining operators inside the integral which yields the following approximation,

$$(\Pi_A^1 \mathcal{I}_o(T_7))(\hat{\mathbf{v}}, \tau) = \mathcal{K}_{o, A}^1\left(\tilde{F}(\hat{\mathbf{v}}, \xi)\right)(\tau) = \int_0^\tau \xi \prod_{i \in \{1, 2, 3\}} u_i d\xi = \frac{\tau^2}{2} v |v|^4,$$

7. Computation of $\Pi_A^1(\mathcal{I}_o(T_8))(\hat{\mathbf{v}}, \tau)$.

We have that,

$$\mathcal{I}_o(T_8) = \begin{array}{c} \bullet \\ \vdots \\ \circ \end{array}$$

encodes the iterated integral

$$\int_0^\tau e^{i(\tau-\xi)\Delta} \left(\left(\int_0^\xi e^{-i(\xi-\xi_1)\Delta} \left((e^{-i\xi_1\Delta} \bar{v}) \bar{V} \right) d\xi_1 \right) (e^{i\xi\Delta} v^2) \right) d\xi.$$

By using the same arguments as made in the above computation of the iterated integral $\mathcal{I}_o(T_7)$, namely by following the Taylor expansion (3.44), we obtain

$$\Pi_A^1(\mathcal{I}_o(T_8))(\hat{\mathbf{v}}, \tau) = \int_0^\tau \xi \prod_{i \in \{1, 2, 3\}} u_i d\xi = \frac{\tau^2}{2} v |v|^2 \bar{V},$$

where $u_1 = \bar{v}$, $u_2 = \bar{V}$, and $u_3 = v^2$. Collecting the above computation together with equation (3.76) yields the second order low-regularity scheme given in (3.75).

Local error analysis. The error for the trees $\mathcal{I}_o^1(\lambda_0)$ and $\mathcal{I}_o^1(\lambda_1)$ follows the same computations as for the first order. One has to go one step further in the Taylor approximation:

$$\begin{aligned} R_{o, A}^1((\tilde{\Pi}_{o, A} \lambda_0)(\hat{\mathbf{v}}, \cdot)) &= \mathcal{C}^2[\mathcal{M}_{\{1, 2\}}, i\Delta](-iv^2, \bar{v}) \\ R_{o, A}^1((\tilde{\Pi}_{o, A} \lambda_1)(\hat{\mathbf{v}}, \cdot)) &= \mathcal{C}^2[\mathcal{M}_{\{1, 2\}}, i\Delta](-iv, \bar{V}). \end{aligned}$$

In the end, we obtain the following contribution to the local error. This produce the following second order commutators:

$$\mathcal{L}_{\text{low}}^1(\mathcal{I}_o(\lambda_0), \hat{\mathbf{v}}, A) = -iv^2 \bar{v} + \mathcal{C}^2[\mathcal{M}_{\{1, 2\}}, i\Delta](-iv^2, \bar{v})$$

$$\mathcal{L}_{\text{low}}^1(\mathcal{I}_o(\lambda_1), \hat{\mathbf{v}}, A) = -ivV + \mathcal{C}^2[\mathcal{M}_{\{1,2\}}, i\Delta](-iv, V),$$

where using the Leibniz rule it follows from Definition 3.1.2 that these second order commutators ask for two spacial derivatives on v and V .

Next, the decorated tree $\mathcal{I}_o(\lambda_0^1)$ contains a polynomial decoration meaning that one has ξ inside the integral. Therefore, applying Definition 3.3.8, one gets

$$\mathcal{L}_{\text{low}}^1(\mathcal{I}_o(\lambda_0^1), \hat{\mathbf{v}}, A) = \mathcal{L}_{\text{low}}^{0,o}(\lambda_0^1, \hat{\mathbf{v}}, A) + R_{o,A}^r \left(\left(\tilde{\Pi}_{o,A} \lambda_0^1 \right) (\hat{\mathbf{v}}, \cdot) \right),$$

where

$$\begin{aligned} \mathcal{L}_{\text{low}}^{r,o}(\lambda_0^1, A) &= \frac{\Upsilon_{\text{root}}^{\Psi_o}[\lambda_0^1]}{S_{\text{root}}(\lambda_0^1)}(\mathbf{v}, 0) V_0 = \mathcal{C}[u^2, i\Delta](-iv)\bar{v} \\ R_{o,A}^1 \left(\left(\tilde{\Pi}_{o,A} \lambda_0^1 \right) (\hat{\mathbf{v}}, \cdot) \right) &= \mathcal{C}[\mathcal{C}[\mathcal{M}_{\{1,2\}}, \Delta](\mathcal{M}_{\{1\}}, \mathcal{M}_{\{1\}})\mathcal{M}_{\{2\}}, i\Delta](-iv, \bar{v}). \end{aligned}$$

It remains to compute the local error for trees with two edges such as $T_3 = \mathcal{I}_o(\lambda_0 \mathcal{I}_o(\lambda_0))$. We proceed with a full derivation for this decorated trees. Two edges mean that we have to go for one extra level of recursivity. One has

$$\mathcal{L}_{\text{low}}^1(T_3, \hat{\mathbf{v}}, A) = \mathcal{L}_{\text{low}}^{0,o}(\lambda_0 \mathcal{I}_o(\lambda_0), \hat{\mathbf{v}}, A) + R_{o,A}^1 \left(\left(\tilde{\Pi}_{o,A}^0 \lambda_0 \mathcal{I}_o(\lambda_0) \right) (\hat{\mathbf{v}}, \cdot) \right). \quad (3.81)$$

Then, for the first term, one gets

$$\mathcal{L}_{\text{low}}^{0,o}(\lambda_0 \mathcal{I}_o(\lambda_0), \hat{\mathbf{v}}, A) = \frac{\Upsilon_{\text{root}}^{\Psi_o}[\lambda_0 \mathcal{I}_o(\lambda_0)]}{S_{\text{root}}(\lambda_0 \mathcal{I}_o(\lambda_0))}(\mathbf{v}, 0) V_0 \mathcal{L}_{\text{low}}^0(\mathcal{I}_o(\lambda_0), \hat{\mathbf{v}}, A).$$

Given that $A = (H^2 \cap H_0^1)(\Omega)^3$, one has from the local error analysis of the first order scheme:

$$\mathcal{L}_{\text{low}}^0(\mathcal{I}_o(\lambda_0), \hat{\mathbf{v}}, A) = -iv^2\bar{v} + \Delta(v^2\bar{v}) + \Delta(v^2)\bar{v} - v^2\Delta\bar{v}.$$

Therefore, one gets

$$\mathcal{L}_{\text{low}}^{0,o}(\lambda_0 \mathcal{I}_o(\lambda_0), \hat{\mathbf{v}}, A) = -v^3\bar{v}^2 - iv\bar{v}\Delta(v^2\bar{v}) - iv\Delta(v^2)\bar{v}^2 + iv^3\bar{v}\Delta\bar{v}.$$

For the second term of (3.81), we Taylor-expand the operators that give:

$$R_{o,A}^1 \left(\left(\tilde{\Pi}_{o,A}^0 \lambda_0 \mathcal{I}_o(\lambda_0) \right) (\hat{\mathbf{v}}, \cdot) \right) = -i\Delta(v^3\bar{v}^2) - i(\Delta v)v^2\bar{v}^2 + i(\Delta\bar{v})v^3\bar{v}.$$

In fact for the approximation of $\mathcal{I}_o(\lambda_0 \mathcal{I}_o(\lambda_0))$, one uses the classical exponential integrators by Taylor-expanding all the operators. We do not ask too much regularity due to the size of the trees which involves two integrations in time. For the other trees $\mathcal{I}_o(T_i)$, $i \in \{4, 5, 6, 7, 8\}$, one can proceed with the same computations and get an error of the same order. \square

Remark 3.5.5 (Error improvement) Note that classical approximation techniques, such as splitting or exponential integrator methods (see, e.g., [CG12, JL00, Lub08]) introduce a local error of type $\mathcal{O}(\Delta^2 v, \Delta^2 V)$ and hence require solution and potential in

$$D(\Delta^2) = \{f \in (H^2 \cap H_0^1)(\Omega); \Delta f \in (H^2 \cap H_0^1)(\Omega)\}.$$

The local error of the second order low regularity GP integrator (3.75) on the other hand only requires the boundedness of second instead of fourth order spatial derivatives of the potential V and solution u , as well as only the classical boundary conditions that the trace vanishes, i.e., $H_0^1(\Omega)$.

Note that the second order low regularity scheme (3.75) involves commutators of the form $\mathcal{C}[f, i\Delta](u^n, \bar{u}^n, V)$ which in general involve spatial derivatives. Indeed, using Definition 3.1.2, one has

$$\begin{aligned} \mathcal{C}[f, i\Delta](v, \bar{v}, V) &= -i\Delta(f(v, \bar{v}, V)) + D_1 f(v, \bar{v}, V) \cdot i\Delta v \\ &+ D_2 f(v, \bar{v}, V) \cdot i\Delta\bar{v} + D_3 f(v, \bar{v}, V) \cdot i\Delta V. \end{aligned} \quad (3.82)$$

For practical computations we need to address the stability issues caused by the inclusion of these commutator terms in the numerical schemes. Different approaches can be made to treat this issue and guarantee the stability of the scheme. One way to overcome the stability issue lies in imposing a CFL condition on the fully discrete scheme, introducing a restriction on the ratio between time step size τ and spatial step size Δx . In this paper we will not impose any CFL type

condition, but stabilize the scheme a posteriori by the use of properly chosen filter operators Ψ . More precisely, instead of considering the second order low regularity integrator (3.75) for the discretisation of the GP equation, we consider its stabilised counterpart

$$\begin{aligned}
u^{n+1} &= e^{i\tau\Delta}u^n - i\tau\left((e^{i\tau\Delta}(u^n)^2)(e^{i\tau\Delta}\varphi_1(-2i\tau\Delta)\bar{u}^n)\right. \\
&\quad \left.+ (e^{i\tau\Delta}u^n)(e^{i\tau\Delta}\varphi_1(-i\tau\Delta)V)\right) \\
&\quad - i\tau^2\Psi\mathcal{C}[(e^{i\tau\Delta}\mathcal{M}_{\{1\}})(e^{i\tau\Delta}(\varphi_1(-2i\tau\Delta) - \varphi_2(-2i\tau\Delta))\mathcal{M}_{\{2\}}), i\Delta]((u^n)^2, \bar{u}^n) \\
&\quad - i\tau^2\Psi\mathcal{C}[(e^{i\tau\Delta}\mathcal{M}_{\{1\}})(e^{i\tau\Delta}(\varphi_1(-i\tau\Delta) - \varphi_2(-i\tau\Delta))\mathcal{M}_{\{2\}}), i\Delta](u^n, V) \\
&\quad - i\tau^2\left(e^{i\tau\Delta}\Psi\mathcal{C}[u^2, i\Delta](u^n)\right)\left(e^{i\tau\Delta}\varphi_2(-2i\tau\Delta)\bar{u}^n\right) \\
&\quad - \frac{\tau^2}{2}(u^n|u^n|^4 + 3u^n|u^n|^2V - |u^n|^2u^n\bar{V} + u^nV^2) \\
&= \Phi_{\text{GP2STAB}}^\tau(u^n),
\end{aligned} \tag{3.83}$$

where we have inserted the filter operator Ψ in front of all commutator terms. This filter function allows us the stabilization of the scheme. In the following section we briefly discuss the appropriate choice of filter function (which allows us to stabilize the scheme without worsening the local error structure) and outline an example. For a general introduction to filter functions in case of ODEs we refer to [HLW10].

3.5.2 Filter functions, commutators and stabilisation

To illustrate the appropriate choice for the filter operator Ψ we place ourselves in the following general framework: to construct a stable scheme at order $p = r + 1$, we wish to stabilize a term of the form

$$\tau^p\mathcal{C}^{p-1}[f, i\Delta](v, \bar{v}, V).$$

In case of the second order scheme for (3.60), the commutator terms are of first order and hence involve first order derivatives (with according boundary conditions), see (3.82), (3.73) and the Remark 3.1.3. This motivates the following choice we make on the filter operator: we denote the filter operator by

$$\Psi = \psi(i\tau|\nabla|),$$

where

$$|\nabla| := (-\Delta)^{1/2}$$

is self-adjoint on the domain $D(|\nabla|) = H_0^1(\Omega)$ and ψ denotes a suitably chosen filter function which allows us to

- (a) stabilize the scheme such that the numerical flow is locally Lipschitz continuous (see Assumption 3 below), while still
- (b) allowing approximations at low regularity (see Assumption 4 below).

Here it is important to note that the main purpose of our new framework lies in reducing the regularity assumptions. Hence, we do not want to introduce a “bad” (classical) error term through the stabilization, otherwise we could use directly classical Taylor series expansion techniques in the construction of our schemes. Thus, we require the filter function ψ to introduce the same optimal local error $O(\tau^{p+1}|\nabla|^p(v + V))$ as is introduced by our low-regularity schemes (see Section 3.4.2).

The two necessary assumptions on the filter operator $\Psi = \psi(i\tau|\nabla|)$ at arbitrary order p reads as follows:

Assumption 3 *Let us denote by X the space endowed with norm $\|\cdot\|$ in which we carry out the error analysis. Then the filter function Ψ should satisfy the following estimate*

$$\|\tau^{p-1}\Psi[\mathcal{C}^{p-1}[f, i\Delta](v, \bar{v}, V)]\| \leq C\|v\|^\sigma$$

for some $\sigma = \sigma(f, p) > 0$.

Assumption 3 guarantees the stability of the scheme, such that (for the appropriate choice of X) we have local Lipschitz continuity of the numerical flow Φ^τ .

Assumption 4 *The filter operator $\Psi = \psi(i\tau|\nabla|)$ shall satisfy the following low regularity expansion*

$$\Psi[\mathcal{C}^{p-1}[f, i\Delta](v, \bar{v}, V)] = \mathcal{C}^{p-1}[f, i\Delta](v, \bar{v}, V) + \mathcal{O}(\tau|\nabla|^p(v + V)). \tag{3.84}$$

Assumption 4 preserves the optimal local error structure $O(\tau^{p+1}|\nabla|^p(v+V))$ of our schemes. This is essential as the inclusion of the filter function should not require more regularity than we assumed in the construction of our low regularity framework.

An example of a possible choice of a filter function in order to stabilize the second order scheme (3.75) is given in the following example.

Example 13 (Filter functions for the GP equation) A possible choice of filter function for the second order low regularity integrator (3.83) is given by

$$\Psi = \psi(i\tau|\nabla|) = \varphi_1(i\tau|\nabla|) = (i\tau|\nabla|)^{-1}(e^{i\tau|\nabla|} - 1), \quad (3.85)$$

where we recall that $|\nabla| = (-\Delta)^{1/2}$ is a self-adjoint operator on the $D(|\nabla|) = H_0^1(\Omega)$. For a detailed analysis made on the torus which justifies the above choice of filter operator to stabilize a low-regularity scheme involving a first order commutator see [AB23a].

For a higher p -th order method we will encounter higher order commutators of the form

$$\tau^p \mathcal{C}^{p-1}[f, i\Delta](u^n, \bar{u}^n, V)$$

in our schemes. In order to stabilize the latter we need to introduce a higher order filter operator Ψ_p . For this purpose, we first note that using the Leibnitz formula, the commutator term $\mathcal{C}^{p-1}[f, i\Delta](v, \bar{v}, V)$ can be written as a combination of terms involving at most $p-1$ derivatives of v and V .

As an example, in the case $p=2$, $\mathcal{C}[f, i\Delta](v, \bar{v}, V)$ has the explicit form (3.82). Hence the role of Ψ_p lies in stabilizing terms which involve the differential operator $|\nabla|^{p-1}$. This motivates the higher order filter operator

$$\Psi_p = \underbrace{\varphi_1(i\tau|\nabla|) \dots \varphi_1(i\tau|\nabla|)}_{p-1 \text{ times}}. \quad (3.86)$$

Note that at first glance another (cheaper) choice of high order filter function would be $\tilde{\Psi}(i\tau|\nabla|) := \varphi_1(i\tau|\nabla|^{p-1})$. The latter, however, introduces a local error of order $\mathcal{O}(\tau|\nabla|^{2(p-1)})$ which at order $p \geq 3$ is not optimal in the sense of our low regularity approximations. Namely, this (cheaper) choice of filter function does not satisfy Assumption 4.

3.5.3 Klein– and Sine–Gordon equations

As a second example we consider a problem with real non-polynomial nonlinearity: the nonlinear Klein–Gordon (KG) equation

$$\begin{aligned} \partial_{tt}z - \Delta z + m^2z &= g(z), & (t, x) \in \mathbf{R} \times \Omega, \\ z(0) &= u_0, \quad \partial_t z(0) = u_1, \end{aligned} \quad (3.87)$$

where for simplicity we assume non zero mass $m \neq 0$ and real-valued solutions $z(t, x) \in \mathbf{R}$. Nevertheless, our framework can also allow for the complex setting $z(t, x) \in \mathbf{C}$ and for the case $m=0$ for wave equations.

First, in order to apply our abstract framework (3.1) to the nonlinear Klein-Gordon model (3.87) we rewrite (3.87) as a first-order complex system. For this purpose we define

$$\langle \nabla \rangle_m = \sqrt{-\Delta + m^2}$$

and assume that our domain Ω (equipped with appropriate boundary conditions) is chosen such that $\langle \nabla \rangle_m$ is well defined and invertible. For instance in the case of periodic boundary conditions the operator $\langle \nabla \rangle_m$ can be expressed as the Fourier multiplier

$$(\langle \nabla \rangle_m)_{k \in \mathbb{Z}^d} = \sqrt{(k_1 + \dots + k_d)^2 + m^2},$$

and is a well defined invertible operator on the space $H^1(\mathbf{T}^d)$, given that $m \neq 0$. While on a sufficiently smooth bounded domain $\Omega \subset \mathbf{R}^d$ equipped with homogeneous Dirichlet boundary conditions, using pseudo-spectral methods we have that the operator $\langle \nabla \rangle_m : (H^2 \cap H_0^1)(\Omega) \rightarrow L^2(\Omega)$ is essentially self-adjoint; its closure is self-adjoint on the domain

$$D(\langle \nabla \rangle_m) = H_0^1(\Omega).$$

See [RS80] for a full discussion on the study of unbounded operators, spectral theorems for self-adjoint operators (pg. 263) and of the notion of closable operators (pg. 250). Next we introduce the transformation

$$u = z - i\langle \nabla \rangle_m^{-1} \partial_t z, \quad (3.88)$$

which allows one to rewrite the Klein-Gordon equation (3.87) as the following first order complex system

$$i\partial_t u = -\langle \nabla \rangle_m u + \langle \nabla \rangle_m^{-1} g\left(\frac{1}{2}(u + \bar{u})\right), \quad (3.89)$$

and where by (3.88) we have that

$$z = \frac{1}{2}(u + \bar{u}) = \operatorname{Re}(u).$$

A natural space to study wave type equations of the form (3.87) is for $(z, \partial_t z) \in H^1 \times L^2$. In terms of u , from the transformation (3.88), we see that a natural space to measure the error in when studying equation (3.89) is H^1 .

In order to illustrate our general theory to the case of a non-polynomial nonlinearity, we choose to study the Sine–Gordon equation. The Sine–Gordon equation corresponds to the following choice of nonlinearity

$$g(z) = -\sin z,$$

which by equation (3.89) yields the first-order complex Sine–Gordon equation:

$$\partial_t u - i\langle \nabla \rangle_m u = i\langle \nabla \rangle_m^{-1} \left(\sin\left(\frac{1}{2}u\right) \cos\left(\frac{1}{2}\bar{u}\right) + \cos\left(\frac{1}{2}u\right) \sin\left(\frac{1}{2}\bar{u}\right) \right). \quad (3.90)$$

We now apply our general framework to the above Sine–Gordon equation. The above equation (3.90) is of the form (3.1) with

$$\begin{aligned} \mathfrak{L}_- &= \{0, 1\}, & \mathfrak{L}_+ &= \mathfrak{L}_+^{o,0} = \mathfrak{L}_+^{o,1} = \mathfrak{L}_+^{\bar{o},0} = \mathfrak{L}_+^{\bar{o},1} = \{o, \bar{o}\}, & V_0 &= V_1 = 1 \\ \mathcal{L}_o &= i\langle \nabla \rangle_m, & \mathcal{L}_{\bar{o}} &= -\mathcal{L}_o, & u_o &= v, & u_{\bar{o}} &= \bar{v} \\ f_{o,o}^0(u) &= \sin\left(\frac{1}{2}u\right), & f_{o,\bar{o}}^0(\bar{u}) &= \cos\left(\frac{1}{2}\bar{u}\right), & f_{o,o}^1(u) &= \cos\left(\frac{1}{2}u\right), & f_{o,\bar{o}}^1(\bar{u}) &= \sin\left(\frac{1}{2}\bar{u}\right), \\ f_{\bar{o},o}^0(u) &= \cos\left(\frac{1}{2}u\right), & f_{\bar{o},\bar{o}}^0(\bar{u}) &= \sin\left(\frac{1}{2}\bar{u}\right), & f_{\bar{o},o}^1(u) &= \sin\left(\frac{1}{2}u\right), & f_{\bar{o},\bar{o}}^1(\bar{u}) &= \cos\left(\frac{1}{2}\bar{u}\right). \end{aligned}$$

Using the above we have that for $(\ell, \bar{\ell}) \in \{o, \bar{o}\} \times \{0, 1\}$ the nonlinearity is given by

$$\Psi_\ell^{\bar{\ell}}(\mathbf{u}_\ell^{\bar{\ell}}) = i\langle \nabla \rangle_m^{-1} \left(f_{\ell,o}^{\bar{\ell}}(u) f_{\bar{\ell},\bar{o}}^{\bar{\ell}}(\bar{u}) \right). \quad (3.91)$$

Before introducing the first order analysis for (3.90), we make the following comparative remark. The decorated trees which will be introduced in the following section for the first order analysis of (3.90) will resemble the ones introduced for the analysis of the Gross–Pitaevskii equation (see Section 3.5.1). The main difference is that the nodes will encode different nonlinearities, given that the nonlinearities associated to V_0 and V_1 for the Sine–Gordon equation are different from the ones for the Gross–Pitaevskii equation. In addition, the Sine–Gordon nonlinearity (3.91) includes the linear operator $\mathcal{B}_o^0 = \mathcal{B}_o^1 = i\langle \nabla \rangle_m^{-1}$. See Section 3.5.1 where for the study of the Gross–Pitaevskii equation we had the more simple case where $\mathcal{B}_o^0 = \mathcal{B}_o^1 = \operatorname{id}$.

First order Duhamel integrator for Sine–Gordon

We seek to provide a first order low-regularity approximation to the following oscillatory integral:

$$\begin{aligned} w_o^0(\hat{v}, \tau) &= e^{i\tau\langle \nabla \rangle_m} v + i\langle \nabla \rangle_m^{-1} \int_0^\tau e^{i(\tau-\xi)\langle \nabla \rangle_m} \\ &\quad \left((e^{i\xi\langle \nabla \rangle_m} \sin\left(\frac{1}{2}v\right))(e^{-i\xi\langle \nabla \rangle_m} \cos\left(\frac{1}{2}\bar{v}\right)) + (e^{i\xi\langle \nabla \rangle_m} \cos\left(\frac{1}{2}v\right))(e^{-i\xi\langle \nabla \rangle_m} \sin\left(\frac{1}{2}\bar{v}\right)) \right) d\xi. \end{aligned}$$

The first order low regularity integrator for the Sine–Gordon equation is given in the following corollary.

Corollary 3.5.6 *At first order our general low regularity scheme (3.57) for the Sine–Gordon equation (3.90) takes the form*

$$\begin{aligned} u^{n+1} &= e^{i\tau\langle \nabla \rangle_m} u^n + i\tau\langle \nabla \rangle_m^{-1} [\\ &\quad \left(e^{i\tau\langle \nabla \rangle_m} \sin\left(\frac{1}{2}u^n\right) \right) \left(e^{i\tau\langle \nabla \rangle_m} (\varphi_1(-2i\tau\langle \nabla \rangle_m) \cos\left(\frac{1}{2}\bar{u}^n\right)) \right) \\ &\quad \left. + \left(e^{i\tau\langle \nabla \rangle_m} \cos\left(\frac{1}{2}u^n\right) \right) \left(e^{i\tau\langle \nabla \rangle_m} (\varphi_1(-2i\tau\langle \nabla \rangle_m) \sin\left(\frac{1}{2}\bar{u}^n\right)) \right) \right] \end{aligned} \quad (3.92)$$

with local error

$$\mathcal{O}(\tau^2 \mathcal{C}[\langle \nabla \rangle_m^{-1} \mathcal{M}_{\{1,2\}}, i\langle \nabla \rangle_m](u, \bar{u}))$$

In case of more regular solutions, we have the following simplified first-order scheme,

$$u^{n+1} = e^{i\tau\langle\nabla\rangle_m} u^n + i\tau\langle\nabla\rangle_m^{-1} \left(\sin\left(\frac{1}{2}u^n\right) \cos\left(\frac{1}{2}\bar{u}^n\right) + \cos\left(\frac{1}{2}u^n\right) \sin\left(\frac{1}{2}\bar{u}^n\right) \right) \quad (3.93)$$

with a local error of order $\mathcal{O}\left(\tau^2\langle\nabla\rangle_m^{-1}((\langle\nabla\rangle_m u)\bar{u})\right)$.

Remark 3.5.7 (Remark on the imposed regularity) In general the local error of type

$$\mathcal{O}\left(\tau^2\mathcal{C}[\langle\nabla\rangle_m^{-1}\mathcal{M}_{\{1,2\}}, i\langle\nabla\rangle_m](u, \bar{u})\right)$$

asks for less regularity assumptions than the local error $\mathcal{O}\left(\tau^2\langle\nabla\rangle_m^{-1}((\langle\nabla\rangle_m u)\bar{u})\right)$, due to the structure of the commutator (see Definition 3.1.2). Indeed, we portray this in the following example, where we measure the error in the space $H^1(\mathbf{T}^d)$.

First, using the commutator estimate established in [RS21, Lemma 27], we have

$$\begin{aligned} \|\mathcal{C}[\langle\nabla\rangle_m^{-1}\mathcal{M}_{\{1,2\}}, i\langle\nabla\rangle_m](u, \bar{u})\|_{H^1} &\lesssim \|\mathcal{C}[\mathcal{M}_{\{1,2\}}, i\langle\nabla\rangle_m](u, \bar{u})\|_{L^2} \\ &\lesssim \|u\|_{H^{\frac{1}{2}+\frac{d}{4}}}^2. \end{aligned}$$

Namely we have that the commutator term asks for solutions in $H^{\frac{1}{2}+\frac{d}{4}}(\mathbf{T}^d)$.

Secondly, using the classical bilinear estimate:

$$\|uv\|_{L^2(\Omega)} \lesssim \|u\|_{L^2(\Omega)} \|v\|_{H^{\frac{d}{2}+\epsilon}(\Omega)}, \quad \epsilon > 0,$$

which follows by the Sobolev injection $H^{\frac{d}{2}+\epsilon} \hookrightarrow L^\infty$, we have,

$$\begin{aligned} \|\langle\nabla\rangle_m^{-1}((\langle\nabla\rangle_m u)\bar{u})\|_{H^1(\Omega)} &\lesssim \|(\langle\nabla\rangle_m u)\bar{u}\|_{L^2(\Omega)} \\ &\lesssim \|\langle\nabla\rangle_m u\|_{L^2(\Omega)} \|u\|_{H^{\frac{d}{2}+\epsilon}(\Omega)}. \end{aligned}$$

It follows from the above that the *classical* local error term asks for solutions in $(H^1 \cap H^{\frac{d}{2}+\epsilon})(\mathbf{T}^d)$ when working on the torus, while when working on a bounded domain equipped with Dirichlet boundary conditions it asks for solutions in $(H_0^1 \cap H^{\frac{d}{2}+\epsilon})(\Omega)$. Hence, the commutator-term asks for less regularity than the classical local error term. For example, when $d = 1$, the low-regularity scheme asks for $H^{\frac{3}{4}}(\mathbf{T})$ -solutions, whereas the classical scheme asks for $u(t) \in D(\langle\nabla\rangle_m) = H^1(\mathbf{T})$.

Proof. The trees we are considering are $\mathcal{T}^1 = \{T_0, T_1\}$, where following the framework given in (3.32) we have that,

$$\begin{aligned} \mathcal{B}_o \left(\prod_{i \in \mathfrak{L}_{+}^{0,0}} e^{\xi \mathcal{L}_i} f_{o,i}^0(v_i) \right) V_0 &= i\langle\nabla\rangle_m^{-1} \left(\left(e^{i\xi\langle\nabla\rangle_m} u_1 \right) \left(e^{-i\xi\langle\nabla\rangle_m} u_2 \right) \right) \\ &\equiv \circ = \lambda_0 = T_0, \\ \mathcal{B}_o \left(\prod_{i \in \mathfrak{L}_{+}^{1,0}} e^{\xi \mathcal{L}_i} f_{o,i}^1(v_i) \right) V_1 &= i\langle\nabla\rangle_m^{-1} \left(\left(e^{i\xi\langle\nabla\rangle_m} u_3 \right) \left(e^{-i\xi\langle\nabla\rangle_m} u_4 \right) \right) \\ &\equiv \bullet = \lambda_1 = T_1, \end{aligned}$$

where $\mathbf{v} = (v, \bar{v})$ and $u_1 = \sin(\frac{1}{2}v)$, $u_2 = \cos(\frac{1}{2}\bar{v})$, $u_3 = \cos(\frac{1}{2}v)$, $u_4 = \sin(\frac{1}{2}\bar{v})$. From equation (3.57) it then follows that the first-order scheme is of the form,

$$u^0(\hat{\mathbf{v}}, \tau) = e^{i\tau\Delta} v + \sum_{T \in \mathcal{T}^1} \Pi_A^0(\mathcal{I}_o(T))(\hat{\mathbf{v}}, \tau), \quad (3.94)$$

where $\mathbf{v} = (v, \bar{v})$. We have, for $i = 0, 1$, that

$$\Pi_A^0 \mathcal{I}_o(\lambda_i)(\hat{\mathbf{v}}, \tau) = \mathcal{K}_{o,A}^0(\tilde{\Pi}_{o,A} \mathcal{D}_{-1}(\lambda_i)(\hat{\mathbf{v}}, \cdot))(\tau) = \mathcal{K}_{o,A}^0 \left(\frac{\Upsilon_{\text{root}}^{\Psi_o}[\lambda_i]}{S_{\text{root}}(\lambda_i)}(\mathbf{v}, \xi) \right)(\tau)$$

where one has,

$$\begin{aligned} S_{\text{root}}(\lambda_0) &= S_{\text{root}}(\lambda_1) = 1, \\ \Upsilon_{\text{root}}^{\Psi_o}[\lambda_0](\mathbf{v}, \xi) &= i\langle \nabla \rangle_m^{-1} \left(\left(e^{i\xi \langle \nabla \rangle_m} \sin\left(\frac{1}{2}v\right) \right) \left(e^{-i\xi \langle \nabla \rangle_m} \cos\left(\frac{1}{2}\bar{v}\right) \right) \right), \\ \Upsilon_{\text{root}}^{\Psi_o}[\lambda_1](\mathbf{v}, \xi) &= i\langle \nabla \rangle_m^{-1} \left(\left(e^{i\xi \langle \nabla \rangle_m} \cos\left(\frac{1}{2}v\right) \right) \left(e^{-i\xi \langle \nabla \rangle_m} \sin\left(\frac{1}{2}\bar{v}\right) \right) \right). \end{aligned}$$

1. When $A \supset (H^1 \cap H^{\frac{d}{2}+\epsilon})(\mathbf{T}^d)^2$ or $A \supset (H_0^1 \cap H^{\frac{d}{2}+\epsilon})(\Omega)^2$.

Given that $r, \ell = 0$, and $v \notin D(G)$, we do not have enough regularity to simply apply the Taylor-expansion (3.44). Instead we perform a low-regularity based approximation of the integrals and apply the first point (i) of Definition 3.3.2. From definition (3.3.2) it then follows that

$$\mathcal{L}_1 = \mathcal{L}_o = i\langle \nabla \rangle_m, \quad \mathcal{L}_2 = -i\langle \nabla \rangle_m, \quad \mathcal{L}_{\text{dom}} = -2i\langle \nabla \rangle_m$$

with $\mathcal{B}_o = \langle \nabla \rangle_m^{-1}$, and hence we have,

$$\begin{aligned} \mathcal{K}_{o,A}^0 \left(\Upsilon_{\text{root}}^{\Psi_o}[\lambda_0](\mathbf{v}, \cdot) \right) (\tau) &= i\tau \langle \nabla \rangle_m^{-1} \left(e^{i\tau \langle \nabla \rangle_m} u_1 \right) \left(e^{i\tau \langle \nabla \rangle_m} (\varphi_1(-2i\tau \langle \nabla \rangle_m) u_2) \right) \\ \mathcal{K}_{o,A}^0 \left(\Upsilon_{\text{root}}^{\Psi_o}[\lambda_1](\mathbf{v}, \cdot) \right) (\tau) &= i\tau \langle \nabla \rangle_m^{-1} \left(e^{i\tau \langle \nabla \rangle_m} u_3 \right) \left(e^{i\tau \langle \nabla \rangle_m} (\varphi_1(-2i\tau \langle \nabla \rangle_m) u_4) \right). \end{aligned}$$

Plugging the above in (3.94) yields the first order low-regularity scheme (3.92) for the Sine-Gordon equation.

2. When $A = (H^1 \cap H^{\frac{d}{2}+\epsilon})(\mathbf{T}^d)^2$ or $A = (H_0^1 \cap H^{\frac{d}{2}+\epsilon})(\Omega)^2$

In this case we apply the Taylor expansion (3.44) with $r = \ell = 0$, to obtain:

$$\begin{aligned} \mathcal{K}_{o,A}^0 \left(\left(\Upsilon_{\text{root}}^{\Psi_o}[\lambda_0] + \Upsilon_{\text{root}}^{\Psi_o}[\lambda_1] \right) (\mathbf{v}, \cdot) \right) (\tau) \\ = i\langle \nabla \rangle_m^{-1} \left(\int_0^\tau u_1 u_2 d\xi + \int_0^\tau u_3 u_4 d\xi \right) \\ = i\tau \langle \nabla \rangle_m^{-1} \left(\sin\left(\frac{1}{2}v\right) \cos\left(\frac{1}{2}\bar{v}\right) + \cos\left(\frac{1}{2}v\right) \sin\left(\frac{1}{2}\bar{v}\right) \right), \end{aligned}$$

which thanks to (3.94) yields the first order scheme (3.93).

Local error analysis: We follow the same steps as for the proof of Corollary 3.5.1. Using the recursive formula in Definition 3.3.8, one gets for $T \in \{\lambda_0, \lambda_1\}$

$$\mathcal{L}_{\text{low}}^0(\mathcal{I}_o(T), \hat{\mathbf{v}}, A) = \mathcal{L}_{\text{low}}^{-1,o}(T, \hat{\mathbf{v}}, A) + R_{o,A}^0 \left(\left(\tilde{\Pi}_{o,A} T \right) (\hat{\mathbf{v}}, \cdot) \right).$$

Then by (3.50), we get for $l \in \{0, 1\}$

$$\mathcal{L}_{\text{low}}^{-1,o}(\lambda_l, \hat{\mathbf{v}}, A) = \frac{\Upsilon_{\text{root}}^{\Psi_o}[T]}{S_{\text{root}}(T)}(\mathbf{v}, 0) V_l$$

which gives

$$\begin{aligned} \mathcal{L}_{\text{low}}^{-1,o}(\lambda_0, \hat{\mathbf{v}}, A) &= i\langle \nabla \rangle_m^{-1} \left(\left(e^{i\xi \langle \nabla \rangle_m} \sin\left(\frac{1}{2}v\right) \right) \left(e^{-i\xi \langle \nabla \rangle_m} \cos\left(\frac{1}{2}\bar{v}\right) \right) \right), \\ \mathcal{L}_{\text{low}}^{-1,o}(\lambda_1, \hat{\mathbf{v}}, A) &= i\langle \nabla \rangle_m^{-1} \left(\left(e^{i\xi \langle \nabla \rangle_m} \cos\left(\frac{1}{2}v\right) \right) \left(e^{-i\xi \langle \nabla \rangle_m} \sin\left(\frac{1}{2}\bar{v}\right) \right) \right). \end{aligned}$$

It remains to compute $R_{o,A}^0((\Pi_A T))$ whose values will depend on A . For $A \supset (H^1 \cap H^{\frac{d}{2}+\epsilon})(\mathbf{T}^d)^2$ or $A \supset (H_0^1 \cap H^{\frac{d}{2}+\epsilon})(\Omega)^2$ one gets

$$\begin{aligned} R_{o,A}^0((\tilde{\Pi}_{o,A} \lambda_0)(\hat{\mathbf{v}}, \cdot)) &= \mathcal{C}[i\langle \nabla \rangle_m^{-1} \mathcal{M}_{\{1,2\}}, i\langle \nabla \rangle_m](\sin\left(\frac{1}{2}v\right), \cos\left(\frac{1}{2}\bar{v}\right)) \\ R_{o,A}^0((\tilde{\Pi}_{o,A} \lambda_1)(\hat{\mathbf{v}}, \cdot)) &= \mathcal{C}[i\langle \nabla \rangle_m^{-1} \mathcal{M}_{\{1,2\}}, i\langle \nabla \rangle_m](\cos\left(\frac{1}{2}v\right), \sin\left(\frac{1}{2}\bar{v}\right)). \end{aligned}$$

For $A = (H^1 \cap H^{\frac{d}{2}+\epsilon})(\mathbf{T}^d)^2$ or $A = (H_0^1 \cap H^{\frac{d}{2}+\epsilon})(\Omega)^2$, one Taylor-expands the operators which give:

$$\begin{aligned}
R_{o,A}^0((\tilde{\Pi}_{o,A}\lambda_0)(\hat{\mathbf{v}}, \cdot)) &= -\sin(\tfrac{1}{2}v) \cos(\tfrac{1}{2}\bar{v}) - \langle \nabla \rangle_m^{-1} \left((\langle \nabla \rangle_m \sin(\tfrac{1}{2}v)) (\cos(\tfrac{1}{2}\bar{v})) \right) \\
&\quad + \langle \nabla \rangle_m^{-1} \left(\sin(\tfrac{1}{2}v) (\langle \nabla \rangle_m \cos(\tfrac{1}{2}\bar{v})) \right) \\
R_{o,A}^0((\tilde{\Pi}_{o,A}\lambda_1)(\hat{\mathbf{v}}, \cdot)) &= -\cos(\tfrac{1}{2}v) \sin(\tfrac{1}{2}\bar{v}) - \langle \nabla \rangle_m^{-1} \left((\langle \nabla \rangle_m \cos(\tfrac{1}{2}v)) (\sin(\tfrac{1}{2}\bar{v})) \right) \\
&\quad + \langle \nabla \rangle_m^{-1} \left(\cos(\tfrac{1}{2}v) (\langle \nabla \rangle_m \sin(\tfrac{1}{2}\bar{v})) \right)
\end{aligned}$$

which concludes the proof. □

Remark 3.5.8 Similarly to Corollary 3.5.6 our general framework (3.4.2) also allows for low regularity approximations at higher order for Klein–Gordon equations.

Part II

The setting of a randomized initial condition

Chapter 4

Approximations of dispersive PDEs in the presence of low-regularity randomness

This chapter is based on the article [ABBS22a] accepted in Foundations of Computational Mathematics.

Abstract. We introduce a new class of numerical schemes which allow for low regularity approximations to the expectation $\mathbb{E}(|u_k(t, v^\eta)|^2)$, where u_k denotes the k -th Fourier coefficient of the solution u of the dispersive equation and $v^\eta(x)$ the associated random initial data. This quantity plays an important role in physics, in particular in the study of wave turbulence where one needs to adopt a statistical approach in order to obtain deep insight into the *generic* long-time behaviour of solutions to dispersive equations. Our new class of schemes is based on Wick's theorem and Feynman diagrams together with a resonance based discretisation [BS22] set in a more general context: we introduce a novel combinatorial structure called paired decorated forests which are two decorated trees whose decorations on the leaves come in pair. The character of the scheme draws its inspiration from the treatment of singular stochastic partial differential equations via Regularity Structures. In contrast to classical approaches, we do not discretize the PDE itself, but rather its expectation. This allows us to heavily exploit the optimal resonance structure and underlying gain in regularity on the finite dimensional (discrete) level.

4.1 Introduction

We consider nonlinear dispersive equations

$$i\partial_t u(t, x) + \mathcal{L}(\nabla)u(t, x) = |\nabla|^\alpha p(u(t, x), \bar{u}(t, x)), \quad (t, x) \in \mathbf{R} \times \mathbf{T}^d \quad (4.1)$$

with random initial data:

$$u(0, x) = v^\eta(x) = \sum_{k \in \mathbf{Z}^d} v_k \eta_k e^{ikx}, \quad (4.2)$$

where $v_k = \overline{v_{-k}}$ and $(\eta_k)_{k \in \mathbf{Z}^d}$ is a family of random variables satisfying

$$\mathbb{E}(\eta_k \eta_{-\ell}) = \delta_{k, \ell}. \quad (4.3)$$

For the condition (4.3) to be satisfied we require η_0 to be a real normalized centered Gaussian, $(\eta_k)_{k>0}$ to be standard complex Gaussians, $(\eta_k)_{k \geq 0}$ to be independent and to satisfy $\eta_k = \overline{\eta_{-k}}$. We first note that the above setting is for real initial conditions. In the complex case, we simply need to take $(\eta_k)_{k \in \mathbf{Z}^d}$ to be independent standard complex Gaussians which satisfy $\mathbb{E}(\eta_k \overline{\eta_\ell}) = \delta_{k, \ell}$, and refer to the Remark 4.1.1. Working with Gaussian random variables allows us to use Wick's formula for computing the second moment of $u_k(\tau, v^\eta)$. Nevertheless, one can go beyond the Gaussian realm. For a discussion on the subject we refer to Remark 4.1.2.

Furthermore, we assume in (4.1) a polynomial nonlinearity p . Moreover, we suppose that there exists a deterministic time $T > 0$ such that the structure of (4.1) implies at least almost-sure local wellposedness of the problem in an appropriate functional space on the finite time interval $]0, T]$. This is a non-trivial assumption since naturally the time of existence is random and not necessarily almost surely bounded from below by a positive time T . We refer to the works on probabilistic Cauchy theory given for instance by [BT08, BT13, SX16, CO12, NS15, CGI22] in the case of nonlinear Schrödinger and wave equations. With the above assumption we have that the solution u admits up until time T a second moment restricted on the almost surely set of its definition. In order to keep notations simple, we will omit such a set in the sequel.

The differential operators $\mathcal{L}(\nabla)$ and $|\nabla|^\alpha$ shall cast in Fourier space into the form

$$\mathcal{L}(\nabla)(k) = k^\sigma + \sum_{\gamma:|\gamma|<\sigma} a_\gamma \prod_j k_j^{\gamma_j}, \quad |\nabla|^\alpha(k) = \sum_{\gamma:|\gamma|\leq\alpha} \prod_{j=1}^d |k_j|^{\gamma_j} \quad (4.4)$$

for some $\alpha \in \mathbf{R}$, $\sigma \in \mathbf{N}$, $\gamma \in \mathbf{Z}^d$ and $|\gamma| = \sum_i \gamma_i$, where for $k = (k_1, \dots, k_d) \in \mathbf{Z}^d$ and $m = (m_1, \dots, m_d) \in \mathbf{Z}^d$ we set

$$k^\sigma = k_1^\sigma + \dots + k_d^\sigma, \quad k \cdot m = k_1 m_1 + \dots + k_d m_d.$$

Concrete examples are discussed in Section 4.5, including the cubic nonlinear Schrödinger (NLS) equation

$$i\partial_t u + \mathcal{L}(\nabla)u = |u|^2 u, \quad \mathcal{L}(\nabla) = \Delta, \quad \alpha = 0, \quad p(u, \bar{u}) = |u|^2 u \quad (4.5)$$

and the Korteweg–de Vries (KdV) equation

$$i\partial_t u + \mathcal{L}(\nabla)u = i\frac{1}{2}\partial_x u^2, \quad \mathcal{L}(\nabla) = i\partial_x^3, \quad \alpha = 1, \quad p(u, \bar{u}) = i\frac{1}{2}u^2. \quad (4.6)$$

Note that one could deal with non-polynomial nonlinearities, and work on more general domains than the periodic one, by combining the present work with the general framework established in [ABBS22b]. Indeed, by introducing nested commutator structures the work [ABBS22b] overcomes the necessity of periodic boundary conditions and polynomial nonlinearities, see also [RS21, AB23a]. One can use the iterated integrals produced in [ABBS22b] and then proceed in Fourier space as in the present work. Doing all the computations in physical space will require a description of the second moment of the random initial data directly in physical space; however, such a randomisation is in general mostly described in Fourier space.

The aim of this paper is to introduce a new class of schemes which, by denoting by τ the time step, allows for a low regularity approximation to

$$\mathbb{E}(|u_k(t, v^\eta)|^2). \quad (4.7)$$

Here, \mathbb{E} denotes the expectation and u_k the k -th Fourier coefficient of the solution u of (4.1) with corresponding initial data v^η defined at equation (4.2). The quantity (4.7) plays an important role in physics, in particular in the study of wave turbulence. A fundamental question in the latter is to derive a rigorous justification of the wave kinetic equation (WKE), an equation which describes the effective dynamics of an interacting wave system in the thermodynamic limit. This yields deep insight into the *generic* long-time behaviour of solutions to dispersive equations. In order to derive this equation one starts with a random initial value and work on a large box of size L . Then under suitable scaling laws which depend on the strength μ of the non-linearity, and the size L of the box, one can show that in the limit of large L and small μ the effective dynamic of $\mathbb{E}(|u_k(t, v^\eta)|^2)$ is given by the WKE over sufficiently long time scales.

A rigorous derivation of the WKE for NLS is performed in [DH21, DH23, ACG21] via a diagrammatic expansion. A similar rigorous derivation result for a high dimensional ($d \geq 14$) discrete KdV-type equation was achieved in [ST21] using also Feynman diagrams, in order to derive its associated wave kinetic equation at the kinetic time under a suitable scaling law. All these works are based on the iteration of Duhamel's formula for (4.1):

$$u(\tau, v^\eta) = e^{i\tau\mathcal{L}(\nabla)} v^\eta - i|\nabla|^\alpha e^{i\tau\mathcal{L}(\nabla)} \int_0^\tau e^{-i\xi\mathcal{L}(\nabla)} p(u(\xi, v^\eta), \bar{u}(\xi, v^\eta)) d\xi \quad (4.8)$$

which in Fourier space cast into the form

$$u_k(\tau, v^\eta) = e^{i\tau\mathcal{L}(\nabla)(k)} \eta_k v_k - i|\nabla|^\alpha(k) e^{i\tau\mathcal{L}(\nabla)(k)} \int_0^\tau e^{-i\xi\mathcal{L}(\nabla)(k)} p_k(u(\xi, v^\eta), \bar{u}(\xi, v^\eta)) d\xi, \quad (4.9)$$

where p_k is given for $p(u, \bar{u}) = |u|^2 u$ by

$$p_k(u, \bar{u}) = \sum_{k=-k_1+k_2+k_3} \bar{u}_{k_1} u_{k_2} u_{k_3}.$$

Iterations of (4.9) produces a tree series, see also [Chr07, Gub12, GKO13] where the series is made explicit for some specific equations. This expansion can also be described via random tensors introduced in [DNY22]. From this tree series, one can compute $\mathbb{E}(|u_k(\tau, v^\eta)|^2)$ using Wick's theorem and Feynman diagrams [DH21, DH23].

The theoretical works mentioned above on the study of wave turbulence, together with the idea of a resonance based discretisation [BS22], set the inspiration for this work. From an algebraic point of view we, however, have to work in a much more general context considering trees with more decorations than introduced in [BS22], with a new combinatorial

structure called *paired decorated forests*. This will allow us to approximate a large class of dispersive PDEs with one general scheme, without the need of treating each and every equation separately.

In contrast to classical approaches, we do not discretize the PDE itself, but rather its expectation. This allows us to heavily exploit the optimal resonance structure and underlying gain in regularity on the discrete level. More precisely, the iteration of Duhamel's formulation (4.8) of (4.1) can be expressed using decorated trees, see [BS22]. Namely, it follows from [BS22, Section 1.2] that the k -th Fourier coefficient of the approximated solution at order r is given by

$$u_k^r(\tau, v^\eta) = \sum_{T \in \mathcal{V}_k^r} \frac{\Upsilon^p(T)(v^\eta)}{S(T)} (\Pi T)(\tau) \quad (4.10)$$

where \mathcal{V}_k^r is a set of decorated trees which incorporate the frequency k , $S(T)$ is the symmetry factor associated to the tree T , $\Upsilon^p(T)$ is the coefficient appearing in the iteration of Duhamel's formulation and $(\Pi T)(\tau)$ represents a Fourier iterated integral. The exponent p corresponds to the nonlinearity appearing in the right hand side of (4.1). The exponent r in \mathcal{V}_k^r means that we consider only trees of size at most $r+1$, these are the trees corresponding to an iterated integral of depth at most $r+1$. These quantities are described in detail in Section 4.4. Generally speaking, the sum (4.10) is the truncation at order r of the infinite series describing formally the solution of (4.1). The low regularity scheme for (4.1) is then obtained by replacing each oscillatory integral $(\Pi T)(\tau)$ appearing in the finite sum (4.10) by a low regularity approximation that embeds the resonance structure into the numerical discretization. We will denote the latter low-regularity approximation operator by $\Pi^{n,r}$. Here, r corresponds to the order of the discretization and n is a formal a priori regularity assumed on the initial data v^η . Namely, we assume that we can differentiate v^η , n -times. The general scheme then takes the form:

$$U_k^r(\tau, v^\eta) = \sum_{T \in \mathcal{V}_k^r} \frac{\Upsilon^p(T)(v^\eta)}{S(T)} (\Pi^{n,r} T)(\tau). \quad (4.11)$$

The local error structure for each approximated iterated integral is given by

$$(\Pi T - \Pi^{n,r} T)(\tau) = \mathcal{O}(\tau^{\tau+2} \mathcal{L}_{\text{low}}^r(T, n)), \quad (4.12)$$

where $\mathcal{L}_{\text{low}}^r$ involves only lower order derivatives. The form of the scheme draws its inspiration from the treatment of singular stochastic partial differential equations (SPDEs) via Regularity Structures in [Hai14, BHZ19, BCCH20, BHZ20]. These decorated trees expansions are generalization of the B-series widely used for ordinary differential equations, we refer to [But72, CCO08, HLW10, MKL13]. In the end, one obtains an approximation of u under much lower regularity assumptions than classical methods (e.g., splitting methods, exponential integrators [CG12, Fao12, HLW10, HO10, Hol10, Law67, Lub08, LR04, MQ02, SSC18]) require, which in general introduce the local error

$$\mathcal{O}(\tau^{\tau+2} \mathcal{L}^r(T, n)) \quad (4.13)$$

involving the full high order differential operator \mathcal{L}^r . Indeed, we have that $\mathcal{D}(\mathcal{L}_{\text{low}}) \supset \mathcal{D}(\mathcal{L})$, meaning that the local error structure (4.12) allows us to deal with a rougher class of solutions than the classical error bound (4.13). The underlying idea behind these low-regularity approximations was initiated by the work of [OS18], and then generalized by [BS22, ABBS22b] to higher order methods, allowing for approximations to large classes of equations. Although the error bound (4.12) derived here are formal, one can obtain rigorous low-regularity error bounds using a classical Sobolev space setting (see [RS21, AB23a]), as well as sharp L^2 error estimates by using discrete Strichartz estimates and discrete Bourgain spaces (see [IZ09, ORS21, ORS22b, RS22, JORS23]). Let us mention that the local error analysis can be nicely understood via a Birkhoff factorisation of the character $\Pi^{n,r}$ (see [BS22, BEF20]) that involves a deformed Butcher-Connes-Kreimer coproduct (see [But72, CK99, CK00, BS22, BM23]). In the present work, we give a recursive description with various Taylor remainders in Definition 4.3.5. This formulation is similar to [ABBS22b] where the Birkhoff factorisation is not available. The Birkhoff factorisation can also be used in our work for a more precise description of the Taylor remainders. We also believe that it could have an impact on the general description of symmetries for low regularity schemes. For the moment, only symmetric and symplectic schemes have been worked out by hand (see [AB23b, MS23]). Lastly, we note that the scheme (4.11) has been generalized to non-polynomial nonlinearities and to parabolic equations in [ABBS22b] with the use of nested commutators first introduced in [RS21].

A natural route to obtain a low regularity approximation to $\mathbb{E}(|u_k(\tau, v^\eta)|^2)$ would be to first compute the low regularity approximation $U_k^{n,r}(\tau, v^\eta)$ given in (4.11) to $u_k(\tau, v^\eta)$, and then to evaluate its expectation $\mathbb{E}(|U_k^{n,r}(\tau, v^\eta)|^2)$ while removing the terms of higher order. By doing so, we would, however, ignore the enhanced resonance structure and gain in regularity introduced by applying the expectation \mathbb{E} . In order to exploit the latter on the discrete level, we will directly compute a low regularity approximation to the second moment of u_k^r , where u_k^r is defined in (4.10), and is the truncation at order r of the tree series describing u_k . Namely, we are interested in computing the following series:

$$V_k^r(\tau, v) = \mathcal{Q}_{\leq r+1} \mathbb{E}(|u_k^r(\tau, v^\eta)|^2) \quad (4.14)$$

$$= \sum_{F=T_1 \cdot T_2 \in \mathcal{G}_k^r} m_F \frac{\tilde{\Upsilon}^p(T_1)(v) \Upsilon^p(T_2)(v)}{S(T_1)S(T_2)} (\bar{\Pi}T_1)(\tau) (\Pi T_2)(\tau)$$

where $\mathcal{Q}_{\leq r+1}$ keeps only the terms of order less than or equal to τ^{r+1} , and m_F is a combinatorial coefficient associated to F . Namely, m_F counts the number of pairings that produce F . It remains to describe the set \mathcal{G}_k^r . For this purpose we introduce a new combinatorial structure called paired decorated forest which are two decorated trees whose decorations on the leaves come in pair. This pairing among the leaves come from the use of Wick's theorem for products of Gaussian random variables that appear in the computation of V_k^r . Similar structures have been used in the theoretical analysis of dispersive PDEs [DH21, DH23, ACG21, ST21] as well as in stochastic differential equations and exotic B-series [LV20, Bro22]. The set \mathcal{G}_k^r consists of all paired forests $F = T_1 \cdot T_2$ of size at most $r+1$, meaning that the term $(\bar{\Pi}T_1)(\tau) (\Pi T_2)(\tau)$ contains at most $r+1$ integrals in time. T_1 and T_2 are the two paired trees and \cdot denotes the forest product. Further, in the above series we have used the following short hand notation:

$$\tilde{\Upsilon}^p(T_1)(v) = \overline{\Upsilon^p(T_1)(v)}, \quad (\bar{\Pi}T_1)(\tau) = \overline{(\Pi T_1)(\tau)},$$

which stands for the complex conjugate, and will be abundantly used throughout the reminder of this article. Notice that the above sum (4.14) is not symmetric, meaning that both $(\bar{\Pi}T_1)(\tau) (\Pi T_2)(\tau)$ and $(\bar{\Pi}T_2)(\tau) (\Pi T_1)(\tau)$ appear when $T_1 \neq T_2$. We then proceed with the discretization in time of (4.14) as is done in [BS22]: we replace $(\Pi T_i)(\tau)$ by their resonance based approximations $(\Pi^{n,r}T_i)$ which yields the following tree series:

$$V_k^{n,r}(\tau, v) = \sum_{F=T_1 \cdot T_2 \in \mathcal{G}_k^r} m_F \frac{\tilde{\Upsilon}^p(T_1)(v) \Upsilon^p(T_2)(v)}{S(T_1)S(T_2)} \mathcal{Q}_{\leq r+1}(\bar{\Pi}^{n,r}T_1 \Pi^{n,r}T_2)(\tau). \quad (4.15)$$

The local error structure is given by

$$(\bar{\Pi}T_1 \Pi T_2 - \mathcal{Q}_{\leq r+1} \Pi^{n,r}T_1 \bar{\Pi}^{n,r}T_2)(\tau) = \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n)). \quad (4.16)$$

The definition of $\mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n)$ is, however, much more involved than in the work of [BS22]. Indeed, given that we consider decorated forests $F = T_1 \cdot T_2$, whose leaves (which encodes the frequency) come in pairs, we have that the same frequencies can appear in both the decorated tree T_1 and that of T_2 . Hence, unlike in the work of [BS22], the set of frequencies appearing on the leaves of T_1 and T_2 are not disjoint, and in consequence a new framework needs to be considered. Moreover, since our calculations are made with these pairings $T_1 \cdot T_2$, cancellations appear when computing the variance (4.7) and the schemes obtained in this work are of simpler form than those obtained in the work of [BS22].

Our main result is the general class of schemes given by (4.15) together with the correct combinatorial structures on paired decorated forests, which yields a low-regularity approximation of (4.7). Our construction is based upon Wick's formula (see Proposition 4.4.1) and is presented in Proposition 4.4.2. The local error structure (4.12) is then given in Theorem 4.4.3. Theorem 4.4.3 is heavily based on Theorem 4.3.6 which introduces a new recursive definition of $\mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n)$ (see Definition 4.3.5) which differs from the one presented in [BS22].

The new scheme (4.15) is an attempt to implement the low regularity integrators introduced in [BS22] when randomness is introduced at the level of the initial data. We expect that the scheme described in [BS22, ABBS22b] will be able to enhance the error structure of classical methods for (dispersive) stochastic PDEs (see, e.g. [BC23, Deb11, LPS14] and the references therein) for low regularity initial data where randomness is added via a stochastic forcing.

Remark 4.1.1 Our assumption on the initial data in (4.3) enforces the initial data to be real. Our scheme is fairly general and works for both real or complex initial data. In the case of a complex initial data the authors [DH23, DH21] use the following assumption. Let $(\eta_k)_{k \in \mathbf{Z}^d}$ be a family of independent identically distributed complex random variables (centered standard Gaussian variables or uniform distributions on the unit circle) satisfying: For all $k, \ell \in \mathbf{Z}^d$

$$\mathbb{E}(|\eta_k|^2) = 1, \quad \mathbb{E}(\eta_k \eta_\ell) = 0.$$

In the Gaussian case see also [CG19]. The second identity in the above simplifies a lot the interactions that need to be considered for building up the Feynman diagrams. Indeed, only the terms $\mathbb{E}(\eta_k \bar{\eta}_\ell)$ from Wick's theorem are potentially non-zero. These terms are the easiest to treat requiring no extra regularity, (see Section 4.1.1 and (4.22) where the pairing $T_0 \cdot T_{1,1}$ is no longer possible, it is the pairing that asks more regularity in the discretisation, see (4.26)).

Remark 4.1.2 In (4.14), the summation is performed on paired decorated forests of the form $T_1 \cdot T_2$. The fact that we have only two trees and not more correspond to the computation of the second moment. For the p -th moment, one will get p paired decorated trees where the leaves will come in pairs. In both cases second moment or higher moments, one uses Wick's theorem applied to product of Gaussian random variables for computing the pairings. One can potentially

go beyond the Gaussian realm by using cumulants for computing the moments of a given random variable. This was extensively used in the context of singular SPDEs (see [CH16] for a general convergence result of renormalised models and [EH21, BN22] for recent works in the discrete setting). In our context, one can imagine to have trees where the leaves are split into different sets of cardinality bigger than two. The scheme will be robust to this case.

Before introducing our general framework we will in the next section illustrate our main idea on an example taken from NLS.

4.1.1 Example

Let us consider the equation:

$$i\partial_t u + \Delta u = |u|^2 u, \quad u(0, x) = v^\eta(x) = \sum_{k \in \mathbf{Z}^d} v_k \eta_k e^{ikx} \quad (4.17)$$

set on the d dimensional torus. We will discuss the approximation of $\mathbb{E}(|u_k(\tau, v^\eta)|^2)$ to first order. We rewrite (4.17) using Duhamel's formula:

$$u(\tau, v^\eta) = e^{i\tau\Delta} v^\eta - ie^{i\tau\Delta} \int_0^\tau e^{-i\xi\Delta} \left(\overline{u(\xi, v^\eta)} u(\xi, v^\eta)^2 \right) d\xi.$$

One obtains the following equation for the Fourier coefficient $u_k(\tau, v^\eta)$:

$$u_k(\tau, v^\eta) = e^{-i\tau k^2} \eta_k v_k - \sum_{\substack{k_1, k_2, k_3 \in \mathbf{Z}^d \\ -k_1 + k_2 + k_3 = k}} ie^{-i\tau k^2} \int_0^\tau e^{i\xi k^2} \overline{u_{k_1}(\xi, v^\eta)} u_{k_2}(\xi, v^\eta) u_{k_3}(\xi, v^\eta) d\xi, \quad (4.18)$$

where the linear operator $e^{i\tau\Delta}$ (resp. $e^{-i\tau\Delta}$) is sent to $e^{-i\tau k^2}$ (resp. $e^{i\tau k^2}$) in Fourier space. The splitting of k into k_1, k_2, k_3 comes from the fact that moving to Fourier space, products become convolution products on the frequencies. We fix $r = 0$ and iterate (4.18) by replacing $u_{k_j}(\tau, v^\eta)$ by

$$u_{k_j}(\tau, v^\eta) = e^{-i\tau k_j^2} \eta_{k_j} v_{k_j} + \mathcal{O}(\tau),$$

with $j \in \{1, 2, 3\}$. We obtain the following first order approximation of the k -th Fourier coefficient $u_k(\tau, v^\eta)$:

$$u_k(\tau, v^\eta) = e^{-i\tau k^2} \eta_k v_k - \sum_{\substack{k_1, k_2, k_3 \in \mathbf{Z}^d \\ -k_1 + k_2 + k_3 = k}} ie^{-i\tau k^2} \int_0^\tau e^{i\xi k^2} (e^{i\xi k_1^2} \eta_{k_1} v_{k_1}) (e^{-i\xi k_2^2} \eta_{k_2} v_{k_2}) (e^{-i\xi k_3^2} \eta_{k_3} v_{k_3}) d\xi + \mathcal{O}(\tau^2).$$

We encode the above Duhamel iterates using the tree series (4.10). Namely, on the continuous level, from (4.10) we have

$$\begin{aligned} u_k^0(\tau, v^\eta) &= u_{k,1}^0(\tau, v^\eta) + u_{k,2}^0(\tau, v^\eta), \\ u_{k,1}^0(\tau, v^\eta) &= \frac{\Upsilon^p(T_0)(v^\eta)}{S(T_0)} (\Pi T_0)(\tau), \\ u_{k,2}^1(\tau, v^\eta) &= \sum_{\substack{k_1, k_2, k_3 \in \mathbf{Z}^d \\ -k_1 + k_2 + k_3 = k}} \frac{\Upsilon^p(T_1)(v^\eta)}{S(T_1)} (\Pi T_1)(\tau), \end{aligned} \quad (4.19)$$

where

$$\begin{aligned} T_0 &= \text{---} \circledast \text{---}, & T_1 &= \text{---} \circledast \begin{array}{c} \circledast \\ \text{---} \circledast \end{array} \text{---}, & S(T_0) &= 1, & S(T_1) &= 2, \\ \Upsilon^p(T_0)(v^\eta) &= \eta_k v_k, & \Upsilon^p(T_1)(v^\eta) &= 2\bar{\eta}_{k_1} \bar{v}_{k_1} \eta_{k_2} v_{k_2} \eta_{k_3} v_{k_3}, \end{aligned} \quad (4.20)$$

$$(\Pi T_0)(\tau) = e^{-i\tau k^2}, \quad (\Pi T_1)(\tau) = -ie^{-i\tau k^2} \int_0^\tau e^{i\xi k^2} e^{i\xi k_1^2} e^{-i\xi k_2^2} e^{-i\xi k_3^2} d\xi.$$

For the decorated trees written above, we have used the following coding: an edge \vdash (resp. \ddagger) corresponds to a factor e^{-itk^2} (resp. e^{itk^2}), while an edge $|$ (resp. \vdash) corresponds to an integral $-i \int_0^\tau e^{i\xi k^2} \dots d\xi$ (resp. $-i \int_0^\tau e^{-i\xi k^2} \dots d\xi$). The dash dotted line introduces a minus sign. The decorations on the leaves correspond to the frequencies that add up in the internal node with a minus sign if one faces a dash edge. In T_1 , the two inner nodes are decorated by $k = -k_1 + k_2 + k_3$ where $-k_1$ comes from the edge \ddagger . The definition of the symmetry factor $S(T)$ and the coefficients $\Upsilon^p(T)$ are defined in Section (4.4). The symmetry factor corresponds to the number of internal symmetries of the tree taking the edge decorations into account but not the node decorations, which explains why $S(T_1) = 2$.

By construction, u_k^0 is a first order truncated approximation of u_k , and it follows from (4.19) that

$$\begin{aligned} \mathbb{E}(|u_k^0(\tau, v^n)|^2) &= \mathbb{E}\left((u_{k,1}^0(\tau, v^n) + u_{k,2}^1(\tau, v^n))(\overline{u_{k,1}^0(\tau, v^n) + u_{k,2}^1(\tau, v^n)})\right) \\ &= \mathbb{E}(|u_{k,1}^0(\tau, v^n)|^2) + 2\text{Re}\mathbb{E}\left(\overline{u_{k,1}^0(\tau, v^n)}u_{k,2}^1(\tau, v^n)\right) + \mathcal{O}(\tau^2). \end{aligned}$$

The main idea is then that we can express on the continuous level the above expansion using the tree series (4.14), and on the discrete level by the tree series (4.15). We show how this is done by detailing the computation of the term

$$\mathbb{E}\left(\overline{u_{k,1}^0(\tau, v^n)}u_{k,2}^1(\tau, v^n)\right).$$

It follows from (4.20) that we need to consider

$$\mathbb{E}\left(\overline{\Upsilon^p(T_0)(v^n)}\Upsilon^p(T_1)(v^n)\right) = 2\bar{v}_k\bar{v}_{k_1}v_{k_2}v_{k_3}\mathbb{E}(\bar{\eta}_k\bar{\eta}_{k_1}\eta_{k_2}\eta_{k_3}). \quad (4.21)$$

Further, we have,

$$\begin{aligned} \mathbb{E}(\bar{\eta}_k\bar{\eta}_{k_1}\eta_{k_2}\eta_{k_3}) &= \mathbb{E}(\bar{\eta}_k\bar{\eta}_{k_1})\mathbb{E}(\eta_{k_2}\eta_{k_3}) + \mathbb{E}(\bar{\eta}_k\eta_{k_2})\mathbb{E}(\bar{\eta}_{k_1}\eta_{k_3}) \\ &\quad + \mathbb{E}(\bar{\eta}_k\eta_{k_3})\mathbb{E}(\bar{\eta}_{k_1}\eta_{k_2}) \\ &= \delta_{k,\bar{k}_1}\delta_{k_2,\bar{k}_3} + \delta_{k,k_2}\delta_{k_1,k_3} + \delta_{k,k_3}\delta_{k_1,k_2} \end{aligned}$$

where we have used Wick's formula (see Proposition 4.4.1) for products of Gaussian random variables. The different $\delta_{\cdot,\cdot}$ correspond to different pairings and fix completely the frequencies on the leaves. We will introduce a new combinatorial object for describing these pairing called *decorated paired forests*. Below, we represent the various pairings coming from (4.21):

$$\begin{aligned} T_0 &= \text{tree with root } k, \\ T_{1,1} &= \text{tree with root } \bar{k}, \text{ children } \bar{k}_1, \bar{k}_1, \\ T_{1,2} &= \text{tree with root } k, \text{ children } \bar{k}_1, \bar{k}_1, \\ T_{1,3} &= \text{tree with root } \bar{k}, \text{ children } \bar{k}_1, k, \end{aligned} \quad (4.22)$$

$$F_i = T_0 \cdot T_{1,i}, \quad i \in \{1, 2, 3\}$$

where $\bar{k}_1 = -k_1$ and \cdot denotes the forest product. The F_i are decorated forests. One can observe that F_2 and F_3 are similar due to the symmetry of the decorated tree T_1 . Hence, we only need to consider one of the decorated forests during the computations, we choose to consider F_2 . Further, it follows in an analogous fashion from (4.19) and (4.20) that there is a single nontrivial pairing when computing $\mathbb{E}(|u_{k,1}^0(\tau, v^n)|^2)$, and that the decorated forest

$$F_0 = T_0 \cdot T_0$$

encodes this pairing and consequently the term $\mathbb{E}(|u_{k,1}^0(\tau, v^n)|^2)$. Therefore, the set \mathcal{G}_k^0 is defined as:

$$\mathcal{G}_k^0 = \{T_0 \cdot T_0, T_0 \cdot T_{1,1}, T_0 \cdot T_{1,2}, k_1 \in \mathbf{Z}^d\}.$$

These decorated forests encode products of iterated integrals, where each iterated integral is encoded by a decorated tree of the form (4.22). Namely, we have

$$(\bar{\Pi}T_0)(\tau) (\Pi T_{1,1})(\tau) = e^{i\tau k^2} \left(-ie^{-i\tau k^2} \int_0^\tau e^{i\xi k^2} e^{i\xi k^2} e^{-i\xi k_2^2} e^{-i\xi k_2^2} d\xi \right)$$

$$\begin{aligned}
&= -i \int_0^\tau e^{2i\xi(k^2 - k_2^2)} d\xi, \\
(\bar{\Pi}T_0)(\tau) (\Pi T_{1,2})(\tau) &= e^{i\tau k^2} \left(-ie^{-i\tau k^2} \int_0^\tau e^{i\xi k^2} e^{i\xi k_1^2} e^{-i\xi k^2} e^{-i\xi k_1^2} d\xi \right) \\
&= -i\tau.
\end{aligned}$$

One observes that for F_2 , due to cancellations in the frequencies, one can perform exact integration in time, and no approximation step is required. The term which requires to be approximated and which asks for some regularity on the initial data is the integral encoded by F_1 . We now discuss how the approximations are made, and how it leads us to the tree series (4.15).

Let us first proceed by describing the idea behind the approximation of ΠT_1 . The main idea of the general resonance based scheme introduced in [BS22] is to split the frequencies in the integrand into the dominant and lower parts:

$$\begin{aligned}
\mathcal{L} &= k^2 + k_1^2 - k_2^2 - k_3^2 = \mathcal{L}_{\text{dom}} + \mathcal{L}_{\text{low}} \\
\mathcal{L}_{\text{dom}} &= 2k_1^2, \quad \mathcal{L}_{\text{low}} = -k_1(k_2 + k_3) + k_2k_3
\end{aligned} \tag{4.23}$$

such that (cf. (4.20))

$$(\Pi T_1)(\tau) = -ie^{-i\tau k^2} \int_0^\tau e^{i\xi \mathcal{L}_{\text{dom}}} e^{i\xi \mathcal{L}_{\text{low}}} d\xi. \tag{4.24}$$

The idea of the splitting (4.23) lies in the observation that k_1^2 asks for two derivatives on the initial data while the cross-terms given in \mathcal{L}_{low} require only one. Moreover, the term $e^{i\xi \mathcal{L}_{\text{dom}}}$ can be integrated out exactly and mapped back into physical space. In order to gain regularity, we will thus only Taylor-expand the lower order part $e^{i\xi \mathcal{L}_{\text{low}}}$ in (4.24) while integrating the dominant part $e^{i\xi \mathcal{L}_{\text{dom}}}$ exactly. This provides the following discretisation:

$$\begin{aligned}
(\Pi T_1)(\tau) &= -ie^{-i\tau k^2} \int_0^\tau e^{2i\xi k_1^2} (1 + \mathcal{O}(\xi \mathcal{L}_{\text{low}})) d\xi \\
&= (\Pi^{1,0} T_1)(\tau) + \mathcal{O}(\tau^2 \mathcal{L}_{\text{low}}) \\
(\Pi^{1,0} T_1)(\tau) &= -ie^{-i\tau k^2} \int_0^\tau e^{2i\xi k_1^2} d\xi
\end{aligned}$$

where the index 0 correspond to the order of the approximation inside the time integral and the index 1 embeds that we ask a priori one derivative on the initial data. If we assume more regularity, such as for instance two derivatives, one can perform the full Taylor expansion and obtains:

$$(\Pi T_1)(\tau) = (\Pi^{2,0} T_1)(\tau) + \mathcal{O}(\tau^2 \mathcal{L}), \quad (\Pi^{2,0} T_1)(\tau) = -i\tau e^{-i\tau k^2}.$$

We would like to proceed in the same manner for the approximation of $(\Pi T_{1,1})(\tau)$. However, we have to choose the splitting as follows:

$$\mathcal{L} = 2k^2 - 2k_2^2, \quad \mathcal{L}_{\text{low}} = \mathcal{L}, \quad \mathcal{L}_{\text{dom}} = 0. \tag{4.25}$$

This is due to the fact that $\frac{1}{k^2 - k_1^2}$ cannot be mapped back into Physical space and hence, we would recover a scheme which needs to be computed fully in Fourier space and where we could not make use of the Fast Fourier Transform (FFT). This would not allow for a practical implementation of the scheme and would lead to high computational and memory costs, in particular in higher spatial dimensions $d \geq 3$. This motivates our choice of dominant and lower order parts (4.25) and leads to the discretization

$$(\Pi T_{1,1})(\tau) = (\Pi^{1,0} T_{1,1})(\tau) + \mathcal{O}(\tau^2 \mathcal{L}), \quad (\Pi^{1,0} T_{1,1})(\tau) = -i\tau e^{-i\tau k^2}. \tag{4.26}$$

The discretization (c.f. (4.15)) is then given by:

$$(\bar{\Pi}^{1,0} T_0)(\tau) (\Pi^{1,0} T_{1,j})(\tau) = -i\tau.$$

The term

$$\mathbb{E} \left(\overline{u_{k,1}^0(\tau, v^\eta)} u_{k,2}^1(\tau, v^\eta) \right)$$

is then well approximated by

$$\begin{aligned} & \frac{\tilde{\Upsilon}^p(T_0)(v^\eta)}{S(T_0)} \left(\sum_{k_1 \in \mathbf{Z}^d} \frac{\Upsilon^p(T_{1,1})(v^\eta)}{S(T_{1,1})} \mathcal{Q}_{\leq 1}(\bar{\Pi}T_0)(\tau)(\Pi T_{1,1})(\tau) \right. \\ & \quad \left. + 2 \sum_{k_1 \in \mathbf{Z}^d} \frac{\Upsilon^p(T_{1,2})(v^\eta)}{S(T_{1,2})} \mathcal{Q}_{\leq 1}(\bar{\Pi}T_0)(\tau)(\Pi T_{1,2})(\tau) \right) \\ & = -3i\tau |v_k|^2 \sum_{k_1 \in \mathbf{Z}^d} |v_{k_1}|^2 \end{aligned}$$

and introduces the following local error

$$\mathcal{O}(\tau^2 \sum_{k_1 \in \mathbf{Z}^d} (k^2 - k_1^2) |v_k|^2 |v_{k_1}|^2).$$

We notice that a term of the form $\frac{k^2 |v_k|^2}{|v_k|^2}$ corresponds (up to a sign) to the Fourier coefficient of $\nabla v * \nabla \tilde{v}$ where $*$ is the space convolution, and $\tilde{v}(x) = v(-x)$. Therefore, in contrast to [BS22], a full Taylor expansion does not ask more than one derivative in space on the initial data. In fact, $T_0 \cdot T_{1,1}$ is the term in \mathcal{G}_k^0 to compute which requires the most regularity on the initial data, namely a factor of k^2 for a first order approximation, and which corresponds in the end to only one derivative due to the previously mentioned convolution structure. In most of the examples in this paper, we end up by considering only full Taylor expansions, as is made in (4.26). This is however not always the case in a general setting. We give an example of a system of PDEs where a more careful resonance analysis (c.f. (4.23)) is needed to obtain an approximation at low regularity. Let us for instance consider the following system:

$$\begin{aligned} i\partial_t u + \Delta u &= |u|^2 u, & u(0) &= v_1, \\ \partial_t v + \partial_x^p v &= |u|^2 u, & v(0) &= v_2. \end{aligned} \tag{4.27}$$

Then depending on the value of p , we may need a resonance based approach. Iterating Duhamel's formula, we get the following oscillatory integrals:

$$I = \int_0^\tau e^{-\xi(i k)^p} e^{-i\xi k_1^2} e^{i\xi k_2^2} e^{i\xi k_3^2} d\xi, \quad k = -k_1 + k_2 + k_3.$$

If we assume that $p \geq 3$, then k^p is clearly the dominant term. Let us compare the local errors depending on the choice of approximation. Using a resonance based discretisation we obtain that

— Resonance scheme:

$$I = \int_0^\tau e^{-\xi(i k)^p} d\xi + \mathcal{O}(\xi^2 P_1), \quad P_1 = -k_1^2 + k_2^2 + k_3^2$$

whereas a classical discretisation leads to

— Classical integrators:

$$I = \xi + \mathcal{O}(\xi^2 P_2), \quad P_2 = k^p - k_1^2 + k_2^2 + k_3^2.$$

As soon as $p \geq 3$, we ask for at least three derivatives on the initial data for a classical integrator (due to the error term $\mathcal{O}(\xi^2 P_2)$) while only requiring two derivatives for the resonance based scheme (thanks to the improved local error term $\mathcal{O}(\xi^2 P_1)$).

4.1.2 Outline of the paper

Let us give a short review of the content of this paper. In Section 4.2, we introduce the combinatorial structures needed for describing oscillatory integrals coming from the iteration of the Duhamel's formula (4.9). We recall the framework introduced in [BS22] by first defining a suitable vector space of decorated trees $\hat{\mathcal{T}}$ and decorated forests $\hat{\mathcal{F}}$. Then, we consider approximated decorated trees and forest which carry an extra decoration r at the root. It corresponds to the order of the approximation of the oscillatory integrals. The main novelty in this section are paired decorated forests which are specific decorated forests with extra constraints. They reflect the computation of the second moment of oscillatory integrals: pairing among the leaves of two trees correspond to the Wick formula applied to product of Gaussian random variables.

In Section 4.3, we construct the approximation of the iterated integrals given by the character $\Pi : \hat{\mathcal{H}} \rightarrow \mathcal{C}$ (see (4.33)) through the character $\Pi^n : \mathcal{H} \rightarrow \mathcal{C}$ (see (4.34)) where n is the a priori regularity assumed on the initial data v . The approximation Π^n is given via a recursive construction involving the operator \mathcal{K} given in Definition 4.3.1. In the definition, we are performing a full Taylor expansion which can be used in the examples mentioned in this paper. It also provides the optimal regularity. In the general case, the resonance approach could be needed. The local error analysis which is the error estimate on the difference between Π and its approximation Π^n is given in Theorem 4.3.6. It is computed via a recursive definition (see Definition 4.3.5) with Taylor remainders of Π^n given in Lemma 4.3.4. Let us mention that Definition 4.3.5 is more involved as the one given in [BS22], as the pairing among the leaves required to be more precise in the estimation of the local error.

In Section 4.4, we introduce truncated series of decorated trees that solve up to order r equation (4.1). Then, we compute the second moment of this series in Proposition 4.4.2 by using Wick's formula (see Proposition 4.4.1). This is where we rely on paired decorated forests for describing the new series obtained. From this series, we built another paired decorated forests series by replacing the character Π by its approximation Π^n . Then, we can write the general scheme (4.49). In the end, we compute its local error structure (see Theorem 4.4.3) based on the local error between Π and Π^n for each paired decorated forest that appears in the expansion of the scheme.

In Section 4.5, we illustrate our general framework on two fundamental examples: the nonlinear Schrodinger (NLS) and the Korteweg–de Vries (KdV) equation.

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4.2 Decorated tree based structures for oscillatory iterated integrals

In this section, we introduce the combinatorial structure for describing oscillatory integrals that stem from Duhamel's formula (4.9). We follow the formalism of decorated trees given in [BS22] which has been used for a low regularity approximation of (4.1). In order to describe $\mathbb{E}(|u_k(t, v^n)|^2)$ we need to introduce a new structure: paired decorated forests which are decorated forests in the sense of [BS22] satisfying extra constraints on the decorations that encode some pairings. These pairings are coming from the Wick formula used for computing $\mathbb{E}(|u_k(t, v^n)|^2)$. Such paired structures have been used in wave turbulence theory in more specific set-ups (see [DH21, DH23, ACG21, ST21]).

4.2.1 Decorated trees

We recall briefly the structure of decorated trees introduced in [BS22, Sec. 2]. We assume a finite set \mathcal{L} and frequencies $k_1, \dots, k_m \in \mathbf{Z}^d$. The set \mathcal{L} parametrizes a set of differential operators with constant coefficients, whose symbols are given by the polynomials $(P_t)_{t \in \mathcal{L}}$. We define the set of decorated trees $\hat{\mathcal{T}}$ as elements of the form $T_\epsilon^{n, \sigma} = (T, n, \sigma, \epsilon)$ where

- T is a non-planar rooted tree with root ϱ_T , node set N_T and edge set E_T . We denote the leaves of T by L_T . T must also be a planted tree which means that there is only one edge connecting the root to the rest of the tree.
- the map $\epsilon : E_T \rightarrow \mathfrak{L} \times \{0, 1\}$ encodes edge decorations. The set $\{0, 1\}$ encodes the action of taking the conjugate, and determines the sign of the frequencies at the top of this edge. Namely, we have that 1 corresponds to a conjugate and to multiplying by (-1) the frequency on the node above and adjacent to this edge.
- the map $n : N_T \setminus \{\varrho_T\} \rightarrow \mathbf{N}$ encodes node decorations. For every inner node v , this map encodes a monomial of the form $\xi^{n(v)}$ where ξ is a time variable.
- the map $\sigma : N_T \setminus \{\varrho_T\} \rightarrow \mathbf{Z}^d$ also encodes node decorations. These decorations are frequencies that satisfy for every inner node u :

$$(-1)^{\mathfrak{p}(e_u)} \sigma(u) = \sum_{e=(u,v) \in E_T} (-1)^{\mathfrak{p}(e)} \sigma(v) \quad (4.28)$$

where $\mathfrak{c}(e) = (\mathfrak{t}(e), \mathfrak{p}(e))$ and e_u is the edge outgoing u of the form (v, u) . From this definition, one can see that the node decorations at the leaves $(\sigma(u))_{u \in L_T}$ determine the decoration of the inner nodes. One can call this identity Kirchoff's law. We assume that the node decorations at the leaves are linear combinations of the k_i with coefficients in $\{-1, 0, 1\}$. In applications, the leaves decoration are either k_i or $-k_i$, the term $-k_i$ is coming from a pairing with the Wick formula.

- we assume that the root of T has no decoration.

When the node decoration \mathbf{n} is zero, we will denote the decorated trees $T_{\mathbf{e}}^{\mathbf{n},\mathbf{o}}$ as $T_{\mathbf{e}}^{\mathbf{o}} = (T, \mathbf{o}, \mathbf{e})$. The set of decorated trees satisfying such a condition is denoted by $\hat{\mathcal{T}}_0$. We set \hat{H} (resp. \hat{H}_0) the (unordered) forests composed of trees in $\hat{\mathcal{T}}$ (resp. $\hat{\mathcal{T}}_0$) with linear spans $\hat{\mathcal{H}}$ and $\hat{\mathcal{H}}_0$. The forest product is denoted by \cdot , the empty forest by $\mathbf{1}$. Elements in $\hat{\mathcal{T}}$ are abstract representation of iterated time integrals and elements in \hat{H} are product of them.

We now introduce how one can represent uniquely decorated trees by using symbolic notations. We denote by \mathcal{I}_o , an edge decorated by $o = (t, \mathbf{p}) \in \mathfrak{L} \times \{0, 1\}$. We introduce the operator $\mathcal{I}_o(\lambda_k^\ell \cdot) : \hat{\mathcal{H}} \rightarrow \hat{\mathcal{H}}$ that merges all the roots of the trees composing the forest into one node decorated by $(\ell, k) \in \mathbf{N} \times \mathbf{Z}^d$. The new decorated tree is then grafted via an edge decorated by o onto a new root with no decoration. If the condition (4.28) is not satisfied on the argument then $\mathcal{I}_o(\lambda_k^\ell \cdot)$ gives zero. If $\ell = 0$, then the term λ_k^ℓ is denoted by λ_k as a short hand notation for λ_k^0 . We have chosen to put no decorations at the root in order to define the operator $\mathcal{I}_o(\lambda_k^\ell \cdot)$, that will assign the decoration k . For us, these decorated trees represent oscillatory iterated integrals and there is no need for having a decoration at the root for encoding them.

The forest product between $\mathcal{I}_{o_1}(\lambda_{k_1}^{\ell_1} F_1)$ and $\mathcal{I}_{o_2}(\lambda_{k_2}^{\ell_2} F_2)$ is given by:

$$\mathcal{I}_{o_1}(\lambda_{k_1}^{\ell_1} F_1) \mathcal{I}_{o_2}(\lambda_{k_2}^{\ell_2} F_2) := \mathcal{I}_{o_1}(\lambda_{k_1}^{\ell_1} F_1) \cdot \mathcal{I}_{o_2}(\lambda_{k_2}^{\ell_2} F_2).$$

Any decorated tree T is uniquely represented as

$$T = \mathcal{I}_o(\lambda_k^\ell F), \quad F \in \hat{H}.$$

Given an iterated integral, its size is given by the number of integrations in time. Therefore, we suppose given a subset \mathfrak{L}_+ of \mathfrak{L} that encodes edge decorations which correspond to time integrals that we have to approximate.

Example 14 We illustrate the definitions introduced above with decorated trees coming from the NLS equation. We consider the following decorated tree:

$$T = \mathcal{I}_{(t_1, 0)} \left(\lambda_k \mathcal{I}_{(t_2, 0)} \left(\lambda_k \mathcal{I}_{(t_1, 1)} \left(\lambda_{k_1} \mathcal{I}_{(t_1, 0)} \left(\lambda_{k_2} \mathcal{I}_{(t_1, 0)} \left(\lambda_{k_3} \right) \right) \right) \right) \right) = \begin{array}{c} \textcircled{k_2} \\ \vdots \\ \textcircled{k_3} \\ \vdots \\ \textcircled{k_1} \end{array},$$

where $k = -k_1 + k_2 + k_3$, $\mathfrak{L} = \{t_1, t_2\}$, $\mathfrak{L}_+ = \{t_2\}$, $P_{t_1}(\lambda) = -\lambda^2$ and $P_{t_2}(\lambda) = \lambda^2$. For the graphical notation, we put the frequencies decorations only on the leaves that determine those on the inner nodes. An edge \vdots (resp. $\ddot{\vdots}$) corresponds to a decoration $(t_1, 0)$ (resp. $(t_1, 1)$) and the operator associated is $e^{itP_{t_1}(k)} = e^{-itk^2}$ (resp. $e^{-itP_{t_1}(k)} = e^{itk^2}$), while an edge \mid (resp. $\dot{\mid}$) corresponds to a decoration $(t_2, 0)$ (resp. $(t_2, 1)$) associated to the integral $-i \int_0^\tau e^{i\xi P_{t_2}(k)} \dots d\xi = -i \int_0^\tau e^{i\xi k^2} \dots d\xi$ (resp. $-i \int_0^\tau e^{-i\xi P_{t_2}(k)} \dots d\xi = -i \int_0^\tau e^{-i\xi k^2} \dots d\xi$). Therefore, T is an abstract version of the following integral:

$$-ie^{-i\tau k^2} \int_0^\tau e^{i\xi k^2} e^{i\xi k_1^2} e^{-i\xi k_2^2} e^{-i\xi k_3^2} d\xi.$$

The next combinatorial structure, we recall from [BS22] is abstract versions of a discretization of an oscillatory integral. We denote by \mathcal{T} the set of decorated trees $T_{\mathbf{e}, r}^{\mathbf{n}, \mathbf{o}} = (T, \mathbf{n}, \mathbf{o}, \mathbf{e}, r)$ where

- $T_{\mathbf{e}, r}^{\mathbf{n}, \mathbf{o}} \in \hat{\mathcal{T}}$
- The decoration of the root is given by $r \in \mathbf{Z}$, $r \geq -1$ such that

$$r + 1 \geq \deg(T_{\mathbf{e}, r}^{\mathbf{n}, \mathbf{o}}) \tag{4.29}$$

where \deg is defined recursively by

$$\begin{aligned} \deg(\mathbf{1}) &= 0, & \deg(F_1 \cdot F_2) &= \max(\deg(F_1), \deg(F_2)), \\ \deg(\mathcal{I}_{(t, \mathbf{p})}(\lambda_k^\ell F_1)) &= \ell + \mathbf{1}_{\{t \in \mathfrak{L}_+\}} + \deg(F_1) \end{aligned}$$

where F_1, F_2 are forests composed of trees in \mathcal{T} . The quantity $\deg(T_{\mathbf{e}, r}^{\mathbf{n}, \mathbf{o}})$ is the maximum number of edges with type in \mathfrak{L}_+ , corresponding to time integrations, and of node decorations \mathbf{n} lying on the same path from one leaf to the root.

We call decorated trees in \mathcal{T} *approximated* decorated trees. We allow in the definition of the approximated decorated trees a new decoration at the root r , which corresponds to the order of the approximation. We now define the symbol $\mathcal{I}_o^r(\lambda_k^\ell \cdot) : \mathcal{H} \rightarrow \mathcal{H}$, which plays the same role as the previously defined symbol $\mathcal{I}_o(\lambda_k^\ell \cdot)$, with the added adjunction of the decoration r which constrains the time-approximations to be of order r . We now define a projection operator \mathcal{D}^r which depends on the order r of the approximation and which is used during the construction of the numerical schemes in order to only retain the terms of order at most r . We define the map $\mathcal{D}^r : \mathcal{H} \rightarrow \mathcal{H}$ which assigns to the root of a decorated tree

a decoration r and performs the projection along the identity (4.29). It is given by

$$\mathcal{D}^r(\mathbf{1}) = \mathbf{1}_{\{0 \leq r+1\}}, \quad \mathcal{D}^r\left(\mathcal{I}_o(\lambda_k^\ell F)\right) = \mathcal{I}_o^r(\lambda_k^\ell F) \quad (4.30)$$

and we extend it multiplicatively to any forest in $\hat{\mathcal{H}}$.

Example 15 We illustrate the action of the map \mathcal{D}^r on the decorated tree T introduced in Example 14. First, we notice that:

$$\deg(T) = 1, \quad \mathcal{D}^r(T) = 0, \quad r > 1.$$

Graphically, we just add r at the root:

$$\mathcal{D}^r(T) = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k_1} \cdots \textcircled{k_3} \\ | \\ \bullet \\ | \\ r \end{array} .$$

4.2.2 Paired decorated forests

Our aim is to discretise the second moment of $u_k^r(\tau, v^\eta)$ which can be expanded as a tree series. By applying the Wick product, one gets products of iterated integrals whose initial data v^η are paired. At the level of the trees, this correspond to a pairing on the leaves. Therefore, one has to introduce a more rigid structure for encoding these new terms. We define $\hat{\mathcal{G}}$ as the set of paired decorated forests F such that:

- F is a forest containing solely two trees denoted by T and \bar{T} .
- One has the following assumptions on the decoration \mathfrak{o} :

$$(-1)^{\mathfrak{p}(e_{\varrho_T})} \mathfrak{o}(u_T) = (-1)^{\mathfrak{p}(e_{\varrho_{\bar{T}}})} \mathfrak{o}(u_{\bar{T}}) \quad (4.31)$$

where u_T (resp. $u_{\bar{T}}$) are the nodes in T (resp. \bar{T}) connected to ϱ_T (resp. $\varrho_{\bar{T}}$). The decoration $\mathfrak{p}(e_{\varrho_T})$ corresponds to the second decoration component on the edge e_{ϱ_T} connecting the root ϱ_T to u_T .

- For any leaf $u \in L_F$, there exists exactly one leaf $v \in L_F$ such that

$$\begin{aligned} (-1)^{\mathfrak{p}(e_u)} \mathfrak{o}(u) &= (-1)^{\mathfrak{p}(e_v)+1} \mathfrak{o}(v), & \text{if } \{u, v\} \subset L_T \text{ or } \{u, v\} \subset L_{\bar{T}} \\ (-1)^{\mathfrak{p}(e_u)} \mathfrak{o}(u) &= (-1)^{\mathfrak{p}(e_v)} \mathfrak{o}(v), & \text{otherwise} \end{aligned} \quad (4.32)$$

where e_u (resp. e_v) is the edge connecting u (resp. v) to the rest of the tree, and $\mathfrak{p}(e) \in \{0, 1\}$ is the second component of the edge decoration associated to e .

Approximated paired decorated forests F are described by

$$F = \mathcal{D}^r(\bar{F}), \quad r \in \mathbf{Z}, \bar{F} \in \hat{\mathcal{G}}.$$

We denote this set as \mathcal{G} and by \mathcal{G}_k^r decorated paired forests having at most r edges with type in \mathfrak{L}_+ and both sides of the identity (4.31) are equal either to k or $-k$.

Example 16 We provide an example of paired decorated forests:

$$F = T_1 \cdot T_2, \quad T_1 = \begin{array}{c} \textcircled{k} \\ | \\ \bullet \\ | \\ r \end{array}, \quad T_2 = \begin{array}{c} \textcircled{k_1} \\ | \\ \textcircled{k_1} \cdots \textcircled{k} \\ | \\ \bullet \\ | \\ r \end{array}$$

Let u denote the single leaf in the tree T_1 , and let \tilde{u}, \tilde{v}, v denote the leaves, from left to right, in the tree T_2 . We have that $\mathfrak{o}(e_u) = \mathfrak{o}(e_v) = k$, and $\mathfrak{o}(e_{\tilde{u}}) = k_1 = \mathfrak{o}(e_{\tilde{v}})$. Moreover, $\mathfrak{p}(e_u) = \mathfrak{p}(e_{\tilde{u}}) = \mathfrak{p}(e_v) = 0$ and $\mathfrak{p}(e_{\tilde{u}}) = 1$ since the edge $e_{\tilde{u}}$ is a dotted brown edge, which encodes that the frequency is preceded by a negative sign. Hence, from (4.32) we read:

$$(-1)^1 k_1 = (-1)^1 k_1, \quad (-1)^0 k = (-1)^0 k.$$

For the first condition (4.31), one has $\mathfrak{p}(e_{\theta T_1}) = 0$ and $\mathfrak{p}(e_{\theta T_2}) = 0$. Therefore, one similarly obtains

$$(-1)^0 k = (-1)^0 k.$$

Remark 4.2.1 In the above definition, paired decorated forests are formed of only two trees with pairings among the leaves. The pairings among the leaves reflect the computation of the second moment of products of Gaussian random variables, dictated by Wick's theorem. One can easily generalise this definition depending on one needs. Indeed, first instead of computing second order moments, one can look at higher order moments, namely moments of order $2p$, and consider forests consisting of $2p$ trees. The pairing on the leaves between the $2p$ trees would follow the same condition (4.31). Secondly, one can consider non-Gaussian random initial conditions together with the use of cumulants to compute second moments, see Remark 4.1.2. In this case, the above definition can be replaced by pairings between bigger clusters of leaves and one has to change (4.32) accordingly, by including more than two leaves.

4.3 Discretizing oscillatory iterated integrals

In this section, we recall the definition of the map $\Pi : \hat{\mathcal{H}} \rightarrow \mathcal{C}$ that interprets decorated forests as oscillatory integrals and its low regularity discretization Π^n introduced both in [BS22]. The main simplification in comparison to the resonance method exposed is the definition of $\mathcal{K}_{o_2}^{k,r}$ which is now performing the full Taylor expansion. This is due to the convolution structures observed in the computation of $\mathbb{E}(|u_k(\tau, v^\eta)|^2)$ (see remark 4.3.2). This will be enough for the examples treated in this paper but in general a resonance analysis could be needed. The local error analysis relies on the error introduced by the operator $\mathcal{K}_{o_2}^{k,r}$ via Lemma 4.3.4. This error is propagated through a recursive definition of the error namely $\mathcal{L}_{\text{low}}^r(F, n)$. This step is more involved in comparison to [BS22]. Indeed, the error introduced by the approximation of a product of iterated integrals needs a more careful treatment, see the new formulation in Definition 4.3.5.

We adopt in this section the following notations: an element of \mathfrak{L}_+ (resp. $\mathfrak{L}_+ \times \{0, 1\}$) is denoted by \mathfrak{t}_2 (resp. o_2) and an element of $\mathfrak{L} \setminus \mathfrak{L}_+$ (resp. $\mathfrak{L} \setminus \mathfrak{L}_+ \times \{0, 1\}$) is denoted by \mathfrak{t}_1 (resp. o_1). We define \mathcal{C} as the space of functions of the form $z \mapsto \sum_j Q_j(z) e^{izP_j(k_1, \dots, k_m)}$ where the $Q_j(z)$ are polynomials in z and the P_j are polynomials in $k_1, \dots, k_n \in \mathbf{Z}^d$. The Q_j may also depend on k_1, \dots, k_m . Equipped with the pointwise product \mathcal{C} is an algebra. Iterated integrals and their discretisation will be characters from decorated forests into \mathcal{C} . For a character $g : \hat{\mathcal{H}} \rightarrow \mathcal{C}$, one has:

$$g(F \cdot \bar{F}) = g(F)g(\bar{F}), \quad F, \bar{F} \in \hat{\mathcal{H}}.$$

We define the character $\Pi : \hat{\mathcal{H}} \rightarrow \mathcal{C}$ by

$$\begin{aligned} \Pi(F \cdot \bar{F})(\tau) &= (\Pi F)(\tau)(\Pi \bar{F})(\tau), \\ \Pi\left(\mathcal{I}_{o_1}(\lambda_k^\ell F)\right)(\tau) &= e^{i\tau P_{o_1}(k)} \tau^\ell (\Pi F)(\tau), \\ \Pi\left(\mathcal{I}_{o_2}(\lambda_k^\ell F)\right)(\tau) &= -i|\nabla|^\alpha(k) \int_0^\tau e^{i\xi P_{o_2}(k)} \xi^\ell (\Pi F)(\xi) d\xi, \end{aligned} \tag{4.33}$$

where $F, \bar{F} \in \hat{\mathcal{H}}$. We have used the short hand notation P_{o_1} given for $o_1 = (\mathfrak{t}_1, \mathfrak{p}_1)$ by:

$$P_{o_1}(k) = (-1)^{\mathfrak{p}_1} P_{\mathfrak{t}_1}((-1)^{\mathfrak{p}_1} k).$$

For the discretisation, we consider a new family of characters defined now on \mathcal{H} and parametrized by $n \in \mathbf{N}$:

$$\begin{aligned} \Pi^n(F \cdot \bar{F})(\tau) &= (\Pi^n F)(\tau)(\Pi^n \bar{F})(\tau), \quad (\Pi^n \lambda^\ell)(\tau) = \tau^\ell, \\ \left(\Pi^n \mathcal{I}_{o_1}(\lambda_k^\ell F)\right)(\tau) &= \tau^\ell e^{i\tau P_{o_1}(k)} \left(\Pi^n \mathcal{D}^{r-\ell}(F)\right)(\tau), \\ \left(\Pi^n \mathcal{I}_{o_2}(\lambda_k^\ell F)\right)(\tau) &= \mathcal{K}_{o_2}^{k,r} \left(\Pi^n \left(\lambda^\ell \mathcal{D}^{r-\ell-1}(F)\right), n\right)(\tau). \end{aligned} \tag{4.34}$$

In the sequel, we will use the short hand notations:

$$\Pi^{n,r} = \Pi^n \mathcal{D}^r, \quad (\bar{\Pi} T)(\tau) = \overline{(\Pi T)(\tau)}, \quad (\bar{\Pi}^{n,r} T)(\tau) = \overline{(\Pi^{n,r} T)(\tau)}.$$

We provide the definition of the approximation operator \mathcal{K} below, when one performs the full Taylor expansion of the oscillatory integrals.

Definition 4.3.1 Assume that $G : \xi \mapsto \xi^q e^{i\xi P(k_1, \dots, k_m)}$ where P is a polynomial in the frequencies k_1, \dots, k_m and let

$o_2 = (t_2, p) \in \mathfrak{L}_+ \times \{0, 1\}$ and $r \in \mathbf{N}$. Let k be a linear map in k_1, \dots, k_m using coefficients in $\{-1, 0, 1\}$. We set

$$\mathcal{K}_{o_2}^{k,r}(G, n)(\tau) = -i|\nabla|^\alpha(k) \sum_{\ell \leq r-q} \frac{\tau^{\ell+q+1}}{\ell!(\ell+q+1)} (iP_{o_2}(k) + iP(k_1, \dots, k_m))^\ell. \quad (4.35)$$

Remark 4.3.2 The definition (4.35) for \mathcal{K} is quite simple and encodes the approximation of the oscillatory integral

$$-i|\nabla|^\alpha(k) \int_0^\tau e^{i\xi P_{o_2}(k)} G(\xi) d\xi$$

by a full Taylor expansion of the operator appearing in the integrand. This approximation does not require a careful resonance based analysis as was the case in [BS22, Def. 3.1]. This is due to the fact that we are not approximating $u_k(\tau)$ but its second moment $\mathbb{E}(|u_k(\tau, v^n)|^2)$. Therefore, our local error terms involve products of two Fourier coefficients. This allows us to repartition half of the regularity on each of the Fourier coefficients, thereby obtaining a similar low-regularity local error structure as in [BS22] without requiring a more delicate analysis. Indeed, to each of the frequencies k_1, \dots, k_m we now consider terms of the form $v_{k_i}^2$, $|v_{k_i}|$ or $\bar{v}_{k_i} v_{k_i}$, instead of v_{k_i} or \bar{v}_{k_i} . The new quadratic terms can be interpreted as convolutions or are better summable. In the case of the convolution, the two following terms ask for the same regularity:

$$k^2 v_k^2 \equiv \partial_x v * \partial_x v, \quad k v_k \equiv \partial_x v$$

where $*$ is the spatial convolution. One can see the difference between the discretization presented here and the one in [BS22] by considering the following oscillatory integral coming from NLS:

$$I = \int_0^\tau e^{-i\xi k^2} e^{-i\xi k_1^2} e^{i\xi k_2^2} e^{i\xi k_3^2} d\xi, \quad k = -k_1 + k_2 + k_3.$$

The idea of the resonance analysis is to split the integrand into the dominant and lower order parts (cf.(4.23))

$$\begin{aligned} \mathcal{L} &= k^2 + k_1^2 - k_2^2 - k_3^2 = \mathcal{L}_{\text{dom}} + \mathcal{L}_{\text{low}} \\ \mathcal{L}_{\text{dom}} &= 2k_1^2, \quad \mathcal{L}_{\text{low}} = -k_1(k_2 + k_3) + k_2 k_3 \end{aligned}$$

and to Taylor expand only the term of lower degree $e^{i\xi \mathcal{L}_{\text{low}}}$. This yields the following discretisation

$$I = \int_0^\tau e^{-2i\xi k_1^2} (1 + \mathcal{O}(\xi P_1)) d\xi, \quad P_1 = k_1(k_2 + k_3) - k_2 k_3$$

with

$$I = \int_0^\tau e^{-2i\xi k_1^2} d\xi + \mathcal{O}(\tau^2 P_1).$$

In contrast, a full classical Taylor expansion gives

$$I = \int_0^\tau e^{-2i\xi k_1^2} d\xi + \mathcal{O}(\tau^2 P_2), \quad P_2 = -2k_1^2 + k_1(k_2 + k_3) - k_2 k_3.$$

The difference between the two approximations is that the second one asks for two derivatives instead of one. In our setting, the latter is, however, absorbed by the convolution of initial data.

Remark 4.3.3 For many equations, the main difference between resonance based and classical integrators lies in the gain of one derivative (at order one). Therefore, there is no need to carry out a resonance based discretization for $\mathbb{E}(|u_k(\tau, v^n)|^2)$ due to the improved resonance structure of the latter. Resonance based schemes are, however, needed if the gap between dominant and lower parts of the resonance is bigger. Then, the full definition [BS22, Def. 3.1] is required. This can happen when one looks at systems of dispersive PDEs as for instance system (4.27).

Example 17 With the aid of (4.33), one can compute recursively the following oscillatory integrals arising in the cubic NLS equation (4.5)

$$\begin{aligned} (\Pi \begin{array}{c} \textcircled{k_2} \\ \vdots \\ \bullet \end{array}) (\tau) &= (\Pi \mathcal{I}_{(t_1, 0)}(\lambda_{k_2})) (\tau) = e^{-i\tau k_2^2}, \\ (\Pi \begin{array}{c} \textcircled{k_1} \\ \vdots \\ \bullet \end{array}) (\tau) &= (\Pi \mathcal{I}_{(t_1, 1)}(\lambda_{k_1})) (\tau) = e^{i\tau k_1^2}, \end{aligned}$$

$$\begin{aligned}
(\Pi \begin{array}{c} \textcircled{k_1} \textcircled{k_2} \textcircled{k_3} \\ \vdots \\ \bullet \end{array})(\tau) &= (\Pi \begin{array}{c} \textcircled{k_1} \\ \vdots \\ \bullet \end{array})(\tau) (\Pi \begin{array}{c} \textcircled{k_2} \\ \vdots \\ \bullet \end{array})(\tau) (\Pi \begin{array}{c} \textcircled{k_3} \\ \vdots \\ \bullet \end{array})(\tau) = e^{i\tau(k_1^2 - k_2^2 - k_3^2)}, \\
(\Pi \begin{array}{c} \textcircled{k_1} \textcircled{k_2} \textcircled{k_3} \\ \vdots \\ \bullet \end{array})(\tau) &= -i \int_0^\tau e^{is(-k_1 + k_2 + k_3)^2} e^{is(k_1^2 - k_2^2 - k_3^2)} ds.
\end{aligned}$$

For a second-order order approximation of the above integral, one has the following discretisation which in the end asks for two derivatives on the initial data,

$$(\Pi^{2,1} \begin{array}{c} \textcircled{k_1} \textcircled{k_2} \textcircled{k_3} \\ \vdots \\ \bullet \end{array})(\tau) = -i\tau + 2\tau^2(k_1^2 - k_1(k_2 + k_3) + k_2k_3).$$

We recall [BS22, Lemma 3.3] for a function G as given in Definition 4.3.1.

Lemma 4.3.4 *We keep the notations of Definition 4.3.1. We suppose that $q \leq r$ then one has*

$$-i|\nabla|^\alpha(k) \int_0^\tau \xi^q e^{i\xi(P_{o_2}(k) + P(k_1, \dots, k_m))} d\xi - \mathcal{K}_{o_2}^{k,r}(G, n)(\tau) = \mathcal{O}(\tau^{r+2} R_{o_2, n}^{k,r}(G))$$

where $R_{o_2, n}^{k,r}(G)$ depends on n , α and the frequencies k_1, \dots, k_m . When $\mathcal{K}_{o_2}^{k,r}$ performs a full Taylor expansions, it is given by

$$(P_{o_2}(k) + P(k_1, \dots, k_m))^{r+1-q} k^\alpha. \tag{4.36}$$

Otherwise, one considers the resonance analysis and decomposes $P_{o_2} + P$ into

$$P_{o_2} + P = \mathcal{L}_{dom} + \mathcal{L}_{low}$$

and one has

$$R_{o_2, n}^{k,r}(G) = k^{\bar{n}}, \quad \bar{n} = \max(n, \alpha + \deg(\mathcal{L}_{low}^{r-q+1})).$$

We define inductively the term $(\Pi \cdot)_0$ on decorated forests:

$$\begin{aligned}
\Pi(F \cdot \bar{F})_0 &= (\Pi F)_0 (\Pi \bar{F})_0, \quad \Pi(\mathcal{I}_{o_1}(\lambda_k^\ell F))_0 = (\Pi F)_0, \\
\Pi(\mathcal{I}_{o_2}(\lambda_k^\ell F))_0 &= |\nabla|^\alpha(k) (\Pi F)_0.
\end{aligned}$$

For every decorated forest, there exists c_F independent of the frequencies k_1, \dots, k_m such that:

$$|(\Pi F)(\tau)| \leq c_F \tau^{\hat{n}_+(F)} (\Pi F)_0$$

where $\hat{n}_+(F) = n_+(F) + \sum_{u \in N_F} \mathbf{n}(u)$, $n_+(F)$ gives the number of edges with decoration $o_2 = (\mathbf{t}_2, \mathbf{p}_2)$ with $\mathbf{t}_2 \in \mathfrak{L}_+$. In the sequel, we will use the following notation: $\Pi^{n,r} = \Pi^n \mathcal{D}^r$. Given a decorated forest, we set $(\Pi^{n,r} F)_\ell$ to be the term of order τ^ℓ in $(\Pi^{n,r} F)(\tau)$ in the sense that one has:

$$\mathcal{Q}_{\leq r+1}(\Pi^{n,r} F)(\tau) = \sum_{\hat{n}_+(F) \leq \ell \leq r+1} (\Pi^{n,r} F)_\ell(\tau) \tau^\ell$$

where each $(\Pi^{n,r} F)_\ell(\tau)$ is bounded, by denoting the bound by $(\Pi^{n,r} F)_\ell$, we have $\forall \tau$, $(\Pi^{n,r} F)_\ell(\tau) \leq (\Pi^{n,r} F)_\ell$.

Definition 4.3.5 Let $n \in \mathbf{N}$, $r \in \mathbf{Z}$. We recursively define $\mathcal{L}_{low}^r(\cdot, n)$ as

$$\mathcal{L}_{low}^r(F, n) = 1, \quad r < 0.$$

Else

$$\begin{aligned}
\mathcal{L}_{low}^r(\mathbf{1}, n) &= 1, \quad \mathcal{L}_{low}^r(\mathcal{I}_{o_1}(\lambda_k^\ell F), n) = \mathcal{L}_{low}^{r-\ell}(F, n) \\
\mathcal{L}_{low}^r(F_1 \cdot F_2, n) &= (\Pi F_2)_0 \mathcal{L}_{low}^{r-\hat{n}_+(F_2)}(F_1, n) \\
&\quad + \sum_{\ell \leq r+1-\hat{n}_+(F_2)} (\Pi^{n,r-\hat{n}_+(F_2)} F_1)_\ell \mathcal{L}_{low}^{r-\ell}(F_2, n)
\end{aligned}$$

$$\mathcal{L}_{\text{low}}^r(\mathcal{I}_{o_2}(\lambda_k^\ell F), n) = k^\alpha \mathcal{L}_{\text{low}}^{r-\ell-1}(F, n) + R_{o_2, n}^{k, r}(\xi^\ell(\Pi^{n, r-\ell-1} F)(\xi)).$$

Example 18 We illustrate Definition 4.3.5 on the following paired trees stemming from the NLS equation:

$$F_2 = T_1 \cdot T_2, \quad T_1 = \mathcal{I}_{o_1}(\lambda_k) = \begin{array}{c} \textcircled{k} \\ | \\ \bullet \end{array}, \quad T_2 = \begin{array}{c} \textcircled{k_2} \\ \vdots \\ \textcircled{k} \\ | \\ \bullet \end{array}, \quad (4.37)$$

where $\bar{k} = -k$. We have,

$$\mathcal{L}_{\text{low}}^0(T_1 \cdot T_2, 1) = (\Pi T_2)_0 \mathcal{L}_{\text{low}}^{-1}(T_1, 1) + (\Pi^{1, -1} T_1)_0 \mathcal{L}_{\text{low}}^0(T_2, 1), \quad (4.38)$$

where $\Pi^{1, -1} = \Pi^1 \mathcal{D}^{-1} = \Pi^1$, $(\Pi^{1, -1} T_1)_0 = e^{-i\tau k^2}$, $\mathcal{L}_{\text{low}}^{-1}(T_1, 1) = 1$ and $(\Pi T_2)_0 = 1$. Next, we have

$$\mathcal{L}_{\text{low}}^0(T_2, 1) = \mathcal{L}_{\text{low}}^0(G_2, 1) + R_{o_2, 1}^{k, 0}(\Pi^{1, -1} G_2),$$

with $T_2 = \mathcal{I}_{o_1}(\lambda_k \mathcal{I}_{o_2}(\lambda_k G_2))$, and $G_2 = \mathcal{I}_{\bar{o}_1}(\lambda_{-k}) \mathcal{I}_{o_1}(\lambda_{-k_2}) \mathcal{I}_{o_1}(\lambda_{k_2})$. A quick computation allow to check that $\mathcal{L}_{\text{low}}^0(G_2, 1)$ is bounded by

$$\mathcal{L}_{\text{low}}^0(\mathcal{I}_{\bar{o}_1}(\lambda_{-k}), 1) + \mathcal{L}_{\text{low}}^0(\mathcal{I}_{o_1}(\lambda_{-k_2}), 1) + \mathcal{L}_{\text{low}}^0(\mathcal{I}_{o_1}(\lambda_{k_2}), 1)$$

and one has:

$$\mathcal{L}_{\text{low}}^0(\mathcal{I}_{\bar{o}_1}(\lambda_{-k}), 1) = \mathcal{L}_{\text{low}}^0(\mathcal{I}_{o_1}(\lambda_{-k_2}), 1) = \mathcal{L}_{\text{low}}^0(\mathcal{I}_{o_1}(\lambda_{k_2}), 1) = \mathcal{L}_{\text{low}}^0(\mathbf{1}, 1) = 1.$$

As in [BS22, Thm. 3.17], we get the following error for our approximation under the assumption:

$$\mathcal{Q}_{\leq r+1} \Pi^{n, r} = \mathcal{Q}_{\leq r+1} \Pi^{n, r'}, \quad r \leq r'. \quad (4.39)$$

Theorem 4.3.6 For every forests F_1 and F_2 , one has,

$$(\Pi(F_1 \cdot F_2) - \mathcal{Q}_{\leq r+1} \Pi^{n, r}(F_1 \cdot F_2))(\tau) = \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(F_1 \cdot F_2, n)) \quad (4.40)$$

where Π is defined in (4.33), Π^n is given in (4.34) and $\Pi^{n, r} = \Pi^n \mathcal{D}^r$ satisfying (4.39).

Proof. The proof follows the same steps given in [BS22, Thm. 3.17]. However, one has to be more precise for dealing with products as now frequencies k_1, \dots, k_m can appear several times. We proceed with the following decomposition:

$$\begin{aligned} & \Pi(F_1 \cdot F_2)(\tau) - \mathcal{Q}_{\leq r+1} \Pi^{n, r}(F_1 \cdot F_2)(\tau) \\ &= \left(\Pi F_1 - \mathcal{Q}_{\leq r+1-\hat{n}_+(F_2)} \Pi^{n, r-\hat{n}_+(F_2)} F_1 \right)(\tau) (\Pi F_2)(\tau) \\ & \quad + \mathcal{Q}_{\leq r+1-\hat{n}_+(F_2)} \left(\Pi^{n, r-\hat{n}_+(F_2)} F_1 \right)(\tau) (\Pi F_2)(\tau) - \mathcal{Q}_{\leq r+1} \Pi^{n, r}(F_1 \cdot F_2)(\tau) \\ &= \left(\Pi F_1 - \mathcal{Q}_{\leq r+1-\hat{n}_+(F_2)} \Pi^{n, r-\hat{n}_+(F_2)} F_1 \right)(\tau) (\Pi F_2)(\tau) \\ & \quad + \sum_{\ell \leq r+1-\hat{n}_+(F_2)} \tau^\ell (\Pi^{n, r} F_1)_\ell(\tau) \left(\Pi F_2 - \mathcal{Q}_{\leq r+1-\ell} \Pi^{n, r-\ell} F_2 \right)(\tau) \end{aligned}$$

where we have used the following identities

$$\begin{aligned} \mathcal{Q}_{\leq r+1-\hat{n}_+(F_2)} \left(\Pi^{n, r-\hat{n}_+(F_2)} F_1 \right)(\tau) &= \sum_{\ell \leq r+1-\hat{n}_+(F_2)} \tau^\ell (\Pi^{n, r-\hat{n}_+(F_2)} F_1)_\ell(\tau) \\ \mathcal{Q}_{\leq r+1} (\Pi^{n, r}(F_1 \cdot F_2))(\tau) &= \sum_{\ell \leq r+1-\hat{n}_+(F_2)} \tau^\ell (\Pi^{n, r} F_1)_\ell(\tau) \mathcal{Q}_{\leq r+1-\ell} (\Pi^{n, r-\ell} F_2)(\tau) \end{aligned}$$

and the fact that by Assumption (4.39), one has:

$$(\Pi^{n, r-\hat{n}_+(F_2)} F_1)_\ell(\tau) = (\Pi^{n, r} F_1)_\ell(\tau).$$

Then, we apply recursively the bounds on F_1 and F_2 to get:

$$\begin{aligned} \left(\Pi F_1 - \mathcal{Q}_{\leq r+1-\hat{n}_+(F_2)} \Pi^{n, r-\hat{n}_+(F_2)} F_1 \right) (\tau) &= \mathcal{O} \left(\tau^{r-\hat{n}_+(F_2)+2} \mathcal{L}_{\text{low}}^{r-\hat{n}_+(F_2)} (F_1, n) \right) \\ \left(\Pi F_2 - \mathcal{Q}_{\leq r+1-\ell} \Pi^{n, r-\ell} F_2 \right) (\tau) &= \mathcal{O} \left(\tau^{r-\ell+2} \mathcal{L}_{\text{low}}^{r-\ell} (F_2, n) \right) \end{aligned}$$

which allows us to conclude. It remains to treat the case when $F = \mathcal{I}_{o_2}(\lambda_k^\ell \bar{F})$. In that case, one has:

$$\begin{aligned} (\Pi - \Pi^{n, r})(F)(\tau) &= -i|\nabla|^\alpha(k) \int_0^\tau \xi^\ell e^{i\xi P_{o_2}(k)} (\Pi - \Pi^{n, r-1-\ell})(\bar{F})(\xi) d\xi \\ &\quad - i|\nabla|^\alpha(k) \int_0^\tau \xi^\ell e^{i\xi P_{o_2}(k)} (\Pi^{n, r-1-\ell} \bar{F})(\xi) d\xi - \mathcal{K}_{o_2}^{k, r}(\xi^\ell (\Pi^{n, r-1-\ell} \bar{F})(\xi))(\tau) \\ &= \int_0^\tau \mathcal{O} \left(\xi^{r+1} k^\alpha \mathcal{L}_{\text{low}}^{r-1-\ell}(\bar{F}, n) \right) d\xi + \mathcal{O}(\tau^{r+2} R_{o_2, n}^{k, r}(\xi^\ell (\Pi^{n, r-1-\ell} \bar{F})(\xi))) \\ &= \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(F, n)). \end{aligned}$$

where the term $R_{o_2, n}^{k, r}(\xi^\ell (\Pi^{n, r-1-\ell} \bar{F})(\xi))$ is obtained by applying Lemma 4.3.4. \square

Remark 4.3.7 An immediate consequence of Theorem 4.3.6, is that for a paired decorated forest $F = T_1 \cdot T_2$, one has

$$(\bar{\Pi} T_1 \Pi T_2 - \mathcal{Q}_{\leq r+1} \bar{\Pi}^{n, r} T_1 \Pi^{n, r} T_2)(\tau) = \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n)) \quad (4.41)$$

Remark 4.3.8 Assumption 4.39 is satisfied by the examples covered in this work as we use mainly full Taylor expansions for describing the numerical scheme. In full generality, Assumption 4.39 does, however, not hold true (see also Remark 4.3.3) and one has to work with a two-parameter family in order to describe the local error. The identity (4.40) becomes:

$$(\Pi(F_1 \cdot F_2) - \mathcal{Q}_{\leq m} \Pi^{n, r}(F_1 \cdot F_2))(\tau) = \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^{r, m}(F_1 \cdot F_2, n)), \quad m \leq r+1$$

where $\mathcal{L}_{\text{low}}^{r, m}(F_1 \cdot F_2, n)$ can be defined in a recursive way as in Definition 4.3.5. The main change occurs in the approximation of a decorated tree given by Lemma 4.3.4. It is changed into

$$\begin{aligned} &-i|\nabla|^\alpha(k) \int_0^\tau \xi^\ell e^{i\xi P_{o_2}(k)} (\Pi^{n, r-1-\ell} \bar{F})(\xi) d\xi - \mathcal{Q}_{\leq m} \mathcal{K}_{o_2}^{k, r}(\xi^\ell (\Pi^{n, r-1-\ell} \bar{F})(\xi))(\tau) \\ &= \mathcal{O}(\tau^{m+1} R_{o_2, n}^{k, r, m}(\xi^\ell (\Pi^{n, r-1-\ell} \bar{F})(\xi))) \end{aligned}$$

The new quantity $R_{o_2, n}^{k, r, m}$ is the new building block for recursively defining $\mathcal{L}_{\text{low}}^{r, m}$.

4.4 Low regularity scheme

The mild solution of (4.1) is given by Duhamel's formula

$$u(\tau, v^\eta) = e^{i\tau \mathcal{L}(\nabla)} v^\eta - i|\nabla|^\alpha e^{i\tau \mathcal{L}(\nabla)} \int_0^\tau e^{-i\xi \mathcal{L}(\nabla)} p(u(\xi), \bar{u}(\xi)) d\xi. \quad (4.42)$$

In the sequel, we will focus on nonlinearities of type

$$p(u, \bar{u}) = u^N \bar{u}^M. \quad (4.43)$$

It has been proven in [BS22, Prop. 4.3] that the following tree series expansion is the k -th Fourier coefficient of a solution of (4.42) up to order $r+1$:

$$u_k^r(\tau, v^\eta) = \sum_{T \in \mathcal{T}_0^{\sigma, k}(R)} \frac{\Upsilon^p(T)(v^\eta)}{S(T)} (\Pi T)(\tau) \quad (4.44)$$

where

— For a decorated tree $T_\epsilon = (T, \epsilon)$ with only edge decorations, we define the symmetry factor $S(T_\epsilon)$ inductively by $S(\mathbf{1})=1$, while if T is of the form

$$\prod_{i, j} \mathcal{I}_{(t_i, p_i)}(T_{i, j})^{\beta_{i, j}},$$

with $T_{i,j} \neq T_{i,\ell}$ for $j \neq \ell$, then

$$S(T) := \left(\prod_{i,j} S(T_{i,j})^{\beta_{i,j}} \beta_{i,j}! \right). \quad (4.45)$$

We extend this definition to any tree $T_\epsilon^{n,\circ}$ in \mathcal{T} by setting:

$$S(T_\epsilon^{n,\circ}) := S(T_\epsilon).$$

— Then, we define the map $\Upsilon^p(T)(v)$ for

$$T = \mathcal{I}_{(t_1,a)} \left(\lambda_k \mathcal{I}_{(t_2,a)} (\lambda_k \prod_{i=1}^n \mathcal{I}_{(t_1,0)} (\lambda_{k_i} T_i) \prod_{j=1}^m \mathcal{I}_{(t_1,1)} (\lambda_{\tilde{k}_j} \tilde{T}_j)) \right), \quad a \in \{0, 1\}$$

by

$$\begin{aligned} \Upsilon^p(T)(v) &:= \partial_v^n \partial_{\bar{v}}^m p_a(v, \bar{v}) \prod_{i=1}^n \Upsilon^p(\mathcal{I}_{(t_1,0)} (\lambda_{k_i} T_i))(v) \\ &\quad \prod_{j=1}^m \Upsilon^p(\mathcal{I}_{(t_1,1)} (\lambda_{\tilde{k}_j} \tilde{T}_j))(v) \end{aligned} \quad (4.46)$$

and

$$\Upsilon^p(\mathcal{I}_{(t_1,0)} (\lambda_k))(v) := v_k, \quad \Upsilon^p(\mathcal{I}_{(t_1,1)} (\lambda_k))(v) := \bar{v}_k.$$

Above, we have used the notation:

$$p_0(v, \bar{v}) = p(v, \bar{v}), \quad p_1(v, \bar{v}) = \overline{p(v, \bar{v})}$$

In the sequel, we will use the following short hand notation:

$$\overline{\Upsilon^p(T)}(v) = \tilde{\Upsilon}^p(T)(v).$$

— We set

$$\begin{aligned} \hat{\mathcal{T}}_0(R) &= \{ \mathcal{I}_{(t_1,0)} (\lambda_k \mathcal{I}_{(t_2,0)} (\lambda_k \prod_{i=1}^N T_i \prod_{j=1}^M \tilde{T}_j)), \mathcal{I}_{(t_1,0)} (\lambda_k) \\ &\quad T_i \in \hat{\mathcal{T}}_0(R), \tilde{T}_j \in \tilde{\mathcal{T}}_0(R), k \in \mathbf{Z}^d \} \\ \tilde{\mathcal{T}}_0(R) &= \{ \mathcal{I}_{(t_1,1)} (\lambda_k \mathcal{I}_{(t_2,1)} (\lambda_k \prod_{i=1}^N T_i \prod_{j=1}^M \tilde{T}_j)), \mathcal{I}_{(t_1,1)} (\lambda_k) \\ &\quad T_i \in \tilde{\mathcal{T}}_0(R), \tilde{T}_j \in \tilde{\mathcal{T}}_0(R), k \in \mathbf{Z}^d \}. \end{aligned}$$

For a fixed $k \in \mathbf{Z}^d$, we denote the set $\hat{\mathcal{T}}_0^k(R)$ (resp. $\tilde{\mathcal{T}}_0^k(R)$) as the subset of $\hat{\mathcal{T}}_0(R)$ (resp. $\tilde{\mathcal{T}}_0(R)$) whose decorated trees have decorations on the node connected to the root given by k . For $r \in \mathbf{Z}$, $r \geq -1$, we set:

$$\hat{\mathcal{T}}_0^{r,k}(R) = \{ T_\epsilon^\circ \in \hat{\mathcal{T}}_0^k(R), n_+(T_\epsilon^\circ) \leq r + 1 \}.$$

In the previous space, we disregard iterated integrals which have more than $r + 1$ integrals and will be of order $\mathcal{O}(\tau^{r+2})$.

We denote by $\mathcal{G}_0^{r,k}(R) \subset \mathcal{G}_k^r$ the paired decorated forests $F = T_1 \cdot T_2$ such that $T_1, T_2 \in \hat{\mathcal{T}}_0^{r,k}(R)$ and $n_+(F) \leq r + 1$.

We want to compute the second moment of the truncated sum (4.44) and then provide a discretisation. Before doing so, let us recall Wick's theorem on the higher order moments of Gaussian random variables that is needed.

Proposition 4.4.1 *Let I be a finite set and $(X_i)_{i \in I}$ a collection of centred jointly Gaussian random variables. Then*

$$\mathbb{E} \left(\prod_{i \in I} X_i \right) = \sum_{P \in \mathcal{P}(I)} \prod_{\{i,j\} \in P} \mathbb{E}(X_i X_j)$$

where $\mathcal{P}(I)$ are partitions of I with two elements of I in each block of the partition.

Proposition 4.4.2 *One has:*

$$\mathcal{Q}_{\leq r+1} \mathbb{E}(|u_k^r(\tau, v^n)|^2) = \sum_{F=T_1 \cdot T_2 \in \mathcal{G}_0^{r,k}(R)} m_F \frac{\tilde{\Upsilon}^P(T_1)(v) \Upsilon^P(T_2)(v)}{S(T_1)S(T_2)} (\bar{\Pi}T_1)(\tau) (\Pi T_2)(\tau).$$

where the m_F belongs to \mathbf{N} .

Proof. We first notice that:

$$\mathbb{E}(|u_k^r(\tau, v^n)|^2) = \sum_{T_1, T_2 \in \tilde{\mathcal{T}}_0^{r,k}(R)} \mathbb{E} \left(\frac{\tilde{\Upsilon}^P(T_1)(v^n) \Upsilon^P(T_2)(v^n)}{S(T_1)S(T_2)} \right) (\bar{\Pi}T_1)(\tau) (\Pi T_2)(\tau) \quad (4.47)$$

Now, we use the fact that for each decorated tree T , one has

$$\Upsilon^P(T)(v^n) = \Upsilon^P(T)(v) \prod_{u \in L_T} \eta_{k_{\sigma(u)}}^u$$

where $\eta_{k_{\sigma(u)}}^u$ is given by

$$\eta_{k_{\sigma(u)}}^u = \overline{\eta_{k_{\sigma(u)}}}, \quad \text{if } \mathfrak{p}(e_u) = 1, \quad \eta_{k_{\sigma(u)}}^u = \eta_{k_{\sigma(u)}}, \quad \text{if } \mathfrak{p}(e_u) = 0,$$

where $\mathfrak{p}(e_u)$ is the second decoration on the edge e_u connecting the leaf u to the rest of the tree T . Then, using the Wick theorem, one gets:

$$\begin{aligned} & \mathbb{E}(\tilde{\Upsilon}^P(T_1)(v^n) \Upsilon^P(T_2)(v^n)) \\ &= \sum_{P \in \mathcal{P}(L_{T_1} \sqcup L_{T_2})} \prod_{\{u, v\} \in P} \mathbb{E}(\tilde{\eta}_{k_{\sigma(u)}}^u \tilde{\eta}_{k_{\sigma(v)}}^v) \tilde{\Upsilon}^P(T_1)(v) \Upsilon^P(T_2)(v). \end{aligned}$$

where

$$\tilde{\eta}_{k_{\sigma(v)}}^v = \begin{cases} \overline{\eta}_{k_{\sigma(v)}}^v, & \text{if } v \in L_{T_1}, \\ \eta_{k_{\sigma(v)}}^v, & \text{if } v \in L_{T_2}, \end{cases}$$

We obtain

$$\mathbb{E}(\tilde{\eta}_{k_{\sigma(u)}}^u \tilde{\eta}_{k_{\sigma(v)}}^v) = \begin{cases} \delta_{(-1)^{\mathfrak{p}(e_u)\sigma(u) + (-1)^{\mathfrak{p}(e_v)\sigma(v)}, 0}, & \text{if } \{u, v\} \subset L_{T_1} \text{ or } \{u, v\} \subset L_{T_2}, \\ \delta_{(-1)^{\mathfrak{p}(e_u)+1\sigma(u) + (-1)^{\mathfrak{p}(e_v)\sigma(v)}, 0}, & \text{otherwise.} \end{cases} \quad (4.48)$$

that fixes the condition (4.32). The map δ_{ℓ_1, ℓ_2} is given by

$$\delta_{\ell_1, \ell_2} = 1 \quad \text{if } \ell_1 + \ell_2 = 0, \text{ and } 0 \text{ otherwise.}$$

The coefficients m_F reflects the number of pairings that can give the same F which allows us to conclude. \square

From Proposition 4.4.2, our general scheme is given by:

$$\begin{aligned} V_k^{n,r}(\tau, v) &= \sum_{F=T_1 \cdot T_2 \in \mathcal{G}_0^{r,k}(R)} m_F \frac{\tilde{\Upsilon}^P(T_1)(v) \Upsilon^P(T_2)(v)}{S(T_1)S(T_2)} \\ & \mathcal{Q}_{\leq r+1}(\bar{\Pi}^{n,r}T_1 \Pi^{n,r}T_2)(\tau) \end{aligned} \quad (4.49)$$

The second moment of the k -th Fourier coefficient u_k of the solution of (4.42) is given by: $V_k = \mathbb{E}(|u_k|^2)$.

Theorem 4.4.3 (Local error) *The numerical scheme (4.49) with initial value $v = u(0)$ approximates the exact second moment $V_k(\tau, v)$ up to a local error of type*

$$V_k^{n,r}(\tau, v) - V_k(\tau, v) = \sum_{T_1 \cdot T_2 \in \mathcal{G}_0^{r,k}(R)} \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n) \tilde{\Upsilon}^P(T_1)(v) \Upsilon^P(T_2)(v))$$

$$+ \mathcal{O}\left(\tau^{r+2}|\nabla|^{\alpha(r+2)}(k) \mathbb{E}(\tilde{p}_k(u(t), v^n))\right)$$

for some polynomial \tilde{p}_k and $0 \leq t \leq \tau$ and where the operator $\mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n)$, given in Definition 4.3.5, embeds the necessary regularity of the solution.

Proof. The second moment of the k -th Fourier coefficient of the solution up to order r is given by

$$V_k^r(\tau, v) = \sum_{F=T_1 \cdot T_2 \in \mathcal{G}_0^{r,k}(R)} m_F \frac{\tilde{\Upsilon}^p(T_1)(v) \Upsilon^p(T_2)(v)}{S(T_1)S(T_2)} (\bar{\Pi} T_1 \Pi T_2)(\tau)$$

which satisfies

$$V_k(\tau, v) - V_k^r(\tau, v) = \mathcal{O}\left(\tau^{r+2}|\nabla|^{\alpha(r+2)}(k) \mathbb{E}(\tilde{p}_k(u(t), v^n))\right) \quad (4.50)$$

for some polynomial \tilde{p}_k and $0 \leq t \leq \tau$. Thanks to Theorem 4.3.6, we furthermore obtain that

$$\begin{aligned} & V_k^{n,r}(\tau, v) - V_k^r(\tau, v) \\ &= \sum_{F=T_1 \cdot T_2 \in \mathcal{G}_0^{r,k}(R)} m_F \frac{\tilde{\Upsilon}^p(T_1) \Upsilon^p(T_2)}{S(T_1)S(T_2)}(v) \\ & \quad (\bar{\Pi} T_1 \Pi T_2 - \mathcal{Q}_{\leq r+1} \bar{\Pi}^{n,r} T_1 \Pi^{n,r} T_2)(\tau) \\ &= \sum_{T_1 \cdot T_2 \in \mathcal{G}_0^{r,k}(R)} \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n) \tilde{\Upsilon}^p(T_1)(v) \Upsilon^p(T_2)(v)). \end{aligned} \quad (4.51)$$

Next we write

$$V_k^{n,r}(\tau, v) - V_k(\tau, v) = V_k^{n,r}(\tau, v) - V_k^r(\tau, v) + V_k^r(\tau, v) - V_k(\tau, v)$$

where by the definition of $\mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n)$ we easily see that the approximation error (4.51) is in general dominant compared to (4.50) (see KdV at order one for a counter-example in Section 4.5.2). \square

We note that generally the terms $\mathcal{L}_{\text{low}}^r(T_1 \cdot T_2, n)$ are the leading terms in the local error analysis.

4.5 Applications

In this section we detail our general numerical scheme (4.49) together with its error analysis (see Theorem 4.4.3) on two concrete examples: The cubic Schrödinger equation (see Section 4.5.1) and the Korteweg–de Vries equation (see Section 4.5.2).

4.5.1 Nonlinear Schrödinger

As a first example let us consider the nonlinear Schrödinger (NLS) equation

$$i\partial_t u(t, x) + \Delta u(t, x) = |u(t, x)|^2 u(t, x) \quad (t, x) \in \mathbf{R} \times \mathbf{T}^d \quad (4.52)$$

together with an initial condition of the form (4.2). The NLS equation (4.52) fits into the general form (4.1) with

$$\mathcal{L}(\nabla) = \Delta, \quad \alpha = 0, \quad \text{and} \quad p(u, \bar{u}) = |u|^2 u.$$

We set $\mathfrak{L} = \{\mathfrak{t}_1, \mathfrak{t}_2\}$, $P_{\mathfrak{t}_1} = -X^2$ and $P_{\mathfrak{t}_2} = X^2$. An edge decorated by $(\mathfrak{t}_1, 0)$ is denoted by \lfloor , while an edge decorated by $(\mathfrak{t}_1, 1)$ is denoted by $\dot{\lfloor}$. Similarly, an edge decorated by $(\mathfrak{t}_2, 0)$ is denoted by \rfloor , and by $\dot{\rfloor}$ an edge decorated by $(\mathfrak{t}_2, 1)$.

First order scheme

We start by expanding the solution as a power series expansion generated by its Duhamel's iterates (see (4.8)). For a first order approximation we have,

$$u(\tau, v^n) = u_1(\tau, v^n) + u_2(\tau, v^n) + \mathcal{O}(\tau^2), \quad (4.53)$$

where $u_m(\tau, v^\eta)$ denotes the m -th Duhamel iterate. Namely we have,

$$u_1(\tau, v^\eta) = e^{i\tau\Delta}v^\eta, \quad u_2(\tau, v^\eta) = e^{i\tau\Delta} \int_0^\tau e^{-i\zeta\Delta} (e^{i\zeta\Delta}v^\eta)^2 (e^{-i\zeta\Delta}\overline{v^\eta}) d\zeta.$$

Using (4.10) one can expand the k -th Fourier coefficient u_k of the above truncated solution (4.53), and of its conjugate, as a sum over all decorated ternary trees of size at most one. As such, using (4.14), we can express a first order truncated approximation of $\mathbb{E}(|u_k(\tau, v^\eta)|^2)$ as a sum over paired couples of decorated trees. We now explain how these pairings are made, and construct the set of paired couples \mathcal{G}_k^0 .

For a first order approximation we fix $r = 0$, and wish to construct an approximation of $\mathbb{E}(|u_k(\tau, v^\eta)|^2)$ with a local error of second order. We have

$$\begin{aligned} \mathbb{E}(|u_k(\tau, v^\eta)|^2) &= \mathbb{E}\left((u_{k,1}(\tau, v^\eta) + u_{k,2}(\tau, v^\eta)) \overline{(u_{k,1}(\tau, v^\eta) + u_{k,2}(\tau, v^\eta))} \right) \\ &\quad + \mathcal{O}(\tau^2) \\ &= \mathbb{E}(|u_{k,1}(\tau, v^\eta)|^2) + 2\text{Re} \left(\mathbb{E} \left(\overline{u_{k,1}(\tau, v^\eta)} u_{k,2}(\tau, v^\eta) \right) \right) \\ &\quad + \mathcal{O}(\tau^2). \end{aligned} \tag{4.54}$$

Each of the above terms involves expectations of products of Gaussians. Hence, their computations revolve around applications of Wick's formula, which we have encoded using a decorated tree formalism at equation (4.32). We start by dealing with the first term $\mathbb{E} \left(\overline{u_{k,1}(\tau, v^\eta)} u_{k,2}(\tau, v^\eta) \right)$. In order for this expectation not to be a trivial one we require the frequencies to be equal. Namely, the couple of paired tree stemming from this pairing is

$$F_1 = T_1 \cdot T_1, \quad T_1 = \mathcal{I}_{(t_1,0)}(\lambda_k) = \begin{array}{c} \circlearrowleft k \\ | \\ \bullet \end{array}. \tag{4.55}$$

We now deal with the computation of the second term $\mathbb{E} \left(\overline{u_{k,1}(\tau, v^\eta)} u_{k,2}(\tau, v^\eta) \right)$. In this case, there are two possible pairings of the frequencies that satisfy equation (4.32), and which yield a nontrivial computation of this second term. See the Example 4.1.1 for more details. The couple of paired trees stemming from these two pairings are:

$$F_2 = T_1 \cdot T_2, \quad T_2 = \begin{array}{c} \circlearrowleft \bar{k} \\ \vdots \\ \circlearrowleft \bar{k} \\ | \\ \bullet \end{array}, \tag{4.56}$$

where $\bar{k} = -k$ and in symbolic notation we have

$$T_2 = \mathcal{I}_{(t_1,0)}\lambda_k \left(\mathcal{I}_{(t_2,0)}(\lambda_k \mathcal{I}_{(t_1,1)}(\lambda_{-k}) \mathcal{I}_{(t_1,0)}(\lambda_{-k_2}) \mathcal{I}_{(t_1,0)}(\lambda_{k_2})) \right). \tag{4.57}$$

Finally the third pairing to consider is,

$$F_3 = T_1 \cdot T_3, \quad T_3 = \begin{array}{c} \circlearrowleft \bar{k} \\ \vdots \\ \circlearrowleft \bar{k} \\ | \\ \bullet \end{array}, \tag{4.58}$$

where in symbolic notation we have,

$$T_3 = \mathcal{I}_{(t_1,0)}\lambda_k \left(\mathcal{I}_{(t_2,0)}(\lambda_k \mathcal{I}_{(t_1,1)}(\lambda_{k_2}) \mathcal{I}_{(t_1,0)}(\lambda_{k_2}) \mathcal{I}_{(t_1,0)}(\lambda_k)) \right).$$

There is another possible pairing which is equivalent to F_3 , and is given by,

$$\tilde{F}_3 = T_1 \cdot T_3, \quad T_3 = \begin{array}{c} \textcircled{k} \\ | \\ \textcircled{k_2} \text{---} \textcircled{k_2} \\ | \\ \textcircled{} \end{array} . \quad (4.59)$$

The above pairing will yield the same quantity to approximate as the pairing of F_3 , since the resonance structure obtained through both pairings are identical: the resonance structure is zero. Hence, we only consider the paired decorated forest F_3 . We keep track of this by setting $m_{F_3} = 2$, while $m_{F_1} = 1 = m_{F_2}$. In conclusion, the set of couples of paired decorated forests is given by

$$\mathcal{G}_0^{0,k} = \{T_1 \cdot T_1, T_1 \cdot T_2, T_1 \cdot T_3\}$$

We are now ready to introduce the first order low-regularity approximation to the second order moments of $u_k(\tau, v^n)$, solution of (4.52) with initial data (4.2).

Corollary 4.5.1 *At first order our general low regularity scheme (4.15) takes the form:*

$$V_k^{1,0}(\tau, v) = v_k \overline{v_k}, \quad (4.60)$$

and is locally of order $\mathcal{O}(\tau^2 |\nabla|v)$. The above is the Fourier coefficient associated to the following scheme written in physical space:

$$u^{\ell+1} = u^\ell * \tilde{u}^\ell \quad (4.61)$$

where $\tilde{u}^\ell(x) = \overline{u^\ell(-x)}$.

Proof. We read from equation (4.15) that the first-order scheme has the general form,

$$V_k^{1,0}(\tau, v) = \sum_{F=T \cdot \tilde{T} \in \mathcal{G}_0^{0,k}(R)} m_F \frac{\tilde{\Upsilon}^P(T)(v) \Upsilon^P(\tilde{T})(v)}{S(T)S(\tilde{T})} \mathcal{Q}_{\leq 1} \left((\bar{\Pi}^{1,0} T)(\Pi^{1,0} \tilde{T}) \right)(\tau), \quad (4.62)$$

Furthermore, we have that,

$$\begin{aligned} \Upsilon^P(T_1)(v) &= v_k, & \Upsilon^P(T_2)(v) &= 2v_k v_{k_2} \overline{v_{k_2}} = \Upsilon^P(T_3)(v), \\ S(T_1) &= 1, & S(T_2) = 2 &= S(T_3). \end{aligned} \quad (4.63)$$

Hence, the first-order scheme (4.62) takes the form

$$\begin{aligned} V_k^{1,0}(\tau, v) &= v_k \overline{v_k} \mathcal{Q}_{\leq 1}(\bar{\Pi}^{1,0}(T_1))(\Pi^{1,0}(T_1)) \\ &+ 2Re \left(v_k \overline{v_k} \sum_{k_2 \in \mathbf{Z}^d} |v_{k_2}|^2 \mathcal{Q}_{\leq 1} \left(\bar{\Pi}^{1,0}(T_1)(\Pi^{1,0}(T_2) + 2\Pi^{1,0}(T_3)) \right) \right)(\tau). \end{aligned} \quad (4.64)$$

We are left to calculate the first-order approximations, encoded in the definition of the character $\Pi^{1,0}$, of each of our decorated trees appearing in the couples defined in $\mathcal{G}_0^{0,k}(R)$. From (4.55) and by Definition 4.34, given that $P_{(t_1,0)}(k) = -k^2$ and $P_{(t_1,1)}(k) = k^2$ we have,

$$(\Pi^{1,0} T_1)(\tau) = e^{i\tau P_{(t_1,0)}(k)} = e^{-i\tau k^2}, \quad (\bar{\Pi}^{1,0} T_1)(\tau) = e^{i\tau P_{(t_1,1)}(k)} = e^{i\tau k^2}. \quad (4.65)$$

Henceforth, for notational convenience we will denote $o_1 = (t_1, 0)$, $\bar{o}_1 = (t_1, 1)$, and $o_2 = (t_2, 0)$. Then again by Definition

4.34 and (4.57) it follows that,

$$\begin{aligned}
& (\Pi^{1,0}T_2)(\tau) \\
&= e^{-i\tau k^2} (\Pi^{1,0}\mathcal{I}_{o_2}(\lambda_k\mathcal{I}_{\bar{o}_1}(\lambda_{-k})\mathcal{I}_{o_1}(\lambda_{-k_2})\mathcal{I}_{o_1}(\lambda_{k_2}))) (\tau) \\
&= e^{-i\tau k^2} \mathcal{K}_{o_2}^{k,0} ((\Pi^{n,-1}\mathcal{I}_{\bar{o}_1}(\lambda_{-k}))(\xi)(\Pi^{n,-1}\mathcal{I}_{o_1}(\lambda_{-k_2}))(\xi) \\
&\quad (\Pi^{n,-1}\mathcal{I}_{o_1}(\lambda_{k_2}))(\xi)) (\tau) \\
&= e^{-i\tau k^2} \mathcal{K}_{o_2}^{k,0} (e^{i\xi(k^2-2k_2^2)}, 1) (\tau) \\
&= -i\tau e^{-i\tau k^2},
\end{aligned} \tag{4.66}$$

where we applied Definition 4.3.1 with $q = \ell = 0$, $P(k_1, \dots, k_n) = k^2 - 2k_2^2$, and $P_{o_2}(k) = k^2$. We note that the resonance structure obtain via this pairing is given by

$$P(k_1, \dots, k_n) + P_{o_2}(k) = 2(k^2 - k_2^2). \tag{4.67}$$

Similarly we have,

$$\begin{aligned}
(\Pi^{1,0}T_3)(\tau) &= e^{-i\tau k^2} (\Pi^{1,0}\mathcal{I}_{o_2}(\lambda_k\mathcal{I}_{\bar{o}_1}(\lambda_{k_2})\mathcal{I}_{o_1}(\lambda_{k_2})\mathcal{I}_{o_1}(\lambda_k))) (\tau) \\
&= e^{-i\tau k^2} \mathcal{K}_{o_2}^{k,0} (e^{i\xi(k_2^2-k_2^2-k^2)}, 1) (\tau) \\
&= -i\tau e^{-i\tau k^2},
\end{aligned} \tag{4.68}$$

where we notice that the resonance structure for the integral ΠT_3 is zero:

$$P(k_1, \dots, k_n) + P_{o_2}(k) = k^2 + (k_2^2 - k_2^2 - k^2) = 0. \tag{4.69}$$

Hence exact integration takes place, and no approximation is necessary when applying the approximation operator \mathcal{K}_{o_2} on the integral corresponding to T_3 . Collecting the above computations, and plugging it in the expansion (4.64) yields the low-regularity scheme (4.60).

Local Error: It remains to show the first order local error bound: $\mathcal{O}(\tau^2|\nabla|v)$. By Theorem 4.4.3 we have

$$V_k^{n,0}(\tau, v) - V_k(\tau, v) = \sum_{T \cdot \tilde{T} \in \mathcal{G}_0^{0,k}(R)} \mathcal{O}(\tau^2 \mathcal{L}_{\text{low}}^0(T \cdot \tilde{T}, 1) \tilde{Y}^p(T)(v) \Upsilon^p(\tilde{T})(v)).$$

We now calculate $\mathcal{L}_{\text{low}}^0(T \cdot \tilde{T}, 1)$, for every pair $T \cdot \tilde{T} \in \mathcal{G}_0^{0,k}(R)$. First, we consider the pair $F_1 = T_1 \cdot T_1$, where we have $n_+(T_1) = 0$ and hence where no time discretization is necessary. By Definition 4.3.5 of $\mathcal{L}_{\text{low}}^r$ we have,

$$\begin{aligned}
\mathcal{L}_{\text{low}}^0(T_1 \cdot T_1, 1) &= (\Pi T_1)_0 \mathcal{L}_{\text{low}}^0(T_1, 1) + (\Pi^{1,0}T_1)_0 \mathcal{L}_{\text{low}}^0(T_1, 1) \\
&\quad + (\Pi^{1,0}T_1)_1 \mathcal{L}_{\text{low}}^{-1}(T_1, 1),
\end{aligned} \tag{4.70}$$

where $\mathcal{L}_{\text{low}}^0(T_1, 1) = \mathcal{L}_{\text{low}}^{-1}(T_1, 1) = 1$. Furthermore, we have $(\Pi T_1)_0 = 1$ and $e^{-i\tau k^2} = (\Pi^{1,0}T_1)_0$, and finally $(\Pi^{1,0}T_1)_1 = 0$ since T_1 corresponds to a term of only zero-th order. Hence, from (4.70) it follows that $\mathcal{L}_{\text{low}}^0(T_1 \cdot T_1, 1) = 2e^{-i\tau k^2}$ and as seen previously $\Upsilon^p(T_1) = v_k$.

Next we consider the pair $F_2 = T_1 \cdot T_2$, where $n_+(T_2) = 1$. Again by Definition 4.3.5 of $\mathcal{L}_{\text{low}}^r$ we have,

$$\mathcal{L}_{\text{low}}^0(T_1 \cdot T_2, 1) = (\Pi T_2)_0 \mathcal{L}_{\text{low}}^{-1}(T_1, 1) + (\Pi^{1,-1}T_1)_0 \mathcal{L}_{\text{low}}^0(T_2, 1), \tag{4.71}$$

where $\Pi^{1,-1} = \Pi^1 \mathcal{D}^{-1} = \Pi^1$, $(\Pi^1 T_1)_0 = e^{-i\tau k^2}$, and $(\Pi T_2)_0 = 1$. Next, we have

$$\mathcal{L}_{\text{low}}^0(T_2, 1) = \mathcal{L}_{\text{low}}^0(G_2, 1) + R_{o_2,1}^{k,0}(\Pi^1 G_2),$$

with $T_2 = \mathcal{I}_{o_1}(\lambda_k \mathcal{I}_{o_2}(\lambda_k G_2))$, and $G_2 = \mathcal{I}_{\bar{o}_1}(\lambda_{-k}) \mathcal{I}_{o_1}(\lambda_{-k_2}) \mathcal{I}_{o_1}(\lambda_{k_2})$. Given that we are performing a full Taylor approximation (4.3.1) of ΠT_2 , we have that the local error $R_{o_2,1}^{k,0}(\Pi^1 G_2)$ is given by (4.36). Given the resonance factor (4.67) it follows that $R_{o_2,1}^{k,0}(\Pi^1 G_2) = R_{o_2,1}^{k,0}(e^{i\xi(k^2-2k_2^2)}) = 2(k^2 - k_2^2)$. Lastly, $\mathcal{L}_{\text{low}}^0(G_2, 1)$ consists of linear combinations involving the propagator $e^{\pm i\tau k^2}$, and not of a polynomial of the frequencies (k_1, \dots, k_n) . This is due to the fact that G_2 only consists of terms of zero-th order, and hence these computations are similar to those already made for $T_1 \cdot T_1$.

Therefore, $\mathcal{L}_{\text{low}}^0(T_2, 1) = \mathcal{O}(\sum_{k_2 \in \mathbf{Z}^d} (k^2 - k_2^2))$, and by (4.71),

$$\mathcal{L}_{\text{low}}^0(T_1 \cdot T_2, 1) \Upsilon^p(T_1) \Upsilon^p(T_2) = \mathcal{O}\left(\sum_{k_2 \in \mathbf{Z}^d} (k^2 - k_2^2) \overline{v_{k_2}} v_k |v_{k_2}|^2\right). \quad (4.72)$$

In physical space this yields an error of $\mathcal{O}(\tau^2 \|\nabla v * \nabla \tilde{v}\|_{L^2}^2 + (v * \tilde{v}) \|\nabla v\|_{L^2}^2)$.

Finally, the computations for the pair $F_3 = T_1 \cdot T_3$ is a simpler case of the above analysis for the pair F_2 . Indeed, with the pairing of F_3 the resonance factor (4.69) is zero and hence, no local error is induced by this term: exact integration takes place. Therefore, the local error is given by (4.84) in Fourier space, and in physical space asks for $\mathcal{O}(\tau |\nabla| v)$, namely requires only one spacial derivative on the initial data thanks to the use of convolutions. \square

Second order schemes

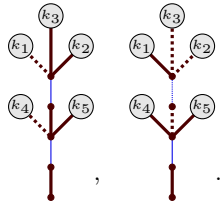
For a second order approximation we have,

$$\begin{aligned} \mathbb{E}(|u_k(\tau, v^\eta)|^2) &= \mathbb{E}\left(\overline{(u_{k,1}(\tau, v^\eta) + u_{k,2}(\tau, v^\eta) + u_{k,3}(\tau, v^\eta))}\right. \\ &\quad \left. (u_{k,1}(\tau, v^\eta) + u_{k,2}(\tau, v^\eta) + u_{k,3}(\tau, v^\eta))\right) + \mathcal{O}(\tau^3) \\ &= \mathbb{E}(|u_{k,1}(\tau, v^\eta)|^2) + 2Re\mathbb{E}\left(\overline{u_{k,1}(\tau, v^\eta)} u_{k,2}(\tau, v^\eta)\right) \\ &\quad + 2Re\mathbb{E}\left(\overline{u_{k,1}(\tau, v^\eta)} u_{k,3}(\tau, v^\eta)\right) + \mathbb{E}(|u_{k,2}(\tau, v^\eta)|^2) + \mathcal{O}(\tau^3), \end{aligned}$$

where $u_{k,3}$ is the k -th coefficient of the term :

$$\begin{aligned} u_3(\tau, v^\eta) &= - \int_0^\tau e^{i(\tau-\xi)\Delta} \left(\int_0^\xi e^{i(\xi-\xi_1)\Delta} \left((e^{i\xi_1\Delta} v^\eta)^2 (e^{-i\xi_1\Delta} \overline{v^\eta}) \right) d\xi_1 \right. \\ &\quad \left. (2(e^{i\xi\Delta} v^\eta) (e^{-i\xi\Delta} \overline{v^\eta})) \right) d\xi \\ &\quad + \int_0^\tau e^{i(\tau-\xi)\Delta} \left(\left(\int_0^\xi e^{-i(\xi-\xi_1)\Delta} (e^{-i\xi_1\Delta} \overline{v^\eta})^2 (e^{i\xi_1\Delta} v^\eta) d\xi_1 \right) (e^{i\xi\Delta} v^\eta)^2 \right) d\xi \\ &:= u_{3,1}(\tau, v^\eta) + u_{3,2}(\tau, v^\eta), \end{aligned} \quad (4.73)$$

and where $u_{3,1}(\tau, v^\eta)$ and $u_{3,2}(\tau, v^\eta)$ are encoded in Fourier by the following two decorated trees respectively:



Using Wick's formula we can once again obtain the possible pairings which come at play when wanting to compute each of the above terms. This determines the set of decorated pair of trees $\mathcal{G}_0^{1,k}(R)$, of size at most two, which we detail below.

From the previous Section 4.5.1, we have that the pair of decorated trees which encodes the first term $\mathbb{E}(|u_{k,1}(\tau, v^\eta)|^2)$ is given by $F_1 = T_1 \cdot T_1$, defined in (4.55). Similarly, we have that the second term $\mathbb{E}[\overline{u_{k,1}(\tau, v^\eta)} u_{k,2}(\tau, v^\eta)]$ is encoded by the pairings $F_2 = T_1 \cdot T_2$ and $F_3 = T_1 \cdot T_3$, defined in (4.56) and (4.58) respectively. Next, we consider the possible pairings we need to take into account for the computation of $\mathbb{E}[\overline{u_{k,1}(\tau, v^\eta)} u_{k,3}(\tau, v^\eta)]$, where u_3 is the sum of two second order terms given in (4.73). We start by considering the different pairings between the frequencies of $\overline{u_{k,1}}$ and $u_{k,3,1}$, those for $u_{k,3,2}$ will then follow. We can classify the different pairings into five groups, which we call the (five) *principal* pairings. This classification is based upon two factors:

- first, whether the frequency pairing is made internally within the same layer/integral in the tree,
- secondly, whether the pairing is made between frequencies of the same or opposite sign.

We start by looking at the pairings which consist of at least one pairing of two frequencies made internally within the same integral. There are then two possibilities to consider, which depend on the sign of the frequency pairing. Namely, we have that a pairing between two frequencies of opposite sign will result in a null resonance factor, as was the case in (4.69) for F_3 , and a pairing between two frequencies of the same sign will result in a resonance structure of the form

(4.67), namely as a difference of the squares of the frequencies. Hence, there are solely four cases of pairings which we need to consider:

- First, the case when the pairings are all of opposite signs: $\{k_1 = k_2, k_4 = k_5, k = k_3\} \cup \{k_1 = k_3, k_2 = k, k_4 = k_5\} \cup \{k_1 = k_2, k_3 = k_4, k = k_5\} \cup \{k_1 = k_3, k_2 = k_4, k = k_5\}$. Without loss of generality we take the first pairing in the union above as the representative of this class, which we include in the set $\mathcal{G}_0^{1,k}(R)$:

$$F_4 = T_1 \cdot T_4, \quad T_1 = \begin{array}{c} \circlearrowleft k \\ \downarrow \end{array}, \quad T_4 = \begin{array}{c} \circlearrowleft k_2 \\ \downarrow \text{---} \circlearrowleft k \\ \downarrow \text{---} \circlearrowleft k_4 \\ \downarrow \text{---} \circlearrowleft k_4 \\ \downarrow \text{---} \circlearrowleft k_2 \end{array}. \quad (4.74)$$

- Secondly, the case where frequencies of opposite signs are paired in the inner-integral (or tree), whereas frequencies of the same signs are paired in the outer-integral (or tree): $\{k_1 = k_2, k_3 = -k_5, k = -k_4\} \cup \{k_1 = k_3, k_2 = -k_5, k = -k_4\}$. We once again take the first pairing in the union above as the representative of this class, which we include in the set $\mathcal{G}_0^{1,k}(R)$:

$$F_5 = T_1 \cdot T_5, \quad T_1 = \begin{array}{c} \circlearrowleft k \\ \downarrow \end{array}, \quad T_5 = \begin{array}{c} \circlearrowleft k_2 \\ \downarrow \text{---} \circlearrowleft k_4 \\ \downarrow \text{---} \circlearrowleft k_4 \\ \downarrow \text{---} \circlearrowleft k_2 \end{array}.$$

- Thirdly, the case where frequencies of the same signs are paired within the inner-integral (or tree), whereas frequencies of opposite signs are paired in the outer-integral (or tree): $\{k_2 = -k_3, k = -k_1, k_4 = k_5\} \cup \{k_2 = -k_3, k_4 = -k_1, k = k_5\}$. We take the first pairing in the union above as the representative of this class:

$$F_6 = T_1 \cdot T_6, \quad T_1 = \begin{array}{c} \circlearrowleft k \\ \downarrow \end{array}, \quad T_6 = \begin{array}{c} \circlearrowleft k_2 \\ \downarrow \text{---} \circlearrowleft k_2 \\ \downarrow \text{---} \circlearrowleft k_4 \\ \downarrow \text{---} \circlearrowleft k_4 \end{array}.$$

- Fourthly, we are left with the case where the internal pairings are of the same sign. The only pairing which corresponds to this case is given by: $\{k_2 = -k_3, k_1 = k_5, k = -k_4\}$.

$$F_7 = T_1 \cdot T_7, \quad T_1 = \begin{array}{c} \circlearrowleft k \\ \downarrow \end{array}, \quad T_7 = \begin{array}{c} \circlearrowleft k_2 \\ \downarrow \text{---} \circlearrowleft k_5 \\ \downarrow \text{---} \circlearrowleft k_5 \\ \downarrow \text{---} \circlearrowleft k_2 \end{array}.$$

Lastly, going back to point (a.) in the above we are left to consider pairings which are all external, meaning that there are no pairings of two frequencies made internally within the same integral. Hence, no simplification will be made at the level of the resonance structure of each of the integrals. This defines the last class to be considered. There are six possibilities of such pairings: $\{k = -k_1, k_2 = k_4, k_3 = -k_5\} \cup \{k = -k_1, k_2 = -k_5, k_3 = k_4\} \cup \{k = k_2, k_1 = -k_4, k_3 = -k_5\} \cup \{k = k_2, k_1 = k_5, k_3 = k_4\} \cup \{k = k_3, k_2 = -k_5, k_1 = -k_4\} \cup \{k = k_3, k_2 = k_4, k_1 = k_5\}$. We take the first pairing

in the union above as the representative of this class:

$$F_8 = T_1 \cdot T_8, \quad T_1 = \begin{array}{c} \textcircled{k} \\ | \\ \bullet \end{array}, \quad T_8 = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k} \text{---} \textcircled{k_4} \\ | \\ \textcircled{k_2} \text{---} \textcircled{k_4} \\ | \\ \bullet \end{array}.$$

Analogously, one can make the analysis for the pairings of $\overline{u_{k,1}}$ and $u_{k,3,2}$ to obtain that five representatives are given by: $F_i = T_1 \cdot T_i$, for $i \in \{9, \dots, 13\}$, where

$$\begin{array}{ccc} T_9 = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k_2} \text{---} \textcircled{k_4} \\ | \\ \textcircled{k} \text{---} \textcircled{k_4} \\ | \\ \bullet \end{array}, & T_{10} = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k_2} \text{---} \textcircled{k} \\ | \\ \textcircled{k_4} \text{---} \textcircled{k_4} \\ | \\ \bullet \end{array}, & T_{11} = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k_4} \text{---} \textcircled{k_2} \\ | \\ \textcircled{k_4} \text{---} \textcircled{k} \\ | \\ \bullet \end{array}, \\ \\ T_{12} = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k} \text{---} \textcircled{k_2} \\ | \\ \textcircled{k_4} \text{---} \textcircled{k_4} \\ | \\ \bullet \end{array}, & T_{13} = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k} \text{---} \textcircled{k_4} \\ | \\ \textcircled{k_2} \text{---} \textcircled{k_4} \\ | \\ \bullet \end{array}. \end{array}$$

Finally, also using the same case analysis as made previously, we can construct the possible pairings between $\overline{u_{k,1}}$ and $u_{k,1}$ in order to compute the last term $\mathbb{E}(|u_{k,1}(\tau, v^\eta)|^2)$. We have the same case figures as seen previously: six possible external pairings, four different possible pairings which are internal and of opposite signs, by symmetry four possibilities of pairings which are internal and one of opposite and the other of the same signs, and finally one possible internal pairing of the same signs. A representative of each of the above four class is given by: $F_i = \tilde{T}_i \cdot T_i$, for $i \in \{14, \dots, 17\}$, where

$$\begin{array}{cccc} \tilde{T}_{14} = \begin{array}{c} \textcircled{k_1} \\ | \\ \textcircled{k_1} \text{---} \textcircled{k} \\ | \\ \bullet \end{array}, & T_{14} = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k_2} \text{---} \textcircled{k} \\ | \\ \bullet \end{array} = T_3, & \tilde{T}_{15} = \begin{array}{c} \textcircled{k_1} \\ | \\ \textcircled{k_1} \text{---} \textcircled{k} \\ | \\ \bullet \end{array}, & T_{15} = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k} \text{---} \textcircled{k_2} \\ | \\ \bullet \end{array} = T_2, \\ \\ \tilde{T}_{16} = \begin{array}{c} \textcircled{k_1} \\ | \\ \textcircled{k} \text{---} \textcircled{k_1} \\ | \\ \bullet \end{array}, & T_{16} = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k} \text{---} \textcircled{k_2} \\ | \\ \bullet \end{array} = T_{15}, & \tilde{T}_{17} = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k_1} \text{---} \textcircled{k_3} \\ | \\ \bullet \end{array} = T_{17}. \end{array}$$

We denote by m_{F_i} , $i \in [4, 17]$ the multiplicative constant representing the number of elements in the class whose representative is F_i . Namely, it follows from the above analysis that

$$\begin{aligned} m_{F_i} &= 6, \text{ for } i \in \{8, 13, 17\}, \\ m_{F_i} &= 2, \text{ for } i \in \{5, 10, 6, 11\}, \\ m_{F_i} &= 1, \text{ for } i \in \{7, 12, 16\}, \\ m_{F_i} &= 4, \text{ for } i \in \{4, 9, 14, 15\}. \end{aligned} \tag{4.75}$$

In conclusion, we have that the set of representatives of approximated paired forests is given by: $\mathcal{G}_0^{1,k}(R) = \{F_i\}_{i=\{1, \dots, 17\}}$. We now present a second order low-regularity approximation to the second order moments of $u_k(\tau, v^\eta)$, solution of (4.52) with initial data (4.2).

Corollary 4.5.2 *At second order our general low regularity scheme (4.15) takes the form:*

$$\begin{aligned} V_k^{2,1}(\tau, v) &= v_k \overline{v_k} + 2\tau^2 v_k \overline{v_k} \left(|k|^2 \sum_{k_2 \in \mathbf{Z}^d} |v_{k_2}|^2 - \sum_{k_2 \in \mathbf{Z}^d} |k_2|^2 |v_{k_2}|^2 \right) \\ &\quad - 6\tau^2 \left(6v_k \overline{v_k} \left(\sum_{k_2 \in \mathbf{Z}^d} |v_{k_2}|^2 \right)^2 - \sum_{\substack{k_1, k_2, k_3 \in \mathbf{Z}^d \\ -k_1 + k_2 + k_3 = k}} |v_{k_1}|^2 |v_{k_2}|^2 |v_{k_3}|^2 \right). \end{aligned} \quad (4.76)$$

The scheme (4.76) is locally of order $\mathcal{O}(\tau^3 |\nabla|^2 v)$. The above is the Fourier coefficient associated to the following scheme written in physical space:

$$\begin{aligned} u^{\ell+1} &= u^\ell * \tilde{u}^\ell + 2\tau^2 \left((\nabla u^\ell * \nabla \tilde{u}^\ell) \|u^\ell\|_{L^2}^2 \right. \\ &\quad \left. - (u^\ell * \tilde{u}^\ell) \|\nabla u^\ell\|_{L^2}^2 \right) - 6\tau^2 \left(6(u^\ell * \tilde{u}^\ell) \|u^\ell\|_{L^2}^4 - (u^\ell * \tilde{u}^\ell)^3 \right), \end{aligned} \quad (4.77)$$

where $\tilde{u}^\ell(x) = \overline{u^\ell(-x)}$.

Remark 4.5.3 (Stabilisation technique) We note that in contrast to the first-order scheme (4.61) the second-order scheme (4.77) involves spatial derivatives on the numerical solution such as for instance in the term $\nabla u^\ell * \nabla \tilde{u}^\ell$. These derivatives cause instability in the discretisation. For practical implementations, one needs to stabilize the scheme in order for it to converge. Different approaches can be taken to stabilize the above scheme, which do not require a Courant-Friedrichs-Lewy (CFL) type condition on the step sizes. Here we propose an approach based on the a posteriori inclusion of well chosen filter functions. We refer to the works of [ABBS22b, AB23a] for more details regarding these questions of stability and of the suitable choice of filter functions used to yield stable schemes with optimal local error. We also refer to [HLW10] for a general introduction to filter function in the case of oscillatory ordinary differential equations.

In this work we introduce the following filter function

$$\text{sinc}^2\left(\tau^{\frac{1}{2}} |\nabla|\right)$$

which in Fourier space takes the form,

$$\Psi(i\tau |k|^2) = \text{sinc}^2\left(\tau^{\frac{1}{2}} |k|\right) = \frac{1}{(i\tau^{\frac{1}{2}} |k|)^2} \left(e^{i\tau^{\frac{1}{2}} |k|/2} - e^{-i\tau^{\frac{1}{2}} |k|/2} \right)^2. \quad (4.78)$$

In order to stabilise our scheme (4.77) we pre-multiply both critical terms in the second line of (4.60) with the filter function (4.78) in the corresponding frequencies k and k_2 respectively. This yields the following stabilised version of (4.76)

$$\begin{aligned} V_k^{2,1}(\tau, v) &= v_k \overline{v_k} \\ &\quad + 2\tau^2 v_k \overline{v_k} \left(\Psi(i\tau |k|^2) |k|^2 \sum_{k_2 \in \mathbf{Z}^d} |v_{k_2}|^2 - \sum_{k_2 \in \mathbf{Z}^d} \Psi(i\tau |k_2|^2) |k_2|^2 |v_{k_2}|^2 \right) + \dots \end{aligned} \quad (4.79)$$

We have that

$$\Psi(i\tau |k|^2) = 1 + \mathcal{O}(\tau |k|^2)$$

and hence the stabilised scheme (4.79) preserves the low regularity error structure of $\mathcal{O}(\tau |\nabla|^2 u)$. This is essential for the local error analysis of the scheme. Furthermore, thanks to the observation that

$$|\Psi(i\tau |k|^2) \tau |k|^2| \leq 1 \quad \text{for all } k \in \mathbf{Z}^d$$

Ψ renders a stabilised version of the scheme (4.77) in physical space given by:

$$\begin{aligned} u^{\ell+1} &= u^\ell * \tilde{u}^\ell \\ &\quad - 2\tau \left((e^{i\tau^{\frac{1}{2}} |\nabla|/2} - e^{-i\tau^{\frac{1}{2}} |\nabla|/2}) u^\ell * (e^{i\tau^{\frac{1}{2}} |\nabla|/2} - e^{-i\tau^{\frac{1}{2}} |\nabla|/2}) \tilde{u}^\ell \right) \|u^\ell\|_{L^2}^2 \\ &\quad - (u^\ell * \tilde{u}^\ell) \left((e^{i\tau^{\frac{1}{2}} |\nabla|/2} - e^{-i\tau^{\frac{1}{2}} |\nabla|/2}) u^\ell \right) \|u^\ell\|_{L^2}^2 \\ &\quad - 6\tau^2 \left(6(u^\ell * \tilde{u}^\ell) \|u^\ell\|_{L^2}^4 - (u^\ell * \tilde{u}^\ell)^3 \right). \end{aligned}$$

Remark 4.5.4 (Practical implementation) In order to allow for a practical implementation of our schemes we want to be able to express the discretization both in physical and Fourier space. This allows us to use the Fast Fourier Transform (FFT) whose computational cost is of order $O(|K|^d \log(|K|^d))$, where K denotes the highest frequency in the discretization and d is the dimension. Namely, we compute the action of the filter functions on the solution in frequency space, while computing the product of functions in physical space.

Remark 4.5.5 In (4.77), the scheme $V_k^{n,r}$ is written in physical space. In fact, one can wonder if it is possible to get a general statement such as [BS22, Prop. 3.18] which shows that low regularity schemes can always be rewritten in physical space. It is not clear how to prove such a statement in full generality when exact integrations are performed instead of a full Taylor expansion. Indeed, the core of the proof [BS22, Prop. 3.18] relies on [BS22, Assumption 1] which is no longer true in our case: Frequencies on the leaves are no longer disjoint. We will have to be more cautious in the scheme and probably Taylor expand a bit more as exact integrations will not allow to move back to physical space. It is a challenging open question. In the case of the present work, we are mostly doing Taylor expansions. They guarantee that we are able to go back to physical space.

Proof. We are considering a second order scheme and hence, we enter the case where $r = 1$. Furthermore, we ask for two derivatives on the initial data, and hence we take the regularity parameter n to take on the value of 2. We read from equation (4.15) that the second-order scheme has the general form,

$$V_k^{2,1}(\tau, v) = \sum_{F=T_1, T_2 \in \mathcal{G}_0^{1,k}(R)} m_F \frac{\tilde{\Upsilon}^p(T_1)(v) \Upsilon^p(T_2)(v)}{S(T)S(T_2)} \mathcal{Q}_{\leq 2}((\bar{\Pi}^{2,1}(T_1))(\Pi^{2,1}(T_2)))(\tau), \quad (4.80)$$

where $\{m_F\}_{F \in \mathcal{G}_0^{1,k}(R)}$ are given in (4.75), and where in the same spirit of (4.63) we have that for all $i \in \{4, \dots, 13\}$,

$$\begin{aligned} \Upsilon^p(T_4)(v) &= 2\Upsilon^p(\mathcal{I}_{(t_1,1)}(\lambda_{k_4}))(v) \Upsilon^p(T_3)(v) \Upsilon^p(\mathcal{I}_{(t_1,0)}(\lambda_{k_4}))(v) \\ &= 2\overline{v_{k_4}}(2\overline{v_{k_2}}v_{k_2}v_k)v_{k_4} \\ &= 4|v_{k_4}|^2|v_{k_2}|^2v_k \\ &= \Upsilon^p(T_i)(v), \end{aligned}$$

and for $i \in \{4, \dots, 8\}$, $S(T_i) = 2$ while for $i \in \{9, \dots, 13\}$, $S(T_i) = 4$. Furthermore, we have that for $i \in \{14, \dots, 17\}$,

$$\tilde{\Upsilon}^p(\tilde{T}_i)(v) \Upsilon^p(T_i)(v) = 4|v_{k_1}|^2|v_{k_2}|^2|v_{k_3}|^2, \quad S(T_i)^2 = 4.$$

Hence, the second order scheme (4.80) takes the form

$$\begin{aligned} V_k^{2,1}(\tau, v) &= v_k \overline{v_k} \\ &+ 2Re \left(v_k \overline{v_k} \sum_{k_2 \in \mathbf{Z}^d} |v_{k_2}|^2 \mathcal{Q}_{\leq 2} \left(\bar{\Pi}^{2,1}(T_1) (\Pi^{2,1}(T_2) + 2\Pi^{2,1}(T_3)) \right) (\tau) \right) \\ &+ 2Re \left(v_k \overline{v_k} \sum_{k_2, k_4 \in \mathbf{Z}^d} |v_{k_2}|^2 |v_{k_4}|^2 \right. \\ &\quad \left. \left(\sum_{4 \leq i \leq 13} m_{F_i} \mathcal{Q}_{\leq 2} (\bar{\Pi}^{2,1}(T_1) \Pi^{2,1}(T_i)) \right) (\tau) \right) \\ &+ v_k \overline{v_k} \sum_{k_1, k_2 \in \mathbf{Z}^d} |v_{k_1}|^2 |v_{k_2}|^2 \left(\sum_{14 \leq i \leq 16} m_{F_i} \mathcal{Q}_{\leq 2} (\bar{\Pi}^{2,1}(\tilde{T}_i) \Pi^{2,1}(T_i)) \right) (\tau) \\ &+ \sum_{\substack{k_1, k_2, k_3 \in \mathbf{Z}^d \\ -k_1 + k_2 + k_3 = k}} |v_{k_1}|^2 |v_{k_2}|^2 |v_{k_3}|^2 \left(m_{F_{17}} \mathcal{Q}_{\leq 2} (\bar{\Pi}^{2,1}(T_{17}) \Pi^{2,1}(T_{17})) \right) (\tau). \end{aligned} \quad (4.81)$$

1. Computation of $\mathcal{Q}_{\leq 2}(\bar{\Pi}^{2,1}(T_1)(\Pi^{2,1}(T_2) + 2\Pi^{2,1}(T_3))$): We apply Definition 4.34 to each of the three decorated trees.

— Computation of $\bar{\Pi}^{2,1}(T_1)$: Given that (4.55) is a zero-th order term, as in (4.65) we have,

$$(\bar{\Pi}^{2,1}T_1)(\tau) = e^{i\tau k^2}.$$

— Computation of $\Pi^{2,1}(T_2)$: It follows from the definition (4.56) and (4.57) of T_2 that,

$$\begin{aligned} (\Pi^{2,1}T_2)(\tau) &= e^{-i\tau k^2} \mathcal{K}_{o_2}^{k,1}((\Pi^{2,0}\mathcal{I}_{\bar{o}_1}(\lambda_{-k}))(\xi)) \\ &= e^{-i\tau k^2} \mathcal{K}_{o_2}^{k,1}(e^{i\xi(k^2-2k_2^2)}, 2)(\tau) \\ &= -i\tau e^{-i\tau k^2} + \tau^2 e^{-i\tau k^2} (k^2 - k_2^2), \end{aligned} \tag{4.82}$$

where we applied Definition 4.3.1 with $\ell = 1$. Namely, up to one additional order then made in (4.66) for the first order analysis.

— Computation of $\Pi^{2,1}(T_3)$: As for the calculations made in (4.68), given that the resonance structure (4.69) of the integrand in $\Pi(T_3)$ is zero it follows that,

$$(\Pi^{2,1}T_3)(\tau) = -i\tau e^{-i\tau k^2}. \tag{4.83}$$

Hence, having only at most second order terms in the above calculations, $\mathcal{Q}_{\leq 2}$ does not play a role and we have:

$$\begin{aligned} \mathcal{Q}_{\leq 2}(\bar{\Pi}^{2,1}(T_1)(\Pi^{2,1}(T_2) + 2\Pi^{2,1}(T_3)))(\tau) &= \bar{\Pi}^{2,1}(T_1)(\Pi^{2,1}(T_2) + 2\Pi^{2,1}(T_3))(\tau) \\ &= -3i\tau + \tau^2(k^2 - k_2^2). \end{aligned}$$

Given that we take the real part of the above approximation, only the second term in the above will contribute to the scheme.

2. Computation of $\mathcal{Q}_{\leq 2}(\bar{\Pi}^{2,1}(T_1)\Pi^{2,1}(T_i))$, for $i \in \{4, \dots, 13\}$:

— Computation of $(\bar{\Pi}^{2,1}(T_1)\Pi^{2,1}(T_4))$: We recall that T_4 is given by (4.74) and in symbolic notation we have,

$$T_4 = \mathcal{I}_{o_1} \left(\lambda_k \left(\mathcal{I}_{o_2} \left(\lambda_k \left(\mathcal{I}_{\bar{o}_1} \left(\lambda_{k_4} T_3 \mathcal{I}_{o_1} \left(\lambda_{k_4} \right) \right) \right) \right) \right) \right),$$

where T_3 is given in (4.58). Hence, it follows that

$$\begin{aligned} (\Pi^{2,1}T_4)(\tau) &= e^{-i\tau k^2} \mathcal{K}_{o_2}^{k,1}((\Pi^{2,0}\mathcal{I}_{\bar{o}_1}(\lambda_{k_4}))(\xi)(\Pi^{2,0}T_3)(\xi)(\Pi^{2,0}\mathcal{I}_{o_1}(\lambda_{k_4}))(\xi))(\tau) \\ &= e^{-i\tau k^2} \mathcal{K}_{o_2}^{k,1} \left(-i\xi e^{i\xi(k_4^2 - k^2 - k_4^2)} \right) (\tau) \\ &= -ie^{-i\tau k^2} \mathcal{K}_{o_2}^{k,1}(\xi e^{-i\xi k^2}, 2)(\tau) \\ &= -\frac{\tau^2}{2} e^{-i\tau k^2}, \end{aligned}$$

where in the second line we used that $(\Pi^{2,0}T_3)(\xi) = -i\xi e^{-i\xi k^2}$, which comes from (4.68), obtained during the first order analysis. We note that when calculating \mathcal{K} in the last line, the resonance structure is as expected equal to zero.

— Computation of $\Pi^{2,1}(T_i)$, for $i \in \{5, \dots, 13\}$: These computations follow exactly the same line as in the above case. We have, $(\Pi^{2,1}T_i)(\tau) = -\frac{\tau^2}{2} e^{-i\tau k^2}$.

The only difference lies in the expression of the resonance factor which will either be of the form (4.67), be equal to zero (as was the case in the above), or finally in the case of an external pairing $(\Pi(T_i), i \in \{8, 13\})$ of the form (4.23). Nevertheless, given that we can make the full Taylor approximation (4.3.1) when approximating the each integral, the approximation of $\Pi^{2,1}(T_i), i \in \{4, \dots, 13\}$ are the same, the difference lies in the local error produced.

Therefore, $\mathcal{Q}_{\leq 2}(\bar{\Pi}^{2,1}(T_1)\Pi^{2,1}(T_i))(\tau) = -\frac{\tau^2}{2}$.

3. Computation of $\mathcal{Q}_{\leq 2}(\bar{\Pi}^{2,1}(T_i)\Pi^{2,1}(T_i))(\tau)$, for $i \in \{14, \dots, 17\}$:

— Computation of $\bar{\Pi}^{2,1}(T_{14})\Pi^{2,1}(T_{14})$. Given that T_{14} has the same null resonance structure as T_3 , it follows as in (4.83) that $(\Pi^{2,1}T_{14})(\tau) = -i\tau e^{-i\tau k^2}$ and hence,

$$(\bar{\Pi}^{2,1}T_{14}\Pi^{2,1}T_{14})(\tau) = \tau^2.$$

For the remaining computations the truncation operator $\mathcal{Q}_{\leq 2}$ will be essential to incorporate the terms of correct order into the scheme.

- Computation of $\mathcal{Q}_{r \leq 2} \bar{\Pi}^{2,1}(\tilde{T}_{15}) \Pi^{2,1}(T_{15})$, $\mathcal{Q}_{r \leq 2} \bar{\Pi}^{2,1}(\tilde{T}_{16}) \Pi^{2,1}(T_{16})$, and $\mathcal{Q}_{r \leq 2} \bar{\Pi}^{2,1}(\tilde{T}_{17}) \Pi^{2,1}(T_{17})$. First, we have that $\Pi(T_{15})$ and $\Pi(T_{16})$ have the same resonance structure as ΠT_2 , and hence following the calculations in (4.82) it follows that,

$$(\Pi T_{15})(\tau) = (\Pi T_{16})(\tau) = -i\tau e^{-i\tau k^2} + \tau^2 e^{-i\tau k^2} (k^2 - k_2^2).$$

Furthermore, we have that $\bar{\Pi}(\tilde{T}_{15})$ has a null resonance structure and hence it follows that $(\bar{\Pi} \tilde{T}_{15})(\tau) = i\tau e^{i\tau k^2}$ and,

$$\begin{aligned} \mathcal{Q}_{r \leq 2}(\bar{\Pi}^{2,1} \tilde{T}_{15} \Pi^{2,1} T_{15})(\tau) &= \mathcal{Q}_{r \leq 2}(\tau^2 + i\tau^3(k^2 - k_2^2)) \\ &= \tau^2. \end{aligned}$$

Similarly, we have

$$\mathcal{Q}_{r \leq 2}(\bar{\Pi}^{2,1} \tilde{T}_{16} \Pi^{2,1} T_{16})(\tau) = \tau^2 = \mathcal{Q}_{r \leq 2}(\bar{\Pi}^{2,1} \tilde{T}_{17} \Pi^{2,1} T_{17})(\tau),$$

where the third and fourth order terms are truncated by the operator $\mathcal{Q}_{\leq 2}$.

Plugging the results obtained in the above computations into (4.81) yields the second order low regularity scheme (4.76), which is given in physical space by (4.77).

Local Error: It remains to show the claimed third order local error bound: $\mathcal{O}(\tau^3 |\nabla|^2 v)$. We follow along the same lines made for the first order local error analysis in Section 4.5.1. By Theorem 4.4.3 we have

$$V_k^{2,1}(\tau, v) - V_k(\tau, v) = \sum_{T_1 \cdot T_2 \in \mathcal{G}_0^{1,k}(R)} \mathcal{O}(\tau^3 \mathcal{L}_{\text{low}}^1(T_1 \cdot T_2, 2) \tilde{\Upsilon}^p(T_1)(v) \Upsilon^p(T_2)(v)).$$

We are left to calculate $\mathcal{L}_{\text{low}}^1(T_1 \cdot T_2, 2)$, for $T_1 \cdot T_2 \in \mathcal{G}_0^{1,k}(R)$. We are interested in the integrals ΠT , $\Pi \tilde{T}$ which have non-zero resonance structure, since oscillatory integrals whose resonance structure is zero are integrated exactly, and hence do not contribute to the local error analysis of the scheme.

- Computation of $\mathcal{L}_{\text{low}}^1(T_1 \cdot T_2, 2)$, where ΠT_2 has the non-zero resonance structure (4.67). Following the analysis made in (4.71) for this pairing we have,

$$R_{o_2,1}^{k,1}(\Pi^{n=2} G_2) = R_{o_2,2}^{k,1}(e^{i\xi(k^2 - 2k_1^2)}) = (2(k^2 - k_1^2))^2,$$

where we applied definition (4.36) up to an additional order. Therefore, it follows from the previously made steps (4.71) that

$$\mathcal{L}_{\text{low}}^1(T_1 \cdot T_2, 2) \tilde{\Upsilon}^p(T_1) \Upsilon^p(T_2) = \mathcal{O}\left(\sum_{k_1 \in \mathbf{Z}^d} (k^2 - k_1^2)^2 \overline{v_k} v_{k_1} |v_{k_1}|^2\right). \quad (4.84)$$

In physical space this yields an error of the form

$$\begin{aligned} &\mathcal{O}\left(\tau^3 \left(\|\nabla|^2 v * |\nabla|^2 \tilde{v}\| \|v\|_{L^2}^2 + \right. \right. \\ &\quad \left. \left. (v * \tilde{v}) \|\nabla|^2 v\|_{L^2}^2 + \|\nabla|v * |\nabla|\tilde{v}\| \|\nabla|v\|_{L^2}^2 \right) \right). \end{aligned} \quad (4.85)$$

The computations for the remaining pairings $F \in \mathcal{G}_0^{1,k}(R)$ can be made in an analogous fashion and can be shown to produce an error term of the form $\mathcal{O}(\tau^3 |\nabla|v)$. In consequence, their approximation requires less regularity on the initial data than that for the above pairing $T_1 \cdot T_2$. We conclude from the above expression (4.85) that the local error in physical space is of the form $\mathcal{O}(\tau^3 |\nabla|^2 v)$, which requires two derivatives on the initial data. \square

Remark 4.5.6 Recently new low-regularity integrators ([AB23b]) and resonance-based discretisations ([FMS23, MS23]) have been introduced, which preserve better the underlying structure of the solution over long-times, and which exhibits improved error constants at low-regularity. Encapsulating the idea behind the construction of these low-regularity structure-preserving schemes into the general framework presented in this article would be of interest in the future. This could yield better insight on the long-time behaviour of the solution on a numerical level.

4.5.2 KdV

Let us next consider the Korteweg–de Vries (KdV) equation

$$\partial_t u + \partial_x^3 u = \frac{1}{2} \partial_x u^2, \quad (t, x) \in \mathbf{R} \times \mathbf{T} \quad (4.86)$$

with a random initial value $u(0) = v$ of the form (4.2). The KdV equation (4.86) fits into the general framework (4.1) with

$$\mathcal{L}(\nabla) = i\partial_x^3, \quad \alpha = 1, \quad \text{and} \quad p(u, \bar{u}) = p(u) = i\frac{1}{2}u^2.$$

One has $\mathcal{L} = \{t_1, t_2\}$, $P_{t_1} = -\lambda^3$ and $P_{t_2} = \lambda^3$. Then, we denoted by \lfloor an edge decorated by $(t_1, 0)$ and by \lceil an edge decorated by $(t_2, 0)$. The general framework (4.49) derived in Section 4.4 builds the foundation of the first- and second-order schemes presented below for the KdV equation (4.86).

Corollary 4.5.7 *For the KdV equation (4.86) the general scheme (4.44) takes at first order the form*

$$u^{\ell+1} = u^\ell * \tilde{u}^\ell \quad (4.87)$$

with a local error of order $\mathcal{O}(\tau^2 \partial_x u)$ and at second-order

$$\begin{aligned} u^{\ell+1} &= u^\ell * \tilde{u}^\ell + \tau^2 \partial_x^2 (u^\ell * \tilde{u}^\ell)^2 \\ &\quad + \frac{\tau^2}{2} \partial_x (u^\ell * \tilde{u}^\ell) \left(\sum_{k_1 \in \mathbf{Z}^d} k_1 |u_{k_1}^\ell|^2 \right) - \frac{\tau^2}{2} (\partial_x u^\ell * \partial_x \tilde{u}^\ell) ((u_0^\ell)^2 + (\overline{u_0^\ell})^2) \end{aligned} \quad (4.88)$$

with a local error of order $\mathcal{O}(\tau^3 \partial_x^2 u)$, and where $\tilde{u}^\ell(x) = \overline{u^\ell(-x)}$.

Remark 4.5.8 (Stability) In view of a practical implementation of the second order scheme (4.88) for KdV, we address the need to stabilize the three terms in the above scheme involving spatial derivatives on the numerical solution. As in the Remark 4.5.3, for the stabilisation of the second order scheme for NLS, we introduce three filter functions which we premultiply in front of each of the last three critical term appearing in the scheme (4.88). We introduce the following three filter functions in Fourier space,

$$\begin{aligned} \Psi_1(k) &= \varphi_1(-i\tau|k|^2) = \frac{1 - e^{-i\tau|k|^2}}{i\tau k^2}, \\ \Psi_2(k, k_1) &= \frac{1}{(i\tau^{\frac{1}{2}}|k|)(i\tau^{\frac{1}{2}}|k_1|)} \left(e^{i\tau^{\frac{1}{2}}|k|/2} - e^{-i\tau^{\frac{1}{2}}|k|/2} \right) \left(e^{i\tau^{\frac{1}{2}}|k_1|/2} - e^{-i\tau^{\frac{1}{2}}|k_1|/2} \right), \\ \Psi_3(k) &= \text{sinc}^2(\tau^{\frac{1}{2}}|k|), \end{aligned}$$

where $\Psi_3(k)$ is the same filter function used for the stabilization of the second order scheme for NLS (see equation (4.78)). We have that

$$\begin{aligned} \Psi_j(k) &= 1 + \mathcal{O}(\tau|k|^2), \quad |\Psi_j(k)\tau|k|^2| \leq 1, \quad j \in \{1, 3\}, \quad k \in \mathbf{Z}, \\ \Psi_2(k, k_1) &= 1 + \mathcal{O}(\tau(|k|^2 + |k_1|^2)), \quad |\Psi_2(k, k_1)\tau|k||k_1|| \leq 1, \quad k, k_1 \in \mathbf{Z}. \end{aligned}$$

Namely, these three filter functions preserve the low regularity error structure of $\mathcal{O}(\tau \partial_x^2 u)$, and provides the following stabilized version of the scheme (4.88) which is given in physical space by,

$$\begin{aligned} u^{\ell+1} &= u^\ell * \tilde{u}^\ell - i\tau (e^{i\tau \partial_x^2} - 1) (u^\ell * \tilde{u}^\ell)^2 \\ &\quad - \frac{\tau}{2} \left((e^{\tau^{\frac{1}{2}} \partial_x / 2} - e^{-\tau^{\frac{1}{2}} \partial_x / 2}) (u^\ell * \tilde{u}^\ell) \right) \left(\sum_{k_1 \in \mathbf{Z}^d} (e^{\tau^{\frac{1}{2}} |k_1| / 2} - e^{-\tau^{\frac{1}{2}} |k_1| / 2}) |u_{k_1}^\ell|^2 \right) \\ &\quad + \frac{\tau}{2} \left((e^{\tau^{\frac{1}{2}} \partial_x / 2} - e^{-\tau^{\frac{1}{2}} \partial_x / 2}) u^\ell * (e^{\tau^{\frac{1}{2}} \partial_x / 2} - e^{-\tau^{\frac{1}{2}} \partial_x / 2}) \tilde{u}^\ell \right) ((u_0^\ell)^2 + (\overline{u_0^\ell})^2). \end{aligned}$$

Proof. We proceed as for the Nonlinear Schrödinger equation. The construction of the schemes is again based on the

general framework (4.44). We consider for $r = 0, 1$ the expansion,

$$V_k^{n,r}(\tau, v) = \sum_{F=T_1 \cdot T_2 \in \mathcal{G}_0^{r,k}(R)} m_F \frac{\tilde{\Upsilon}^p(T_1)(v) \Upsilon^p(T_2)(v)}{S(T_1)S(T_2)} \mathcal{Q}_{\leq r+1}(\bar{\Pi}^{n,r} T_1 \Pi^{n,r} T_2)(\tau). \quad (4.89)$$

For the first-order scheme ($r = 0$) we need only to consider the single paired decorated forest:

$$\mathcal{G}_0^{0,k}(R) = \{T_0 \cdot T_0\}, \quad T_0 = \begin{array}{c} \textcircled{k} \\ | \\ \text{---} \end{array}. \quad (4.90)$$

Indeed, we recall the first order expansion (4.54), where for the KdV equation we have,

$$u_1(\tau, v^\eta) = e^{-\tau \partial_x^3} v^\eta, \quad u_2(\tau, v^\eta) = e^{-\tau \partial_x^3} \int_0^\tau e^{\zeta \partial_x^3} \partial_x (e^{-\zeta \partial_x^3} v^\eta)^2 d\zeta.$$

Given that for the KdV equation the term $\mathbb{E}[\overline{u_{k,1}(\tau, v^\eta) u_{k,2}(\tau, v^\eta)}]$ consists of a product of three Gaussians, we have that this term is equal to zero. Hence, the only term to compute in the expansion (4.54) is

$$\mathbb{E}[\overline{u_{k,1}(\tau, v^\eta) u_{k,1}(\tau, v^\eta)}],$$

and the pairing to consider is (4.90).

A straightforward calculation yields,

$$S(T_0) = 1, \quad \Upsilon^p(T_0)(v) = v_k, \quad m_{T_0 \cdot T_0} = 1,$$

and

$$(\Pi^{n,0} T_0)(\tau) = e^{-i\tau k^3}.$$

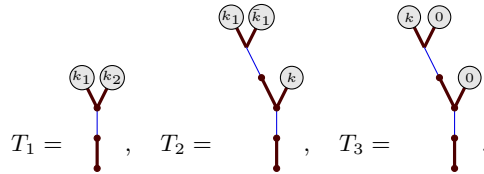
In the end, the first order scheme takes on the simple form:

$$V_k^{n,0}(\tau, v) = |v_k|^2.$$

One can notice that the only approximation error made comes from the first-order truncation of the tree series (4.49). Namely, by noting that $\alpha = 1$, it follows from (4.50) that $(V_k^{n,0} - V_k)(\tau, v) = \mathcal{O}(\tau^2 k^2 v_k \bar{v}_k)$. Therefore, in physical space the local error is of order $\mathcal{O}(\tau^2 (\partial_x v * \partial_x \bar{v}))$, which solely requires one additional derivative on the initial data.

For a second order scheme, one has to compute more terms. The set of paired decorated forests is given by:

$$\mathcal{G}_0^{1,k}(R) = \{T_0 \cdot T_0, T_1 \cdot T_1, T_0 \cdot T_2, T_0 \cdot T_3, k_i \in \mathbf{Z}^d\},$$



A straightforward computation gives:

$$\begin{aligned} S(T_1) &= 2, \quad S(T_2) = S(T_3) = 2, \quad \Upsilon^p(T_1)(v) = v_{k_1} v_{k_2}, \\ \Upsilon^p(T_2)(v) &= |v_{k_1}|^2 v_k, \quad \Upsilon^p(T_3)(v) = v_0^2 v_k \\ m_{T_1 \cdot T_1} &= 2, \quad m_{T_0 \cdot T_2} = 1, \quad m_{T_0 \cdot T_3} = 2. \end{aligned}$$

Further, due to cancellations in the resonance, the integrals encoded by the trees T_2 and T_3 have a null resonance structure, and hence it follows that

$$\begin{aligned} (\Pi^{n,1} T_0)(\tau) &= e^{-i\tau k^3}, \quad (\Pi^{n,1} T_2)(\tau) = -\frac{\tau^2}{2} k_1 k e^{-i\tau k^3}, \\ (\Pi^{n,1} T_3)(\tau) &= -\frac{\tau^2}{2} k^2 e^{-i\tau k^3}. \end{aligned}$$

For the computation of $(\Pi^{n,1}T_1)(\tau)$, we proceed by a full Taylor expansion which yields

$$\begin{aligned} (\Pi^{n,1}T_1)(\tau) &= e^{-i\tau k^3} \mathcal{K}_{(t_2,1)}^{k,1} \left(e^{i\xi(-k_1^3 - k_2^3)}, n \right) (\tau) \\ &= e^{-i\tau k^3} \left(i\tau k + \frac{3}{2}\tau^2 k_1 k_2 k^2 \right), \end{aligned}$$

where we used the fact that the resonance structure is given by,

$$P_{(t_2,0)}(k) - k_1^3 - k_2^3 = k^3 - k_1^3 - k_2^3 = 3k_1 k_2 (k_1 + k_2) = 3k_1 k_2 k.$$

Then, by taking the product and making the truncation, we obtain:

$$\begin{aligned} \mathcal{Q}_{\leq 2}(\bar{\Pi}^{n,1}T_1)(\tau)(\Pi^{n,1}T_1)(\tau) &= \mathcal{Q}_{\leq 2} \left((-i\tau k + \frac{3}{2}\tau^2 k_1 k_2 k^2)(i\tau k + \frac{3}{2}\tau^2 k_1 k_2 k^2) \right) \\ &= \tau^2 k^2. \end{aligned}$$

The local error introduced is of order $\mathcal{O}(\tau^3 k^4)$ which corresponds to two derivatives due to the convolution structure. In the end, the scheme in Fourier space is given by:

$$\begin{aligned} V_k^{n,1}(\tau, v) &= |v_k|^2 + \tau^2 k^2 \sum_{k=k_1+k_2} |v_{k_1}|^2 |v_{k_2}|^2 \\ &\quad - \sum_{k_1 \in \mathbf{Z}^d} \frac{\tau^2}{2} k_1 k |v_{k_1}|^2 |v_k|^2 - \frac{\tau^2}{2} k^2 |v_k|^2 (v_0^2 + \overline{v_0^2}). \end{aligned}$$

By writing the above scheme in physical space we recover the scheme (4.88), which induces a local error of $\mathcal{O}(\tau^3 \partial_x^2 v)$. \square

Part III

Structure preserving schemes suited for low-regularity approximations

Chapter 5

A symmetric low-regularity integrator for the nonlinear Schrödinger equation

This chapter is based on the article [AB23b] published in the IMA Journal of Numerical Analysis.

Abstract. We introduce and analyze a symmetric low-regularity scheme for the nonlinear Schrödinger (NLS) equation beyond classical Fourier-based techniques. We show fractional convergence of the scheme in L^2 -norm, from first up to second order, both on the torus \mathbb{T}^d and on a smooth bounded domain $\Omega \subset \mathbb{R}^d$, $d \leq 3$, equipped with homogeneous Dirichlet boundary condition. The new scheme allows for a symmetric approximation to the NLS equation in a more general setting than classical splitting, exponential integrators, and low-regularity schemes (i.e. under lower regularity assumptions, on more general domains, and with fractional rates). We motivate and illustrate our findings through numerical experiments, where we witness better structure preserving properties and an improved error-constant in low-regularity regimes.

5.1 Introduction

We consider the nonlinear Schrödinger (NLS) equation,

$$i\partial_t u(t, x) = -\Delta u(t, x) + |u(t, x)|^2 u(t, x), \quad (t, x) \in \mathbb{R} \times \Omega \quad (5.1)$$

with $\Omega \subset \mathbb{R}^d$ or $\Omega = \mathbb{T}^d$, $d \leq 3$, and an initial condition

$$u|_{t=0} = u_0. \quad (5.2)$$

When $\partial\Omega \neq \emptyset$, we assume that Ω is a smooth bounded domain and we assign homogeneous boundary conditions which will be encoded in the choice of the domain of the operator $i\Delta$. In the convergence analysis we will consider either periodic or homogeneous Dirichlet boundary conditions. Nevertheless, one could also consider different types of boundary conditions such as homogeneous Neumann boundary conditions by defining the functional spaces accordingly (see Section 5.2).

Throughout this article we will be interested in providing a reliable approximation of (5.1) when the initial data u_0 are non-smooth, in the sense that they belong to Sobolev spaces of low order. Namely, we will be interested in studying numerical schemes which approximate the time dynamics of (5.1) at low regularity. The numerical study of low-regularity approximations to nonlinear evolution equations has gained lots of attention in the past years, and numerous contributions have been made in this direction. The first results were established on the torus for the Korteweg-De Vries (KdV) equation and then the NLS equation with the pioneering works of [HS17b] and [OS18]. These results could be further greatly extended, see for instance [WZ22b, NWZ22, RS22, LW22] and [ORS22b, WY22, LW21, OWY22] for the KdV and NLS equations respectively. More types of dispersive equations could be dealt with, including for example the Dirac equation [SWZ21] or the “good” Boussinesq equation ([LS23]), and a general framework for constructing low-regularity approximations up to arbitrary order and for a class of dispersive equations on the torus was obtained in [BS22].

The construction of these time integrators (called *resonance-based schemes*, *exponential-type low-regularity integrators*, or *Fourier integrators*) strongly depended on Fourier-based expansions, and hence were restricted to periodic boundary conditions. Recently, this restriction was withdrawn to treat more general domains $\Omega \subset \mathbb{R}^d$ and boundary conditions, as well as more general nonlinearities (see [RS21, AB23a, ABBS22b, BLW23, LMS21]).

The general aim of low-regularity integrators is that they converge under lower regularity assumptions, contrarily to classical methods (see [ABBS22b] for a comparative analysis on general smooth domains). Their major drawback is

that they do not preserve the geometric structure of the underlying system. The NLS equation (5.1) is time reversible, meaning that $\overline{u(-t, x)}$ is again solution of (5.1), and both the density and the energy are conserved quantities:

$$\begin{cases} \|u(t)\|_{L^2} &= \|u_0\|_{L^2}, \\ E(t) &= E_0, \end{cases} \quad t \in I, \quad (5.3)$$

where I is the interval of existence of the solution, and where for H^1 -solutions we have

$$E(t) = \frac{1}{2} \int |\nabla u|^2(t, x) dx + \frac{1}{4} \int |u|^4(t, x) dx.$$

Hence, when designing a numerical scheme it is natural to take into account both of these conserved quantities, and to retain (as much as possible) these properties also on the discrete level by introducing so-called structure preserving schemes, see [HLW10] for an extensive introduction on the subject. The latter has received great interest thanks to their good long-time near-preservation of the actions of the integrable properties of the equation, and have been successfully studied in the past for the approximation of the NLS equation (5.1). Examples of such schemes are splitting schemes ([Lub08], [Fao12]), relaxation finite difference type schemes ([Bes04]), symmetric exponential integrators ([CCO08]) or Crank-Nicolson Galerkin methods ([HP17]), just to name a couple of them. For an overview of symmetric methods for NLS see [CCO08, Fao12, ABB13]. While these classical structure preserving schemes provide excellent approximations to smooth solutions in general even up to long times, they often break down and lead to severe loss of convergence for non-smooth solutions. Low-regularity integrators which are suited for non-smooth solutions on the other hand do not preserve the structure of the underlying equation. The natural question which thus arises is: *What about low-regularity structure preserving schemes for solving the NLS equation (5.1)?* Only very little is known in this direction, see the work of [MS22] on the KdV equation, [WZ22a] on the cubic Klein-Gordon equation, and [BMS22] on the isotropic Landau-Lifschitz equation. Also worth to be mentioned is the work of [WY22] which introduces for the first time a first-order Fourier integrator for the NLS equation (5.1) set on \mathbb{T} which almost conserves the mass.

In this article, we introduce a *symmetric* low-regularity integrator for solving the NLS equation (5.1) which allows for low-regularity approximation while maintaining good long-time preservation of the two conserved properties (5.3) on the discrete level. We carry-out a rigorous convergence analysis in $L^2(\Omega)$ on smooth domains $\Omega \subset \mathbb{R}^d$ and obtain improved error estimates at low-regularity compared to classical symmetric methods. Our numerical findings not only show better structure preservation properties but also show a much better error constant at low-regularity than previously proposed methods (see Figure 5.1).

In the finite dimensional ODE setting it is well-known that symmetric methods are of even order. In the context of PDEs this is a much more delicate question as convergence is met only when sufficient regularity assumptions are imposed on the solution. Thanks to the gain of symmetry, we show second order L^2 -convergence of the symmetric scheme under less regularity assumptions than what is required by classical symmetric schemes ([Lub08, Bes04, BDDL21, HP17]), while asking for slightly more regularity than asymmetric second-order low-regularity schemes ([AB23a]) which however do not preserve the structure of the system (see Figures 5.2 and 5.3). Optimal first order low-regularity convergence rates could be obtained. See Section 5.1.2 for a detailed discussion on the subject.

The scheme we present here is based on the first-order low-regularity scheme first introduced in [OS18] which is given by,

$$\Phi_\tau(u^n) := e^{i\tau\Delta}(u^n - i\tau(u^n)^2\varphi_1(-2i\tau\Delta)\overline{u^n}), \quad u^0 = u_0, \quad (5.4)$$

where $\varphi_1(z) = \frac{e^z - 1}{z}$, and τ is the time step. In order to symmetrize the above scheme we introduce the adjoint method as the map

$$\hat{\Phi}_\tau = \Phi_{-\tau}^{-1},$$

and compute (see [HLW10])

$$\hat{\Phi}_{\tau/2} \circ \Phi_{\tau/2}.$$

This yields the following implicit symmetric low-regularity scheme,

$$\begin{aligned} u^{n+1} = \varphi^\tau(u^n) &= e^{i\tau\Delta}u^n - i\frac{\tau}{2}e^{i\tau\Delta}((u^n)^2\varphi_1(-i\tau\Delta)\overline{u^n}) - i\frac{\tau}{2}((u^{n+1})^2\varphi_1(i\tau\Delta)\overline{u^{n+1}}) \\ &= e^{i\tau\Delta}u^n + \psi_E^{\tau/2}(u^n) + \psi_I^{\tau/2}(u^{n+1}) \\ &= e^{i\tau\Delta}u^n + \Psi^\tau(u^n, u^{n+1}), \end{aligned} \quad (5.5)$$

which satisfies the discrete analogue of the time-reversible property of (5.1).

We highlight the properties which the scheme (5.5) inherits through numerical experiments, where we couple the time-integrators with the standard Fourier pseudo-spectral method which encodes periodic boundary conditions. The case of homogeneous Dirichlet boundary conditions remains very similar, yet for completeness we also include a convergence plot in this case where we expand the solution as a sine series expansion. First, in the case of periodic boundary

conditions, we observe in Figures 5.1a and 5.1b the favorable convergence properties of the scheme (5.5) for H^1 and H^2 data respectively. We notice that the error constant of the symmetric scheme is much better than the asymmetric first-order low-regularity integrator (Low-reg 1), and is also better than the asymmetric second-order low-regularity integrator (Low-reg 2). Figure 5.1c similarly shows the favorable convergence behavior when considering homogeneous Dirichlet boundary conditions. Secondly, we study in Figures 5.2 and 5.3 the structure preserving properties of the new symmetric low-regularity integrator (5.5) against previous asymmetric low-regularity integrators. We witness that the asymmetric first and second-order low-regularity integrators (Low-reg 1, Low-reg 2) are unable to preserve the density and energy (see (5.3)), whereas the symmetric integrator (5.5) appears to nearly-preserve both conserved properties over long-times. We note that in the finite dimensional ODE setting a general theory for symmetric methods applied to integrable reversible systems has been established in [HLW10] allowing for long-time near-conservation of first-integrals. In the infinite dimensional case the understanding of the long-time behavior of numerical solutions is an ongoing challenge in the field of geometric integration and few results are known, see for example [Fao12, FGP10a, GL10b, CHL08]. We expect that it would be possible to prove long-time near-preservation of the density and energy of the scheme (5.5) by using the results of [HLW10], and by benefitting of an analysis using modulated Fourier expansions (see [CHL08, GL10b]) or using normal form techniques ([FGP10a, BG22]) to show near-conservation of the energy. This delicate analysis is out of scope for this paper, where here we focus on the low-regularity error estimates on the solution itself. Finally, we refer

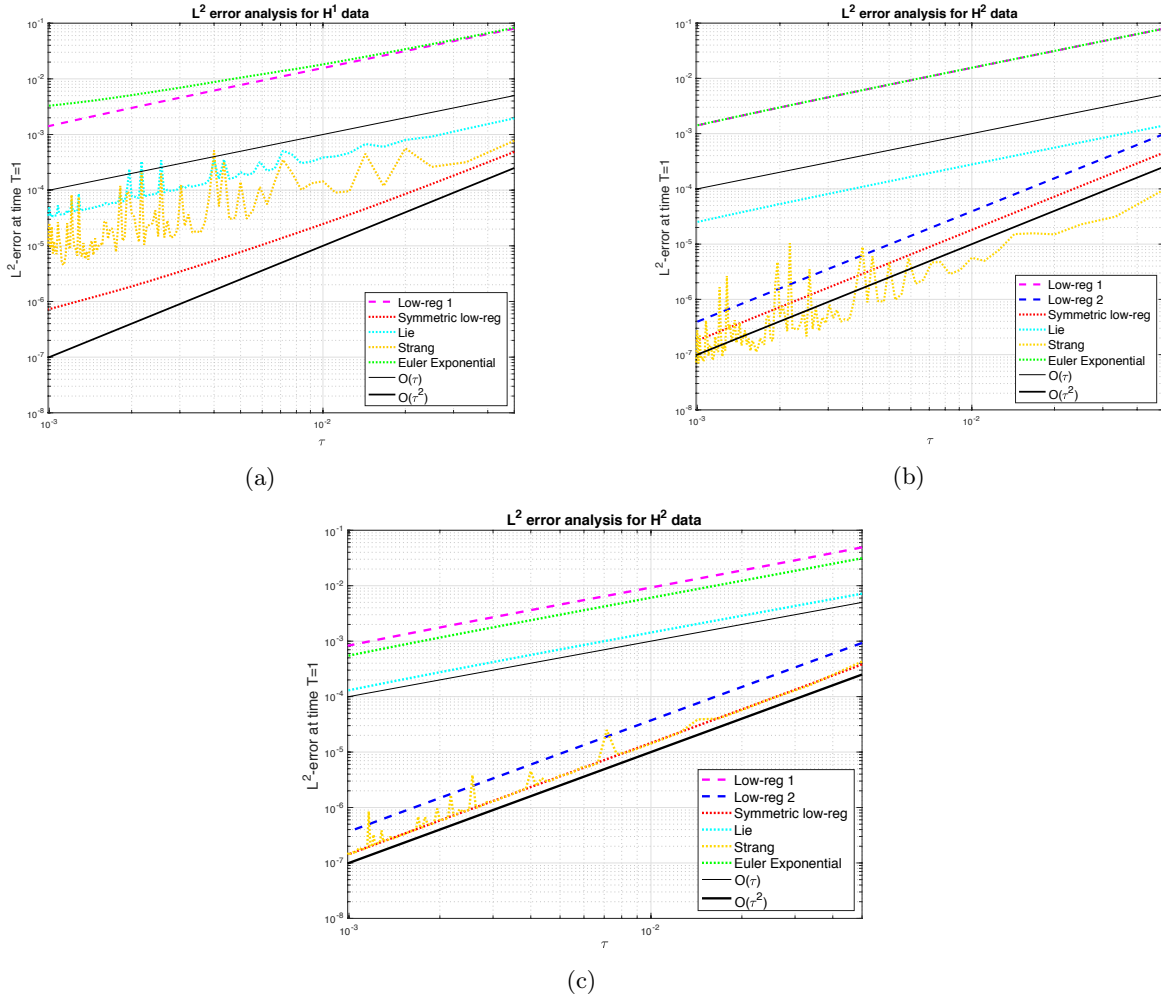


Figure 5.1 – Convergence plot for data in H^1 (Figure (a)) and data in H^2 (Figure (b) and (c)) of the asymmetric first and second-order low-regularity integrators (pink, dark blue), the symmetric method (5.5) (red), the classical Lie splitting, Strang splitting, and Euler Exponential method (light blue, yellow, and green). We observe order reduction of the classical Euler Exponential and Lie and Strang splitting methods (Figure (a), $H^1(\mathbb{T})$ -data), and of the Strang splitting method (Figure (b), $H^2(\mathbb{T})$ -data, and Figure (c), $H^2([0,1])$ -data). Figures (a) and (b) are with periodic boundary conditions, while Figure (c) is with homogeneous Dirichlet boundary conditions. The slopes of the continuous black lines are one and two, respectively. We took the final time $T = 1$, and the number of Fourier modes $K = 2^{11}$. The figure is taken from [AB23b].

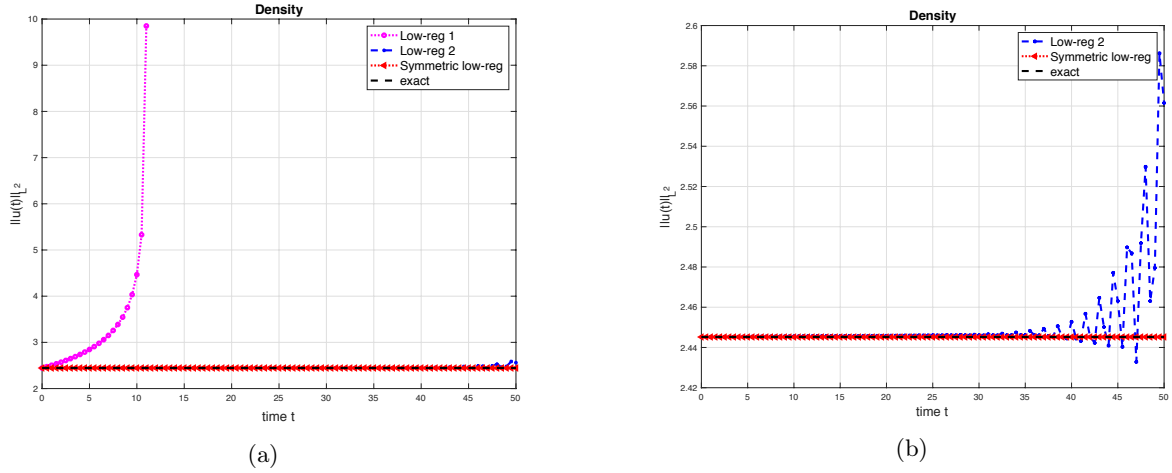


Figure 5.2 – Plot (a) : We graph the L^2 -norm $\|u(t)\|_{L^2(\mathbb{T})}$ up until time $T = 50$ of three low-regularity integrators. The asymmetric first and second-order low-regularity integrators (pink, blue), and the new symmetric low-regularity integrator (red). We also graph the exact value $\|u_0\|_{L^2(\mathbb{T})}$ (black). Plot (b): We only graph the asymmetric second-order low-regularity integrators (blue), and the symmetric low-regularity integrator (red) together with the exact L^2 -norm of the initial value (black). We fixed the number of Fourier modes $K = 2^9$, the time step $\tau = 0.05$, and took an initial data $u_0 \in H^2$. The figures is taken from [AB23b].

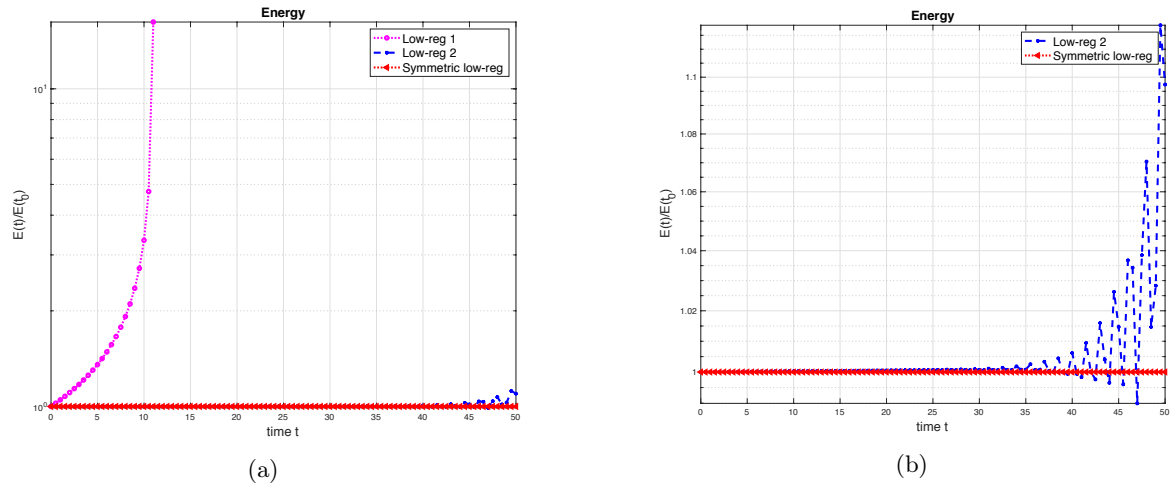


Figure 5.3 – Plot (a) : We graph the relative energy $E(t)/E(t_0)$ (see (5.3)) up to $T = 50$ of the same three low-regularity integrators as in Figures 5.2a and 5.2b. Plot (b): We only graph the relative energy of the asymmetric second order low-regularity integrators (blue), and the symmetric low-regularity integrator (red). We again fixed the number of Fourier modes $K = 2^9$, the time step $\tau = 0.05$, and took an initial data $u_0 \in H^2$.

to Figure 5.4 for a broad indication of the relative computational cost of each of the three low-regularity integrators, and discuss the added cost of implementing the symmetric implicit scheme (5.5). We observe that the asymmetric second-order low-regularity integrator (Low-reg 2) costs in CPU-time approximately the same as the symmetric integrator (5.5). Whereas when comparing with the asymmetric first-order scheme (Low-reg 1) we have that the improved convergence properties of the scheme (5.5) make up for the extra cost of solving the implicit system (5.5) at every time step.

This numerical study motivates the use of the scheme (5.5), which conserves better the underlying geometric structure of the equation, exhibits a better error constant, and can be implemented at relatively low additional cost despite its implicit nature.

Remark 5.1.1 (Implicit versus explicit low-regularity schemes) We make the important remark that unlike the previous (asymmetric) low-regularity integrators [OS18, BS22, ORS21, ORS22b, RS21, AB23a, ABBS22b] the above symmetrized scheme (5.5) is an *implicit* one. We have witnessed that the implicit nature of the scheme does not adversely affect the computational cost of the method (see Figure 5.4). Nevertheless, one could query on the necessity of the

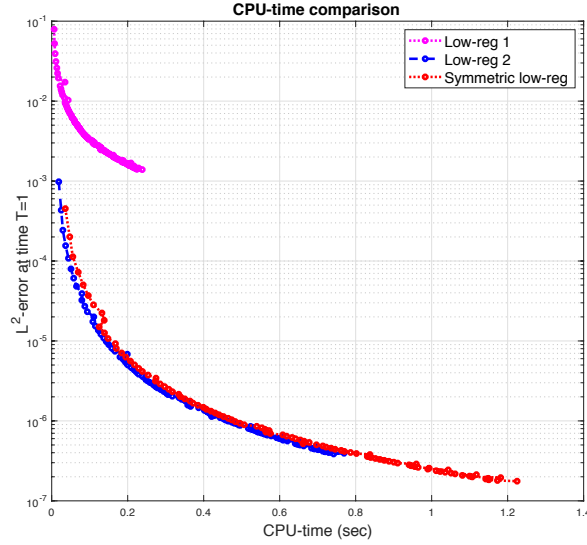


Figure 5.4 – We plot the CPU time versus the L^2 -error. Namely, we compare the computational cost for running the first and second-order low-regularity scheme (pink, dark blue), with the low-regularity symmetric integrator (5.5) (red). We took the same parameter values as in Figure 5.1. The figure is taken from [AB23b].

implicit nature of the symmetric low-regularity scheme. In the case of second-order wave-type equations, instead of considering implicit symmetrized schemes one could study explicit three-time step symmetric schemes using Gautschi-type methods. Indeed, for the cubic Klein-Gordon equation set on \mathbb{T} , an *explicit* symmetric *three time-step* low-regularity integrator could be obtained by [WZ22a]. While this approach is suited to second order equations, by combining the work of [WZ22a] together with the uniformly accurate low-regularity integrator [CS22a] adapted to the non-relativistic regime, an interesting open problem would be to obtain in the non-relativistic limit an *explicit* symmetric *three time-step* low-regularity approximation to the NLS equation (5.1).

Having motivated the scheme (5.5) we now provide the underlying idea behind its construction. To provide a better intuition to the reader we will work in the twisted variable and place ourselves on the torus $\Omega = \mathbb{T}$ in order to make use of Fourier-based expansions (see also [OS18]).

5.1.1 Derivation of the scheme

We switch to the twisted variable $v = e^{-it\Delta}u$. We observe that v satisfies

$$i\partial_t v = e^{-it\Delta}(|e^{it\Delta}v|^2 e^{it\Delta}v), \quad v_0 = u_0.$$

Equivalently, by integrating the above and mapping Duhamel's formula in Fourier space we have

$$v(t_{n+1}) = v(t_n) - i \sum_{k=-k_1+k_2+k_3} e^{ikx} e^{it_n(k^2+k_1^2-k_2^2-k_3^2)} I^\tau, \quad (5.6)$$

where the oscillatory integral is given by

$$I^\tau = \int_0^\tau e^{i\omega_1 s} h(s) ds, \quad (5.7)$$

and $h(s) = e^{i\omega_2 s} g(s)$, $\omega_1 = 2k_1^2$, $\omega_2 = k^2 - k_1^2 - k_2^2 - k_3^2 = -2k_1(k_2 + k_3) + k_2k_3$ and

$$g(s) = \bar{v}_{k_1}(t_n + s)v_{k_2}(t_n + s)v_{k_3}(t_n + s).$$

The central question revolves around making a suitable choice of discretization of the oscillatory integral I^τ , with the aim of minimizing the regularity assumption required by this approximation. The underlying idea behind the construction of the previous (asymmetric) low-regularity integrators (or *resonance-based schemes*) is to choose an approximation of the integral I^τ which allows for a practical implementation (by not performing exact integration), while optimizing the local error in the sense of regularity. Namely, by recalling that $2k_1^2$ corresponds to second order derivatives in Fourier space while the terms $k_m k_j$ (for $m \neq j$) correspond to product of first order derivatives, the idea is to separate the dominant

(ω_1) and lower-order (ω_2) frequencies. The lower-order and non-oscillatory part $h(s)$ is then approximated by a Taylor series expansion centered at $s = 0$,

$$h(s) = h(0) + O(sw_2g),$$

and the dominant part $e^{i\omega_1 s}$ is integrated exactly. This yields the first-order low-regularity scheme (5.4) with a local error of $O(\tau^2 \partial_x v)$. At low regularity this is more advantageous than classical techniques (such as exponential integrators [HO10] or splitting methods [Lub08]) which do not embed the dominant frequency interactions into the scheme and obtain a local error of $O(\tau^2 \partial_x^2 v)$.

The key idea behind obtaining the symmetric scheme (5.1) is to make a different Taylored discretization of the lower-order and non-oscillatory part $h(s)$. Namely, we again integrate exactly and embed the dominant part $e^{i\omega_1 s}$ into the numerical scheme, while this time approximating the non-dominant part in the following symmetric fashion,

$$h(s) \approx h(0)\mathbb{1}_{[0, \tau/2]} + h(\tau)\mathbb{1}_{(\tau/2, \tau]}, \quad s \in [0, \tau], \quad (5.8)$$

where $\mathbb{1}_A$ is the indicator function on the set A . By plugging this approximation for h into the oscillatory integral (5.7) yields two terms: an explicit and an implicit one. The explicit term is given by,

$$\int_0^{\tau/2} e^{i\omega_1 s} h(0) ds = \tau \frac{e^{i\omega_1 \tau/2} - 1}{i\omega_1 \tau} v_{k_1}^n(t_n) v_{k_2}^n(t_n) v_{k_3}^n(t_n) = \frac{\tau}{2} \varphi_1(ik_1^2 \tau) \overline{v_{k_1}^n(t_n)} v_{k_2}^n(t_n) v_{k_3}^n(t_n).$$

Using the definition of the twisted variable, equation (5.6), and by mapping the above back to physical space yields the explicit nonlinear term $\psi_E^{\tau/2}(u^n)$ in the scheme (5.5). Similarly, one obtains the nonlinear implicit term in (5.5) by using the definitions $\omega_1 = 2k_1^2$, $\omega_2 = k^2 - k_1^2 - k_2^2 - k_3^2$ and noticing that

$$h(\tau) = e^{ik^2 \tau} \left(\left(e^{-ik_2^2 \tau} v_{k_2}^n(t_{n+1}) \right) \left(e^{-ik_3^2 \tau} v_{k_3}^n(t_{n+1}) \right) \left(e^{-ik_1^2 \tau} \overline{v_{k_1}^n(t_{n+1})} \right) \right)$$

and

$$\begin{aligned} \int_{\tau/2}^{\tau} e^{i\omega_1 s} h(\tau) ds &= e^{ik^2 \tau} \left(\left(e^{-ik_2^2 \tau} v_{k_2}^n(t_{n+1}) \right) \left(e^{-ik_3^2 \tau} v_{k_3}^n(t_{n+1}) \right) \int_0^{\tau/2} e^{2ik_1^2(\tau-s)} ds \left(e^{-ik_1^2 \tau} \overline{v_{k_1}^n(t_{n+1})} \right) \right) \\ &= e^{ik^2 \tau} \left(\left(e^{-ik_2^2 \tau} v_{k_2}^n(t_{n+1}) \right) \left(e^{-ik_3^2 \tau} v_{k_3}^n(t_{n+1}) \right) \frac{\tau}{2} \varphi_1(-i\tau k_1^2) \left(e^{+ik_1^2 \tau} \overline{v_{k_1}^n(t_{n+1})} \right) \right). \end{aligned}$$

We note that a general approach to obtain the approximation (5.8) is to first give a symmetric approximation to the non-oscillatory part $g(s)$ by iterating Duhamel's formula inside $v_k(t_n + s)$ in a symmetric fashion. Namely, $v_k(t_n + s)$ is approximated on $[0, \frac{\tau}{2}]$ by the linear term in the *Duhamel formula centered about $s = 0$* (yielding the approximation $g(0)$, see (5.6)). While on $(\frac{\tau}{2}, \tau]$, $v_k(t_n + s)$ is approximated by the linear term in the *Duhamel formula centered about $s = \tau$* (yielding the approximation $g(\tau)$). We then proceed by approximating the lower-order oscillatory part $e^{i\omega_2 s}$ in a symmetric fashion. In order to obtain higher-order symmetric low-regularity approximations, we would iterate inside $g(s)$ both of these Duhamel expansions (centered about $s = 0$ on $[0, \frac{\tau}{2}]$ and about $s = \tau$ on $(\frac{\tau}{2}, \tau]$) up to higher order. The construction of higher-order low-regularity symmetric integrators will be dealt with in future work.

Remark 5.1.2 (Third order local error bound) We make an important point related to the third-order local error structure of the scheme (5.5). Thanks to the symmetry of the scheme (5.5) we can expect to have second-order convergence under suitable regularity assumptions on the solution. From the above calculations in Fourier one easily observes that we naturally need three additional derivatives in order to obtain a third-order local error bound of the scheme (5.5). Indeed, by Taylor expanding around the midpoint one observes that the error induced by the discretization (5.8) of I^τ requires the boundedness of a term of the form,

$$\begin{aligned} &\int_{-\tau}^0 e^{i\omega_1(\frac{s+\tau}{2})} \left(e^{i\omega_2(\frac{s+\tau}{2})} - 1 \right) ds g(0) \\ &+ \int_0^{\tau} e^{i\omega_1(\frac{s+\tau}{2})} \left(e^{i\omega_2(\frac{s+\tau}{2})} - e^{i\omega_2 \tau} \right) ds g(0). \end{aligned} \quad (5.9)$$

For the above to yield a third order term one needs to bound a term of order $O(\tau^3 \omega_1 \omega_2 \bar{v}_{k_1} v_{k_2} v_{k_3})$ which corresponds in physical space to asking for three additional derivatives on \bar{v} . This is to be compared with classical (symmetric) schemes which usually have a local error of $O(\tau^3 \partial_x^4 v)$ (see for example [Lub08] for splitting schemes), and to asymmetric resonance-based schemes which merely asks for $O(\tau^3 \partial_x^2 v)$, ([BS22, OWY22]).

While we motivated this symmetric low-regularity integrator on a periodic domain, we show that it also allows for a low-regularity approximation on general smooth domains by establishing its convergence at low-regularity (see Section

5.1.2). Throughout the remainder of this article we will work on general smooth domains $\Omega \subset \mathbb{R}^d$ and make use of semi-group theory to derive our scheme and establish our convergence result on general domains (see Section 5.4). This differs from the first structure preserving low-regularity integrators [MS22, BMS22] which are restricted to periodic boundary conditions.

We now enter the main bulk of this paper, which answers the question of what can be rigorously proven on the L^2 -convergence of the scheme (5.5) when set on a general smooth domain.

We state and prove L^2 -fractional convergence results, from first to second order, both on the torus \mathbb{T}^d and on a smooth bounded domain $\Omega \subset \mathbb{R}^d$, under moderate regularity assumptions on the solution u . These are stronger convergence results than the more typical $H^\sigma(\mathbb{T}^d)$ ($\sigma > \frac{d}{2}$)-convergence analysis, which is restricted to an analysis in smooth Sobolev spaces and to periodic boundary conditions. We state our results in the next subsection.

5.1.2 Result

Theorem 5.1.1 ($\Omega = \mathbb{T}^d$) *Let $T > 0$, $d \leq 3$, and $u_0 \in H^\alpha(\mathbb{T}^d)$ with $\alpha \in [1 + \frac{d}{4}, 3]$. Let $u \in \mathcal{C}([0, T], H^\alpha(\mathbb{T}^d))$ be the unique solution of (5.1). Then there exist $\tau_{\min} > 0$ depending on T and on $\|u_0\|_{H^\alpha}$, and C_T a positive function depending on T and $\sup_{[0, T]} \|u(t)\|_{H^\alpha}$, such that for every time step size $\tau \leq \tau_{\min}$ the numerical solution u^n given in equation (5.5) has the following error bound:*

$$\|u(n\tau) - u^n\|_{L^2} \leq C_T (\sup_{[0, T]} \|u(t)\|_{H^\alpha}) \tau^{1+\gamma}, \quad 0 \leq n\tau \leq T, \quad (5.10)$$

for α and $\gamma \in [0, 1]$ which satisfy

$$\begin{cases} \alpha > 1 + \frac{d}{2} \text{ and } 0 \leq \gamma \leq \frac{\alpha-1}{2}, \\ \alpha = 1 + \frac{d}{2} \text{ and } 0 \leq \gamma < \frac{d}{4}, \\ \alpha < 1 + \frac{d}{2} \text{ and } 0 \leq \gamma \leq \alpha - 1 - \frac{d}{4}. \end{cases} \quad (5.11)$$

We now consider the case where Ω is a smooth bounded domain. Given that in this case the space X^s (see Section 5.2) in which the solution belongs depends not only on Sobolev regularity but also on compatibility conditions which the solution must satisfy on the boundary, we divide the statement of our results depending on the compatibility conditions imposed on $u|_{\partial\Omega}$, (and on the order of convergence).

Theorem 5.1.2 ($\Omega \subset \mathbb{R}^d$ smooth bounded domain) *Let Ω be a smooth bounded domain of \mathbb{R}^d . We consider the NLS equation (5.1), equipped with homogeneous Dirichlet boundary conditions. Given any $T > 0$, and $d \leq 3$, there exists $\tau_{\min} > 0$ depending on T and the norm of the initial data such that we have the following:*

1. *Given any $u_0 \in (H^{1+d/4} \cap H_0^1)(\Omega)$ we have first-order convergence of the symmetric scheme (5.5),*

$$\|u^n - u(n\tau)\|_{L^2} \leq C_T \tau,$$

for all $\tau \leq \tau_{\min}$, and $0 \leq n\tau \leq T$.

2. *More generally, given any $u_0 \in (H^\alpha \cap H_0^1)(\Omega)$ with $\alpha \in [1 + \frac{d}{4}, 2]$ we have the fractional convergence estimates (5.10) for α and γ which satisfies (5.26). In particular, we have*

$$\|u(n\tau) - u^n\|_{L^2} \leq C_T \begin{cases} \tau^{1+\frac{\alpha-1}{2}} & \text{if } 1 + \frac{d}{2} < \alpha \leq 2, \\ \tau^{1+\frac{d}{4}-\epsilon} & \text{for } \alpha = 1 + \frac{d}{2}, \\ \tau^{\alpha-d/4}, & \text{for } 1 + \frac{d}{4} \leq \alpha < 1 + \frac{d}{2}, \end{cases}$$

for $0 \leq n\tau \leq T$, $\tau \leq \tau_{\min}$, and for any $\epsilon > 0$.

3. *By allowing for more compatibility condition on the boundary we have the following second-order convergence result for an initial data $u_0 \in X^3 = \{u \in H^3(\Omega) : u|_{\partial\Omega} = 0, \Delta u|_{\partial\Omega} = 0 \text{ in } L^2(\partial\Omega)\}$,*

$$\|u^n - u(n\tau)\|_{L^2} \leq C_T \tau^2,$$

for all $\tau \leq \tau_{\min}$, and $0 \leq n\tau \leq T$.

We start by making a few remarks on Theorem 5.1.1, set on the torus \mathbb{T}^d . Let us first mention that the symmetric low-regularity integrator (5.5) requires less regularity assumptions than classical symmetric schemes (see [ESS16, Lub08, BDDL21, HP17]). Indeed, for example the authors [ESS16] require H^2 solutions to obtain first order convergence of a Lie splitting scheme for NLS, and the author [Lub08] requires H^4 -solutions for second-order convergence of a Strang splitting method, whereas we require $H^{1+\frac{d}{4}}$ and H^3 to obtain first and resp. second order convergence.

We compare this result to previous convergence results of explicit low-regularity integrators for the NLS equation (5.1), which are not symmetric and hence do not have good structure preservation properties (see Figures 5.2, 5.3). To the best of our knowledge, this is the first fractional convergence results of a low-regularity schemes to be obtained from first to second order. We compare our full first and second-order convergence result with the work of [AB23a], which also obtains first order convergence in $L^2(\mathbb{T}^d)$ for solutions $u(t) \in H^{1+d/4}(\mathbb{T}^d)$. For the second order convergence in L^2 of their asymmetric second-order low-regularity integrator the author [AB23a] asks for solutions $u(t) \in H^{2+d/4}$, whereas the symmetric low-regularity integrator (5.5) requires a bit more regularity, namely H^3 solutions. Moreover, convergence of order $\tau^{1+\gamma}$ in H^r -norm, $r > d/2$, for $u_0 \in H^{2\gamma+r+1}(\mathbb{T}^d)$ easily follows from the proof of Theorem 5.1.1. This is to be compared with asymmetric resonance-based schemes which would typically ask for $u_0 \in H^{\gamma+r+1}(\mathbb{T}^d)$, $r > \frac{d}{2}$. See [OS18, OWY22] for a first and resp. second order analysis. We refer to Remark 5.1.2 which discusses the necessity of requiring three additional derivatives on the solution to obtain second-order convergence of the scheme (5.5).

We finish by comparing our result with the work of [BMS22], which introduced a symmetrized low-regularity integrator for the Schrödinger map (SM), where they relate the SM flow to the NLS equation set on 1-d torus \mathbb{T} via the Hasimoto transform. The analysis of their scheme is however restricted to the 1-d torus, and to first order convergence in smooth Sobolev spaces $H^r(\mathbb{T})$, $r > 1/2$. The results we present here go beyond the more typical $H^r(\mathbb{T})$ error analysis ($r > \frac{1}{2}$), by pushing down the error analysis to L^2 for first and up to second order convergence. Furthermore, we do not restrict ourselves to Fourier-based techniques, and hence to periodic boundary conditions, as is testified by Theorem 5.1.2. Using the techniques presented in this article, one can also obtain a symmetric low-regularity approximation to the Schrödinger map in a more general setting than [BMS22].

We now comment upon Theorem 5.1.2. To our knowledge, this is the first convergence result which goes beyond the first-order convergence analysis of a low-regularity integrator when set on a smooth bounded domain $\Omega \subset \mathbb{R}^d$. We refer to [RS21, Corollary 20] where the authors show first order convergence in $L^2(\Omega)$ of the asymmetric low-regularity scheme (5.4) while analogously asking for $(H^{1+\frac{d}{4}} \cap H_0^1)(\Omega)$ solutions.

We also compare our result to the work of [HP17] which introduces a mass and energy conserving variant of the Crank-Nicolson method as its time-discretization. They show first order convergence on a smooth bounded domain $\Omega \subset \mathbb{R}^d$ under -among other assumptions- $u_t \in L^2(0, T; H^2(\Omega))$, and obtain second order convergence under -among other assumptions- $u_{tt} \in L^2(0, T; H^2(\Omega))$, while assuming $u \in C([0, T], H^2(\Omega))$ throughout their analysis. In contrast to the above classical results Theorem 5.1.2 permits less regularity assumptions on $u(t)$, namely less than H^2 -solutions for first order, and less than H^4 -solutions for second order. We note that the analysis presented here works analogously when adding a potential term uV to equation (5.1), as is considered in [HP17]. One would need to ask for the same regularity assumption (and boundary conditions) on V as is required on u in the above theorem. This follows exactly as done in [AB23a]. The case of a rougher potential ($V \in L^\infty(\Omega)$) is dealt in the works of [HP17, BW23b, BMW23, MWZ24].

We also mention that for the 1-d NLS equation with Neumann boundary conditions a low-regularity integrator has been introduced by [BLW23], where using harmonic analysis techniques they could prove up to almost first order convergence with H^1 -data.

5.1.3 Outline of the paper

In Section 5.2 we set the scene and introduce the spaces and norms, together with crucial nonlinear estimates, which we will work with throughout the error analysis section. In Section 5.3 we analyze the implicit nature of the scheme; we show that it is well-defined and establish a crucial a priori estimate on the numerical solution. Finally, in Section 5.4 we prove the fractional global error estimates presented in Theorems 5.1.1 and 5.1.2. First, in Section 5.4.1 the fractional local error bounds are obtained, followed by Section 5.4.2 where the stability estimate is shown, and from which the convergence results then naturally follow.

5.2 Norms, spaces, and nonlinear estimates

The norm and space used during the error analysis will depend on the domain Ω and boundary conditions imposed. We will treat the case where $\Omega = \mathbb{T}^d$ with periodic boundary conditions, and the case of homogeneous Dirichlet boundary conditions when placed on a smooth bounded domain of \mathbb{R}^d . In the case where $\Omega = \mathbb{T}^d$ the domain of the operator $\mathcal{L} = -\Delta$ is $D(\mathcal{L}) = H^2(\mathbb{T}^d)$, whereas for Dirichlet boundary conditions we have that $D(\mathcal{L}) = (H^2 \cap H_0^1)(\Omega)$. We can define powers of \mathcal{L} , \mathcal{L}^s , for $s \geq 0$ using the spectral resolution, and define the space $X^s(\Omega) = \mathcal{D}(\mathcal{L}^{s/2})$ as the domain of the operator $\mathcal{L}^{s/2}$, where $X^0(\Omega) = L^2(\Omega)$. We define the norm on $X^s(\Omega)$ by the usual graph norm

$$\|u\|_s^2 = \|u\|^2 + \|\mathcal{L}^{s/2}u\|^2, \quad s \geq 0,$$

where $\|u\| = \|u\|_{L^2}$ is the $L^2(\Omega)$ -norm. We will be interested in characterizing the space $X^s(\Omega)$ depending on the domain Ω at study.

5.2.1 The case of periodic boundary conditions

In the case of periodic boundary conditions we have that

$$X^s(\mathbb{T}^d) = H^s(\mathbb{T}^d) := \left\{ u = \sum_{k \in \mathbb{Z}^d} u_k \frac{e^{ikx}}{\sqrt{(2\pi)^d}} \in L^2(\mathbb{T}^d) : |u|_s^2 \triangleq \sum_{k \in \mathbb{Z}^d} |k|^{2s} |u_k|^2 < \infty \right\}$$

with equivalence of norms

$$\|u\|_s^2 = \|u\|_{L^2(\mathbb{T}^d)}^2 + \|(-\Delta)^{s/2} u\|_{L^2(\mathbb{T}^d)}^2 = \sum_{k \in \mathbb{Z}^d} (1 + |k|^{2s}) |u_k|^2 = \|u\|_{H^s}^2,$$

where $u_k = \frac{1}{\sqrt{(2\pi)^d}} \int_{\mathbb{T}^d} u e^{-ikx} dx$.

5.2.2 The case of Dirichlet boundary conditions

We will be interested in characterizing the domain $X^s(\Omega)$ for $s \in [0, 2] \cup \mathbb{N}$ (see Theorem 5.1.2).

In the case where $s = m \in \mathbb{N}$ we have the following characterization (see [Tho07, Lemma 3.1])

$$X^m = \{u \in H^m(\Omega) : \Delta^j u = 0 \text{ in } L^2(\partial\Omega) \text{ for } j < m/2\},$$

with equivalence of the norms on $H^m(\Omega)$ and X^m for functions in X^m .

To treat the case where s is not an integer we first introduce the following fractional Sobolev-type spaces known as the *Sobolev-Slobodetskij*, *Gagliardo* or *Aronszajn* space. Given any $s > 0$ of the form $s = m + \sigma$, with $m \in \mathbb{N}$ and $\sigma \in (0, 1)$, we define

$$H^s(\Omega) = \{u \in H^m(\Omega) : D^\alpha u \in H^\sigma(\Omega) \text{ for any } \alpha \text{ s.t. } |\alpha| = m\},$$

endowed with the norm

$$\|u\|_{H^s}^2 = \sum_{|\alpha|=0}^m \|D^\alpha u\|^2 + \sum_{|\alpha|=m} |D^\alpha u|_{H^\sigma}^2.$$

For $s = m$ an integer the space $H^s(\Omega)$ coincides with the usual Sobolev space $H^m(\Omega)$, and for $\sigma \in (0, 1)$ we have

$$H^\sigma(\Omega) = \left\{ u \in L^2(\Omega) : |u|_{H^\sigma}^2 := \int_{\Omega} \int_{\Omega} \frac{|u(x) - u(y)|^2}{|x - y|^{d+2\sigma}} dx dy < \infty \right\}.$$

We note that all of the fractional Sobolev spaces which we introduce here can also be defined by using interpolation theory. Indeed, the above space is an intermediary Banach space between $L^2(\Omega)$ and $H^1(\Omega)$, and can be defined by interpolation as

$$H^\sigma(\Omega) = [L^2(\Omega), H^1(\Omega)]_\sigma,$$

see [BSV15, Appendix 1] and [Yag09]. Finally, for $s \in (1/2, 2]$ we define

$$H_D^s(\Omega) = \{u \in H^s(\Omega) : u|_{\partial\Omega} = 0 \text{ in } L^2(\partial\Omega)\},$$

it follows from the above that $D(\mathcal{L}) = H_D^2(\Omega)$. We can now express X^s in terms of Sobolev spaces for $s \in [0, 2] \setminus \frac{1}{2}$ (see [Yag09, Theorem 16.12]),

$$X^s(\Omega) = \begin{cases} H^s(\Omega) & \text{if } 0 \leq s < \frac{1}{2} \\ H_D^s(\Omega) & \text{if } \frac{1}{2} < s \leq 2 \end{cases},$$

with norm equivalence

$$C^{-1} \|u\|_{H^s} \leq \|u\|_s \leq C \|u\|_{H^s}, \quad u \in X^s, \quad (5.12)$$

for some constant $C > 0$. In the special case where $s = 1/2$ we have that $X^{1/2} = H_{00}^{1/2}$ is the intermediate space defined by

$$H_{00}^{1/2}(\Omega) := \{u \in H^{1/2}(\Omega) : |u|_{H_{00}^{1/2}}^2 := \int_{\Omega} \frac{u^2(x)}{\text{dist}(x, \partial\Omega)} dx < \infty\},$$

with equivalence of norms on $X^{1/2}$ as in (5.12), see [APR18, Prop 2.2].

Bilinear and nonlinear estimates

In this section we introduce bilinear estimates that are fundamental for the global error analysis, which we now motivate. The results we present in this article go beyond the more typical H^s error analysis ($s > \frac{d}{2}$), by pushing down the analysis to L^2 and obtaining fractional rates of convergence, from first up to second order. In particular, to obtain these fractional rates when $\gamma < d/4$, we need to work in the low-order Sobolev spaces $H^{2\gamma}$ (see Section 5.4). In order to obtain sharp low-regularity error estimates in these spaces we call upon three bilinear estimates (see equations (5.14), (5.15), and (5.16) below) which are tailored to require the least regularity assumptions on u when bounding the local error terms (see also Remark 5.2.1).

Let $\gamma \geq 0$ and $\epsilon > 0$. Throughout the error analysis we will use the following bilinear estimates, depending on the values of γ . In the regime $\gamma > d/4$ we call upon the classical bilinear estimate

$$\|uv\|_{H^{2\gamma}} \lesssim \|u\|_{H^{2\gamma}} \|v\|_{H^{2\gamma}}, \text{ for } \gamma > \frac{d}{4}, \quad (5.13)$$

whereas in the regime $\gamma \in [0, d/4)$ we exploit the following three bilinear estimates,

$$\|uv\| \lesssim \|u\|_{H^{\frac{d}{4}+\gamma}} \|v\|_{H^{\frac{d}{4}-\gamma}} \text{ for } 0 \leq \gamma < \frac{d}{4}, \quad (5.14)$$

$$\|uv\|_{H^{2\gamma}} \lesssim \|u\|_{H^{\frac{d}{4}+\gamma}} \|v\|_{H^{\frac{d}{4}+\gamma}} \text{ for } 0 \leq \gamma < \frac{d}{4}, \quad (5.15)$$

and

$$\|uv\|_{H^{2\gamma}} \lesssim \|u\|_{H^{\frac{d}{2}+\epsilon}} \|v\|_{H^{2\gamma}} \text{ for } 0 \leq \gamma \leq \frac{d}{4}, \quad (5.16)$$

for any $\epsilon > 0$. The above estimates are particular cases of [Hör97, Theorem 8.3.1], valid either on \mathbb{R}^d or \mathbb{T}^d . Furthermore, for a smooth bounded domain $\Omega \subset \mathbb{R}^d$, Stein's extension theorem ([AF03, p.154]) guarantees the existence of a total extension operator, bounded both from $L^2(\Omega)$ to $L^2(\mathbb{R}^d)$ and from $H^m(\Omega)$ to $H^m(\mathbb{R}^d)$, for any $m \in \mathbb{N}$. By interpolation, this operator is bounded from $H^s(\Omega)$ to $H^s(\mathbb{R}^d)$ for any $s \leq m$ (see [AF03, p. 208]). The estimates (5.13), (5.14), (5.15) and (5.16) consequently hold on Ω by extending u and v to \mathbb{R}^d , applying the estimates on their extensions, and restricting their product to Ω .

Remark 5.2.1 (Bilinear estimates in low-order Sobolev spaces $H^{2\gamma}$, $\gamma < d/4$) A natural bilinear estimate which is essential for an analysis in the spaces $H^{2\gamma}$, $\gamma < d/4$, is the estimate (5.16). This estimate is an analogue of the estimate (5.13) in the smooth case where $\gamma > d/4$. These two estimates allow to start and fall back on the same space $H^{2\gamma}$. However, the estimate (5.16) requires more regularity on u than on v ($\frac{d}{2} + \epsilon > 2\gamma$, for $\gamma < d/4$), and asks for $H^{\frac{d}{2}+\epsilon}$ -regularity on the solution. One can obtain more optimal bounds which require less regularity assumptions by equally distributing the regularity on u and on v . Indeed, by assuming that u and v have the same regularity, applying the estimate (5.15) requires $\frac{d}{4} + \gamma$ additional derivatives, which is better than $\frac{d}{2} + \epsilon$ for $\gamma < d/4$. While the estimate (5.14) is used when v requires 2γ derivatives more than u , and balances the regularity requirement to again ask for $\frac{d}{4} + \gamma$ on both u and v (see Proposition 5.4.2).

We now consider the nonlinearity, which we denote by

$$f(u, \bar{u})(t, x) = -iu^2(t, x)\bar{u}(t, x). \quad (5.17)$$

One can easily deduce from the inequalities (5.13) and (5.16) together with the equivalence of norms on X^s the following estimates on the nonlinearity (5.17)

$$\|f(w, \bar{w})\|_s \leq c_{s,\sigma} \|w\|_\sigma^2 \|w\|_s \leq C_{s,\sigma} (\|w\|_\sigma) \|w\|_s, \quad (5.18)$$

$$\|f(v, \bar{v}) - f(w, \bar{w})\|_s \leq c_{s,\sigma} \|v - w\|_s \sum_{k=0}^2 \|v\|_\sigma^k \|w\|_\sigma^{2-k} \leq C_{s,\sigma} (\|v\|_\sigma, \|w\|_\sigma) \|v - w\|_s$$

where $\sigma = \frac{d}{2} + \epsilon$, $c_{s,\sigma} > 0$, and $C_{s,\sigma}(\|u\|, \|v\|)$ denotes a generic constant which depends continuously on the bounded arguments $\|u\|$ and $\|v\|$. In the regime $s > \frac{d}{2}$ the above holds with $\sigma = s$.

Remark 5.2.2 (An analysis for very rough solutions) The main ingredient throughout the error analysis section of this article rests upon the crucial bilinear estimates given above, and restricts the solution to belong to the Sobolev space H^s , $s > d/2$. In order to consider very rough solutions $u \in H^s$, $s \leq d/2$ one needs to call upon more refined tools such as discrete Bourgain spaces when working on the torus ([ORS22b]), and discrete Strichartz estimates when working on the full space ([ORS21]). This delicate error-analysis is out of scope for this paper.

Lastly, as we are interested in obtaining fractional error estimates we will call upon the following estimate several times throughout the error analysis section. For $\gamma \in [0, 1]$, we have,

$$\left\| \frac{(e^{it\Delta} - 1)}{(-it\Delta)^\gamma} u \right\| \leq 2^{1-\gamma} \|u\|. \quad (5.19)$$

The above estimate easily follows from the usual bound

$$|e^{ix} - 1| \leq 2^{1-\gamma} |x|^\gamma, \quad \gamma \in [0, 1],$$

and using the discrete spectral decomposition of the operator $\mathcal{L} = -\Delta$.

We finish this section by stating the definition of a commutator-type term, which is used in order to obtain low-regularity error estimates (see Section 5.4.1). For $H(v_1, \dots, v_n)$, $n \geq 1$, a function and L a linear operator, we define the commutator-type term $\mathcal{C}[H, L]$ as

$$\mathcal{C}[H, L](v_1, \dots, v_n) = -L(H(v_1, \dots, v_n)) + \sum_{j=1}^n \partial_{v_j} H(v_1, \dots, v_n) \cdot Lv_j.$$

In our setting, $H(v_1, v_2) = f(v_1, v_2) = -iv_1^2 v_2$ is the nonlinearity given in (5.17), $L = i\Delta$, and hence

$$\partial_{v_1} f(v_1, v_2) = -2iv_1 v_2 \quad \text{and} \quad \partial_{v_2} f(v_1, v_2) = -iv_1^2 \quad (5.20)$$

and

$$\mathcal{C}[f, i\Delta](v_1, v_2) = -\Delta(v_1^2 v_2) + 2v_1 v_2 \Delta v_1 + v_1^2 \Delta v_2 = -2(|\nabla v_1|^2 v_2 + 2v_1 \nabla v_1 \cdot \nabla v_2). \quad (5.21)$$

5.3 The implicit nature of the scheme

In this section we deal with the question of solving the nonlinear equation (5.5) at a given time step. We also provide an a priori bound on the numerical solution $\varphi^\tau(v)$ in terms of v , which is crucial for the convergence analysis. We recall from Figure 5.4 that the implicit nature of the scheme does not adversely affect the computational cost of the method.

In the following, we fix $v \in X^\sigma$ for some $\sigma > d/2$. We note that v will play the role of the element u^n in the scheme (5.5). We then introduce the map

$$z \mapsto S(z) = e^{i\tau\Delta} v + \psi_E^{\tau/2}(v) + \psi_I^{\tau/2}(z),$$

and wish to prove that it admits a unique fixed point given by $\varphi^\tau(v)$.

We start by introducing some useful estimates on the map S .

Proposition 5.3.1 *Given any $\sigma > d/2$ we have*

$$\|S(z_1) - S(z_2)\|_\sigma \leq \tau M(\|z_1\|_\sigma, \|z_2\|_\sigma) \|z_1 - z_2\|_\sigma, \quad \text{and} \quad \|S(e^{i\tau\Delta} z_1) - e^{i\tau\Delta} z_1\|_\sigma \leq \tau \widetilde{M}(\|z_1\|_\sigma),$$

where $M(\|z_1\|, \|z_2\|)$ and $\widetilde{M}(\|z_1\|)$ denote generic constants which depend continuously on their arguments $\|z_1\|$ and $\|z_2\|$.

Proof of Proposition 5.3.1. The proof follows directly from the definition of the map S , the scheme (5.5) and of the estimate (5.18). \square

The following theorem shows that the implicit scheme (5.5) is well-defined, and admits an a priori bound.

Theorem 5.3.1 *Let $R > 0$ and $\sigma > d/2$. There exists $\tau_R > 0$ such that, for all $\tau \leq \tau_R$ and $v \in X^\sigma$ with $\|v\|_\sigma \leq R$, we have that $\varphi^\tau(v)$ defined in (5.5) is given by*

$$\varphi^\tau(v) \stackrel{H^\sigma}{=} \lim_{j \rightarrow +\infty} S^j(e^{i\tau\Delta} v). \quad (5.22)$$

Moreover, under the same conditions, we have

$$\|\varphi^\tau(v)\|_\sigma \leq 2R. \quad (5.23)$$

Proof of Theorem 5.3.1. For notational convenience we let $x_j = S^j(x_0)$, with $x_0 = e^{i\tau\Delta} v$. We first show by induction that for sufficiently small τ we have the bound

$$\|x_j\|_\sigma \leq 2R, \quad j \geq 0. \quad (5.24)$$

We choose $\tau_R > 0$ such that $\tau_R M(2R, 2R) \leq 1/2$ and $\tau_R \widetilde{M}(R) \leq R/2$, with M and \widetilde{M} from Proposition 5.3.1. We assume that $\|x_j\|_\sigma \leq 2R$, $\forall j \leq J$. It follows that for $\tau \leq \tau_R$ we have,

$$\begin{aligned} \|x_{J+1} - x_0\|_\sigma &\leq \sum_{j=1}^J \|S(x_j) - S(x_{j-1})\|_\sigma + \|S(x_0) - x_0\|_\sigma \\ &\leq \sum_{j=0}^J \left(\prod_{k=1}^j \tau M(\|x_k\|_\sigma, \|x_{k-1}\|_\sigma) \right) \|S(x_0) - x_0\|_\sigma \\ &\leq \frac{R}{2} \sum_{j=0}^J \frac{1}{2^j} \\ &\leq R. \end{aligned}$$

By recalling that, by assumption, $\|x_0\| = \|v\| \leq R$, we conclude from the above that

$$\|x_{J+1}\|_\sigma \leq 2R,$$

and hence by induction bound (5.24) holds.

It then follows that for all $\tau \leq \tau_R$, $(x_j)_{j \in \mathbb{N}}$ is a Cauchy sequence. Indeed, for $m > p$ we have

$$\|x_m - x_p\|_\sigma \leq \sum_{j=p}^{m-1} \|S(x_j) - S(x_{j-1})\|_\sigma \leq \frac{R}{2} \sum_{j=p}^{\infty} \frac{1}{2^j} \xrightarrow{p \rightarrow \infty} 0.$$

This implies that the sequence $(x_j)_{j \in \mathbb{N}}$ converges in X^σ to the unique fixed-point $\varphi^\tau(v)$ of S , and the characterization (5.22) follows. Finally, by passing to the limit in (5.24) we obtain the desired a priori bound (5.23) on $\varphi^\tau(v)$, which concludes the proof. \square

5.4 Error Analysis

In this section we will prove the following proposition.

Proposition 5.4.1 *Let $T > 0$, and $\gamma \in [0, 1] \setminus \{\frac{d}{4}\}$. Then there exists $\tau_{\min} > 0$ such that for every time step $\tau \leq \tau_{\min}$ the numerical solution u^n given in equation (5.5) has the following error bound:*

$$\|u(n\tau) - u^n\|_{L^2} \leq C_T (\sup_{[0, T]} \|u(t)\|_{H^\alpha}) \tau^{1+\gamma}, \quad 0 \leq n\tau \leq T, \quad (5.25)$$

where α is given by

$$\begin{cases} \alpha = 2\gamma + 1 & \text{if } \frac{d}{4} < \gamma \leq 1 \\ \alpha = \gamma + 1 + \frac{d}{4} & \text{if } 0 \leq \gamma < \frac{d}{4} \end{cases} \quad (5.26)$$

and where τ_{\min} depends on T and on $\|u_0\|_{H^\alpha}$, and C_T is a positive function of its argument, depending on T .

Given a fixed convergence rate this proposition expresses the regularity assumptions needed in order to obtain this rate, while on the other hand given a fixed regularity assumption on the initial data Theorems 5.1.1 and 5.1.2 express the convergence rates one can attain with the method (5.5). We now link these results.

Proof of Theorem 5.1.1 and Theorem 5.1.2. By writing the convergence rate γ in terms of the regularity assumptions needed on the solution, it directly follows from the above proposition that the convergence rate (5.10) holds for α and γ which satisfy:

$$\begin{cases} 1 + \frac{d}{2} < \alpha \leq 3, & \gamma = \frac{\alpha-1}{2} \\ 1 + \frac{d}{4} \leq \alpha < 1 + \frac{d}{2}, & \gamma = \alpha - 1 - \frac{d}{4}. \end{cases} \quad (5.27)$$

The proof of Theorem 5.1.1 then follows by using the fact that if (5.10) holds for some $\tilde{\alpha} \in [1 + \frac{d}{4}, 3]$, $\tilde{\gamma} \in [0, 1]$, then the error bound also holds for any $\alpha \geq \tilde{\alpha}$, and $\gamma \leq \tilde{\gamma}$. In particular, we recover the case $\alpha = 1 + \frac{d}{2}$ in Theorem 5.1.1 by applying the second line in (5.27) with $(\tilde{\alpha}, \tilde{\gamma}) = (1 + \frac{d}{2} - \epsilon, \frac{d}{4} - \epsilon)$ to obtain convergence for $0 \leq \gamma < \frac{d}{4}$. See Figure 5.5 which illustrates graphically the convergence result.

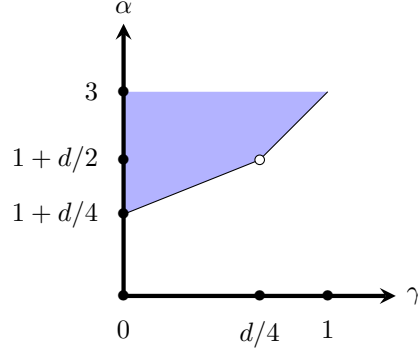


Figure 5.5 – Illustration of the interplay between the regularity parameter α and the convergence rate parameter γ in the convergence result stated in Proposition (5.4.1) and Theorem 5.1.1. We plot the regularity assumption $(u(t) \in H^\alpha)$ needed in order to obtain convergence of order $\tau^{1+\gamma}$.

The proof of Theorem 5.1.2 follows in the same manner, with the added constraint of the boundary conditions. Namely, we require $u \in C([0, T], X^s)$ and $s = 2\gamma + 1$ or $\gamma + 1 + d/4$, where the boundary conditions are imposed in the definition of the space X^s . See Section 5.2 for the definition of the spaces X^s .

□

In order to prove Proposition 5.4.1 we combine local error bounds together with a stability argument to conclude via a Lady Windermere's fan argument. We start by showing the local error bound of order $\tau^{2+\gamma}$ with the regularity assumptions stated in Proposition 5.4.1.

5.4.1 Local error analysis

We decompose the local error term as follows,

$$\begin{aligned} u(t_n + \tau) - \varphi^\tau(u(t_n)) &= \int_0^\tau e^{i(\tau-s)\Delta} f(u(t_n + s), \bar{u}(t_n + s)) ds - \psi_E^{\tau/2}(u(t_n)) - \psi_I^{\tau/2}(\varphi^\tau(u(t_n))) \\ &= \mathcal{R}_1(\tau, t_n) + \mathcal{R}_2(\tau, t_n) + \mathcal{R}_3(\tau, t_n), \end{aligned}$$

with

$$\begin{aligned} \mathcal{R}_1(\tau, t_n) &= \left(\int_0^{\tau/2} e^{i(\tau-s)\Delta} f(e^{is\Delta}u(t_n), e^{-is\Delta}\bar{u}(t_n)) ds - \psi_E^{\tau/2}(u(t_n)) \right) \\ &\quad + \left(\int_{\tau/2}^\tau e^{i(\tau-s)\Delta} f(e^{is\Delta}u(t_n), e^{-is\Delta}\bar{u}(t_n)) ds - \psi_I^{\tau/2}(e^{i\tau\Delta}u(t_n)) \right), \end{aligned} \quad (5.28)$$

$$\mathcal{R}_2(\tau, t_n) = \psi_I^{\tau/2}(e^{i\tau\Delta}u(t_n)) - \psi_I^{\tau/2}(\varphi_\tau(u(t_n))), \quad (5.29)$$

and

$$\mathcal{R}_3(\tau, t_n) = \int_0^\tau e^{i(\tau-s)\Delta} \left(f(u(t_n + s), \bar{u}(t_n + s)) - f(e^{is\Delta}u(t_n), e^{-is\Delta}\bar{u}(t_n)) \right) ds.$$

We start by estimating the first error term $\mathcal{R}_1(\tau, t_n)$. This term is the one which asks for the most regularity, and hence dictates the regularity assumptions required on the solution, and thereby the initial data. We then proceed by estimating each of the terms $\mathcal{R}_2(\tau, t_n)$ and $\mathcal{R}_3(\tau, t_n)$, to obtain a cancelation in their sum thanks to the symmetry of the scheme, yielding the desired local error estimate.

Proposition 5.4.2 *The error term $\mathcal{R}_1(\tau, t_n)$ satisfies the following bound,*

$$\|\mathcal{R}_1(\tau, t_n)\| \leq \begin{cases} C_T \left(\sup_{t \in [0, T]} \|u(t)\|_{X^{2\gamma+1}} \right) \tau^{2+\gamma} & \text{if } \gamma > \frac{d}{4} \\ C_T \left(\sup_{t \in [0, T]} \|u(t)\|_{X^{\gamma+1+\frac{d}{4}}} \right) \tau^{2+\gamma} & \text{if } 0 \leq \gamma < \frac{d}{4} \end{cases}, \quad (5.30)$$

for $0 \leq t_n \leq T$.

Proof of Proposition 5.4.2. We define the filtered function as

$$\begin{aligned} \mathcal{N}(\tau, s, \zeta, \Delta, v) &= -ie^{i(\tau-s)\Delta} [(e^{is\Delta}v)^2 (e^{is\Delta}e^{-2i\zeta\Delta}\bar{v})] \\ &= e^{i(\tau-s)\Delta} f(e^{is\Delta}v, e^{i(s-2\zeta)\Delta}\bar{v}) \end{aligned} \quad (5.31)$$

which plays a fundamental role in the derivation and analysis of our scheme on general domains. In the above expression we duplicate the time variable into s and ζ , pulling out a factor $e^{is\Delta}$ in front of the conjugate term $e^{i(s-2\zeta)\Delta}\bar{v}$. Taylor expanding in the variable s yields the right cancellation with the factor $e^{i(\tau-s)\Delta}$ to recover, after integrating in the variable ζ , the explicit term $\psi_E^{\tau/2}(v)$ in the scheme (5.5), as is detailed below. Similar filtering techniques are used in [RS21, AB23a, ABBS22b].

Let $v = u(t_n)$. By Taylor expanding the filtering function (5.31) around $s = 0$, we obtain that the first term in (5.28) satisfies

$$\begin{aligned} \int_0^{\tau/2} e^{i(\tau-\zeta)\Delta} f(e^{i\zeta\Delta}v, e^{-i\zeta\Delta}\bar{v}) d\zeta &= \int_0^{\tau/2} \mathcal{N}(\tau, \zeta, \zeta, \Delta, v) d\zeta \\ &= \int_0^{\tau/2} \mathcal{N}(\tau, 0, \zeta, \Delta, v) d\zeta + \int_0^{\tau/2} \int_0^\zeta \partial_s \mathcal{N}(\tau, s, \zeta, \Delta, v) ds d\zeta \\ &= \psi_E^{\tau/2}(v) + \int_0^{\tau/2} \int_0^\zeta e^{i(\tau-s)\Delta} \mathcal{C}[f, i\Delta](e^{is\Delta}v, e^{i(s-2\zeta)\Delta}\bar{v}) ds d\zeta, \end{aligned} \quad (5.32)$$

where to obtain the last line we used the definition of the φ_1 function (see (5.4)) to obtain that

$$\int_0^{\tau/2} e^{-2i\zeta\Delta} d\zeta = \frac{\tau}{2} \frac{e^{-i\tau\Delta} - 1}{-i\tau\Delta} = \frac{\tau}{2} \varphi_1(-i\tau\Delta)$$

and the definition of commutator term $\mathcal{C}[f, i\Delta](u, v)$ given in (5.21).

Similarly, using the filtering function (5.31), we can treat the second line in (5.28) by Taylor expanding around $s = \tau$. This yields

$$\begin{aligned} \int_{\tau/2}^\tau e^{i(\tau-\zeta)\Delta} f(e^{i\zeta\Delta}v, e^{-i\zeta\Delta}\bar{v}) d\zeta &= \int_{\tau/2}^\tau \mathcal{N}(\tau, \zeta, \zeta, \Delta, v) d\zeta \\ &= \int_{\tau/2}^\tau \mathcal{N}(\tau, \tau, \zeta, \Delta, v) d\zeta - \int_{\tau/2}^\tau \int_\zeta^\tau \partial_s \mathcal{N}(\tau, s, \zeta, \Delta, v) ds d\zeta \\ &= \psi_I^{\tau/2}(e^{i\tau\Delta}v) - \int_{\tau/2}^\tau \int_\zeta^\tau e^{i(\tau-s)\Delta} \mathcal{C}[f, i\Delta](e^{is\Delta}v, e^{i(s-2\zeta)\Delta}\bar{v}) ds d\zeta, \end{aligned} \quad (5.33)$$

where to go from the second line in the above to the third we used that

$$\begin{aligned} \int_{\tau/2}^\tau \mathcal{N}(\tau, \tau, \zeta, \Delta, v) d\zeta &= -i(e^{i\tau\Delta}v)^2 \left(\left(\int_{\tau/2}^\tau e^{-2i\zeta\Delta} d\zeta \right) e^{i\tau\Delta}\bar{v} \right) \\ &= -i(e^{i\tau\Delta}v)^2 \left(\left(\int_0^{\tau/2} e^{-2i(\tau-\zeta)\Delta} d\zeta \right) e^{i\tau\Delta}\bar{v} \right) \\ &= -i\frac{\tau}{2}(e^{i\tau\Delta}v)^2 \varphi_1(i\tau\Delta)(e^{-i\tau\Delta}\bar{v}), \\ &= \psi_I^{\tau/2}(e^{i\tau\Delta}v). \end{aligned}$$

By definition of $\mathcal{R}_1(\tau, t_n)$ and by using (5.32) and (5.33) we have that

$$\begin{aligned}
\mathcal{R}_1(\tau, t_n) &= \int_0^{\tau/2} \int_0^\zeta e^{i(\tau-s)\Delta} \mathcal{C}[f, i\Delta](e^{is\Delta} v, e^{is\Delta} e^{-2i\zeta\Delta} \bar{v}) ds d\zeta \\
&\quad - \int_{\tau/2}^\tau \int_\zeta^\tau e^{i(\tau-s)\Delta} \mathcal{C}[f, i\Delta](e^{is\Delta} v, e^{is\Delta} e^{-2i\zeta\Delta} \bar{v}) ds d\zeta \\
&= \int_0^{\tau/2} \int_0^\zeta e^{i(\tau-s)\Delta} \mathcal{C}[f, i\Delta](e^{is\Delta} v, e^{is\Delta} e^{-2i\zeta\Delta} \bar{v}) \\
&\quad - e^{is\Delta} \mathcal{C}[f, i\Delta](e^{i(\tau-s)\Delta} v, e^{i(\tau-s)\Delta} e^{-2i(\tau-\zeta)\Delta} \bar{v}) ds d\zeta.
\end{aligned} \tag{5.34}$$

Note that the local error structure lead by the commutator-type terms in the above expression requires less regularity assumptions than what is required by classical methods, such as exponential integrators of splitting methods (see [HO10, Lub08]). Indeed, from the explicit form (5.21) of the commutator term we see that this error term requires only one additional derivative on the initial datum rather than two (see also [AB23a, ABBS22b]).

We now show that thanks to the symmetry of the scheme, we obtain a cancelation in the second-order error term (5.34) yielding (up to) a third-order remainder. For notational convenience we let $w_1(s) = e^{is\Delta} v$, $w_2(s, \zeta) = e^{i(s-2\zeta)\Delta} \bar{v}$, $z_1(s) = e^{i(\tau-s)\Delta} v$, and $z_2(s, \zeta) = e^{i(2\zeta-\tau-s)\Delta} \bar{v}$ and we denote the integrand by

$$R_r(\tau, s, \zeta, v) = e^{i(\tau-s)\Delta} \mathcal{C}[f, i\Delta](w_1(s), w_2(s, \zeta)) - e^{is\Delta} \mathcal{C}[f, i\Delta](z_1(s), z_2(s, \zeta)). \tag{5.35}$$

It follows from the above equations (5.34) and (5.35) that

$$\|\mathcal{R}_1(\tau, t_n)\| \leq \frac{\tau^2}{4} \sup_{s, \zeta \in [0, \tau/2]} \|R_r(\tau, s, \zeta, v)\|.$$

It remains to show that

$$\sup_{s, \zeta \in [0, \tau/2]} \|R_r(\tau, s, \zeta, v)\| \leq \begin{cases} C(\|v\|_{2\gamma+1})\tau^\gamma & \text{if } \gamma > d/4 \\ C(\|v\|_{\gamma+1+\frac{d}{4}})\tau^\gamma & \text{if } \gamma < d/4 \end{cases}. \tag{5.36}$$

We first approximate the exponentials appearing in front of both commutator terms in (5.35) to obtain the following first approximation result on R_r .

Lemma 5.4.3 *We have*

$$R_r(\tau, s, \zeta, v) = R_r^1(\tau, s, \zeta, v) + R_r^2(\tau, s, \zeta, v),$$

with

$$R_r^1(\tau, s, \zeta, v) = (e^{i(\tau-s)\Delta} - 1)\mathcal{C}[f, i\Delta](w_1(s), w_2(s, \zeta)) - (e^{is\Delta} - 1)\mathcal{C}[f, i\Delta](z_1(s), z_2(s, \zeta))$$

and

$$R_r^2(\tau, s, \zeta, v) = \mathcal{C}[f, i\Delta](w_1(s), w_2(s, \zeta)) - \mathcal{C}[f, i\Delta](z_1(s), z_2(s, \zeta)),$$

which satisfy

$$\sup_{s, \zeta \in [0, \tau/2]} \|R_r^i(\tau, s, \zeta, \tau, v)\| \leq \begin{cases} C(\|v\|_{2\gamma+1})\tau^\gamma & \text{if } \gamma > d/4, \\ C(\|v\|_{\gamma+1+\frac{d}{4}})\tau^\gamma & \text{if } \gamma < d/4, \end{cases} \tag{5.37}$$

for $i = 1, 2$.

Proof of Lemma 5.4.3. We write the error term R_r^1 as

$$\begin{aligned}
R_r^1(s, \zeta, \tau, v, \bar{v}) &= (\tau - s)^\gamma \left(\frac{e^{i(\tau-s)\Delta} - 1}{(\tau - s)^\gamma (-\Delta)^\gamma} \right) (-\Delta)^\gamma \mathcal{C}[f, i\Delta](w_1(s), w_2(s, \zeta)) \\
&\quad - s^\gamma \left(\frac{e^{is\Delta} - 1}{s^\gamma (-\Delta)^\gamma} \right) (-\Delta)^\gamma \mathcal{C}[f, i\Delta](z_1(s), z_2(s, \zeta)).
\end{aligned} \tag{5.38}$$

Using the bound given in equation (5.19), and the boundedness of $e^{it\Delta}$ on Sobolev spaces, it follows from equation (5.38) that we are left to provide a bound on $\mathcal{C}[f, i\Delta](v, \bar{v})$ of the form

$$\|\mathcal{C}[f, i\Delta](v, \bar{v})\|_{2\gamma} \leq \begin{cases} C(\|v\|_{2\gamma+1}) & \text{if } \gamma > d/4 \\ C(\|v\|_{\gamma+1+\frac{d}{4}}) & \text{if } \gamma < d/4 \end{cases}. \tag{5.39}$$

From the definition of the commutator (5.21), and by using the equivalence of norms $\|\cdot\|_s$ and $\|\cdot\|_{H^s}$ on X^s (see

Section 5.2), it follows that for $d/4 < \gamma \leq 1$

$$\begin{aligned} \|\nabla v|^2 \bar{v}\|_{2\gamma} &\lesssim \|\nabla v\|^2 \bar{v}\|_{H^{2\gamma}} \\ &\lesssim \|v\|_{H^{2\gamma}} \|\nabla v \cdot \nabla v\|_{H^{2\gamma}} \\ &\lesssim \|v\|_{H^{2\gamma}} \|v\|_{H^{2\gamma+1}}^2 \\ &\lesssim C(\|v\|_{2\gamma+1}), \end{aligned}$$

where we used the estimate (5.13). Similarly, in the case $0 \leq \gamma < d/4$ we have

$$\begin{aligned} \|\nabla v|^2 \bar{v}\|_{2\gamma} &\lesssim \|v\|_{H^{d/2+\epsilon}} \|\nabla v \cdot \nabla v\|_{H^{2\gamma}} \\ &\lesssim \|v\|_{H^{d/2+\epsilon}} \|v\|_{H^{\gamma+1+\frac{d}{4}}}^2 \\ &\lesssim C(\|v\|_{\gamma+1+\frac{d}{4}}), \end{aligned}$$

where to obtain the first line we used estimate (5.16), to go from the first to the second line we used the estimate (5.15) and concluded using the fact that $d/2 + \epsilon < \gamma + 1 + \frac{d}{4}$ together with the equivalence of norms on $X^{\gamma+1+\frac{d}{4}}$.

We can bound the second term in the commutator-type term (5.21) in the same manner to obtain the desired bound (5.39). The estimate (5.37) on R_r^\pm follows immediately.

We now deal with the approximation of the second error term R_r^2 by approximating each of the exponentials appearing in the arguments of the commutator terms, namely on w_1, w_2, z_1 and z_2 . Given the form of the commutator (5.21) and of w_1, w_2, z_1, z_2 , each term to approximate will either be of the form

$$\left\| w \nabla ((e^{i\xi\Delta} - 1)u) \cdot \nabla z \right\| \quad (5.40)$$

or

$$\left\| ((e^{i\xi\Delta} - 1)w) \nabla u \cdot \nabla z \right\| \quad (5.41)$$

for $\xi \in [0, \tau]$, and where we use the boundedness of $e^{it\Delta}$ on Sobolev spaces ($t \in \mathbb{R}$). We can approximate (5.40) as follows, given any $\epsilon > 0$,

$$\begin{aligned} \left\| w \nabla ((e^{i\xi\Delta} - 1)u) \cdot \nabla z \right\| &\lesssim \xi^\gamma \begin{cases} \|w\|_{H^{2\gamma}} \left\| \nabla (-\Delta)^\gamma \left(\frac{e^{i\xi\Delta} - 1}{(-\xi\Delta)^\gamma} u \right) \right\| \|\nabla z\|_{H^{2\gamma}} & \text{if } \gamma > d/4 \\ \|w\|_{H^{\frac{d}{2}+\epsilon}} \left\| \nabla (-\Delta)^\gamma \left(\frac{e^{i\xi\Delta} - 1}{(-\xi\Delta)^\gamma} u \right) \right\|_{H^{\frac{d}{4}-\gamma}} \|\nabla z\|_{H^{\frac{d}{4}+\gamma}} & \text{if } \gamma < d/4 \end{cases} \\ &\leq \xi^\gamma \begin{cases} C(\|w\|_{2\gamma}, \|u\|_{2\gamma+1}, \|z\|_{2\gamma+1}) & \text{if } \gamma > d/4 \\ C(\|w\|_{\frac{d}{2}+\epsilon}, \|u\|_{\gamma+1+\frac{d}{4}}, \|z\|_{\gamma+1+\frac{d}{4}}) & \text{if } \gamma < d/4 \end{cases}, \end{aligned}$$

where we used the Sobolev embedding $H^\sigma \hookrightarrow L^\infty$, for $\sigma > \frac{d}{2}$, and the estimate (5.14) to obtain the first inequality. To obtain the second line in the above we used the equivalence of norms, thanks to the fact that u, v, w belong to $X^{2\gamma+1}$ or $X^{\gamma+1+d/4}$ respectively, as well as the estimate (5.19). Hence, given that $\frac{d}{2} + \epsilon < \gamma + 1 + \frac{d}{4}$, the term above satisfies the desired bound of the form (5.37).

Furthermore, for the expression (5.41) we have,

$$\begin{aligned} \left\| ((e^{i\xi\Delta} - 1)w) \nabla u \cdot \nabla z \right\| &\lesssim \xi^\gamma \begin{cases} \left\| (-\Delta)^\gamma \frac{e^{i\xi\Delta} - 1}{(-\xi\Delta)^\gamma} w \right\| \|\nabla u \cdot \nabla z\|_{H^{2\gamma}} & \text{if } \gamma > d/4 \\ \left\| (-\Delta)^\gamma \frac{e^{i\xi\Delta} - 1}{(-\xi\Delta)^\gamma} w \right\|_{H^{1+\frac{d}{4}-\gamma}} \|\nabla u \cdot \nabla z\|_{H^{2\gamma}} & \text{if } \gamma < d/4 \end{cases} \\ &\lesssim \xi^\gamma \begin{cases} \left\| (-\Delta)^\gamma \frac{e^{i\xi\Delta} - 1}{(-\xi\Delta)^\gamma} w \right\| \|\nabla u\|_{H^{2\gamma}} \|\nabla z\|_{H^{2\gamma}} & \text{if } \gamma > d/4 \\ \left\| (-\Delta)^\gamma \frac{e^{i\xi\Delta} - 1}{(-\xi\Delta)^\gamma} w \right\|_{H^{1+\frac{d}{4}-\gamma}} \|\nabla u\|_{H^{\frac{d}{4}+\gamma}} \|\nabla z\|_{H^{\frac{d}{4}+\gamma}} & \text{if } \gamma < d/4 \end{cases} \\ &\leq \xi^\gamma \begin{cases} C(\|w\|_{2\gamma}, \|u\|_{2\gamma+1}, \|z\|_{2\gamma+1}) & \text{if } \gamma > d/4 \\ C(\|w\|_{\gamma+1+\frac{d}{4}}, \|u\|_{\gamma+1+\frac{d}{4}}, \|z\|_{\gamma+1+\frac{d}{4}}) & \text{if } \gamma < d/4, \end{cases} \end{aligned}$$

where to obtain the first line we used the Sobolev embedding $H^\sigma \hookrightarrow L^\infty$, $\sigma > \frac{d}{2}$, and the estimate $\|uz\| \lesssim \|u\|_{H^{1+\frac{d}{4}-\gamma}} \|z\|_{H^{2\gamma}}$, $\gamma \in [0, 1]$, (see [Hör97, Theorem 8.3.1]). In order to obtain the second line in the above we again used the estimates (5.13) and (5.15), and to obtain the third line we used the equivalence of norms on the spaces X^s together with the

estimate (5.19).

By approximating each of the exponentials in the commutator terms defining R_r^2 and by collecting the error terms which are either of the form (5.40) or (5.41) we recuperate the desired τ^γ bound in (5.37). \square

We can conclude from Lemma 5.4.3 that we have the desired bound (5.36), and hence the bound (5.30) on $\mathcal{R}_1(\tau, t_n)$. \square

We now continue with the bound on the two remaining terms $(\mathcal{R}_2 + \mathcal{R}_3)(\tau, t_n)$, which asks for less regularity assumptions than the boundedness of $\mathcal{R}_1(\tau, t_n)$, as shown below.

Proposition 5.4.4 *For $\gamma \in [0, 1]$, we have the following fractional bound,*

$$\|(\mathcal{R}_2 + \mathcal{R}_3)(\tau, t_n)\| \leq C \left(\sup_{[0, T]} \|u(t)\|_{2\gamma}, \sup_{[0, T]} \|u(t)\|_\sigma \right) \tau^{2+\gamma}, \quad (5.42)$$

given any $\sigma > \frac{d}{2}$. In particular we have the bound,

$$\|(\mathcal{R}_2 + \mathcal{R}_3)(\tau, t_n)\| \leq \begin{cases} C_{T, \gamma} \left(\sup_{t \in [0, T]} \|u(t)\|_{2\gamma+1} \right) \tau^{2+\gamma}, & \text{if } \gamma > \frac{d}{4} \\ C_{T, \gamma} \left(\sup_{t \in [0, T]} \|u(t)\|_{\gamma+1+\frac{d}{4}} \right) \tau^{2+\gamma}, & \text{if } 0 \leq \gamma < \frac{d}{4} \end{cases}, \quad (5.43)$$

for $0 \leq t_n \leq T$.

Proof of Proposition 5.4.4. First, we rewrite the error term $\mathcal{R}_3(\tau, t_n)$ by making suitable Taylor expansions on f . We start by expanding $u(t_n + \zeta)$ locally up to second order :

$$u(t_n + \zeta) = e^{i\zeta\Delta} u(t_n) + \zeta f^n + \tilde{R}(\zeta, t_n) \quad (5.44)$$

where $f^n = f(u(t_n), \bar{u}(t_n))$ and

$$\tilde{R}(\zeta, t_n) = \int_0^\zeta e^{i(\zeta-s)\Delta} f(u(t_n + s), \bar{u}(t_n + s)) ds - \zeta f^n. \quad (5.45)$$

Using the above expansion for u we rewrite the error term as

$$\begin{aligned} \mathcal{R}_3(\tau, t_n) = & \int_0^\tau e^{i(\tau-\zeta)\Delta} \left(f \left(e^{i\zeta\Delta} u(t_n) + \zeta f^n + \tilde{R}(\zeta, t_n), e^{-i\zeta\Delta} \bar{u}(t_n) + \zeta \bar{f}^n + \overline{\tilde{R}(\zeta, t_n)} \right) \right. \\ & \left. - f \left(e^{i\zeta\Delta} u(t_n), e^{-i\zeta\Delta} \bar{u}(t_n) \right) \right) d\zeta. \end{aligned} \quad (5.46)$$

For notational convenience we let $a_1 := e^{i\zeta\Delta} u(t_n) + \zeta f^n$. By Taylor expanding f around (a_1, \bar{a}_1) and $(e^{i\zeta\Delta} u(t_n), e^{-i\zeta\Delta} \bar{u}(t_n))$ respectively we obtain,

$$\begin{aligned} f \left(a_1 + \tilde{R}(\zeta, t_n), \bar{a}_1 + \overline{\tilde{R}(\zeta, t_n)} \right) &= f(a_1, \bar{a}_1) + E_1(\zeta) \\ f \left(a_1, \bar{a}_1 \right) &= f \left(e^{i\zeta\Delta} u(t_n), e^{-i\zeta\Delta} \bar{u}(t_n) \right) + E_2(\zeta) \end{aligned} \quad (5.47)$$

where

$$\begin{aligned} E_1(\zeta) = & \int_0^1 \partial_{v_1} f \left(a_1 + \theta \tilde{R}(\zeta, t_n), \bar{a}_1 + \theta \overline{\tilde{R}(\zeta, t_n)} \right) \cdot \tilde{R}(\zeta, t_n) \\ & + \partial_{v_2} f \left(a_1 + \theta \tilde{R}(\zeta, t_n), \bar{a}_1 + \theta \overline{\tilde{R}(\zeta, t_n)} \right) \cdot \overline{\tilde{R}(\zeta, t_n)} d\theta \end{aligned} \quad (5.48)$$

$$\begin{aligned} E_2(\zeta) = & \zeta \int_0^1 [\partial_{v_1} f \left(e^{i\zeta\Delta} u(t_n) + \theta \zeta f^n, e^{-i\zeta\Delta} \bar{u}(t_n) + \theta \zeta \bar{f}^n \right) \cdot f^n \\ & + \partial_{v_2} f \left(e^{i\zeta\Delta} u(t_n) + \theta \zeta f^n, e^{-i\zeta\Delta} \bar{u}(t_n) + \theta \zeta \bar{f}^n \right) \cdot \bar{f}^n] d\theta, \end{aligned} \quad (5.49)$$

and $\partial_{v_1} f$ together with $\partial_{v_2} f$ are given in (5.20). Hence, plugging the above into equation (5.46) yields,

$$\begin{aligned}\mathcal{R}_3(\tau, t_n) &= \int_0^\tau e^{i(\tau-\zeta)\Delta} E_1(\zeta) d\zeta + \int_0^\tau e^{i(\tau-\zeta)\Delta} E_2(\zeta) d\zeta \\ &= \mathcal{E}_1(\tau, t_n) + \mathcal{E}_2(\tau, t_n).\end{aligned}\quad (5.50)$$

We first deal with the term in the decomposition above which is of highest order and hence is the simplest to bound, namely the third order term $\mathcal{E}_1(\tau, t_n)$. In view of obtaining the bound (5.42) on $(\mathcal{R}_2 + \mathcal{R}_3)(\tau, t_n)$, we first show that $\mathcal{E}_1(\tau, t_n)$ satisfies this bound.

Lemma 5.4.5 *We have the following fractional bound on $\mathcal{E}_1(\tau, t_n)$,*

$$\|\mathcal{E}_1(\tau, t_n)\| \leq C(\sup_{[0, T]} \|u(t)\|_\sigma, \sup_{[0, T]} \|u(t)\|_{2\gamma}) \tau^{2+\gamma},$$

for any $\gamma \in [0, 1]$, and $\sigma > d/2$.

Proof. It follows from (5.48) that in order to obtain the above bound we need to show that

$$\|E_1(\zeta)\| \leq C(\sup_{[0, T]} \|u(t)\|_\sigma, \sup_{[0, T]} \|u(t)\|_{2\gamma}) \zeta^{1+\gamma}.$$

By equation (5.48) and by using the Sobolev embedding $H^\sigma \hookrightarrow L^\infty$ we have that for all $\sigma > \frac{d}{2}$,

$$\begin{aligned}\|E_1(\zeta)\| &\leq \sup_{\theta \in]0, 1[} \left(\|\partial_{v_1} f(a_1 + \theta \tilde{R}(\zeta, t_n), \bar{a}_1 + \theta \overline{\tilde{R}(\zeta, t_n)})\|_\sigma \right. \\ &\quad \left. + \|\partial_{v_2} f(a_1 + \theta \tilde{R}(\zeta, t_n), \bar{a}_1 + \theta \overline{\tilde{R}(\zeta, t_n)})\|_\sigma \right) \|\tilde{R}(\zeta, t_n)\| \\ &\leq C \left(\sup_{t \in [0, T]} \|u(t)\|_\sigma, \sup_{(\zeta, t) \in [0, \tau] \times [0, T]} \|\tilde{R}(\zeta, t)\|_\sigma \right) \|\tilde{R}(\zeta, t_n)\|,\end{aligned}\quad (5.51)$$

where the last inequality follows by using the explicit form of the derivatives (5.20), the bilinear inequality (5.13), the first estimate of equation (5.18), and the fact that $e^{i\zeta\Delta}$ is an isometry on Sobolev spaces. Next, we show that

$$\sup_{(\zeta, t) \in [0, \tau] \times [0, T]} \|\tilde{R}(\zeta, t)\|_\sigma < \infty, \quad \text{and} \quad \|\tilde{R}(\zeta, t_n)\| \leq C_T (\sup_{[0, T]} \|u(t)\|_\sigma, \sup_{[0, T]} \|u(t)\|_{2\gamma}) \zeta^{1+\gamma}.\quad (5.52)$$

We obtain the first bound by using the first estimate of equation (5.18) on f with $r = \sigma$,

$$\sup_{(\zeta, t) \in [0, \tau] \times [0, T]} \|\tilde{R}(\zeta, t)\|_\sigma \leq \tau C (\sup_{t \in [0, T]} \|u(t)\|_\sigma) < +\infty.$$

Next, we obtain the second fractional estimate of equation (5.52) by making the following decomposition,

$$\tilde{R}(\zeta, t_n) = \tilde{R}_1(\zeta, t_n) + \tilde{R}_2(\zeta, t_n),\quad (5.53)$$

with

$$\tilde{R}_1(\zeta, t_n) = \int_0^\zeta (\zeta - s)^\gamma \frac{(e^{i(\zeta-s)\Delta} - 1)}{(-(\zeta - s)\Delta)^\gamma} (-\Delta)^\gamma f(u(t_n + s), \bar{u}(t_n + s)) ds$$

and

$$\tilde{R}_2(\zeta, t_n) = \int_0^\zeta f(u(t_n + s), \bar{u}(t_n + s)) ds - \zeta f^n.$$

Using the fractional bound (5.19) and the nonlinear estimate (5.18) we have that $\tilde{R}_1(\zeta, t_n)$ is bounded by

$$\|\tilde{R}_1(\zeta, t_n)\| \leq \zeta^{1+\gamma} C (\sup_{t \in [0, T]} \|u(t)\|_\sigma, \sup_{t \in [0, T]} \|u(t)\|_{2\gamma}).$$

Next, by iterating Duhamel's formula in the first term of $\tilde{R}_2(\zeta, t_n)$ we obtain the following expansion for $\tilde{R}_2(\zeta, t_n)$,

$$\tilde{R}_2(\zeta, t_n) = \tilde{R}_{2,1}(\zeta, t_n) + \tilde{R}_{2,2}(\zeta, t_n),\quad (5.54)$$

where

$$\tilde{R}_{2,1}(\zeta, t_n) = \int_0^\zeta f(e^{is\Delta} u(t_n), e^{-is\Delta} \bar{u}(t_n)) ds - \zeta f^n,$$

$$\begin{aligned} \tilde{R}_{2,2}(\zeta, t_n) = & \int_0^\zeta \int_0^1 \partial_{v_1} f \left(e^{is\Delta} u(t_n) + \theta \tilde{R}_{2,2}^r(s), e^{-is\Delta} \bar{u}(t_n) + \theta \overline{\tilde{R}_{2,2}^r(\zeta)} \right) \cdot \tilde{R}_{2,2}^r(s) \\ & + \partial_{v_2} f \left(e^{is\Delta} u(t_n) + \theta \tilde{R}_{2,2}^r(s), e^{-is\Delta} \bar{u}(t_n) + \theta \overline{\tilde{R}_{2,2}^r(s)} \right) \cdot \overline{\tilde{R}_{2,2}^r(s)} d\theta ds, \end{aligned}$$

and $\tilde{R}_{2,2}^r(s) = \int_0^s e^{i(s-s_1)\Delta} f(u(t_n + s_1), \bar{u}(t_n + s_1)) ds_1$.

Using the nonlinear estimate (5.18), one easily obtains the bound

$$\|\tilde{R}_{2,2}(\zeta, t_n)\| \leq C(\sup_{[0,T]} \|u(t)\|_\sigma) \zeta^2,$$

and hence in particular the $\zeta^{1+\gamma}$ bound for $\gamma \in [0, 1]$.

In order to deal with the first term in the decomposition (5.54), we Taylor expand the exponentials appearing in $\tilde{R}_{2,1}(\zeta, t_n)$ which yields,

$$\begin{aligned} \tilde{R}_{2,1}(\zeta, t_n) = & \int_0^\zeta \int_0^1 \partial_{v_1} f \left(u(t_n) + \theta(e^{is\Delta} - 1)u(t_n), \bar{u}(t_n) + \theta(e^{-is\Delta} - 1)\bar{u}(t_n) \right) \cdot \tilde{R}_{2,1}^r(s) \\ & + \partial_{v_2} f \left(u(t_n) + \theta(e^{is\Delta} - 1)u(t_n), \bar{u}(t_n) + \theta(e^{-is\Delta} - 1)\bar{u}(t_n) \right) \cdot \overline{\tilde{R}_{2,1}^r(s)} d\theta ds, \end{aligned}$$

with $\tilde{R}_{2,1}^r(s) = s^\gamma \frac{(e^{is\Delta} - 1)}{(-s\Delta)^\gamma} (-\Delta)^\gamma u(t_n)$. Using the fractional estimate (5.19) we obtain the bound

$$\|\tilde{R}_{2,1}^r(s)\| \leq C_T(\sup_{[0,T]} \|u(t)\|_{2\gamma}) s^\gamma.$$

Therefore, by using the usual bilinear inequality (5.13) we achieve the desired bound on $\tilde{R}_{2,1}$;

$$\|\tilde{R}_{2,1}(\zeta)\| \leq C(\sup_{[0,T]} \|u(t)\|_\sigma, \sup_{[0,T]} \|u(t)\|_{2\gamma}) \zeta^{1+\gamma},$$

which concludes the proof of Lemma 5.4.5. □

Now that we have dealt with the third order term $\mathcal{E}_1(t_n, \tau)$ in the decomposition (5.50) of $\mathcal{R}_3(t_n, \tau)$, we are left to consider the term $\mathcal{E}_2(t_n, \tau)$, together with the term $\mathcal{R}_2(t_n, \tau)$ defined at equation (5.29). First, we rewrite $\mathcal{E}_2(t_n, \tau)$ as a second order term with a third order remainder. The goal being that this second order term cancels with the second order part of the term $\mathcal{R}_2(t_n, \tau)$, thereby only leaving third order remainders.

By using the definition of $\partial_{v_1} f$ and $\partial_{v_2} f$ given in (5.20) we have that

$$E_2(\zeta) = -i\zeta \int_0^1 [2(e^{i\zeta\Delta} u(t_n) + \theta\zeta f^n)(e^{-i\zeta\Delta} \bar{u}(t_n) + \theta\zeta \bar{f}^n) f^n + (e^{i\zeta\Delta} u(t_n) + \theta\zeta f^n)^2 \bar{f}^n] d\theta.$$

We can separate the first order terms in the above with the higher order ones to obtain the following decomposition for $E_2(\zeta)$,

$$E_2(\zeta) = \tilde{E}_2(\zeta) + E_2^r(\zeta),$$

with

$$\tilde{E}_2(\zeta) = -i\zeta \left(2(e^{i\zeta\Delta} u(t_n))(e^{-i\zeta\Delta} \bar{u}(t_n)) f^n + (e^{i\zeta\Delta} u(t_n))^2 \bar{f}^n \right),$$

and where one can easily show using the nonlinear estimate (5.18) with $r = \sigma$ that $E_2^r(\zeta)$ has the following bound: $\|E_2^r(\zeta)\| \leq C_T(\sup_{[0,T]} \|u(t)\|_\sigma) \zeta^2$.

We let

$$\tilde{\mathcal{E}}_2(\tau, t_n) = \int_0^\tau e^{i(\tau-\zeta)\Delta} \tilde{E}_2(\zeta) d\zeta \quad \text{and} \quad \tilde{\mathcal{E}}_2^r(\tau, t_n) = \int_0^\tau e^{i(\tau-\zeta)\Delta} E_2^r(\zeta) d\zeta,$$

where the error term produced has the bound $\|\tilde{\mathcal{E}}_2^r(\tau, t_n)\| \leq C(\sup_{[0,T]} \|u(t)\|_\sigma) \tau^3$, which in particular satisfies the $\tau^{2+\gamma}$ bound for $\gamma \in [0, 1]$.

It remains to show that the sum of the remaining terms to bound $(\mathcal{R}_2 + \tilde{\mathcal{E}}_2)(\tau, t_n)$ also satisfy the $\tau^{2+\gamma}$ bound given in equation (5.42). In view of this, one last approximation step is made on the term $\tilde{\mathcal{E}}_2(\tau, t_n)$ before estimating its sum with the term $\mathcal{R}_2(\tau, t_n)$. By Taylor expanding around $\zeta = \tau$ the function $\zeta \mapsto e^{i(\tau-\zeta)\Delta} (\tilde{E}_2(\zeta)/\zeta)$ we obtain the following approximation of $\tilde{\mathcal{E}}_2$,

$$\tilde{\mathcal{E}}_2(\tau, t_n) = \tilde{\mathcal{E}}_{2,1}(\tau, t_n) + \tilde{\mathcal{E}}_{2,1}^r(\tau, t_n),$$

with

$$\tilde{\mathcal{E}}_{2,1}(\tau, t_n) = -i\frac{\tau^2}{2} \left(2(e^{i\tau\Delta}u(t_n))(e^{-i\tau\Delta}\bar{u}(t_n))f^n + (e^{i\tau\Delta}u(t_n))^2\bar{f}^n \right), \quad (5.55)$$

and where $\tilde{\mathcal{E}}_{2,1}^r(\tau)$ satisfies

$$\|\tilde{\mathcal{E}}_{2,1}^r(\tau)\| \leq C(\sup_{[0,T]} \|u(t)\|_\sigma, \sup_{[0,T]} \|u(t)\|_{2\gamma})\tau^{2+\gamma}.$$

The above estimate follows from the definition of \tilde{E}_2 , the estimate (5.19), and the expansion

$$e^{i\tau\Delta}v + (e^{i\zeta\Delta} - e^{i\tau\Delta})v = e^{i\tau\Delta}v + \left(\zeta^\gamma \frac{(e^{i\zeta\Delta} - 1)}{(-\zeta\Delta)^\gamma} + \tau^\gamma \frac{(1 - e^{i\tau\Delta})}{(-\tau\Delta)^\gamma} \right) (-\Delta)^\gamma v.$$

The first estimate (5.42) of Proposition 5.4.4 then follows directly once the following lemma is established.

Lemma 5.4.6 *The remaining error terms have the following bound,*

$$\|\mathcal{R}_2(\tau, t_n) + \tilde{\mathcal{E}}_{2,1}(\tau, t_n)\| \leq C(\sup_{[0,T]} \|u(t)\|_\sigma, \sup_{[0,T]} \|u(t)\|_{2\gamma})\tau^{2+\gamma}, \quad (5.56)$$

for any $\sigma > d/2$.

Proof. We perform a very similar analysis as was done on the term $\mathcal{R}_3(\tau, t_n)$ to the term $\mathcal{R}_2(\tau, t_n)$ to show that it can be decomposed as a second and third order term. We then conclude by showing that this second order part coincides with the second order term $-\tilde{\mathcal{E}}_{2,1}(\tau, t_n)$.

First, we expand $\varphi^\tau(u(t_n))$ as follows,

$$\varphi^\tau(u(t_n)) = e^{i\tau\Delta}u(t_n) + \tau f^n + R^1(\tau, t_n), \quad (5.57)$$

where

$$R^1(\tau, t_n) = \Psi^\tau(u(t_n), \varphi^\tau(u(t_n))) - \tau f^n,$$

and Ψ^τ is the nonlinear part of the numerical scheme (5.5). We show the same bounds in X^σ and L^2 given in equation (5.52) on the error term $R^1(\tau, t_n)$. First, using the estimate (5.18) with $r = \sigma$ we have that

$$\sup_{t \in [0, T]} \|R^1(\tau, t)\|_\sigma \leq \tau C(\sup_{[0, T]} \|u(t)\|_\sigma, \sup_{[0, T]} \|\varphi^\tau(u(t))\|_\sigma) \leq C(\sup_{[0, T]} \|u(t)\|_\sigma) < \infty,$$

where we use the bound

$$\|\varphi^\tau(u(t))\|_\sigma \leq 2\|u(t)\|_\sigma, \quad (5.58)$$

which follows from equation (5.23). We note that in what follows we will always use the above a priori bound (5.58) when bounding the term $\varphi^\tau(u(t_n))$, and hence will not show its explicit dependence. In order to obtain the L^2 -bound on $R^1(\tau, t_n)$ we use the following expansion

$$\begin{aligned} R^1(\tau, t_n) &= -i\frac{\tau}{2} e^{i\tau\Delta} \left((u(t_n))^2 \varphi_1(-i\tau\Delta) \overline{u(t_n)} \right) - i\frac{\tau}{2} \left(\left(e^{i\tau\Delta}u(t_n) + \Psi^\tau(u(t_n), \varphi^\tau(u(t_n))) \right)^2 \right. \\ &\quad \left. \varphi_1(i\tau\Delta) \left(e^{-i\tau\Delta} \overline{u(t_n)} + \overline{\Psi^\tau(u(t_n), \varphi^\tau(u(t_n)))} \right) \right) - \tau f^n \end{aligned} \quad (5.59)$$

where we used equation (5.5) and simply inserted into the term $\Psi^\tau(u(t_n), \varphi^\tau(u(t_n)))$ the definition of the scheme

$$\varphi^\tau(u(t_n)) = e^{i\tau\Delta}u(t_n) + \Psi^\tau(u(t_n), \varphi^\tau(u(t_n))).$$

By expanding about $e^{i\tau\Delta}u(t_n)$ the second term in (5.59), and then by approximating the remaining exponentials using the usual fractional estimate (5.19), we obtain that the first-order terms cancel leaving the following bound on $R^1(\tau, t_n)$,

$$\begin{aligned} \|R^1(\tau, t_n)\| &\leq \tau^{1+\gamma} C(\sup_{[0, T]} \|u(t)\|_{2\gamma}, \sup_{[0, T]} \|u(t)\|_\sigma) + \tau C(\sup_{n\tau \leq T} \|\Psi^\tau(u(t_n), \varphi^\tau(u(t_n)))\|_\sigma) \\ &\leq \tau^{1+\gamma} C(\sup_{[0, T]} \|u(t)\|_{2\gamma}, \sup_{[0, T]} \|u(t)\|_\sigma), \end{aligned}$$

where in order to obtain the second line we used the estimate

$$\|\Psi^\tau(u(t_n), \varphi^\tau(u(t_n)))\| \leq C(\sup_{[0, T]} \|u(t)\|_\sigma)\tau.$$

We make note that in order to approximate the φ_1 functions appearing in (5.59) we use the following expansion

$$\tau\varphi_1(i\tau\Delta)v = \int_0^\tau e^{is\Delta} ds v = \tau v + \int_0^\tau \frac{(e^{is\Delta} - 1)}{(-s\Delta)^\gamma} s^\gamma ds (-\Delta)^\gamma v. \quad (5.60)$$

We conclude from the above calculations that the error term $R^1(\tau, t_n)$ satisfies the X^σ and L^2 bounds,

$$\sup_{t \in [0, T]} \|R^1(\tau, t)\|_\sigma < \infty \quad \text{and} \quad \|R^1(\tau, t_n)\| \leq C(\sup_{[0, T]} \|u(t)\|_\sigma, \sup_{[0, T]} \|u(t)\|_{2\gamma}) \tau^{1+\gamma}. \quad (5.61)$$

We now return to the definition (5.29) of $\mathcal{R}_2(\tau, t_n)$ and to the expansion (5.57). By letting $b_1 = e^{i\tau\Delta}u(t_n) + \tau f^n$ we have

$$\begin{aligned} \psi_I^{\tau/2}(b_1 + R^1(\tau, t_n)) &= \psi_I^{\tau/2}(b_1) + \mathcal{E}_3(\tau, t_n) \\ \psi_I^{\tau/2}(b_1) &= \psi_I^{\tau/2}(e^{i\tau\Delta}u(t_n)) + \mathcal{E}_4(\tau, t_n), \end{aligned} \quad (5.62)$$

where using the estimates in equation (5.61) and the definition of $\psi_I^{\tau/2}$ it follows that

$$\|\mathcal{E}_3(\tau, t_n)\| \leq \tau^{2+\gamma} C(\sup_{[0, T]} \|u(t)\|_\sigma, \sup_{[0, T]} \|u(t)\|_{2\gamma}).$$

Furthermore, it follows from equation (5.62) that by isolating the second order terms with the higher order ones we have the following expansion for $\mathcal{E}_4(\tau, t_n)$,

$$\begin{aligned} \mathcal{E}_4(\tau, t_n) &= -i\frac{\tau^2}{2} \left(2f^n(e^{i\tau\Delta}u(t_n))(\varphi_1(i\tau\Delta)(e^{-i\tau\Delta}\overline{u(t_n)})) \right. \\ &\quad \left. + (e^{i\tau\Delta}u(t_n))^2 \varphi_1(i\tau\Delta)\overline{f^n} \right) + \mathcal{E}_4^r(\tau, t_n), \end{aligned} \quad (5.63)$$

where from a simple calculation one obtains that $\mathcal{E}_4^r(\tau, t_n)$ satisfies

$$\|\mathcal{E}_4^r(\tau, t_n)\| \leq C(\sup_{[0, T]} \|u(t)\|_\sigma) \tau^3 \leq C_T \tau^{2+\gamma}.$$

By approximating the φ_1 functions in (5.63) following the expansion given in equation (5.60), and by using once again the fractional estimate (5.19) we conclude from the above equations together with definition (5.55) of $\tilde{\mathcal{E}}_{2,1}$ that the bound (5.56) is met. This concludes the proof of Lemma 5.4.6. \square

The proof of the above lemma concludes the proof of the first estimate (5.42) on $(\mathcal{R}_2 + \mathcal{R}_3)(\tau, t_n)$ of Proposition 5.4.4.

The second estimate (5.43) of Proposition 5.4.4 follows directly from the first estimate (5.42) by noticing that for some small $\epsilon > 0$ and with $\sigma = d/2 + \epsilon$, we have that 2γ and σ are smaller than $2\gamma + 1$ for $\gamma > d/4$, and are also smaller than $\gamma + 1 + d/4$ for $d \leq 3$ (and $\gamma \in [0, 1]$). \square

Remark 5.4.7 Another way of writing the local error terms is as follows,

$$u(t_n + \tau) - \varphi^\tau(u(t_n)) = \mathcal{R}(\tau, t_n) + \tilde{\mathcal{R}}(\tau, t_n), \quad (5.64)$$

with

$$\begin{aligned} \mathcal{R}(\tau, t_n) &= \int_0^{\tau/2} e^{i(\tau-s)\Delta} \left(f(u(t_n+s), \bar{u}(t_n+s)) - f(e^{is\Delta}u(t_n), e^{-is\Delta}\bar{u}(t_n)) \right) ds \\ &\quad + \int_{\tau/2}^\tau e^{i(\tau-s)\Delta} \left(f(u(t_n+s), \bar{u}(t_n+s)) - f(e^{i(s-\tau)\Delta}u(t_{n+1}), e^{-i(s-\tau)\Delta}\bar{u}(t_{n+1})) \right) ds \end{aligned}$$

and

$$\begin{aligned} \tilde{\mathcal{R}}(\tau, t_n) &= \left(\int_0^{\tau/2} e^{i(\tau-s)\Delta} f(e^{is\Delta}u(t_n), e^{-is\Delta}\bar{u}(t_n)) ds - \psi_E^{\tau/2}(u(t_n)) \right) \\ &\quad + \left(\int_{\tau/2}^\tau e^{i(\tau-s)\Delta} f(e^{i(s-\tau)\Delta}u(t_{n+1}), e^{-i(s-\tau)\Delta}\bar{u}(t_{n+1})) ds - \psi_I^{\tau/2}(\varphi^\tau(u(t_n))) \right). \end{aligned}$$

The above error decomposition uses the fact that on $[0, \frac{\tau}{2}]$ we center the approximation at the left-end point and on $(\frac{\tau}{2}, \tau]$

at the right-end point. Hence, on each interval respectively we iterate the Duhamel expansions

$$\begin{aligned} u(t_n + s) &= e^{is\Delta} u(t_n) + \int_0^s e^{i(s-s_1)\Delta} f(u(t_n + s_1), \bar{u}(t_n + s_1)) ds_1, \quad s \in [0, \frac{\tau}{2}], \\ u(t_n + s) &= e^{i(s-\tau)\Delta} u(t_{n+1}) - \int_s^\tau e^{i(s-s_1)\Delta} f(u(t_n + s_1), \bar{u}(t_n + s_1)) ds_1, \quad s \in (\frac{\tau}{2}, \tau]. \end{aligned}$$

Using the tools in Section 5.4.1 one can bound the local error terms (5.64) in an analogous manner.

5.4.2 Stability

Theorem 5.4.1 *Let $R > 0$, $s \geq 0$. There exists $\tau_R > 0$ and $\sigma > d/2$ such that for any $\tau \leq \tau_R$ and $w, v \in X^\sigma$, such that $\|w\|_\sigma \leq R$ and $\|v\|_\sigma \leq R$ we have,*

$$\|\varphi^\tau(v) - \varphi^\tau(w)\|_s \leq e^{\tau C_R} \|v - w\|_s,$$

where C_R denotes a generic constant depending on R (and on s).

Proof of Theorem 5.4.1. Using the second estimate in equation (5.18) we have

$$\|\varphi^\tau(v) - \varphi^\tau(w)\|_s \leq (1 + \tau C_s(\|v\|_\sigma, \|w\|_\sigma)) \|v - w\|_s + \tau C_s(\|\varphi^\tau(v)\|_\sigma, \|\varphi^\tau(w)\|_\sigma) \|\varphi^\tau(v) - \varphi^\tau(w)\|_s,$$

with $\sigma = d/2 + \epsilon$ if $s \leq d/2$ and $\sigma = s$ if $s > d/2$. By Theorem 5.3.1 we have that there exists $\tau_R > 0$ such that for all $\tau \leq \tau_R$ we have the bounds: $\|\varphi^\tau(v)\|_\sigma \leq 2R$ and $\|\varphi^\tau(w)\|_\sigma \leq 2R$. Hence, it follows from the above that,

$$\|\varphi^\tau(v) - \varphi^\tau(w)\|_s \leq \frac{(1 + \tau C_s(R, R))}{(1 - \tau C_s(2R, 2R))} \|v - w\|_s \leq e^{\tau C_R} \|v - w\|_s,$$

for some $C_R > 0$. □

It remains to combine the stability argument presented in Section 5.4.2 together with the local error bounds of Section 5.4.1 to prove the global convergence result stated in Proposition 5.4.1.

Proof of Proposition 5.4.1. We let $e^n = u^n - u(t_n)$, with $e^0 = 0$. First, thanks to Proposition 5.4.2 and 5.4.4 we have the local error bound in L^2 required for the global convergence analysis, where the regularity requirements on u have been optimized depending on the fractional order of convergence desired. In order to apply the stability bound stated in Theorem 5.4.1 and to conclude with a Lady Windermere's fan type argument, one needs to show the following uniform bound on the numerical solution,

$$\|u^n\|_\sigma \leq M_T, \quad \forall n\tau \leq T, \tag{5.65}$$

for some $\sigma > d/2$ and $M_T > 0$.

We let $\sigma = d/2 + \epsilon$, for some small $\epsilon > 0$. To obtain the bound (5.65) we show that there exists $\delta > 0$, a constant $C_{R_n} = C_T(\|u^n\|_\sigma)$ depending on $\|u^n\|_\sigma$ and on $\sup_{[0, T]} \|u(t)\|_\sigma$, and some $\tau_{R_n} > 0$ also depending on $\|u^n\|_\sigma$ such that the following global error bound is met,

$$\|e^{n+1}\|_\sigma \leq \|\varphi^\tau(u(t_n)) - u(t_{n+1})\|_\sigma + \|\varphi^\tau(u^n) - \varphi^\tau(u(t_n))\|_\sigma \leq C_{T, \gamma} \tau^{1+\delta} + e^{\tau C_{R_n}} \|e^n\|_\sigma \tag{5.66}$$

for all $\tau \leq \tau_{R_n}$. One can obtain the second term in the above estimate for $\tau \leq \tau_{R_n}$, where τ_{R_n} depends on $\|u^n\|_\sigma$ and on $\sup_{[0, T]} \|u(t)\|_\sigma$, by applying Theorem 5.4.1 with $s = \sigma$. Hence, it remains to obtain the first term in the above estimate, which corresponds to the local error bound in X^σ . Namely, by letting $\mathcal{R}(\tau, t_n) = u(t_{n+1}) - \varphi^\tau(u(t_n))$ we show that there exists $\delta > 0$ such that

$$\|\mathcal{R}(\tau, t_n)\|_\sigma \leq C_{T, \gamma} \tau^{1+\delta}, \tag{5.67}$$

where $C_{T, \gamma}$ is a constant depending on T and on the regularity assumptions on u (which in turn depend on γ , the fractional order of convergence required). We establish the above local error estimate (5.67) by using the following interpolation bound,

$$\|\mathcal{R}(\tau, t_n)\|_\sigma \leq \begin{cases} \|\mathcal{R}(\tau, t_n)\|^\theta \|\mathcal{R}(\tau, t_n)\|_{2\gamma+1}^{1-\theta} & \text{if } \gamma > \frac{d}{4} \\ \|\mathcal{R}(\tau, t_n)\|^{\tilde{\theta}} \|\mathcal{R}(\tau, t_n)\|_{\gamma+1+\frac{d}{4}}^{1-\tilde{\theta}} & \text{if } 0 \leq \gamma < \frac{d}{4} \end{cases}, \tag{5.68}$$

where $(\theta, \tilde{\theta}) \in (0, 1)^2$ satisfies $\sigma = (1 - \theta)(2\gamma + 1) = (1 - \tilde{\theta})(\gamma + 1 + d/4)$. We have already established the L^2 -bound on

$\mathcal{R}(\tau, t_n)$ in Section 5.4.1, which is given by,

$$\|\mathcal{R}(\tau, t_n)\| \leq \tau^{2+\gamma} \begin{cases} C_{T,\gamma} \left(\sup_{t \in [0, T]} \|u(t)\|_{2\gamma+1} \right) & \text{if } \gamma > \frac{d}{4} \\ C_{T,\gamma} \left(\sup_{t \in [0, T]} \|u(t)\|_{\gamma+1+\frac{d}{4}} \right) & \text{if } 0 \leq \gamma < \frac{d}{4} \end{cases}. \quad (5.69)$$

To obtain the $X^{2\gamma+1}$ and $X^{\gamma+1+\frac{d}{4}}$ bound on $\mathcal{R}(\tau, t_n)$ we simply express the local error using Duhamel's formula and the scheme (5.5),

$$\begin{aligned} \mathcal{R}(\tau, t_n) = & \int_0^\tau e^{i(\tau-s)\Delta} f(u(t_n+s), \bar{u}(t_n+s)) ds - i \frac{\tau}{2} e^{i\tau\Delta} ((u(t_n))^2 \varphi_1(-i\tau\Delta) \bar{u}(t_n)) \\ & - i \frac{\tau}{2} \left((\varphi^\tau(u(t_n)))^2 \varphi_1(i\tau\Delta) \overline{\varphi^\tau(u(t_n))} \right). \end{aligned}$$

One can bound each of the above terms separately using the first estimate in equation (5.18) with $s = 2\gamma + 1$ and $s = \gamma + 1 + \frac{d}{4}$ together with equation (5.23) (with $R = \sup_{[0, T]} \|u(t)\|_s$) to obtain that there exists some $\tilde{\tau}_0 > 0$ depending on u_0 and T such that for all $\tau \leq \tilde{\tau}_0$

$$\|\mathcal{R}(\tau, t_n)\|_s \leq C(\sup_{[0, T]} \|u(t)\|_s) \tau \leq C_{T,s} \tau. \quad (5.70)$$

We conclude that the bound (5.67) follows from equation (5.68) (with $\delta = (1 + \gamma)\theta$ for $\gamma > d/4$ and $\delta = (1 + \gamma)\tilde{\theta}$ for $\gamma < d/4$), and where the constant $C_{T,\gamma}$ is given in equation (5.69) by the L^2 local error bound. We then proceed by induction on (5.66) to obtain that there exists a $\tau_0 > 0$ which depends on T and u_0 for which the uniform bound (5.65) is true for all $\tau \leq \tau_0$.

Finally, by taking $s = 0$, $\sigma = d/2 + \epsilon$, and $R = \max\{M_T, \sup_{[0, T]} \|u(t)\|_\sigma\}$ in Theorem 5.4.1 yields the existence of a τ_R which depends on T and u_0 such that for all $\tau \leq \tau_R$,

$$\|e^{n+1}\| \leq C_{T,\gamma} \tau^{2+\gamma} + e^{\tau C_R} \|e^n\|, \quad n\tau \leq T,$$

where $C_{T,\gamma}$ is given in equation (5.69). The global error bound of Proposition 5.4.1 follows by iterating the above estimate and taking $\tau_{\min} = \min\{\tau_0, \tau_R\}$, which concludes the proof. \square

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Chapter 6

Symmetric resonance based integrators and forest formulae

This chapter is based on the article [ABBMS23], and the numerical simulations presented here are taken from that article.

Abstract. In the present work we introduce a unified framework that allows for the very first systematic construction of symmetric resonance-based integrators to approximate a wide class of nonlinear dispersive equations at low-regularity. The inclusion of symmetries in the construction of resonance-based schemes presents serious challenges and induces a need for a significant extension of prior approaches to allow for sufficient number of degrees of freedom in the resulting schemes while preserving the favorable low-regularity convergence properties of prior constructions. Motivated by recent work [BS22], we achieve this by introducing a novel formalism based on forest formulae that allows us to encode a wider range of possibilities of iterating Duhamel’s formula and interpolatory approximations of lower order parts in the construction of these time-stepping methods. The forest formulae allow for a simple characterisation of symmetric schemes and provides a fascinating algebraic structure in its own right which echo those used in Quantum Field Theory for renormalising Feynman diagrams and those used for the renormalisation of singular SPDEs via the theory of Regularity Structures. Our constructions lead to the development of several new symmetric resonance-based integrators that exhibit remarkable structure preservation and convergence properties which are witnessed in numerical experiments.

6.1 Introduction

We consider a general class of dispersive differential equations of the form

$$\begin{aligned} i\partial_t u(t, x) + \mathcal{L}(\nabla, \frac{1}{\varepsilon})u(t, x) &= |\nabla|^\alpha p(u(t, x), \bar{u}(t, x)), \\ u(0, x) &= v(x), \end{aligned} \tag{6.1}$$

equipped with periodic boundary conditions $x \in \mathbb{T}^d$. Throughout, we assume that p is a polynomial nonlinearity, and that the structure of (6.1) implies at least local well-posedness of the problem on a finite time interval $[0, T]$, $T < \infty$, in an appropriate functional space. This class of equations captures a number of physically important models, including the Korteweg de Vries (KdV) equation

$$\partial_t u - i\mathcal{L}(\nabla)u = \frac{1}{2}\partial_x u^2, \quad \mathcal{L}(\nabla) = i\partial_x^3, \quad |\nabla|^\alpha = \partial_x, \quad x \in \mathbb{T}, \tag{6.2}$$

and the nonlinear Schrödinger (NLS) equation,

$$i\partial_t u + \mathcal{L}(\nabla)u = |u|^2 u, \quad \mathcal{L}(\nabla) = \Delta, \quad x \in \mathbb{T}^d. \tag{6.3}$$

Like those two examples many physical equations in this class possess conservation laws, or are indeed integrable systems (for example the KdV equation is a completely integrable parity-time invariant system). It is known that symmetric numerical schemes have favourable long-time behaviour when applied to such reversible integrable systems, such as linear (slow) growth in error as a function of the integration time, and near conservation of first integrals over long times [HL04, HLW10, BG94]. At the same time the numerical approximation of the Cauchy problem in low-regularity regimes requires the design of designated methods, amongst which resonance-based schemes have seen significant success over recent years. Firstly developed for specific equations, including the KdV equation [HS17b, WZ22b, LW22], the NLS

equation [OS18, OWY22, AB23b, ORS21, ORS22b, WY22, BLW23], the Gross–Pitaevskii equation [AB23a] and the Navier–Stokes equations [NS15], more recent work has started to establish a more general framework for resonance based low-regularity integrators [ABBS22b, ABBS22a, RS22]. The key idea of these schemes lies in embedding the underlying structure of resonances - triggered by the nonlinear frequency interactions between the leading differential operator $\mathcal{L}(\nabla, \frac{1}{\varepsilon})$ and the nonlinearity $p(u(t, x), \bar{u}(t, x))$ - into the numerical discretisation. These nonlinear interactions are in general neglected by classical approximation techniques such as Runge–Kutta methods, splitting methods or exponential integrators. While for smooth solutions these nonlinear interactions are indeed negligible, they do play a central role at low regularity and high oscillations. The accurate resolution of these interactions has been achieved in broad generality only in the recent few years in [BS22, RS21, ABBS22b]. Yet, while the design of such schemes has seen a wide range of developments, prior work has focussed mostly on explicit schemes with desired convergence properties. A few recent results [BMS22, AB23b, FMS23, MS22] have introduced first or second order implicit symmetric integrators at low-regularity fitting the particular structure of the equation with better conservation properties. Nevertheless, a central question remained unanswered: *Can we systematically construct structure preserving resonance based schemes up to arbitrary order which preserve central symmetries of the underlying continuous equation?*

For ordinary differential equations (ODEs) the theory of *structure preservation* in numerical schemes is thoroughly established [HLW10], specifically there is a extensive amount of literature on the characterisation of symmetric and symplectic Runge–Kutta methods [Kul03, SS88, IZ00] and, more broadly, B-series methods [BS94, CM07]; on the favourable long-time behaviour of such methods when applied for finite-dimensional integrable reversible systems and Hamiltonian systems [HL04, HLW10, BG94] respectively; and even on the limitations on types of structure that can be preserved with B-series methods [IQT07]. Even though the long-time analysis of such methods in the case of PDEs is much less straightforward [Fao12, GL10b], these favourable structure preservation properties have motivated the study of symmetric methods for PDEs, for example in the classification of symmetric splitting methods [MQ02] and symmetric exponential integrators [CCO08].

In general, resonance based schemes are *not* structure preserving and do not preserve the symmetries in the system. We can consider for example the second order resonance based scheme introduced by [BS22, Section 5.1.2], referred to henceforth as ‘Bruned & Schratz 2022’, and given by

$$\begin{aligned} u^{n+1} = & e^{i\tau\Delta} u^n - i\tau e^{i\tau\Delta} \left((u^n)^2 (\varphi_1(-2i\tau\Delta) - \varphi_2(-2i\tau\Delta)) \overline{u^n} \right) \\ & - i\tau \left(e^{i\tau\Delta} u^n \right)^2 \varphi_2(-2i\tau\Delta) (e^{i\tau\Delta} \overline{u^n}) - \frac{\tau^2}{2} e^{i\tau\Delta} (|u^n|^4 u^n), \end{aligned} \quad (6.4)$$

where $\varphi_1(\sigma) = \frac{e^\sigma - 1}{\sigma}$ and $\varphi_2(\sigma) = \frac{e^\sigma - \varphi_1(\sigma)}{\sigma}$. Symmetry of a numerical scheme is defined by considering its adjoint method: For a given method $u^n \mapsto u^{n+1} = \Phi_\tau(u^n)$ its adjoint method is defined as $\widehat{\Phi}_\tau := \Phi_{-\tau}^{-1}$.

Definition 1 (See for example Definition V.1.4 in [HLW10]) *The method Φ_τ is called symmetric if $\Phi_\tau = \widehat{\Phi}_\tau$.*

The scheme (6.4) is not symmetric in the sense of definition (1) because the adjoint method is given by

$$\begin{aligned} u^{n+1} = & e^{i\tau\Delta} u^n - i\tau \left((u^{n+1})^2 (\varphi_1(2i\tau\Delta) - \varphi_2(2i\tau\Delta)) \overline{u^{n+1}} \right) \\ & - i\tau e^{i\tau\Delta} \left((e^{-i\tau\Delta} u^{n+1})^2 \varphi_2(2i\tau\Delta) (e^{-i\tau\Delta} \overline{u^{n+1}}) \right) \\ & + \frac{\tau^2}{2} (|u^{n+1}|^4 u^{n+1}), \end{aligned}$$

which is implicit as opposed to the original scheme (6.4), which is explicit.

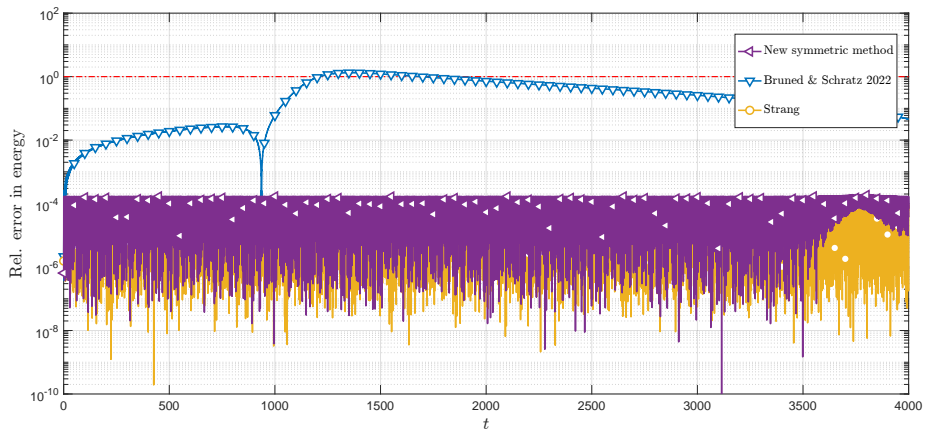
The derivation of new schemes which are structure preserving and at the same time allow for low-regularity approximations was first addressed in the specific case of the KdV, the Klein–Gordon (KG), the NLS equation and the isotropic Landau–Lifschitz equation in the recent work of [MS23], [WZ22a], [AB23b] and [BMS22] respectively. A further symmetric low-regularity integrator with good long time behaviour was introduced in [FMS23]; see also [MS23] for the construction of symplectic resonance-based schemes. Let us also highlight the work [WY22] which was the first low regularity method which allowed for high order mass conservation (for fixed time). However, all these results are yet again tailored to the particular structure of the equation, and bespoke calculations made on individual resonance structure of the equation at hand. Furthermore, they are restricted to second order and not always optimal in the sense of regularity.

This motivates the study of systematic constructions of symmetric resonance based schemes that we address in the present work. In particular, we develop a unified framework of symmetric resonance based schemes which preserve central symmetries of the system (6.1) while allowing for good approximation in the regimes treated by [BS22]. We extend the resonance decorated trees approach introduced in [BS22] to a richer framework by exploring different ways of iterating Duhamel’s formula, capturing the dominant parts while interpolating the lower parts of the resonances in a symmetric

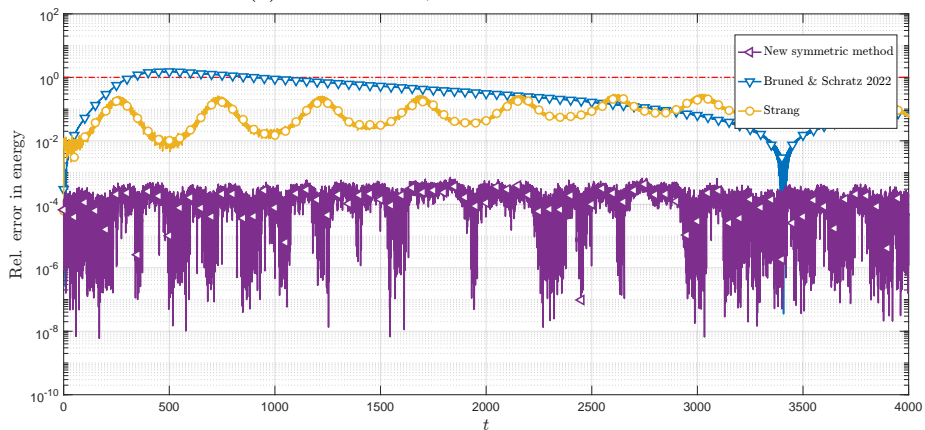
manner. This gives a range of new numerical schemes with more degrees of freedom than the original framework from [BS22]. Our new framework allows us to recover previously constructed low-regularity symmetric schemes such as [AB23b], but also introduce new symmetric low regularity schemes which are optimal in the sense of regularity - in the spirit of [BS22]. An example of such a method introduced in the present work is (6.63) matching the regularity obtained for the non-symmetric scheme given in [BS22]. In addition, as opposed to the previous works [BS22, ABBS22a, ABBS22b] the schemes we introduce here do not need to be accompanied by well-chosen filter functions in order to obtain stability of the scheme. Indeed, our construction based on interpolation rather than Taylor series expansion of the non-dominant parts of the nonlinear frequency interactions directly leads to stable schemes, see also [RS21, AB23a].

Our main result is the new general resonance based scheme presented in Definition (6.3.9), with its error structure given in Theorem (6.3.15), the latter of which is a consequence of [BS22]. We show that this scheme is symmetric in Theorem (6.4.3) and that it is contained within a forest formula in Theorem (6.3.11). Our general framework is illustrated on concrete examples in Section (6.4.3) and simulations show the better structure preserving properties as well as the convergence properties of the scheme. This was only possible through a significant extension of the algebraic structures proposed in [BS22] by introducing a new forest formula in Theorem (6.3.6). This formula is used for finding new symmetric schemes and have their own interest by providing a new parametrisation of low regularity schemes allowing for implicitness in the schemes and thus resembling more closely the formulation of classical schemes such as Runge–Kutta methods or exponential integrators. We derive conditions on the coefficients of these formulae for having a symmetric scheme, see Proposition (6.4.7).

Remark 6.1.1 Up to now we were faced with a choice between structure preservation and low-regularity approximation properties. This is exhibited in Figure (6.1) where we study the cubic NLS equation and compare the preservation of energy of the Strang splitting (a symmetric splitting method) against previous resonance based integrators (Bruned & Schratz 2022 [BS22]) for smooth C^∞ and H^2 data.



(a) Smooth data, $u_0 \in C^\infty$ and $M = 64$.

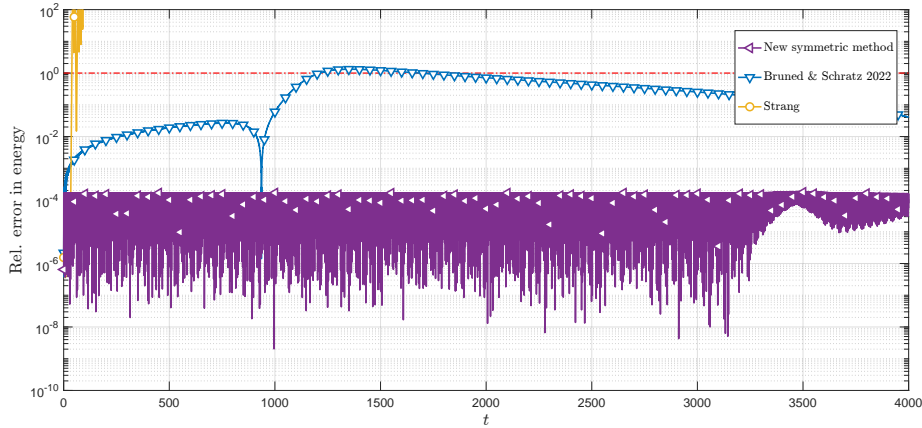


(b) Low regularity data, $u_0 \in H^2$ and $M = 64$.

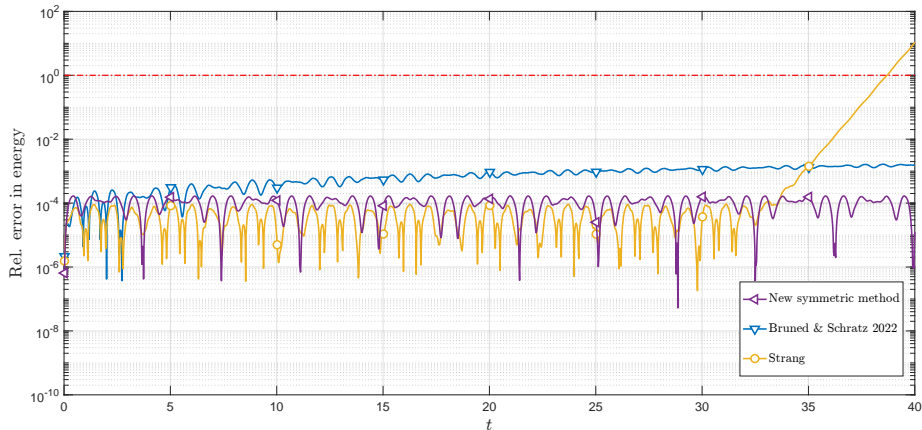
Figure 6.1 – Long-time relative error in the energy of the NLS equation with time-step $\tau = 0.02$.

The Strang splitting almost preserves the energy over long times for smooth solutions, but suffers from numerical energy blow up for rougher data. The resonance based integrator Bruned & Schratz 2022 [BS22] on the other hand only achieves approximate energy preservation up to short times (for both smooth and rougher data). Our novel resonance based midpoint method (6.63) bridges this gap allowing for numerical long-time approximate energy conservation even at low regularity, see Figure (6.1b).

Let us now take a closer look at smooth solutions, where we find a surprising additional characteristic of our new scheme (6.63). Note that long-time structure preservation properties apply only subject to a CFL condition for Strang splitting methods applied to the NLS equation. More precisely the time step size τ has to be chosen such that $\tau \lesssim M^{-2}$ where M is the number of degrees of freedom in the spatial discretisation, see for instance [Fao12] and references therein for a detailed discussion. This step size restriction is not only a theoretical technicality, but also observed in numerical experiments. The long-time energy preservation in the Strang splitting drastically breaks down if we start to increase the number of Fourier modes M , i.e., move from “ODE to PDE”, see Figure (6.1a) versus Figure (6.2), where we double the Fourier modes in our discretisation. A very interesting feature of our new resonance-based constructions appears to be that in numerical experiments the long-time behaviour of the method seemingly does not depend on the number M of spatial modes used.



(a) Long time interval $t \in [0, 4000]$, smooth data $u_0 \in C^\infty$ and $M = 256$.

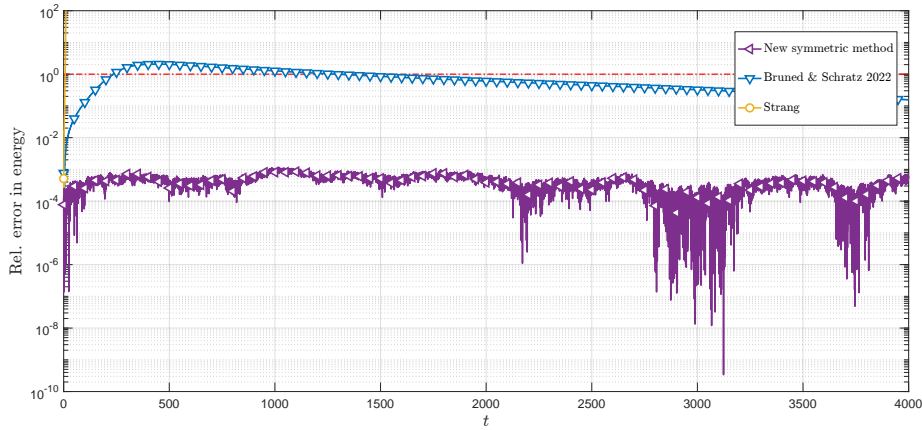
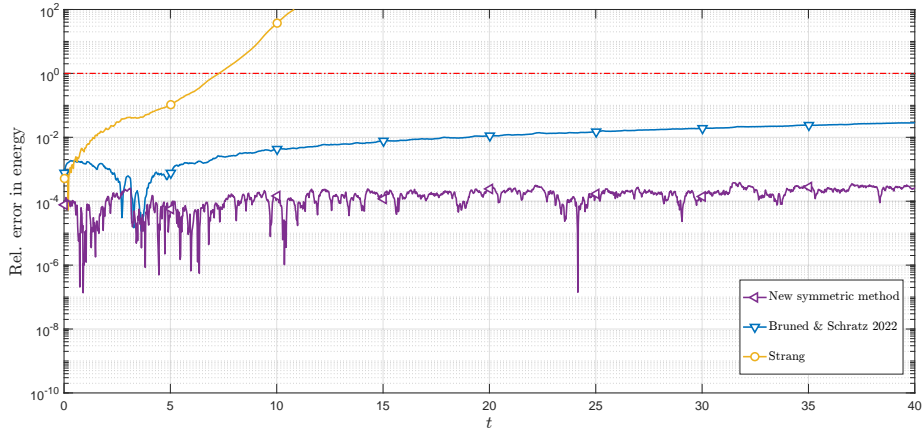


(b) Zoom on time interval $t \in [0, 40]$, smooth data $u_0 \in C^\infty$ and $M = 256$.

Figure 6.2 – Long-time relative error in the energy of the NLS equation with time-step $\tau = 0.02$.

In summary, the long-time dynamics shown in Figures (6.1)-(6.3) is representative of the behaviour of these methods and is observed in a large number of numerical experiments. Namely, we have that the Strang splitting is able to approximately preserve the energy over long times only for a small number of spatial discretisation points and for smooth initial data ($M \ll \tau^{-1/2}$). In contrast, our proposed symmetric low-regularity integrators can achieve this feat even for low regularity solutions and with a large number of spatial discretisation points.

Outline of the article

(a) Long time interval $t \in [0, 4000]$, low-regularity data $u_0 \in H^2$ and $M = 256$.(b) Zoom on time interval $t \in [0, 40]$, low-regularity data $u_0 \in H^2$ and $M = 256$.Figure 6.3 – Long-time relative error in the energy of the NLS equation with time-step $\tau = 0.02$.

The remainder of this manuscript is structured as follows. To begin with, in section (6.2), we outline the main ideas in the construction of symmetric resonance based schemes, before formalising those ideas more rigorously in the subsequent sections. In particular, in section (6.3) we firstly recall the decorated tree framework introduced in [BS22] for non-symmetric resonance based schemes. We then generalise this framework in order to capture a broader class of resonance based integrators allowing for polynomial interpolation of lower order parts in the approximation (cf. section (6.3.1)). This leads to a general framework taking the form of a forest formula that can capture a wide class of implicit and explicit resonance based schemes and which is introduced in section (6.3.2). This forest formula motivates our consideration of a particular way of iterating Duhamel’s formula to generate a subclass of resonance based schemes described by this general framework in section (6.3.3) which turns out to be sufficiently general to allow us to find symmetric resonance based schemes of arbitrary order in this class. In section (6.4) we then describe how symmetric interpolation in the construction from section (6.3.3) leads to symmetric schemes before classifying all symmetric schemes captured by the general forest formula in section (6.4.2). We conclude the section with examples of the new symmetric resonance based integrators that can be found using our novel framework in section (6.4.3). In section (6.5), we provide numerical experiments demonstrating the favorable practical performance of the new symmetric resonance based schemes that we were able to develop using our formalism.

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6.2 Main ideas of the derivation of symmetric resonance based schemes

Before diving into a more abstract construction of the algebraic structures describing our novel resonance based schemes let us begin by outlining the main assumptions on the type of equation we consider as well as the blueprint for the construction of implicit (and specifically symmetric) resonance based integrators for equations of the form (6.1).

Assumptions

We impose periodic boundary conditions, i.e. $x \in \mathbf{T}^d$. We assume that the differential operator \mathcal{L} is real and that the differential operators $\mathcal{L}(\nabla)$ and $|\nabla|^\alpha$ shall cast in Fourier space into the form

$$\mathcal{L}(\nabla)(k) = k^\sigma + \sum_{\gamma:|\gamma|<\sigma} a_\gamma \prod_j k_j^{\gamma_j}, \quad |\nabla|^\alpha(k) = \sum_{\gamma:|\gamma|\leq\alpha} \prod_{j=1}^d k_j^{\gamma_j} \quad (6.5)$$

for some $\alpha \in \mathbf{R}$, $\sigma \in \mathbf{N}$, $\gamma \in \mathbf{Z}^d$ and $|\gamma| = \sum_i \gamma_i$, where for $k = (k_1, \dots, k_d) \in \mathbf{Z}^d$ and $m = (m_1, \dots, m_d) \in \mathbf{Z}^d$ we set

$$k^\sigma = k_1^\sigma + \dots + k_d^\sigma, \quad k \cdot m = k_1 m_1 + \dots + k_d m_d.$$

Construction of implicit resonance based schemes

We first rewrite (6.1) in Duhamel's form

$$u(t, x) = e^{it\mathcal{L}} v(0, x) - ie^{it\mathcal{L}} \int_0^t e^{-is\mathcal{L}} |\nabla|^\alpha p(u(s, x), \bar{u}(s, x)) ds$$

where we have used $\mathcal{L} = \mathcal{L}(\nabla, \frac{1}{\varepsilon})$ as a short hand notation. Then, if we move to Fourier space by denoting u_k and v_k the k -th Fourier coefficients of u and v , one obtains:

$$u_k(t) = e^{it\mathcal{L}(k)} v_k(0) - ie^{it\mathcal{L}(k)} \int_0^t e^{-is\mathcal{L}(k)} |\nabla|^\alpha(k) p_k(u(s, x), \bar{u}(s, x)) ds \quad (6.6)$$

where $\mathcal{L}(k)$ and $|\nabla|^\alpha(k)$ are the differential operators \mathcal{L} and $|\nabla|^\alpha$ mapped in Fourier space. The term $p_k(u(s, x), \bar{u}(s, x))$ stands for the Fourier transform of the product. For example, in the case of NLS we have $\alpha = 0$, $\mathcal{L} = \Delta$, and $p(u, \bar{u}) = u^2 \bar{u}$. The equation (6.6) becomes

$$u_k(t) = e^{-itk^2} v_k(0) - ie^{-itk^2} \int_0^t e^{isk^2} \left(\sum_{k=-k_1+k_2+k_3} \bar{u}_{k_1}(s) u_{k_2}(s) u_{k_3}(s) \right) ds.$$

The product $|u|^2 u$ becomes a convolution on the coefficients in Fourier space, where we note that the minus pre-multiplying k_1 is due to the conjugate. We have also used the fact that the Fourier transform of $e^{it\Delta}$ is e^{-itk^2} . The first step in the construction of resonance based schemes consists in iterating (6.6) inside the nonlinearity which produces a sum of oscillatory integrals that can be described by decorated trees as introduced in [BS22]. Namely, in [BS22] we iterate only with (6.6) which corresponds to a left end point iteration, meaning that given a time step τ , we always take the left end point approximation in the linear part $\exp(-itk^2)v_k(0)$ on the interval $[0, \tau]$. Hence, in general we do not obtain a symmetric scheme. Indeed, one has the possibility to write Duhamel's formula around any point in the interval $[0, \tau]$. In particular, if we set for $s \in [0, \tau]$

$$I(k, u, s, t) = e^{i(t-s)\mathcal{L}(k)} u_k(s) - ie^{it\mathcal{L}(k)} \int_s^t e^{-i\tilde{s}\mathcal{L}(k)} |\nabla|^\alpha(k) p_k(u(\tilde{s}, x), \bar{u}(\tilde{s}, x)) d\tilde{s} \quad (6.7)$$

then we have the identity:

$$u_k(t) = I(k, u, v, s, t).$$

From the identity (6.7), we will obtain implicit schemes. We can take a weighted sum of the various Duhamel's iterations (6.7) ultimately to arrive at schemes with a large number of additional degrees of freedom. The sum that we will use for a large part of this paper is the midpoint rule, that is:

$$u_k(t) = \frac{1}{2} (I(k, u, 0, t) + I(k, u, \tau, t)). \quad (6.8)$$

For example, to construct a symmetric resonance based scheme of a desired order we can start the first iteration for $u_k(\tau)$ with the left end point Duhamel's formula and then we iterate the midpoint rule (6.8). We can express this iteration in terms of the following tree series

$$U_{\text{mid},k}^r(\tau) = e^{i\tau\mathcal{L}}u_k(0) + \sum_{T \in \mathcal{V}_k^r} \frac{\Upsilon_{\text{mid}}^p(T)(u, \tau)}{S(T)} (\Pi_{\text{mid}}T)(\tau) \quad (6.9)$$

where \mathcal{V}_k^r is a set of decorated trees of size at most $r + 1$ which incorporate the frequency k . These trees encode via $(\Pi_{\text{mid}}T)(\tau)$, iterated integrals of depth at most $r + 1$. The coefficient $S(T)$ is the symmetry factor associated to the tree T and $\Upsilon_{\text{mid}}^p(T)(u, \tau)$ is the coefficient appearing in the iteration of Duhamel's formulation depending on the nonlinearity p . The coefficients $\Upsilon_{\text{mid}}^p(T)(u, \tau)$ depend on τ as with our midpoint iteration, we finish always on terms of the form:

$$\frac{1}{2} \left(e^{is\mathcal{L}}u_{k_j}(0) + e^{i(s-\tau)\mathcal{L}}u_{k_j}(\tau) \right) = e^{is\mathcal{L}} \frac{1}{2} \left(u_{k_j}(0) + e^{-i\tau\mathcal{L}}u_{k_j}(\tau) \right).$$

It is natural to absorb the term $e^{is\mathcal{L}}$ in the definition of $(\Pi_{\text{mid}}T)(\tau)$ and

$$\frac{1}{2} \left(u_{k_j}(0) + e^{-i\tau\mathcal{L}}u_{k_j}(\tau) \right)$$

into the definition of $\Upsilon_{\text{mid}}^p(T)(u, \tau)$. These aforementioned quantities are described in detail in Section (6.3.3). The sum (6.9) can be viewed as a first numerical approximation by keeping only the iterated integrals of order below r of the infinite series describing formally the solution of (6.1). In Proposition (6.4.1), we show that (6.9) is a symmetric scheme.

In order for the scheme to have a suitable local error when applied to low-regularity solutions, it is necessary to replace each oscillatory integral $(\Pi_{\text{mid}}T)(\tau)$ appearing in the finite sum (6.9) by a low regularity approximation that embeds the resonance structure into the numerical discretization. Our novel approach is to try and perform this approximation in a symmetric manner. Let us explain briefly how it works. Suppose we aim to discretise an oscillatory integral of the form

$$\int_0^t e^{is\mathcal{L}} ds, \quad \mathcal{L} = \mathcal{L}_{\text{dom}} + \mathcal{L}_{\text{low}},$$

where we have split the operator into a dominant part \mathcal{L}_{dom} that we will integrate exactly and a lower part \mathcal{L}_{low} that we will approximate (cf. section (6.3.1) for a definition of these quantities). A typical example arising in the case of NLS is

$$\mathcal{L} = k^2 + k_1^2 - k_2^2 - k_3^2, \quad \mathcal{L}_{\text{dom}} = 2k_1^2 \quad \mathcal{L}_{\text{low}} = -2k_1(k_2 + k_3) + 2k_2k_3,$$

where $k = -k_1 + k_2 + k_3$. We see that the exact integration of

$$\int_0^t e^{is\mathcal{L}_{\text{dom}}} ds = \frac{e^{2isk_1^2} - 1}{2ik_1^2}$$

can be mapped back to physical space as $1/k^2$ corresponds to Δ^{-1} . This property of being able to write the scheme in physical space is crucial for efficient numerical implementation: If we have an expression in physical space the differential operators can be computed quickly in *frequency* space using the Fast Fourier Transform (FFT) while any polynomial-type nonlinear term can be computed quickly in *physical* space since it corresponds to a local operation on the function values on a grid. Now, it remains to approximate the lower part. For this task, we use a polynomial interpolation with $m + 1$ points on $[0, \tau]$ denoted by $a_j\tau$. We note that the error incurred by this polynomial interpolation will be one of the determining factors of the convergence order of our overall numerical scheme, and thus we highlight that this interpolation can be done to any given order. We take $r + 1$ distinct interpolation points $0 \leq a_0 < a_1 < \dots < a_r \leq 1$ which are symmetrically distributed such that $a_j = 1 - a_{r-j}$, $j = 0, \dots, r$. Let us denote the corresponding nodal polynomials by $p_{j,r}$ such that

$$p_{j,r}(a_m\tau) = \delta_{j,m}.$$

Then, we define the following approximation

$$\tilde{p}_r(f, \xi) = \sum_{j=0}^r f(a_j)p_{j,r}(\xi), \quad f(a_j) = e^{ia_j\tau\mathcal{L}_{\text{low}}}.$$

We have the following local error

$$f(\xi) - \tilde{p}_r(f, \xi) = \mathcal{O}\left(\prod_{j=0}^r (\xi - a_j \tau)(i\mathcal{L}_{\text{low}})^{r+1}\right) \quad (6.10)$$

which requires less regularity than if we had chosen to base our approximation on \mathcal{L} instead of \mathcal{L}_{low} as classical schemes do.

In order to arrive at a numerical scheme, we will in the following introduce the low-regularity symmetric approximation operator of Π_{mid} denoted by $\Pi_{\text{mid}}^{n,r}$. Here, r corresponds to the order of the discretization and n is the a priori regularity assumed on the initial data v . Namely, we assume $v \in H^n$, where H^n is a Sobolev space. The general scheme then takes the form:

$$U_{\text{mid},k}^{n,r}(\tau, u) = \sum_{T \in \mathcal{V}_k^r} \frac{\Upsilon_{\text{mid}}^p(T)(u, \tau)}{S(T)} (\Pi_{\text{mid}}^{n,r} T)(\tau). \quad (6.11)$$

We will show in Theorem (6.4.3) that this scheme is symmetric. The local error structure for each approximated iterated integral is given by

$$(\Pi_{\text{mid}} T - \Pi_{\text{mid}}^{n,r} T)(\tau) = \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T, n)), \quad (6.12)$$

where $\mathcal{L}_{\text{low}}^r$ involves only lower order derivatives. Its proof is exactly the same as in [BS22]. The local error does not depend on the choice of Duhamel's iteration and polynomial interpolations. The form of the scheme draws its inspiration from the treatment of singular stochastic partial differential equations (SPDEs) via Regularity Structures in [Hai14, BHZ19, BCCH20, BHZ20]. These decorated tree expansions are generalization of the B-series widely used for ordinary differential equations, we refer to [But72, CCO08, HLW10, MKL13] and tree series used for dispersive equations [Chr07, GKO13, Gub12, LO13, HLO20]. In the end, one obtains an approximation of u under much lower regularity assumptions than classical methods (e.g., splitting methods, exponential integrators [CG12, Fao12, HLW10, HO10, Hol10, Law67, Lub08, LR04, MQ02, SSC18]) require, which in general introduce the local error

$$\mathcal{O}(\tau^{r+2} \mathcal{L}^r(T, n)) \quad (6.13)$$

involving the full high order differential operator \mathcal{L}^r . Indeed, denoting by $\mathcal{D}(\cdot)$ the domain of a given operator, we have that $\mathcal{D}(\mathcal{L}_{\text{low}}) \supset \mathcal{D}(\mathcal{L})$, meaning that the local error structure (6.12) allows us to deal with a rougher class of solutions than the classical error bound (6.13). Let us mention that the local error analysis can be nicely understood via a Birkhoff factorisation of the character $\Pi_{\text{mid}}^{n,r}$ (see [BS22, BEF20]) that involves a deformed Butcher-Connes-Kreimer coproduct (see [But72, CK99, CK00, BS22, BM23]). In the present work, we push further the algebraic perspective by writing several forest formulae that can be used to represent a larger class of low regularity schemes. These forest formulae take the following form:

$$\begin{aligned} u_k^{\ell+1} &= e^{i\tau\mathcal{L}} u_k^\ell + e^{i\tau\mathcal{L}} \sum_{T \in \tilde{\mathcal{V}}_k^r} \sum_{\mathbf{a} \in [0,1]^{\tilde{E}_T}} \sum_{\chi \in \{0,1\}^{L_T}} \sum_{T_0 \cdot T_1 \dots \cdot T_m \subset T} C_T \\ &\quad b_{\mathbf{a}, \chi, T, T_0 \dots T_m}(\tau, i\tau \mathcal{F}_{\text{dom}}(T_j), j \in \{0, \dots, m\}) \\ &\quad \prod_{e \in \tilde{E}_{T_j}} e^{i\tau a_e \mathcal{F}_{\text{low}}(T_j^e)} \frac{\Upsilon_\chi^p(T)(u_{k_v}^{\ell+\chi_v}, v \in L_T, \tau)}{S(T)}. \end{aligned} \quad (6.14)$$

Below, we give a brief description of the notation of this forest formula before introducing each term in full detail in section (6.3). Here, \mathcal{L} is the full operator of (6.1), $\tilde{\mathcal{V}}_k^r$ is a finite set of decorated trees, \tilde{E}_T denotes the edges of T that correspond to a time integration. These time integrals are discretised with a low regularity approximation. Therefore, we have to use a map \mathbf{a} on these edges that specifies which interpolation points have been used. This corresponds to the following term

$$\prod_{e \in \tilde{E}_{T_j}} e^{i\tau a_e \mathcal{F}_{\text{low}}(T_j^e)}$$

Here $\mathcal{F}_{\text{low}}(T_j^e)$ denote the lower part of the various discretisations where T_j^e is included into T_j . The set L_T are the leaves of T associated to some u_{k_u} and the map χ specifies if they are evaluated at the right ($u_{k_u}^\ell$) or left end point ($u_{k_u}^{\ell+1}$). The coefficients $\Upsilon_\chi^p(T)(u_{k_v}^{\ell+\chi_v}, v \in L_T, \tau)$ depend on the structure of the equation and the way one iterates Duhamel's formula. One essential choice of this forest formula is the splitting of T into a forest $T_0 \cdot \dots \cdot T_m$ where the T_i are decorated trees. This allows us to encode all the lower parts of the resonances $\mathcal{F}_{\text{low}}(T_j^e)$ and all their dominant

parts $\mathcal{F}_{\text{dom}}(T_j)$ that appear in the low regularity discretisation. As we shall see below, this forest splitting is a crucial novelty necessary for the construction and classification of symmetric low-regularity integrators. For the splitting, one can use a Butcher-Connes-Kreimer coproduct (see Section (6.3.2)) or a deformed Butcher-Connes-Kreimer coproduct used for the local error analysis. In our applications so far, the forest formula without deformation is enough for finding symmetric schemes hence this is the one presented in this article. We derive a condition on the coefficients $b_{\mathbf{a},\chi,T,T_0,\dots,T_m}$ in Proposition(6.4.7) that allows to find symmetric schemes. The coefficients $b_{\mathbf{a},\chi,T,T_0,\dots,T_m}$ do not depend on the frequencies that are node decorations of the trees T, T_j . One can see them only as functions of the dominant parts of the various operators encountered during the discretisation. The term C_T is a structure term depending on the frequencies that encode the various operators that appear in the iterated integral given by T . We conclude this section with a few remarks concerning the structures introduced and the properties of the resulting low-regularity schemes.

Remark 6.2.1 The forest formula appear in the BPHZ algorithm [BP57, Hep69, Zim69] for renormalising Feynman diagrams and was later used for renormalising singular SPDEs in [BHZ19, CH16] with an extension of the algebraic structure.

Remark 6.2.2 The scheme (6.11) has been generalized to non-polynomial nonlinearities and to parabolic equations in [ABBS22b] with the use of nested commutators first introduced in [RS21]. The Birkhoff factorisation discovered in [BS22] is not available in this case. It is also not obvious to translate forest formulae into this context. Indeed, due to the fact that the formula is written in Fourier space, there is no order on the operators written in Fourier space. This is not the case in physical space. But one can repeat the construction of the scheme $U_k^{n,r}$ in this context and this scheme should be symmetric as the recursive proofs in Section (6.4.1) seem robust to this case.

Remark 6.2.3 The schemes presented in [BS22] have been adapted to a probabilistic setting by proposing a low regularity approximation [ABBS22a] of the second moment of the Fourier coefficient of the solution, i.e. $\mathbb{E}(|u(v^\eta, \tau)|^2)$ where v^η is a random initial data. In this context, one has to work with paired decorated trees. It possible to write symmetric schemes for approximating this second moment using our approach. Also, one can set up an equivalent forest formula on these paired decorated trees. One open direction is to understand the connection between the algebraic tools developed for these numerical schemes and the tools used for the rigorous derivation of the wave kinetic equation (WKE) for NLS is performed in [DH21, DH23, ACG21]

Remark 6.2.4 The central novelty of the present work is the structured understanding of implicit and, in particular, symmetric low-regularity integrators. The local error bounds we use in this paper often rely on the previous local error derivations first introduced in [BS22]. Indeed, the scheme $U_k^{n,r}(\tau, u)$ is of the form (6.14) but the local error analysis comes from the fact that it is defined recursively via the character $\Pi_{\text{mid}}^{n,r}$ and therefore the tools from [BS22] are available. If one found a new scheme by choosing the coefficients $b_{\mathbf{a},\chi,T,T_0,\dots,T_m}$, it is not clear how to get directly the local error analysis and check that the scheme is optimal in terms of regularity.

We also make the important remark that given that we derive schemes which are of implicit nature, an additional fixed-point argument needs to be performed on the numerical flow in order to rigorously buckle the local error bounds, we refer to the works of [MS22, AB23b] where this analysis is made in detail.

Remark 6.2.5 On this forest formula, we have identified symmetric schemes and, in addition, we have provided a general recursive mechanism to derive symmetric schemes for a large class of PDEs. One can wonder if such an approach could be repeated for other symmetries. Indeed, we believe that our techniques are fairly general. The degrees of freedom offered by different Duhamel's iterations and interpolations should allow us to capture other symmetries at low regularity using variants of the recursive scheme $U_k^{n,r}(\tau, u)$. One degree of freedom which has not been used in full generality is the splitting of the operator into dominant and lower part :

$$\mathcal{L} = \mathcal{L}_{\text{dom}} + \mathcal{L}_{\text{low}}.$$

Right now, it is governed by Definition 6.3.1 that guarantees to get a resonance-based scheme and a scheme which can be written in physical space. For symplectic schemes, one expects to have symmetries between the frequencies of \mathcal{L}_{dom} and those \mathcal{L}_{low} . One should have the possibility of refining this splitting for encapsulating some symmetries as has been done for the 1D NLSE and the KdV equation in recent work [MS23]. The rest of the construction of the scheme remains unchanged. Consequently, a natural line of future research is the study of such symmetries (ρ -reversibility, preservation of quadratic invariants, etc.) directly on a structured tree or forest expansion of the numerical schemes comparable to the use of B-series in the study of structure preservation properties of methods for ODEs. We believe that the forest formulae presented in the current work take a first step in this direction.

Remark 6.2.6 Let us close this section with an interesting, but crucial observation: In the context of ODEs it is well known that symmetric methods are of even order (cf. [HLW10, Theorem IX.2.2]). In general this is, however, *not* the case for PDEs as the rate of convergence depends intrinsically on the regularity of the solution, and hence convergence at even order only holds if sufficient regularity requirements are met by the solution. For instance, the resonance based midpoint method for the NLS equation takes the form (see Section (6.4.3) below for its derivation)

$$\begin{aligned} u^{n+1} &= e^{i\tau\Delta} u^n \\ &\quad - i\frac{\tau}{16} e^{i\tau\Delta} \left((u^n + e^{-i\tau\Delta} u^{n+1})^2 \varphi_1(-2i\tau\Delta) \left(\overline{u^n} + e^{i\tau\Delta} \overline{u^{n+1}} \right) \right) \\ &\quad - i\frac{\tau}{16} \left((e^{i\tau\Delta} u^n + u^{n+1})^2 \varphi_1(2i\tau\Delta) \left(e^{-i\tau\Delta} \overline{u^n} + \overline{u^{n+1}} \right) \right). \end{aligned} \quad (6.15)$$

This scheme is symmetric and first order with optimal local error structure in the sense of [BS22], as its first order local error structure $\mathcal{O}(\tau^2 \nabla u)$ does not require more regularity on the solution than the asymmetric first order resonance based schemes of [BS22, OS18]. As the scheme (6.15) is symmetric it is, for C^∞ solutions, naturally of even order, hence, not only of order one, but also of order two. However, a closer look shows that its second order convergence is only attained for sufficiently regular solutions: With a similar error analysis as introduced in [AB23b] one can show that at second order the symmetric scheme (6.15) introduces a local error of type $\mathcal{O}(\tau^3 \nabla \Delta u)$ which requires the boundedness of three additional derivatives in order to attain second order convergence. For initial data in lower order spaces than H^3 , one can obtain fractional convergence of order *less than two*, see [AB23b]. We make the additional remark that in view of [BS22], requiring a local error of $\mathcal{O}(\tau^3 \nabla \Delta u)$ is not optimal in the sense of regularity. Indeed, we recall that the second-order non-symmetric resonance based integrators [BS22] obeys the favourable error structure $\mathcal{O}(\tau^3 \Delta u)$, hence asking for one less derivative on the solution.

6.3 Decorated trees and generalised resonance based schemes

The main object of this manuscript is to formalise the construction of symmetric resonance based schemes as outlined in section (6.2). To achieve this we resort to a new, generalised tree formalism which has already seen (in much simpler version) significant success in the construction of explicit (asymmetric) resonance based schemes (cf. [BS22]). In the present section we will begin by recalling some of the main definitions in this framework before generalising the construction to incorporate the possibility of implicit low-regularity integrators before ultimately culminating in a forest formula (6.31) which captures a broad class of resonance based numerical schemes in such way that we can later characterise those schemes in this class which are symmetric in the sense of definition (1).

We recall briefly the structure of decorated trees introduced in [BS22, Sec. 2]. Let \mathfrak{L} a finite set and frequencies $k_1, \dots, k_m \in \mathbf{Z}^d$. We suppose we are given a fixed time step $\tau > 0$. The set \mathfrak{L} parametrizes a set of differential operators with constant coefficients, whose symbols are given by the polynomials $(P_i)_{i \in \mathfrak{L}}$. These operators are given in Fourier space and therefore the polynomials will be evaluated in the frequencies k_i . We define the set of decorated trees $\hat{\mathcal{T}}$ as elements of the form $T_\epsilon^{n, \circ} = (T, n, \circ, \epsilon)$ where

- T is a non-planar rooted tree with root ϱ_T , node set N_T and edge set E_T . We denote the leaves of T by L_T . T must also be a planted tree which means that there is only one edge connecting the root to the rest of the tree.
- the map $\epsilon : E_T \rightarrow \mathfrak{L} \times \{0, 1\}$ are edge decorations. The set $\{0, 1\}$ encodes the action of taking the conjugate, and determines the sign of the frequencies at the top of this edge. Namely, we have that 1 corresponds to a conjugate and to multiplying by (-1) the frequency on the node above and adjacent to this edge.
- the map $\mathfrak{n} : N_T \setminus \{\varrho_T\} \rightarrow \mathbf{N}^2$ are node decorations. For every inner node v , this map encodes a monomial of the form $\xi^{n_1(v)} \tau^{n_2(v)}$ where ξ is a free time variable belonging to $[0, \tau]$. This is a novelty from [BS22] where we do not have factors in τ . We need it as in the sequel, we will consider integrals of the form $\int_\tau^\xi \dots ds$.
- the map $\circ : N_T \setminus \{\varrho_T\} \rightarrow \mathbf{Z}^d$ are node decorations. These decorations are frequencies that satisfy for every inner node u :

$$(-1)^{\mathfrak{p}(e_u)} \circ(u) = \sum_{e=(u,v) \in E_T} (-1)^{\mathfrak{p}(e)} \circ(v) \quad (6.16)$$

where $\epsilon(e) = (\mathfrak{t}(e), \mathfrak{p}(e))$ is the edge decoration of e with $\mathfrak{t}(e) \in \mathfrak{L}$ and $\mathfrak{p}(e) \in \{0, 1\}$ and e_u is the unique edge outgoing from u which is part of the path connecting u to the root. We denote this edge by (v, u) . From this definition, one can see that the node decorations at the leaves $(\circ(u))_{u \in L_T}$ determine the decoration of the inner nodes. One can call this identity Kirchhoff's law. We assume that the node decorations at the leaves are linear combinations of the k_i with coefficients in $\{-1, 0, 1\}$.

- we assume that the root of T has no decoration.

When the node decoration \mathfrak{n} is zero, we will denote the decorated trees $T_\epsilon^{n, \circ}$ as $T_\epsilon^\circ = (T, \circ, \epsilon)$. The set of decorated

at the root r . We denote by \mathcal{H} the vector space spanned by forests composed of trees in \mathcal{T} and λ^ℓ , $\ell \in \mathbf{N}^2$ where λ^ℓ is the tree with one node decorated by ℓ . When the decoration ℓ is equal to zero we identify this tree with the empty forest: $\lambda^0 = \mathbf{1}$. We now define the symbol $\mathcal{I}_o^r(\lambda_k^\ell \cdot) : \mathcal{H} \rightarrow \mathcal{H}$, as the same as $\mathcal{I}_o(\lambda_k^\ell \cdot)$, with the added adjunction of the decoration r which constrains the time-approximations to be of order r . It is given by:

$$\mathcal{I}_o^r(\lambda_k^\ell (\prod_j \lambda^{m_j} \prod_i \mathcal{I}_{o_i}^{r_i}(\lambda_{k_i}^{\ell_i} F_i))) := \mathcal{I}_o^r(\lambda_k^{\ell + \sum_j m_j} (\prod_i \mathcal{I}_{o_i}(\lambda_{k_i}^{\ell_i} F_i))).$$

We define a projection operator \mathcal{D}^r which depends on r and which is used during the construction of the numerical schemes in order to only retain the terms of order at most r . We define the map $\mathcal{D}^r : \hat{\mathcal{H}} \rightarrow \mathcal{H}$ which assigns r to the root of a decorated tree. This implies a projection along the identity (6.17). It is given by

$$\mathcal{D}^r(\mathbf{1}) = \mathbf{1}_{\{0 \leq r+1\}}, \quad \mathcal{D}^r(\mathcal{I}_o(\lambda_k^\ell F)) = \mathcal{I}_o^r(\lambda_k^\ell F) \quad (6.18)$$

and we extend it multiplicatively to any forest in $\hat{\mathcal{H}}$.

Example 20 We illustrate the action of the map \mathcal{D}_r on the decorated tree T introduced in Example (19). One has:

$$\deg(T) = 1, \quad \mathcal{D}_r(T) = 0, \quad r > 1, \quad \mathcal{D}_r(T) = \begin{array}{c} \textcircled{k_2} \\ | \\ \textcircled{k_1} \cdots \textcircled{k_3} \\ | \\ r \end{array}$$

6.3.1 Dominant part and polynomial interpolation

Let us now introduce the operations used when approximating integrals represented by tree formalism as described above. We first recall [BS22, Def.2.2] that select higher degree terms in a polynomial of the frequencies.

Definition 6.3.1 Let $P(k_1, \dots, k_n)$ a polynomial in the k_i . If the highest-degree monomials of P are of the form

$$a \sum_{i=1}^n (a_i k_i)^m, \quad a_i \in \{0, 1\}, \quad a \in \mathbf{Z},$$

then we define $\mathcal{P}_{\text{dom}}(P)$ as

$$\mathcal{P}_{\text{dom}}(P) = a \left(\sum_{i=1}^n a_i k_i \right)^m. \quad (6.19)$$

Otherwise, it is zero.

This definition is used for splitting an operator between a lower part and a dominant part. Indeed, if we consider the polynomial

$$P(k_1, k_2, k_3) = k^2 + k_1^2 - k_2^2 - k_3^2, \quad k = -k_1 + k_2 + k_3.$$

coming from the NLS equation, we observe that P can be rewritten into the form:

$$P(k_1, k_2, k_3) = 2k_1^2 - 2k_1(k_2 + k_3) + 2k_2k_3.$$

Then, we set

$$\mathcal{L}_{\text{dom}} = \mathcal{P}_{\text{dom}}(P) = 2k_1^2, \quad \mathcal{L}_{\text{low}} = (\text{id} - \mathcal{P}_{\text{dom}})(P).$$

We note that \mathcal{L}_{dom} asks for boundedness of two derivatives due to the factor k_1^2 and \mathcal{L}_{low} only one because the latter consists only of cross products $k_i k_j$, $i \neq j$. Another main reason for this splitting is to be able to map back to physical space the following integral:

$$\int_0^t e^{is\mathcal{L}_{\text{dom}}} ds = \frac{e^{it\mathcal{L}_{\text{dom}}} - 1}{i\mathcal{L}_{\text{dom}}}.$$

We observe that it is essential to map back to physical space the term $\frac{1}{\mathcal{L}_{\text{dom}}}$ equal to $\frac{1}{2k_1^2}$. Such a term is given by Δ^{-1} in physical space.

The next definition extracted from [BS22, Def. 2.6] allows us to compute recursively the various frequency interactions by extracting dominant and lower parts. Such a definition is required for the local error analysis and the forest formula given in the sequel.

Definition 6.3.2 We recursively define $\mathcal{F}_{\text{dom}}, \mathcal{F}_{\text{low}} : \hat{H}_0 \rightarrow \mathbb{R}[\mathbf{Z}^d]$ as:

$$\begin{aligned} \mathcal{F}_{\text{dom}}(\mathbf{1}) &= 0 & \mathcal{F}_{\text{dom}}(F \cdot \bar{F}) &= \mathcal{F}_{\text{dom}}(F) + \mathcal{F}_{\text{dom}}(\bar{F}) \\ \mathcal{F}_{\text{dom}}(\mathcal{I}_{(\mathfrak{t}, \mathfrak{p})}(\lambda_k F)) &= \begin{cases} \mathcal{P}_{\text{dom}}(P_{(\mathfrak{t}, \mathfrak{p})}(k) + \mathcal{F}_{\text{dom}}(F)), & \text{if } \mathfrak{t} \in \mathfrak{L}_+, \\ P_{(\mathfrak{t}, \mathfrak{p})}(k) + \mathcal{F}_{\text{dom}}(F), & \text{otherwise} \end{cases} \\ \mathcal{F}_{\text{low}}(\mathcal{I}_{(\mathfrak{t}, \mathfrak{p})}(\lambda_k F)) &= (\text{id} - \mathcal{P}_{\text{dom}})(P_{(\mathfrak{t}, \mathfrak{p})}(k) + \mathcal{F}_{\text{dom}}(F)), \end{aligned}$$

where we recall that \mathfrak{L}_+ is a subset of \mathfrak{L} that encodes edge decorations which correspond to time integrals. We extend these two maps to \hat{H} by ignoring the node decorations \mathfrak{n} .

In a nutshell the above recursive definition means that in the set $\mathfrak{L} \setminus \mathfrak{L}_+$, i.e. operators that do not correspond to integration, we collect all frequency contributions, and in the set \mathfrak{L}_+ , i.e. operators that correspond to integration, we extract the dominant frequencies of the full integrand.

Example 21 We illustrate the previous definition on a simple decorated tree coming from the NLS equation.

$$T = \begin{array}{c} \textcircled{k_2} \\ \textcircled{k_1} \quad \textcircled{k_3} \\ \vdots \\ \bullet \end{array} = \mathcal{I}_{(\mathfrak{t}_2, 0)}(\lambda_k F), \quad F = \mathcal{I}_{(\mathfrak{t}_1, 1)}(\lambda_{k_1}) \mathcal{I}_{(\mathfrak{t}_1, 0)}(\lambda_{k_2}) \mathcal{I}_{(\mathfrak{t}_1, 0)}(\lambda_{k_3}).$$

with $k = -k_1 + k_2 + k_3$. One has

$$\mathcal{F}_{\text{dom}}(T) = \mathcal{P}_{\text{dom}}(P_{(\mathfrak{t}_2, 0)}(k) + \mathcal{F}_{\text{dom}}(F))$$

because $\mathfrak{t}_2 \in \mathfrak{L}_+$. Then, we use the fact that

$$P_{(\mathfrak{t}_2, 0)}(k) = k^2, \quad P_{(\mathfrak{t}_1, 0)}(k) = -k^2, \quad P_{(\mathfrak{t}_1, 1)}(k) = k^2$$

and

$$\begin{aligned} \mathcal{F}_{\text{dom}}(F) &= \mathcal{F}_{\text{dom}}(\mathcal{I}_{(\mathfrak{t}_1, 1)}(\lambda_{k_1})) + \mathcal{F}_{\text{dom}}(\mathcal{I}_{(\mathfrak{t}_1, 0)}(\lambda_{k_2})) + \mathcal{F}_{\text{dom}}(\mathcal{I}_{(\mathfrak{t}_1, 0)}(\lambda_{k_3})) \\ &= P_{(\mathfrak{t}_2, 1)}(k_1) + P_{(\mathfrak{t}_2, 0)}(k_2) + P_{(\mathfrak{t}_2, 0)}(k_3) \\ &= k_1^2 - k_2^2 - k_3^2. \end{aligned}$$

Therefore,

$$\begin{aligned} \mathcal{F}_{\text{dom}}(T) &= \mathcal{P}_{\text{dom}}(k^2 + k_1^2 - k_2^2 - k_3^2) \\ &= \mathcal{P}_{\text{dom}}(2k_1^2 - 2k_1(k_2 + k_3) + 2k_2k_3) \\ &= 2k_1^2 \end{aligned}$$

One observes that the projection \mathcal{P}_{dom} projects to zero the cross terms $k_i k_j$ with $i \neq j$.

A central novel idea which we introduce in our present work is that we proceed to interpolate the exponential of the lower part of the operator in place of a direct Taylor series expansion. The advantage of this procedure is firstly that it allows us to immediately arrive at stable schemes without the need for filter functions (the spectrum of $i\mathcal{P}_{\text{low}} = i\mathcal{P} - i\mathcal{P}_{\text{dom}}$ typically lies on the imaginary axis so terms involving the exponential of the operator are all bounded). Secondly, through this interpolation process we are able to arrive at numerical schemes whose adjoint has the same functional form which is essential in the construction of symmetric methods. Classical Taylor expansion for the lower part gives:

$$e^{i\xi \mathcal{L}_{\text{low}}} = \sum_{\ell \leq r} \frac{\xi^\ell}{\ell!} (i\mathcal{L}_{\text{low}})^\ell + \mathcal{O}(\xi^{r+1} (i\mathcal{L}_{\text{low}})^{r+1})$$

Now, for reasons of stability, we would like to use a polynomial interpolation that will give the same local error analysis. We suppose given $r + 1$ distinct interpolation points $0 \leq a_0 < a_1 < \dots < a_r \leq 1$ associated to the polynomials $p_{j,r}(\cdot, \tau)$ such that

$$p_{j,r}(a_m \tau, \tau) = \delta_{j,m}.$$

Then, we define the following approximation

$$\tilde{p}_r(f, \xi) = \sum_{j=0}^r f(a_j \tau) p_{j,r}(\xi, \tau), \quad f(a_j \tau) = e^{ia_j \tau \mathcal{L}_{\text{low}}}, j = 0, \dots, r,$$

where we have suppressed the implicit τ -dependency of $\tilde{p}_r(f, \xi)$ for notational simplicity. One has the following local error

$$f(\xi) - \tilde{p}_r(f, \xi) = \mathcal{O}\left(\prod_{j=0}^r (\xi - a_j \tau) (i\mathcal{L}_{\text{low}})^{r+1}\right). \quad (6.20)$$

In the sequel, we will write the polynomial interpolation as:

$$\tilde{p}_r(f, \xi) = \sum_{j=0}^r \hat{p}_{j,r}(f, \tau) \xi^j \quad (6.21)$$

where the $\hat{p}_{j,r}(f, \tau)$ are bounded in τ because they correspond to linear combinations of terms of the form $\exp(ia_j \tau \mathcal{L}_{\text{low}})$. We provide below one example with two points 0 and τ

$$\tilde{p}_1(f, \xi) = 1 + \frac{s}{\tau} (e^{is\mathcal{L}_{\text{low}}} - 1), \quad (6.22)$$

and

$$\begin{aligned} \hat{p}_{0,1}(f, \tau) &= 1, & \hat{p}_{1,1}(f, \tau) &= \frac{e^{is\mathcal{L}_{\text{low}}} - 1}{\tau}, \\ p_{0,1}(f, \xi) &= \frac{\tau - s}{\tau}, & p_{1,1}(f, \xi) &= \frac{s}{\tau} e^{is\mathcal{L}_{\text{low}}}. \end{aligned}$$

When $r = 0$ we can, for example, pick

$$p_0(f, \xi) = \hat{p}_{0,0}(f, \tau) = p_{0,0}(f, \xi) = f\left(\frac{\tau}{2}\right).$$

In practice, we will also consider

$$\hat{p}_{0,0}(f, \xi) = \frac{f(0) + f(\xi)}{2}.$$

The next definition is a slight modification of [BS22, Def. 3.1] where Taylor expansions around zero are replaced by an interpolation on the interval $[0, \tau]$ and we take into account monomials in τ for the discretisation.

Definition 6.3.3 Assume that $G : \xi \mapsto \tau^m \xi^q e^{i\xi P(k_1, \dots, k_n)}$ where P is a polynomial in the frequencies k_1, \dots, k_n and let $o_2 = (t_2, p) \in \mathfrak{L}_+ \times \{0, 1\}$ and $r \in \mathbf{N}$. Let k be a linear combination of k_1, \dots, k_n using coefficients in $\{-1, 0, 1\}$ and

$$\begin{aligned} \mathcal{L}_{\text{dom}} &= \mathcal{P}_{\text{dom}}(P_{o_2}(k) + P), & \mathcal{L}_{\text{low}} &= \mathcal{P}_{\text{low}}(P_{o_2}(k) + P) \\ f(\xi) &= e^{i\xi \mathcal{L}_{\text{dom}}}, & g(\xi) &= e^{i\xi \mathcal{L}_{\text{low}}}, & \tilde{g}(\xi) &= e^{i\xi (P_{o_2}(k) + P)}. \end{aligned}$$

Then, we define for $n \in \mathbf{N}$, $r \geq q$, $\tilde{r} = r - q - m$ and $\bar{n} = \deg(\mathcal{L}_{\text{dom}}^{r+1}) + \alpha$

$$\mathcal{K}_{o_2}^{k,r}(G, n)(s) = \begin{cases} -i|\nabla|^\alpha(k) \sum_{\ell \leq \tilde{r}} \hat{p}_{\ell, \tilde{r}}(\tilde{g}, \tau) \int_0^s \tau^m \xi^{q+\ell} d\xi, & \text{if } n \geq \bar{n}, \\ -i|\nabla|^\alpha(k) \sum_{\ell \leq \tilde{r}} \tau^m \hat{p}_{\ell, \tilde{r}}(g, \tau) \Psi_{n,q}^r(\mathcal{L}_{\text{dom}}, \ell)(s), & \text{otherwise.} \end{cases} \quad (6.23)$$

Thereby we set for $(r - q - m - \ell + 1) \deg(\mathcal{L}_{\text{dom}}) + \ell \deg(\mathcal{L}_{\text{low}}) + \alpha > n$

$$\Psi_{n,q}^r(\mathcal{L}_{\text{dom}}, \ell)(s) = \int_0^s \xi^{q+\ell} f(\xi) d\xi. \quad (6.24)$$

Otherwise,

$$\Psi_{n,q}^r(\mathcal{L}_{\text{dom}}, \ell)(s) = \sum_{j \leq \hat{r}} \hat{p}_{j,\hat{r}}(f, \tau) \int_0^s \xi^{q+\ell+j} d\xi. \quad (6.25)$$

Here $\hat{r} = r - q - m - \ell$, $\deg(\mathcal{L}_{\text{dom}})$ and $\deg(\mathcal{L}_{\text{low}})$ denote the degree of the polynomial \mathcal{L}_{dom} and \mathcal{L}_{low} , respectively and $|\nabla|^\alpha(k) = \prod_{\alpha=\sum \gamma_j < \deg(\mathcal{L})} k_j^{\gamma_j}$. If $r < q + m$, the map $\mathcal{K}_{o_2}^{k,r}(G, n)(s)$ is equal to zero.

We perform an example to illustrate the polynomial interpolation.

Example 22 We consider $P_{t_2}(\lambda) = -\lambda^2$, $p = 0$, $\alpha = 0$, $k = -k_1 + k_2 + k_3$ and

$$G(\xi) = \xi e^{i\xi(k_1^2 - k_2^2 - k_3^2)}.$$

With the notation of Definition (6.3.3) we observe that

$$\mathcal{L}_{\text{dom}} = 2k_1^2, \quad \mathcal{L}_{\text{low}} = -2k_1(k_2 + k_3) + 2k_2k_3,$$

Furthermore, we observe as $\deg(\mathcal{L}_{\text{dom}}) = 2$, $\deg(\mathcal{L}_{\text{low}}) = 1$ and $q = 1$ that

$$(r - q - \ell + 1) \deg(\mathcal{L}_{\text{dom}}) + \ell \deg(\mathcal{L}_{\text{low}}) > n \quad \text{if} \quad 2r - n > \ell. \quad (6.26)$$

We consider the polynomial interpolation given in (6.22) and focus on some cases

— **Case $r = 1$ and $n = 1$** : We obtain

$$\begin{aligned} \mathcal{K}_{o_2}^{k,1}(G, n)(s) &= -i\hat{p}_{0,0}(f, \tau) \Psi_{n,1}^1(\mathcal{L}_{\text{dom}}, 0)(s) \\ &= -i\hat{p}_{0,0}(f, \tau) \int_0^s \xi f(\xi) d\xi \\ &= \frac{1}{2ik_1^2} \left(se^{2isk_1^2} - \frac{e^{2isk_1^2} - 1}{2ik_1^2} \right) \left(\frac{1 + e^{is\mathcal{L}_{\text{low}}}}{2} \right) \end{aligned}$$

as condition (6.26) takes for $\ell = 0$ the form $2 - n > 0$.

— **Case $r = 2$ and $n = 2$** : We have that

$$\mathcal{K}_\alpha^{k,2}(G, n)(s) = -i(\hat{p}_{0,1}(g, \tau) \Psi_{n,1}^2(\mathcal{L}_{\text{dom}}, 0)(s) + \hat{p}_{1,1}(g, \tau) \Psi_{n,1}^2(\mathcal{L}_{\text{dom}}, 1)(s))$$

and condition (6.26) takes the form $4 - n > \ell$.

If $\ell = 1$ we thus obtain

$$\Psi_{n,1}^2(\mathcal{L}_{\text{dom}}, 1)(s) = \int_0^s \xi^2 f(\xi) d\xi = \frac{s^2}{2ik_2^2} \left(e^{2isk_1^2} - 2\Psi_{1,1}^1(\mathcal{L}_{\text{dom}}, 0) \right).$$

If $\ell = 0$, on the other hand, condition (6.26) holds. Henceforth, we have that

$$\Psi_{n,1}^2(\mathcal{L}_{\text{dom}}, 0)(s) = \int_0^s \xi f(\xi) d\xi.$$

Following a similar proof as for [BS22, Lem. 3.3] by using (6.20), one gets

Lemma 6.3.4 *We keep the notations of Definition (6.3.3). We suppose that $q + m \leq r$ then one has for $s \in [0, \tau]$*

$$-i|\nabla|^\alpha(k) \int_0^s \tau^m \xi^q e^{i\xi(\mathcal{L}_{\text{dom}} + \mathcal{L}_{\text{low}})} d\xi - \mathcal{K}_{o_2}^{k,r}(G, n)(s) = \mathcal{O}(\tau^{r+2} k^{\bar{n}}) \quad (6.27)$$

where $\bar{n} = \max(n, \deg(\mathcal{L}_{\text{low}}^{r-q-m+1}) + \alpha)$.

6.3.2 A forest formula for resonance based schemes

We recall the characters defined now on \mathcal{H} and parametrised by $n \in \mathbf{N}$ where n here the a priori regularity assumed on the initial value, that is $v \in H^n$ where H^n is the periodic Sobolev space of order n . These characters give a low regularity discretisation of some iterated integrals:

$$\begin{aligned} \Pi^n(F \cdot \bar{F})(s, \tau) &= (\Pi^n F)(s, \tau)(\Pi^n \bar{F})(s, \tau), \quad (\Pi^n \lambda^\ell)(s, \tau) = s^{\ell_1} \tau^{\ell_2}, \\ (\Pi^n \mathcal{I}_{o_1}^r(\lambda_k^\ell F))(s, \tau) &= s^{\ell_1} \tau^{\ell_2} e^{isP_{o_1}(k)} (\Pi^n \mathcal{D}^{r-|\ell|}(F))(s, \tau), \\ (\Pi^n \mathcal{I}_{o_2}^r(\lambda_k^\ell F))(s, \tau) &= \mathcal{K}_{o_2}^{k,r} \left(\Pi^n \left(\lambda^\ell \mathcal{D}^{r-|\ell|-1}(F) \right) (\cdot, \tau), n \right) (s). \end{aligned} \tag{6.28}$$

where $o_2 = (t_2, p_2)$ with $t_2 \in \mathfrak{L}_+$ and $o_1 = (t_1, p_1)$ with $t_1 \in \mathfrak{L} \setminus \mathfrak{L}_+$ and $\ell = (\ell_1, \ell_2) \in \mathbf{N}^2$. We will use frequently the notations o_i in the sequel. The main difference with [BS22] is the use of the polynomial interpolation in Definition (6.3.3). In the next theorem, we state a forest formula for the resonance scheme in the sense that we exhibit a general formula for the terms $(\Pi^{n,r} F)(t)$ where $\Pi^{n,r}$ is short hand notation for $\Pi^n \mathcal{D}_r$. This new forest formula is a significant extension of contributions in [BS22] since it incorporates not just the aforementioned polynomial interpolants but also allows for implicit discretisations in the unknown v . We first need to introduce some notations that are needed for its formulation. We denote by \tilde{E}_T the edges of T associated to an integration in time. They carry a decoration of the type o_2

$$\tilde{E}_T = \{e \in E_T \mid \mathfrak{c}(e) \in \mathfrak{L}_+ \times \{0, 1\}\}.$$

The notation T^e means that we consider the planted tree above the edge e in T . This tree has its root connected to the rest of its nodes by the edge e . By $F_0 \cdot T_1 \dots \cdot T_m \subset F$, we mean that the forest

$$F_0 \cdot T_1 \dots \cdot T_m \subset F \tag{6.29}$$

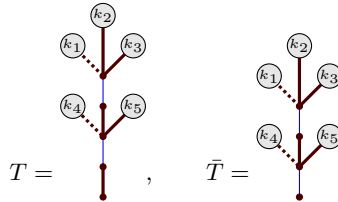
is a splitting of F where :

- The T_i are planted trees with the edge connecting the root decorated by an edge decoration of type o_2 .
- F_0 is a forest either empty or taking the form:

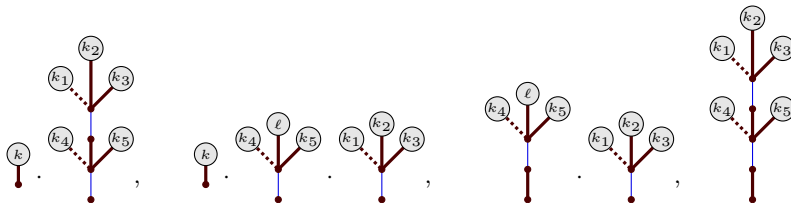
$$F_0 = \prod_{j=1}^{m_0} T_{0,j}$$

where the $T_{0,j}$ are subtrees at the root of some trees appearing in the decomposition of the forest F into product of planted trees.

Example 23 We provide an example of the forests such that $F_0 \cdot T_1 \dots \cdot T_m \subset F$. Let us consider F to be the following decorated trees coming from the NLS equation

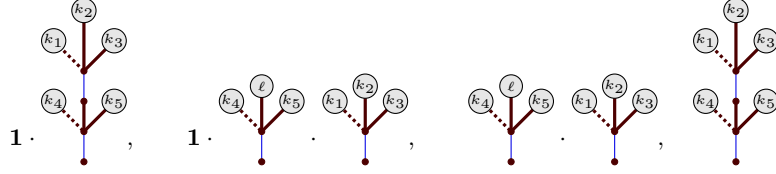


Because T starts with a brown edge that is an edge decorated by $(t_1, 0)$, F_0 is not empty. Below, we list all the possible splitting respecting this rule and also that the T_i with $i \geq 1$ must be planted trees with a blue edge (decorated by $(t_2, 0)$) at their root.



where $\ell = -k_1 + k_2 + k_3$ and $k = -k_4 + \ell + k_5$. We also give below the decomposition for the decorated tree \bar{T} . Notice

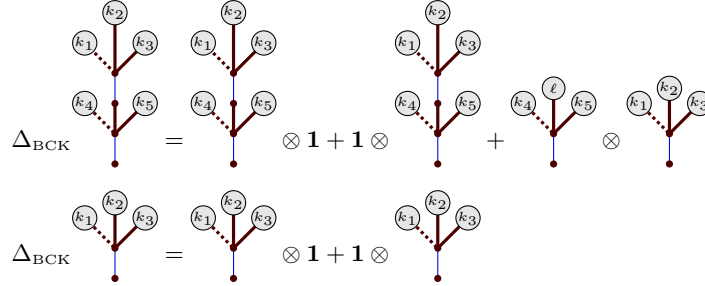
that now \bar{T}_0 could be empty.



We can obtain these terms by iterating a Butcher-Connes-Kreimer type coproduct $\Delta_{\text{BCK}} : \hat{\mathcal{H}}_0 \rightarrow \hat{\mathcal{H}}_0 \otimes \hat{\mathcal{H}}_0$, a simple version of the one introduced in [BS22]. It is defined recursively by

$$\begin{aligned} \Delta_{\text{BCK}} \mathcal{I}_{O_1}(\lambda_k^\ell F) &= \left(\mathcal{I}_{O_1}(\lambda_k^\ell \cdot) \otimes \text{id} \right) \Delta_{\text{BCK}} F, \\ \Delta_{\text{BCK}} \mathcal{I}_{O_2}(\lambda_k^\ell F) &= \left(\mathcal{I}_{O_2}(\lambda_k^\ell \cdot) \otimes \text{id} \right) \Delta_{\text{BCK}} F + \mathbf{1} \otimes \mathcal{I}_{O_2}(\lambda_k^\ell F). \end{aligned}$$

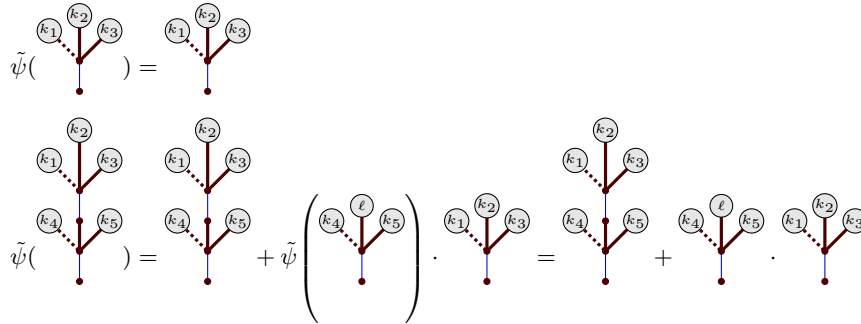
and then extended multiplicatively for the forest product. Below, we provide some examples of computations:



Below, we introduce recursive maps ψ_{BCK} and $\tilde{\psi}_{\text{BCK}}$ that can compute the splitting describe above with the coproduct Δ_{BCK} :

$$\begin{aligned} \psi_{\text{BCK}} &= \left(\text{id} \otimes \tilde{\psi}_{\text{BCK}} \right) \Delta_{\text{BCK}}, \\ \tilde{\psi}_{\text{BCK}} &= \mathcal{M} \left(\tilde{\psi}_{\text{BCK}} \otimes P_1 \right) \Delta_{\text{BCK}}, \quad \tilde{\psi}_{\text{BCK}}(\mathbf{1}) = \mathbf{1} \end{aligned} \tag{6.30}$$

where \mathcal{M} is the forest product and $P_1 = \text{id} - \mathbf{1}^*$ is the augmentation projector. Here $\mathbf{1}^*$ is the co-unit which is non-zero and equal to one only on the empty forest. The projector P_1 forces at least one cut at each iteration and therefore the recursion is well-defined. If we apply ψ to T , we obtain a linear combination of the terms of the form $T_0 \otimes T_1 \dots \otimes T_m$ that corresponds exactly to the splitting described above. We do not get a forest in the end but a term with a tensor product. This is for distinguishing the root as it is needed in our splitting. As an example of computation of those maps, one has



Theorem 6.3.5 For every forest $F \in \hat{H}_0$, $(\Pi^{n,r} F)(t, \tau)$ takes the form:

$$\begin{aligned} \sum_{\mathbf{a} \in [0,1]^{\bar{E}_F}} \sum_{F_0 \cdot T_1 \dots \cdot T_m \subset F} C_F e^{it \mathcal{F}_{\text{dom}}(F_0)} \prod_{j=0}^m \prod_{e \in \bar{E}_{T_j}} e^{i\tau a_e \mathcal{F}_{\text{low}}(T_j^e)} \\ b_{\mathbf{a}, F, F_0 \dots \cdot T_m}(t, \tau, i\tau \mathcal{F}_{\text{dom}}(T_j), i\tau \mathcal{F}_{\text{dom}}(T_{0,\bar{j}})) \end{aligned} \tag{6.31}$$

with the convention $T_0 = F_0$. The coefficients C_F depend only on the node decorations of F . The coefficients b are polynomial in t and are non zero only for a finite number of values of \mathbf{a} . They are uniformly bounded in τ . Moreover, they do not depend on the node decorations of the T_i, F_0 and F that correspond to the frequencies.

We recall that in the above notation the parameters n and r in $(\Pi^{n,r}F)(t, \tau)$ denote the regularity requirements and maximum length of trees in the approximation respectively.

Proof. We proceed by induction on the size of the forest F . For the empty forest, the sum is equal to one by convention and

$$(\Pi^{n,r}\mathbf{1})(t, \tau) = 1.$$

Let F_1, F_2 two decorated forests with $F = F_1 \cdot F_2$ for which we have (6.31). We apply the induction hypothesis and get

$$\begin{aligned} (\Pi^{n,r}F)(s, \tau) &= (\Pi^{n,r}F_1)(s, \tau)(\Pi^{n,r}F_2)(s, \tau) \\ &= \sum_{\mathbf{a}_1 \in [0,1]^{\tilde{E}_{F_1}}} \sum_{\mathbf{a}_2 \in [0,1]^{\tilde{E}_{F_2}}} \sum_{F_{1,0} \cdot T_{1,1} \cdots T_{1,m_1} \subset F_1} \sum_{F_{2,0} \cdot T_{2,1} \cdots T_{2,m_2} \subset F_2} C_{F_1} C_{F_2} \\ &e^{it(\mathcal{F}_{\text{dom}}(F_{1,0}) + \mathcal{F}_{\text{dom}}(F_{2,0}))} \prod_{j=0}^{m_1} \prod_{e \in \tilde{E}_{T_{1,j}}} e^{i\tau a_{1,e} \mathcal{F}_{\text{low}}(T_{1,j}^e)} \times \prod_{j=0}^{m_2} \prod_{e \in \tilde{E}_{T_{2,j}}} e^{i\tau a_{2,e} \mathcal{F}_{\text{low}}(T_{2,j}^e)} \\ &b_{\mathbf{a}_1, F_1, F_{1,0} \cdots T_{1,m_1}} \times b_{\mathbf{a}_2, F_2, F_{2,0} \cdots T_{2,m_2}}. \end{aligned}$$

By using Definition (6.3.2), we have

$$\mathcal{F}_{\text{dom}}(F_{1,0}) + \mathcal{F}_{\text{dom}}(F_{2,0}) = \mathcal{F}_{\text{dom}}(F_0), \quad F_0 = F_{1,0} \cdot F_{2,0}.$$

Then, we can perform the disjoint sum of \mathbf{a}_1 and \mathbf{a}_2 :

$$\mathbf{a} = \mathbf{a}_1 + \mathbf{a}_2$$

by extending \mathbf{a}_1 (resp. \mathbf{a}_2) on the edges of F_2 (resp. F_1) by zero. Then, \mathbf{a} is defined on the edges of F . We can gather the sum on the forests by:

$$\begin{aligned} \sum_{F_{1,0} \cdot T_{1,1} \cdots T_{1,m_1} \subset F_1} \sum_{F_{2,0} \cdot T_{2,1} \cdots T_{2,m_2} \subset F_2} &= \sum_{F_0 \cdot T_{1,1} \cdots T_{1,m_1} \cdot T_{2,1} \cdots T_{2,m_2} \subset F} \\ &= \sum_{F_0 \cdot T_1 \cdots T_m \subset F} \end{aligned}$$

and we can also set

$$\begin{aligned} b_{\mathbf{a}, F, F_0 \cdots T_1 \cdots T_m} &= b_{\mathbf{a}_1, F_1, F_{1,0} \cdots T_{1,m_1}} \times b_{\mathbf{a}_2, F_2, F_{2,0} \cdots T_{2,m_2}} \\ C_F &= C_{F_1} \times C_{F_2} \end{aligned}$$

and see that the properties of the coefficient b are preserved by multiplication. Indeed, we have a bijection between partitions of $F = F_1 \cdot F_2$ into a product of trees and the forest product of partitions of F_i . For a tree of the form $\mathcal{I}_{o_1}(\lambda_k^\ell F)$, one has

$$(\Pi^n \mathcal{I}_{o_1}^r(\lambda_k^\ell F))(t, \tau) = t^{\ell_1} \tau^{\ell_2} e^{itP_{o_1}(k)} (\Pi^{n,r-\ell} F)(t, \tau).$$

We multiply the formula for F obtained by the induction hypothesis by $e^{itP_{o_1}(k)}$:

$$\begin{aligned} \sum_{\mathbf{a} \in [0,1]^{\tilde{E}_F}} \sum_{F_0 \cdot T_1 \cdots T_m \subset F} C_F e^{it(\mathcal{F}_{\text{dom}}(F_0) + P_{o_1}(k))} \prod_{j=0}^m \prod_{e \in \tilde{E}_{T_j}} e^{i\tau a_e \mathcal{F}_{\text{low}}(T_j^e)} \\ t^\ell b_{\mathbf{a}, F, F_0 \cdots T_m}(t, \tau, i\tau \mathcal{F}_{\text{dom}}(T_j), i\tau \mathcal{F}_{\text{dom}}(T_{0,j})). \end{aligned}$$

From Definition (6.3.2), we have

$$\mathcal{F}_{\text{dom}}(F_0) + P_{o_1}(k) = \mathcal{F}_{\text{dom}}(\mathcal{I}_{o_1}(\lambda_k^\ell F_0)).$$

Moreover, for $\mathcal{I}_{o_1}(\lambda_k^\ell F)$, the forest at the root must be of the form $\mathcal{I}_{o_1}(\lambda_k^\ell F_0)$. For the coefficients b , we have

$$t^{\ell_1} \tau^{\ell_2} b_{\mathbf{a}, F, F_0, \dots, T_m} = b_{\mathbf{a}, \mathcal{I}_{o_1}(\lambda_k^\ell F), \mathcal{I}_{o_1}(\lambda_k^\ell F_0), \dots, T_m}, \quad C_{\mathcal{I}_{o_1}(\lambda_k^\ell F)} = C_F$$

It remains to prove the forest formula for a tree of the form $\mathcal{I}_{o_2}(\lambda_k^\ell F)$. We have

$$\left(\Pi^n \mathcal{I}_{o_2}^r(\lambda_k^\ell F) \right)(t, \tau) = \mathcal{K}_{o_2}^{k,r} \left(\Pi^n \left(\lambda^\ell \mathcal{D}^{r-|\ell|-1}(F) \right)(\cdot, \tau), n \right)(t).$$

We apply the induction hypothesis on $\Pi^{n,r-|\ell|-1}$. Then, the proof boils down to understand how the operator $\mathcal{K}_{o_2}^{k,r}$ acts on the forest formula. This operator computes first the dominant part of the oscillation. It is given for a fixed forest $F_0 \cdot T_1 \dots \cdot T_m \subset F$ by

$$\mathcal{P}_{\text{dom}}(P_{o_2}(k) + \mathcal{F}_{\text{dom}}(F_0)) = \mathcal{F}_{\text{dom}}(\mathcal{I}_{o_2}(\lambda_k^\ell F_0)).$$

If this dominant part is integrated exactly, we obtain a factor of the form

$$e^{it \mathcal{F}_{\text{dom}}(\mathcal{I}_{o_2}(\lambda_k^\ell F_0))}.$$

This will correspond to forests $\mathcal{I}_{o_2}(\lambda_k^\ell F_0) \cdot \dots \cdot T_m$. In this exact integration, we have terms without this factor which corresponds to the forest $\mathbf{1} \cdot \mathcal{I}_{o_2}(\lambda_k^\ell F_0) \cdot \dots \cdot T_m$ as the forest connected to the root could be the empty forest. For the lower part given by

$$(\text{id} - \mathcal{P}_{\text{dom}})(P_{o_2}(k) + \mathcal{F}_{\text{dom}}(F)) = \mathcal{F}_{\text{low}}(\mathcal{I}_{o_2}(\lambda_k^\ell F_0))$$

we perform an interpolation that produces terms of the form

$$e^{i\tau a \mathcal{F}_{\text{low}}(\mathcal{I}_{o_2}(\lambda_k^\ell F_0))}, \quad a \in [0, 1].$$

The operator $\mathcal{K}_{o_2}^{k,r}$ depends on n which is the a priori regularity assumed on the initial data. With this information, if n is sufficiently big, we can perform a full Taylor expansion via an interpolation that will produce terms of the form:

$$e^{i\tau a \mathcal{F}_{\text{low}}(\mathcal{I}_{o_2}(\lambda_k^\ell F_0))} e^{i\tau a' \mathcal{F}_{\text{dom}}(\mathcal{I}_{o_2}(\lambda_k^\ell F_0))}, \quad a, a' \in [0, 1].$$

These terms will be associated to a forest of the form $\mathbf{1} \cdot \mathcal{I}_{o_2}(\lambda_k^\ell F_0) \cdot \dots \cdot T_m$. The factor $e^{i\tau a' \mathcal{F}_{\text{dom}}(\mathcal{I}_{o_2}(\lambda_k^\ell F_0))}$ will be inside the coefficients b . The interpolation also produces monomials in t and τ which implies the polynomial structure of the coefficients b in t . Also, it produces coefficients bounded in τ such as the $\hat{p}_{j,r}(f, \tau)$ given in (6.21). The choice of the $a \in [0, 1]$ are fixed by the interpolation method and one uses only a finite number of them which implies that the coefficients b are non-zero on a finite set of the \mathbf{a} . Finally, we have

$$C_{\mathcal{I}_{o_2}(\lambda_k^\ell F)} = -i|\nabla|^\alpha(k) C_F.$$

□

Theorem 6.3.6 *For every decorated tree $T = \mathcal{I}_{o_2}(\lambda_k F)$, $(\Pi^{n,r} T)(\tau, \tau)$ takes the form:*

$$\sum_{\mathbf{a} \in [0,1]^{\tilde{E}_F}} \sum_{T_0 \cdot T_1 \dots \cdot T_m \subset T} C_T \prod_{j=0}^m \prod_{e \in \tilde{E}_{T_j}} e^{i\tau a_e \mathcal{F}_{\text{low}}(T_j^e)} b_{\mathbf{a}, T, T_0, \dots, T_m}(\tau, i\tau \mathcal{F}_{\text{dom}}(T_j)) \quad (6.32)$$

where the coefficients b are polynomial in τ with bounded coefficient in τ and are non zero for finite values of \mathbf{a} . Moreover, they do not depend on the nodes decorations of the T_i, F_0 and F that correspond to the frequencies.

Proof. The proof works mostly in the same way as for Theorem (6.3.5) but with $t = \tau$. The main difference is that when we apply the operator $\mathcal{K}_{o_2}^{k,r}$, we put factors of the form $e^{it \mathcal{F}_{\text{dom}}(\mathcal{I}_{o_2}(\lambda_k F_0))}$ in the coefficients b . □

6.3.3 Midpoint general resonance based schemes

In this section, we introduce new resonance based schemes where we iterate Duhamel's formula in slightly different manner. The iteration chosen follows the mid point rule. These schemes turn out to be a subclass of the general forest formula (6.45). In this subclass it is also possible to work with a fairly general framework more closely aligned with [BS22] which allows for an automatic handle on the local error of these schemes. In particular, in order to incorporate the midpoint iterations and subsequent lower part interpolations we need to add more edge decorations on the trees

representing the iterated integrals. For example, we can consider decorated trees of the form $T_{\mathfrak{e}, \chi}^{n, \mathfrak{o}} = (T, \mathbf{n}, \mathfrak{o}, \mathfrak{e}, \chi)$ where $\chi : E_T \rightarrow \mathfrak{D}$. Here \mathfrak{D} is a finite set and encodes the following information for an edge $e \in N_T$ decorated by (t, p) :

- For $t \notin \mathfrak{L}_+$, the edge e is associated with a term of the form $e^{iP_{(t,p)}(k_v)}$. Then, $\chi(e)$ corresponds of a way of iterating Duhamel's formula not only using the leftmost point of the interval but a weighted sum of iterations on various points in $[0, \tau]$.
- For $t \in \mathfrak{L}_+$, the edge e is associated with a term of the form $\int_{a\tau}^t e^{iP_{(t,p)}(k_v)} \dots ds$ where $a \in [0, 1]$ and it corresponds to a different Duhamel's iteration. Now, $\chi(e)$ gives a choice of a polynomial interpolation for the lower part of the resonance in the discretisation.

For reasons of presentation we focus on the midpoint rule, however, we could also follow other types of Duhamel iterations. Moreover, in this subclass we take the polynomial interpolation to be fixed.

To illustrate the central idea of a different way of iterating Duhamel's formula, let us first consider the Nonlinear Schrödinger equation. The usual iteration is given by

$$u(t_n + s) = e^{i\tau\Delta} u(t_n) - ie^{i\tau\Delta} \int_0^\tau e^{-is\Delta} (|u(t_n + s)|^2 u(t_n + s)) ds.$$

In Fourier space, we obtain

$$\begin{aligned} u_k(t_n + \tau) &= e^{-i\tau k^2} u_k(t_n) \\ &\quad - ie^{-i\tau k^2} \sum_{k=-k_1+k_2+k_3} \int_0^\tau e^{isk^2} \overline{\hat{u}_{k_1}(t_n + s)} u_{k_2}(t_n + s) u_{k_3}(t_n + s) ds. \end{aligned} \quad (6.33)$$

We can now choose to iterate this expression using two possible ways:

$$\begin{aligned} u_k(t_n + s) &= e^{-isk^2} u_k(t_n) \\ &\quad - ie^{-isk^2} \sum_{k=-k_1+k_2+k_3} \int_0^s e^{isk^2} \overline{\hat{u}_{k_1}(t_n + \tilde{s})} u_{k_2}(t_n + \tilde{s}) u_{k_3}(t_n + \tilde{s}) d\tilde{s}. \end{aligned} \quad (6.34)$$

and

$$\begin{aligned} u_k(t_n + s) &= e^{-i(s-\tau)k^2} u_k(t_n + \tau) \\ &\quad - ie^{-isk^2} \sum_{k=-k_1+k_2+k_3} \int_\tau^s e^{isk^2} \overline{\hat{u}_{k_1}(t_n + \tilde{s})} u_{k_2}(t_n + \tilde{s}) u_{k_3}(t_n + \tilde{s}) d\tilde{s}. \end{aligned} \quad (6.35)$$

The iteration (6.34) corresponds to the left end point of the interval $[0, \tau]$ while (6.35) is the right end point. We now have a choice over each term in (6.33) if we want the iteration of Duhamel's formula to begin with (6.34) or (6.35). The average of the two iterations gives the midpoint rule.

There are quite a lot of degrees of freedom as one can choose various linear combinations of Duhamel's formulae in different points. Let us mention that the tree structure is not modified if one changes the iteration but the definition of Π has to reflect this new formulation. The midpoint rule oscillatory integrals are given by

$$\begin{aligned} \Pi_{\text{mid}}(F \cdot \bar{F})(s, \tau) &= (\Pi_{\text{mid}} F)(s, \tau) (\Pi_{\text{mid}} \bar{F})(s, \tau), \\ (\Pi_{\text{mid}} \mathcal{I}_{o_1}(\lambda_k F))(s, \tau) &= \frac{1}{2} e^{isP_{o_1}(k)} ((\Pi_{\text{mid},1} F)(s, \tau) + (\Pi_{\text{mid},2} F)(s, \tau)), \\ (\Pi_{\text{mid},1} \mathcal{I}_{o_2}(\lambda_k F))(s, \tau) &= -i|\nabla|^\alpha(k) \int_\tau^s e^{i\xi P_{o_2}(k)} (\Pi_{\text{mid}} F)(\xi, \tau) d\xi, \\ (\Pi_{\text{mid},2} \mathcal{I}_{o_2}(\lambda_k F))(s, \tau) &= -i|\nabla|^\alpha(k) \int_0^s e^{i\xi P_{o_2}(k)} (\Pi_{\text{mid}} F)(\xi, \tau) d\xi. \end{aligned} \quad (6.36)$$

We notice that, in this definition, we have to keep track of the time step τ in order to remember the interval $[0, \tau]$. In this definition, we have assumed that the Duhamel iteration corresponds to edges decorated by \mathfrak{t}_1 . Moreover, we have supposed that F is not empty for $(\Pi_{\text{mid}} \mathcal{I}_{o_1}(\lambda_k F))(s, \tau)$ and $s \neq \tau$. If F is empty, we set

$$(\Pi_{\text{mid}} \mathcal{I}_{o_1}(\lambda_k \mathbf{1}))(s, \tau) = e^{isP_{o_1}(k)}. \quad (6.37)$$

If $\tau = s$, we set

$$(\Pi_{\text{mid}} \mathcal{I}_{o_1}(\lambda_k F))(\tau, \tau) = (\Pi_{\text{mid}} \mathcal{I}_{o_1}(\lambda_k F))(\tau) = e^{i\tau P_{o_1}(k)} (\Pi_{\text{mid},2} F)(\tau, \tau). \quad (6.38)$$

The last two specific cases are necessary for building up the scheme. Indeed, (6.37) corresponds to the leaves of our trees or when we terminate on an initial data u_{k_i} . Here, we will apply the midpoint rule in the sequel (see (6.41) in the definition of $\Upsilon_{\text{mid}}^p(T)(v, \tau)$)

$$\frac{1}{2}u_{k_j}(0) + e^{-i\tau P_{o_1}(k_j)}\frac{1}{2}u_{k_j}(\tau).$$

The second condition (6.38) corresponds to the fact that the first is not the midpoint rule approximation as we do not need to perform it as $\tau = s$.

Remark 6.3.7 This approach also works for the more general scheme given in [ABBS22b]. The main difference is that now $\Upsilon_{\text{mid}}^p(T)(v, \tau)$ defined in the sequel is part of the definition of Π_{mid} .

The scheme $\Pi_{\text{mid}}^{n,r}$ is defined as the same as for Π_{mid} but now we discretise the time integrals:

$$(\Pi_{\text{mid},j}^{n,r}\mathcal{I}_{o_2}(\lambda_k F))(s, \tau) = \mathcal{K}_{o_2,j}^{k,r}(\Pi_{\text{mid}}^{n,r}(F)(\cdot, \tau), n)(s, \tau), \quad j \in \{1, 2\}$$

where the map $\mathcal{K}_{o_2,1}^{k,r}(\cdot)(s, \tau)$ uses the exact integration $\int_s^\tau \dots d\xi$ and $\mathcal{K}_{o_2,2}^{k,r}$ the one given by $\int_0^s \dots d\xi$. We first introduce some notations:

Definition 2 — For a decorated tree $T_\mathfrak{c} = (T, \mathfrak{c})$ with only edge decorations, we define the symmetry factor $S(T_\mathfrak{c})$ inductively by $S(\mathbf{1})=1$, while if T is of the form

$$\prod_{i,j} \mathcal{I}_{(t_i, p_i)}(T_{i,j})^{\beta_{i,j}},$$

with $T_{i,j} \neq T_{i,\ell}$ for $j \neq \ell$, then

$$S(T) := \left(\prod_{i,j} S(T_{i,j})^{\beta_{i,j}} \beta_{i,j}! \right). \quad (6.39)$$

We extend this definition to any tree $T_\mathfrak{c}^{n,o}$ in \mathcal{T} by setting:

$$S(T_\mathfrak{c}^{n,o}) := S(T_\mathfrak{c}).$$

Let us stress that the symmetric factor depends only on the edges decorations but not on the nodes decorations given by the frequencies.

— Then, we define the map $\Upsilon_{\text{mid}}^p(T)(v, \tau)$ for

$$T = \mathcal{I}_{(t_1, a)} \left(\lambda_k \mathcal{I}_{(t_2, a)} (\lambda_k \prod_{i=1}^n \mathcal{I}_{(t_1, 0)} (\lambda_{k_i} T_i) \prod_{j=1}^m \mathcal{I}_{(t_1, 1)} (\lambda_{\tilde{k}_j} \tilde{T}_j)) \right), \quad a \in \{0, 1\}$$

by

$$\begin{aligned} \Upsilon_{\text{mid}}^p(T)(v, \tau) &:= \partial_v^n \partial_{\bar{v}}^m p_a(v, \bar{v}) \prod_{i=1}^n \Upsilon_{\text{mid}}^p(\mathcal{I}_{(t_1, 0)} (\lambda_{k_i} T_i))(v, \tau) \\ &\prod_{j=1}^m \Upsilon_{\text{mid}}^p(\mathcal{I}_{(t_1, 1)} (\lambda_{\tilde{k}_j} \tilde{T}_j))(v, \tau) \end{aligned} \quad (6.40)$$

and

$$\begin{aligned} \Upsilon_{\text{mid}}^p(\mathcal{I}_{(t_1, 0)} (\lambda_k))(v, \tau) &:= \frac{1}{2}v_k(0) + \frac{1}{2}e^{-iP_{o_1}(k)\tau}v_k(\tau) \\ \Upsilon_{\text{mid}}^p(\mathcal{I}_{(t_1, 1)} (\lambda_k))(v, \tau) &:= \frac{1}{2}\bar{v}_k(0) + \frac{1}{2}e^{iP_{o_1}(k)\tau}\bar{v}_k(\tau). \end{aligned} \quad (6.41)$$

Above, we have used the notation:

$$p_0(v, \bar{v}) = p(v, \bar{v}), \quad p_1(v, \bar{v}) = \overline{p(v, \bar{v})}$$

In the sequel, we will use the following short hand notation:

$$\overline{\Upsilon_{\text{mid}}^p(T)}(v, \tau) = \bar{\Upsilon}_{\text{mid}}^p(T)(v, \tau).$$

— We set

$$\begin{aligned}\hat{\mathcal{T}}_0(R) &= \{\mathcal{I}_{(\mathfrak{t}_1,0)}(\lambda_k \mathcal{I}_{(\mathfrak{t}_2,0)}(\lambda_k \prod_{i=1}^N T_i \prod_{j=1}^M \tilde{T}_j)), \mathcal{I}_{(\mathfrak{t}_1,0)}(\lambda_k) \\ &\quad T_i \in \hat{\mathcal{T}}_0(R), \tilde{T}_j \in \tilde{\mathcal{T}}_0(R), k \in \mathbf{Z}^d\} \\ \tilde{\mathcal{T}}_0(R) &= \{\mathcal{I}_{(\mathfrak{t}_1,1)}(\lambda_k \mathcal{I}_{(\mathfrak{t}_2,1)}(\lambda_k \prod_{i=1}^N T_i \prod_{j=1}^M \tilde{T}_j)), \mathcal{I}_{(\mathfrak{t}_1,1)}(\lambda_k) \\ &\quad T_i \in \tilde{\mathcal{T}}_0(R), \tilde{T}_j \in \hat{\mathcal{T}}_0(R), k \in \mathbf{Z}^d\} \\ \hat{\mathcal{T}}_2(R) &= \{\mathcal{I}_{(\mathfrak{t}_2,0)}(\lambda_k \prod_{i=1}^N T_i \prod_{j=1}^M \tilde{T}_j), T_i \in \hat{\mathcal{T}}_0(R), \tilde{T}_j \in \tilde{\mathcal{T}}_0(R), k \in \mathbf{Z}^d\}\end{aligned}$$

For a fixed $k \in \mathbf{Z}^d$, we denote the set $\hat{\mathcal{T}}_0^k(R)$ (resp. $\tilde{\mathcal{T}}_0^k(R)$ and $\hat{\mathcal{T}}_2^k(R)$) as the subset of $\hat{\mathcal{T}}_0(R)$ (resp. $\tilde{\mathcal{T}}_0(R)$ and $\hat{\mathcal{T}}_2(R)$) whose decorated trees have decorations on the node connected to the root given by k . For $r \in \mathbf{Z}$, $r \geq -1$, we set:

$$\hat{\mathcal{T}}_0^{r,k}(R) = \{T_c^o \in \hat{\mathcal{T}}_0^k(R), n_+(T_c^o) \leq r + 1\}.$$

In the previous space, we disregard iterated integrals which have more than $r + 1$ integrals and will be of order $\mathcal{O}(\tau^{r+2})$. The set $\hat{\mathcal{T}}_2^{r,k}(R)$ is defined as the same from $\hat{\mathcal{T}}_2^k(R)$. In the sequel, we will use the short hand notation for $T \in \hat{\mathcal{T}}_2^k(R)$:

$$\Upsilon_{mid}^p(T)(v, \tau) = \Upsilon_{mid}^p(\mathcal{I}_{(\mathfrak{t}_1,0)}(\lambda_k T))(v, \tau).$$

This truncation leads exactly to the current local error behaviour as shown in the following proposition which forms the basis of our local error analysis in Theorem (6.3.15).

Proposition 6.3.8 *The tree series given by*

$$U_{mid,k}^r(\tau, v) = \sum_{T \in \hat{\mathcal{T}}_0^{r,k}(R)} \frac{\Upsilon_{mid}^p(T)(v, \tau)}{S(T)} (\Pi_{mid} T)(\tau) \quad (6.42)$$

where $o_1 = (\mathfrak{t}_1, 0)$, is the k -th Fourier coefficient of a solution of (6.33) with the midpoint rule expansion up to order $r + 1$.

Proof. The proof follows the same lines as the one given in [BS22, Prop. 4.3]. \square

We are now able to define the main resonance based scheme:

Definition 6.3.9 The midpoint resonance based scheme is given by:

$$U_{mid,k}^{n,r}(\tau, v) = \sum_{T \in \hat{\mathcal{T}}_0^{r,k}(R)} \frac{\Upsilon_{mid}^p(T)(v, \tau)}{S(T)} (\Pi_{mid}^{n,r} T)(\tau) \quad (6.43)$$

It is obtained by replacing the character Π_{mid}^r by $\Pi_{mid}^{n,r}$ in (6.42).

The new scheme (6.43) can be described by the same type of forest formula introduced before.

Proposition 6.3.10 *For every forest F , $(\Pi_{mid}^{n,r} F)(t, \tau)$ is of the form of (6.31). For every decorated tree $T = \mathcal{I}_{o_1}(\lambda_k \mathcal{I}_{o_2}(\lambda_k F))$, $(\Pi_{mid}^{n,r} T)(\tau)$ is of the form (6.32).*

Proof. The proof follow by induction as in Theorem-(6.3.5) and Theorem (6.3.6). \square

Before stating our main result connecting the midpoint resonance based schemes to our earlier forest formula, we need to introduce a new map

$$\Upsilon_\chi^p(T)(u_{k_v}^{n+\chi_v}, v \in L_T, \tau)$$

defined as the same as $\Upsilon_{mid}^p(T)(v, \tau)$ except that for the leaves we use

$$e^{-i\chi_u \tau P_{o_{e_u}}(k_u)} u_{k_u}^{n+\chi_u}, \quad (6.44)$$

where e_u is the outgoing edge of u in T and o_{e_u} corresponds to the edge decoration of e_u . The map $\Upsilon_\chi^p(T)$ allows to parametrise implicit schemes as the scheme given by the midpoint rule.

Theorem 6.3.11 *The low regularity scheme $U_{mid,k}^{n,r}$ is of the form:*

$$u_k^{n+1} = e^{i\tau P_{o_1}(k)} u_k^n + e^{i\tau P_{o_1}(k)} \sum_{T \in \hat{\mathcal{T}}_2^{r,k}(R)} \sum_{\mathbf{a} \in [0,1]^{\tilde{E}_T}} \sum_{\chi \in \{0,1\}^{L_T}} \sum_{T_0, T_1, \dots, T_m \subset T} C_T b_{\mathbf{a}, \chi, T, T_0, \dots, T_m}(\tau, i\tau \mathcal{F}_{dom}(T_j), j \in \{0, \dots, m\}) \prod_{e \in \tilde{E}_{T_j}} e^{i\tau a_e \mathcal{F}_{low}(T_j^e)} \frac{\Upsilon_{\chi}^p(T)(u_{k_v}^{n+\chi_v}, v \in L_T, \tau)}{S(T)}, \quad (6.45)$$

where $\hat{\mathcal{T}}_2^{r,k}(R)$ was introduced in Definition (2).

Proof. First, we notice that

$$U_{mid,k}^{n,r}(\tau, v) = e^{i\tau P_{o_1}(k)} u_k^n + e^{i\tau P_{o_1}(k)} \sum_{T \in \hat{\mathcal{T}}_2^{r,k}(R)} \frac{\Upsilon_{mid}^p(T)(v, \tau)}{S(T)} (\Pi_{mid}^{n,r} T)(\tau).$$

Then, the result is just a consequence of Theorem (6.3.6) applied to each of the $(\Pi_{mid}^{n,r} T)(\tau)$. Indeed, one multiplies the coefficients for a decorated trees (6.32) with $\Upsilon_{mid}^p(T)(v, \tau)$. \square

For the local error, we can adapt [BS22, Def. 3.11].

Definition 6.3.12 Let $n \in \mathbf{N}$, $r \in \mathbf{Z}$. We recursively define $\mathcal{L}_{low}^r(\cdot, n)$ as

$$\mathcal{L}_{low}^r(F, n) = 1, \quad r < 0.$$

Else, when $r \geq 0$, we let:

$$\begin{aligned} \mathcal{L}_{low}^r(\mathbf{1}, n) &= 1, & \mathcal{L}_{low}^r(F \cdot \bar{F}, n) &= \mathcal{L}_{low}^r(F, n) + \mathcal{L}_{low}^r(\bar{F}, n) \\ \mathcal{L}_{low}^r(\mathcal{I}_{o_1}(\lambda_k^\ell F), n) &= \mathcal{L}_{low}^{r-|\ell|}(F, n) \\ \mathcal{L}_{low}^r(\mathcal{I}_{o_2}(\lambda_k^\ell F), n) &= k^\alpha \mathcal{L}_{low}^{r-|\ell|-1}(F, n) + \mathbf{1}_{\{r-|\ell| \geq 0\}} \sum_j k^{\bar{n}_j} \end{aligned}$$

where

$$\bar{n}_j = \max_m \left(n, \deg \left(P_{(F_j^{(1)}, F_j^{(2)}, m)} \mathcal{F}_{low}(\mathcal{I}_{(t_2, p)}(\lambda_k^\ell F_j^{(1)}))^{r-|\ell|+1-m} + \alpha \right) \right)$$

with

$$\begin{aligned} \Delta \mathcal{D}^{r-|\ell|-1}(F) &= \sum_j F_j^{(1)} \otimes F_j^{(2)}, \\ A^n(F_j^{(2)}) B^n(F_j^{(1)})(\xi, \tau) &= \sum_{|m| \leq r-|\ell|-1} \frac{P_{(F_j^{(1)}, F_j^{(2)}, m)}}{Q_{(F_j^{(1)}, F_j^{(2)}, m)}} \xi^{m_1} \tau^{m_2} \end{aligned}$$

and \mathcal{F}_{low} is defined in Definition (6.3.2).

Remark 6.3.13 The main difference between the definition above and [BS22, Def. 3.11] is the fact that we deal with monomials of the form $s^{m_1} \tau^{m_2}$ due to the fact that τ appears in the exact integrations. These modifications are minor from the original structure as the formalism is robust from moving from decorations on the edges in \mathbf{N} to \mathbf{N}^2 .

With the previous definition, one is able to give the local error of the approximations of the oscillatory integrals and for the schemes. The proofs are exactly the same as in [BS22, Section 3.3].

Theorem 6.3.14 *For every $T \in \mathcal{T}$ one has,*

$$(\Pi_{mid} T - \Pi_{mid}^{n,r} T)(\tau) = \mathcal{O}(\tau^{r+2} \mathcal{L}_{low}^r(T, n)).$$

The numerical scheme (6.42) approximates the exact solution locally up to order $r + 2$. More precisely, the following Theorem holds:

Theorem 6.3.15 (Local error) *The numerical scheme (6.42) with initial value $v = u(0)$ approximates the exact solution $U_k(\tau, v)$ up to a local error of type*

$$U_{\text{mid},k}^{n,r}(\tau, v) - U_k(\tau, v) = \sum_{T \in \hat{\mathcal{T}}_0^{r,k}(R)} \mathcal{O}(\tau^{r+2} \mathcal{L}_{\text{low}}^r(T, n) \Upsilon_{\text{mid}}^p(\lambda_k T)(v, \tau))$$

where the operator $\mathcal{L}_{\text{low}}^r(T, n)$, given in Definition (6.3.12), embeds the necessary regularity of the solution.

Remark 6.3.16 The local error of the resonance based low regularity schemes does not depend on the choice of the polynomial interpolation and the iteration of Duhamel's formula but only on the structure of the resonances.

Remark 6.3.17 As in [BS22, Prop. 3.18], one can always map back to physical space the scheme $U_{\text{mid},k}^{n,r}$. This due to the fact that the structure of the resonances and their exact integration is the same in this context.

6.4 Symmetric schemes

Having introduced the general forest formula (6.31) and the general subclass of midpoint general resonance based schemes, we now seek to answer the central question of this manuscript: "Which schemes in these classes are symmetric in the sense of definition (1)?" For this we take two routes: Firstly, for the subclass of midpoint general resonance based schemes it turns out that symmetry of the interpolation nodes is sufficient for the symmetry of the schemes. Secondly, for schemes captured by the forest formula (6.31) we can study the form of their adjoint method and find conditions on the coefficients of these schemes under which the methods are symmetric. We recall the adjoint method of a numerical scheme $v^{n+1} = \Phi_\tau v^n$ is defined by $\hat{\Phi}_\tau := \Phi_{-\tau}^{-1}$ and the method is said to be symmetric if $\hat{\Phi}_\tau = \Phi_\tau$. We can find the adjoint method of a scheme simply by the operations $n \leftrightarrow n+1$ and $\tau \leftrightarrow -\tau$. The swapping of n and $n+1$ corresponds in our case to changing $v_k(0)$ into $v_k(\tau)$. We define $\tilde{\Upsilon}_{\text{mid}}^p(T)(v, \tau)$ as the same as $\Upsilon_{\text{mid}}^p(T)(v, \tau)$ except that we exchange $v_k(0)$ and $v_k(\tau)$ in the definition:

$$\begin{aligned} \tilde{\Upsilon}_{\text{mid}}^p(\mathcal{I}_{(t_1,0)}(\lambda_k))(v, \tau) &:= \frac{1}{2}v_k(\tau) + \frac{1}{2}e^{iP_{o_1}(k)\tau}v_k(0) \\ \tilde{\Upsilon}_{\text{mid}}^p(\mathcal{I}_{(t_1,1)}(\lambda_k))(v, \tau) &:= \frac{1}{2}\bar{v}_k(\tau) + \frac{1}{2}e^{-iP_{o_1}(k)\tau}\bar{v}_k(0). \end{aligned}$$

6.4.1 Symmetric interpolation

We prove in the next proposition that the Duhamel's midpoint iteration truncated up to order $r+1$ gives a symmetric scheme. The proof uses the recursive construction of the iterated integrals.

Proposition 6.4.1 *The scheme defined by (6.42) is symmetric.*

Proof. We first observe that the scheme is given by

$$u_k(\tau) = e^{i\tau P_{o_1}(k)}u_k(0) + \sum_{T \in \hat{\mathcal{T}}_0^{r,k}(R) \setminus \{\mathcal{I}_{(t_1,0)}(\lambda_k \mathbf{1})\}} \frac{\Upsilon_{\text{mid}}^p(T)(u, \tau)}{S(T)} (\Pi_{\text{mid}} T)(\tau).$$

Now we swap n and $n+1$, and we also send τ onto $-\tau$, we obtain

$$u_k(\tau) = e^{i\tau P_{o_1}(k)}u_k(0) - e^{i\tau P_{o_1}(k)} \sum_{T \in \hat{\mathcal{T}}_0^{r,k}(R) \setminus \{\mathcal{I}_{(t_1,0)}(\lambda_k \mathbf{1})\}} \frac{\tilde{\Upsilon}_{\text{mid}}^p(T)(u, -\tau)}{S(T)} (\Pi_{\text{mid}} T)(-\tau).$$

Then, one has to show that two sums coincide for proving that the scheme is symmetric. We prove that this is the case for each term of the sum namely, one has:

$$-e^{-i\tau P_{o_1}(k)} \frac{\tilde{\Upsilon}_{\text{mid}}^p(T)(u, -\tau)}{S(T)} (\Pi_{\text{mid}} T)(-\tau) = \frac{\Upsilon_{\text{mid}}^p(T)(u, \tau)}{S(T)} (\Pi_{\text{mid}} T)(\tau). \quad (6.46)$$

We proceed by induction on the construction of the trees for showing (6.46). Decorated trees in $\hat{\mathcal{T}}_0^{r,k}(R) \setminus \{\mathcal{I}_{(t_1,0)}(\lambda_k \mathbf{1})\}$ are necessarily of the form

$$T = \mathcal{I}_{(t_1,0)}(\lambda_k \mathcal{I}_{(t_2,0)}(\lambda_k F)).$$

We notice that

$$(\Pi_{\text{mid}}T)(-\tau) = -i|\nabla|^\alpha(k)e^{i\tau P_{(\mathfrak{t}_1,0)}(k)} \int_0^{-\tau} e^{-isP_{(\mathfrak{t}_1,0)}(k)} (\Pi F)_{\text{mid}}(s, -\tau) ds.$$

By performing the change of variable $s = s + \tau$, one gets

$$(\Pi_{\text{mid}}T)(-\tau) = i|\nabla|^\alpha(k) \int_0^\tau e^{isP_{(\mathfrak{t}_1,0)}(k)} (\Pi_{\text{mid}}F)(s - \tau, -\tau) ds.$$

It remains to show that

$$\frac{\tilde{\Upsilon}_{\text{mid}}^p(T_j)(u, -\tau)}{S(T_j)} (\Pi_{\text{mid}}T_j)(s - \tau, -\tau) = \frac{\Upsilon_{\text{mid}}^p(T_j)(u, \tau)}{S(T_j)} (\Pi_{\text{mid}}T_j)(s, \tau),$$

where $T_j = \mathcal{I}_{o_1}(\lambda_{k_j} F_j)$ is a decorated tree appearing in the decomposition of F into a product of planted trees. If $F_j = \mathbf{1}$, with loss of generality, we suppose that $o_1 = (\mathfrak{t}_1, 0)$, then

$$\begin{aligned} \frac{\Upsilon_{\text{mid}}^p(T_j)(u, \tau)}{S(T_j)} (\Pi_{\text{mid}}T_j)(s, \tau) &= \left(\frac{1}{2} e^{-i\tau P_{o_1}(k_j)} u_{k_j}(\tau) + \frac{1}{2} u_{k_j}(0) \right) e^{isP_{o_1}(k_j)} \\ &= \frac{1}{2} e^{i(s-\tau)P_{o_1}(k_j)} u_{k_j}(\tau) + \frac{1}{2} e^{isP_{o_1}(k_j)} u_{k_j}(0) \end{aligned}$$

and

$$\begin{aligned} \frac{\tilde{\Upsilon}_{\text{mid}}^p(T_j)(u, -\tau)}{S(T_j)} (\Pi_{\text{mid}}T_j)(s - \tau, -\tau) &= \left(\frac{1}{2} e^{i\tau P_{o_1}(k_j)} u_{k_j}(0) + \frac{1}{2} u_{k_j}(\tau) \right) e^{i(s-\tau)P_{o_1}(k_j)} \\ &= \frac{1}{2} e^{i(s-\tau)P_{o_1}(k_j)} u_{k_j}(\tau) + \frac{1}{2} e^{isP_{o_1}(k_j)} u_{k_j}(0). \end{aligned}$$

For $(\mathfrak{t}_1, 1)$, we proceed analogously with the conjugate. For a more general F_j , we have:

$$(\Pi_{\text{mid}}T_j)(s - \tau, -\tau) = \frac{1}{2} e^{i(s-\tau)P_{o_1}(k_j)} ((\Pi_{\text{mid},1}F_j)(s - \tau, -\tau) + (\Pi_{\text{mid},2}F_j)(s - \tau, 0)).$$

Then F_j is of the form $\mathcal{I}_{o_2}(\lambda_{k_j} \hat{F}_j)$. Thus, we have

$$\begin{aligned} \left((\Pi_{\text{mid},1}\mathcal{I}_{o_2}(\lambda_{k_j} \hat{F}_j)) \right) (s - \tau, -\tau) &= -i|\nabla|^\alpha(k_j) \int_{-\tau}^{s-\tau} e^{i\xi P_{o_2}(k_j)} (\Pi_{\text{mid}}\hat{F}_j)(\xi, -\tau) d\xi, \\ &= -i|\nabla|^\alpha(k_j) \int_0^s e^{i(\xi-\tau)P_{o_2}(k_j)} (\Pi_{\text{mid}}\hat{F}_j)(\xi - \tau, -\tau) d\xi \end{aligned}$$

and

$$\begin{aligned} \left((\Pi_{\text{mid},2}\mathcal{I}_{o_2}(\lambda_{k_j} \hat{F}_j)) \right) (s - \tau, 0) &= -i|\nabla|^\alpha(k_j) \int_0^{s-\tau} e^{i\xi P_{o_2}(k_j)} (\Pi_{\text{mid}}\hat{F}_j)(\xi, -\tau) d\xi \\ &= -i|\nabla|^\alpha(k_j) \int_\tau^s e^{i(\xi-\tau)P_{o_2}(k_j)} (\Pi_{\text{mid}}\hat{F}_j)(\xi - \tau, -\tau) d\xi. \end{aligned}$$

We conclude by applying the induction hypothesis on \hat{F}_j that is

$$\frac{\tilde{\Upsilon}_{\text{mid}}^p(F_j)(u, -\tau)}{S(F_j)} (\Pi_{\text{mid}}\hat{F}_j)(s - \tau, -\tau) = \frac{\Upsilon_{\text{mid}}^p(F_j)(u, \tau)}{S(F_j)} (\Pi_{\text{mid}}\hat{F}_j)(s, \tau).$$

□

We recall the scheme given by the midpoint rule (6.43)

$$U_{\text{mid},k}^{n,r}(\tau, v) = \sum_{T \in \hat{\mathcal{T}}_0^{r,k}(R)} \frac{\Upsilon_{\text{mid}}^p(T)(v, \tau)}{S(T)} (\Pi_{\text{mid}}^n T)(\tau). \quad (6.47)$$

The terms $(\Pi_{\text{mid}}^{n,r}T)(\tau)$ are constructed in a similar way as $(\Pi_{\text{mid}}T)(\tau)$. The main difference happens for the computation of the time integrals. Indeed, $(\Pi_{\text{mid}}^{n,r}T)(\tau)$ performs an approximation with a polynomial interpolation and we need to do it in a symmetric way. We need the following lemma on the polynomial interpolation in order to guarantee this property:

Lemma 6.4.2 *If the interpolation nodes $a_j \in [0, 1], j = 0, \dots, r$ are symmetrically distributed, i.e. $a_j = 1 - a_{r-j}, j = 0, \dots, r$, then*

$$\tilde{p}_r(s - \tau, -\tau) = \sum_{j=0}^r e^{-ia_j\tau\mathcal{L}_{\text{low}}} p_j(s - \tau, -\tau) = e^{-i\tau\mathcal{L}_{\text{low}}} \tilde{p}_r(s, \tau), \quad (6.48)$$

where we have used the short hand notation

$$\tilde{p}_r(s, \tau) := \tilde{p}_r(\exp(is\mathcal{L}_{\text{low}}), \tau).$$

Proof. To begin with, for any $j = 0, \dots, r$ we have by definition of the interpolating polynomials $\tilde{p}_r(s, \tau)$ and $\tilde{p}_r(s, -\tau)$

$$\tilde{p}_r(a_j\tau, \tau) = e^{ia_j\tau\mathcal{L}_{\text{low}}}, \quad \tilde{p}_r(-a_j\tau, -\tau) = e^{ia_j\tau\mathcal{L}_{\text{low}}}.$$

Thus in particular we have

$$\begin{aligned} \tilde{p}_r(a_j\tau - \tau, -\tau) &= \tilde{p}_r(-a_{r-j}\tau, -\tau) = e^{ia_{r-j}\tau\mathcal{L}_{\text{low}}} \\ &= e^{i\tau\mathcal{L}_{\text{low}}} e^{-ia_j\tau\mathcal{L}_{\text{low}}} = e^{i\tau\mathcal{L}_{\text{low}}} \tilde{p}_r(a_j\tau, \tau), \end{aligned}$$

for each $j = 0, \dots, r$. Thus, for any given τ , $\tilde{p}_r(s - \tau, -\tau)$ and $e^{-i\tau\mathcal{L}_{\text{low}}} \tilde{p}_r(s, \tau)$ are two polynomials in s of degree $\leq r$ which match at $r + 1$ distinct points, so they are identical. \square

Theorem 6.4.3 *The scheme given by (6.43) is symmetric.*

Proof. The proof works in the same manner as for Proposition (6.4.1). The main difference is the use of the operator $\mathcal{K}_{o_2, j}^{k, r}$. We suppose that

$$\frac{\tilde{\Upsilon}_{\text{mid}}^p(F_j)(u, -\tau)}{S(F_j)} (\Pi_{\text{mid}}^{n, r} \hat{F}_j)(s - \tau, -\tau) = \frac{\Upsilon_{\text{mid}}^p(F_j)(u, \tau)}{S(F_j)} (\Pi_{\text{mid}}^{n, r} \hat{F}_j)(s, \tau) \quad (6.49)$$

and we consider

$$\left(\Pi_{\text{mid}, 1}^{n, r} \mathcal{I}_{o_2}(\lambda_{k_j} \hat{F}_j) \right) (s - \tau, -\tau) = \mathcal{K}_{o_2, 1}^{k_j, r} \left((\Pi_{\text{mid}}^{n, r} \hat{F}_j)(\cdot, -\tau), n \right) (s - \tau, -\tau).$$

From (6.49), we know that $\Pi_{\text{mid}}^{n, r} \hat{F}_j$ is of the form

$$(\Pi_{\text{mid}}^{n, r} \hat{F}_j)(s, \tau) = e^{i(s-\tau)\mathcal{F}_{\text{dom}}(\hat{F}_j)} A(s - \tau) + e^{is\mathcal{F}_{\text{dom}}(\hat{F}_j)} A(s).$$

Now, when we apply the operator $\mathcal{K}_{o_2, j}^{k, r}$, we get among various cases the exact integration

$$\begin{aligned} & \sum_{\ell=0}^r \int_{-\tau}^{s-\tau} e^{i\xi\mathcal{L}_{\text{dom}}} e^{-ia_j\tau\mathcal{L}_{\text{low}}} p_{\ell, r}(\xi, -\tau) \left(e^{i\tau\mathcal{F}_{\text{dom}}(\hat{F}_j)} A(\xi + \tau) + A(\xi) \right) d\xi \\ &= \sum_{\ell=0}^r \int_0^s e^{i(\xi-\tau)\mathcal{L}_{\text{dom}}} e^{-ia_j\tau\mathcal{L}_{\text{low}}} p_{\ell, r}(\xi - \tau, -\tau) \left(e^{i\tau\mathcal{F}_{\text{dom}}(\hat{F}_j)} A(\xi) + A(\xi - \tau) \right) d\xi \\ &= \int_0^s e^{i(\xi-\tau)\mathcal{L}_{\text{dom}}} e^{-i\tau\mathcal{L}_{\text{low}}} \tilde{p}_r(s, \tau) \left(e^{i\tau\mathcal{F}_{\text{dom}}(\hat{F}_j)} A(\xi) + A(\xi - \tau) \right) d\xi \end{aligned}$$

where from the second to the third line, we have used the assumption (6.48) and we have

$$\mathcal{L}_{\text{dom}} + \mathcal{L}_{\text{low}} = P_{o_2}(k_j) + \mathcal{F}_{\text{dom}}(\hat{F}_j).$$

Therefore, we obtain in the end

$$e^{-i\tau P_{o_2}(k_j)} \int_0^s e^{i\xi\mathcal{L}_{\text{dom}}} \tilde{p}_r(s, \tau) \left(A(\xi) + e^{-i\tau\mathcal{F}_{\text{dom}}(\hat{F}_j)} A(\xi - \tau) \right) d\xi$$

which allows us to conclude the symmetry of the method. \square

6.4.2 Conditions for symmetry

Based on the general expression of the scheme (6.45) we can arrive at sufficient conditions for the methods to be symmetric. The following observation is crucial:

Lemma 6.4.4 *Let T a decorated tree in $\widehat{\mathcal{T}}_0^k(\mathbb{R})$ as introduced in (6.29). We have*

$$\mathcal{F}_{\text{dom}}(T) + \sum_{e \in \tilde{E}_T} \mathcal{F}_{\text{low}}(T^e) = \sum_{v \in L_T} P_{o_{e_v}}(k_v)$$

where e_v is the outgoing edge of v in T and o_{e_v} corresponds to the edge decoration of e_v . The k_v are the leaves decorations corresponding to the frequencices. The dominant part $\mathcal{F}_{\text{dom}}(T)$ and the lower parts $\mathcal{F}_{\text{low}}(T^e)$ depend on them.

Before proving this statement let us briefly exhibit the meaning based on a simple example already introduced in Example (21).

Example 24 We consider the simple decorated tree from the NLSE

$$T = \mathcal{I}_{(t_1,0)}(\lambda_k \tilde{T}) = \begin{array}{c} \begin{array}{c} \circlearrowleft k_1 \\ \circlearrowleft k_2 \\ \circlearrowleft k_3 \end{array} \\ \vdots \\ \color{blue} \text{---} \\ \color{red} \text{---} \end{array},$$

with $k = -k_1 + k_2 + k_3$ we use the fact that

$$P_{(t_1,0)}(k) = -k^2, \quad P_{(t_1,1)}(k) = k^2$$

to find

$$\sum_{v \in L_T} P_{o_{e_v}}(k_v) = P_{(t_1,1)}(k_1) + P_{(t_1,0)}(k_2) + P_{(t_1,0)}(k_3) = k_1^2 - k_2^2 - k_3^2.$$

Moreover we have already established in Example (21) that

$$\mathcal{F}_{\text{dom}}(T) = \mathcal{F}_{\text{dom}}(\tilde{T}) + P_{(t_1,0)}(k) = 2k_1^2 - k^2$$

On the other hand, we have

$$\mathcal{F}_{\text{low}}(\tilde{T}) = k^2 - k_1^2 - k_2^2 - k_3^2$$

and the set \tilde{E}_T is composed of only one edge which is the only blue edge in T . We have $T^e = \tilde{T}$. In the end

$$\begin{aligned} \mathcal{F}_{\text{dom}}(T) + \sum_{e \in \tilde{E}_T} \mathcal{F}_{\text{low}}(T^e) &= \mathcal{F}_{\text{dom}}(T) + \mathcal{F}_{\text{low}}(T) \\ &= 2k_1^2 - k^2 + k^2 - k_1^2 - k_2^2 - k_3^2 \\ &= k_1^2 - k_2^2 - k_3^2 \\ &= \sum_{v \in L_T} P_{o_{e_v}}(k_v). \end{aligned}$$

Proof of Lemma (6.4.5). We proceed by induction on the size of the trees. If T is of the form $\mathcal{I}_{(t_1,a)}(\lambda_k \mathbf{1})$ then

$$\mathcal{F}_{\text{dom}}(\mathcal{I}_{(t_1,a)}(\lambda_k \mathbf{1})) = P_{(t_1,a)}(k)$$

which allows us to conclude the desired result since \tilde{E}_T is empty and this tree has only one leaf giving a contribution $P_{(t_1,a)}(k)$. If T is of the form $\mathcal{I}_{(t_1,a)}(\lambda_k \mathcal{I}_{(t_2,a)}(\lambda_k F))$ then

$$\begin{aligned} \mathcal{F}_{\text{dom}}(T) + \sum_{e \in \tilde{E}_T} \mathcal{F}_{\text{low}}(T^e) &= P_{(t_1,a)}(k) + \mathcal{F}_{\text{dom}}(\mathcal{I}_{(t_2,a)}(\lambda_k F)) \\ &\quad + \mathcal{F}_{\text{low}}(\mathcal{I}_{(t_2,a)}(\lambda_k F)) + \sum_{e \in \tilde{E}_T \setminus \{\bar{e}\}} \mathcal{F}_{\text{low}}(T^e) \end{aligned}$$

where \bar{e} denotes the edge such that $T^{\bar{e}} = \mathcal{I}_{(t_2,a)}(\lambda_k F)$. Now, we use Definition (6.3.2) to notice that

$$\mathcal{F}_{\text{dom}}(\mathcal{I}_{(t_2,a)}(\lambda_k F)) + \mathcal{F}_{\text{low}}(\mathcal{I}_{(t_2,a)}(\lambda_k F)) = P_{(t_2,a)}(k) + \mathcal{F}_{\text{dom}}(F).$$

By definition, we have also

$$P_{(t_2,a)}(k) + P_{(t_1,a)}(k) = 0. \tag{6.50}$$

We got in the end

$$\begin{aligned} \mathcal{F}_{\text{dom}}(T) + \sum_{e \in \tilde{E}_T} \mathcal{F}_{\text{low}}(T^e) &= \mathcal{F}_{\text{dom}}(F) + \sum_{e \in \tilde{E}_T \setminus \{\bar{e}\}} \mathcal{F}_{\text{low}}(T^e) \\ &= \mathcal{F}_{\text{dom}}(F) + \sum_{e \in \tilde{E}_F} \mathcal{F}_{\text{low}}(F^e). \end{aligned}$$

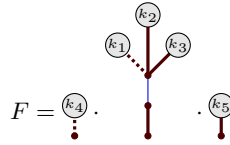
We continue the induction by observing that F is a product of trees in $\tilde{\mathcal{T}}_0^{r,k}(R)$. We apply the induction hypothesis on each of these trees and use the fact that \mathcal{F}_{dom} is additive for the forest product in order to conclude. \square

Lemma 6.4.5 *Let $T_0 \cdot T_1 \dots \cdot T_m \subset \mathcal{I}_{(t_2,0)}(\lambda_k F) \in \hat{\mathcal{T}}_2^k(R)$ be a splitting of F as introduced in (6.29). Then we have*

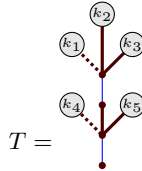
$$\sum_{j=0}^m \left(\mathcal{F}_{\text{dom}}(T_j) + \sum_{e \in \tilde{E}_{T_j}} \mathcal{F}_{\text{low}}(T_j^e) \right) = \sum_{v \in L_F} P_{o_{e_v}}(k_v) + P_{(t_2,0)}(k). \quad (6.51)$$

Proof. This is a consequence of Lemma (6.4.4) applied to each of the T_j . In the end, we do not get all the leaves of the T_j but only the ones in F because the root of the T_j ($j \geq 0$) is associated with a leaf in a T_i . Indeed, this introduced a cancellation of the type (6.50). \square

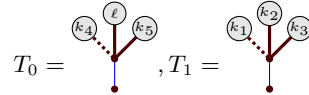
Example 25 Let us consider the following forest



such that $T = \mathcal{I}_{(t_2,0)}(\lambda_k F)$ is identified with



with $k = -k_1 - k_4 + k_2 + k_3 + k_5$. We consider the following forest splitting of T , with $T_0 \cdot T_1 \subset T$:



with $k = k_4 - \ell - k_5$ and $\ell = -k_1 + k_2 + k_3$. Let us compute both sides of the identity (6.51) for this forest splitting: Beginning with the left hand side where we have

$$\mathcal{F}_{\text{dom}}(T_0) = 2k_4^2.$$

Moreover, since the tree has just one single blue edge the sum simplifies and we find

$$\sum_{e \in \tilde{E}_{T_0}} \mathcal{F}_{\text{low}}(T_0^e) = \mathcal{F}_{\text{low}}(T_0^e) = -k_4^2 - k_5^2 - \ell^2 + k^2,$$

and, similarly for T_1 we have

$$\begin{aligned} \mathcal{F}_{\text{dom}}(T_1) &= 2k_1^2, \\ \sum_{e \in \tilde{E}_{T_1}} \mathcal{F}_{\text{low}}(T_1^e) &= -k_1^2 - k_2^2 - k_3^2 + \ell^2. \end{aligned}$$

For the right hand side on the other hand we obtain

$$\sum_{v \in L_F} P_{o_{e_v}}(k_v) = k_4^2 + k_1^2 - k_2^2 - k_3^2 - k_5^2,$$

$$P_{(t_2,0)}(k) = -k^2.$$

Combining all of the above expressions clearly shows that the identity (6.51) is indeed satisfied in the present example.

Remark 6.4.6 The appearance of the term $P_{(t_2,0)}(k)$ in (6.51) is due to the fact that here we consider forest splittings of trees inside $\hat{\mathcal{T}}_2^k(R)$. Had we instead chosen to work with trees inside $\hat{\mathcal{T}}_0^k(R)$ this term would disappear from the above identity. Essentially, like in the previous proof, if we want to express the sum of the dominant and lower order parts in a forest splitting we can take advantage of cancellations of the form (6.50), meaning as soon as a blue dotted and brown solid edge are adjacent this leads to cancellation of the contribution from the nodal decoration in the overall identity. This means the only terms left are those which cannot be paired with an edge of conjugate colour, in particular the root and all the leaves of the resulting tree.

Proposition 6.4.7 *If the coefficients b , satisfy the following simple relation*

$$-\left(\prod_{j=0}^m e^{z_j}\right) b_{\mathbf{a}, \chi, T, T_0, \dots, T_m}(-\tau, -z_j) = b_{1-\mathbf{a}, 1-\chi, T, T_0, \dots, T_m}(\tau, z_j) \quad (6.52)$$

for every $\mathbf{a} \in [0, 1]^{\tilde{E}_F}$, $\chi \in \{0, 1\}^{L_T}$ and any splitting $T_0 \cdot T_1 \dots \cdot T_m \subset T$, then the method (6.45) is symmetric.

Proof. Let us consider the adjoint method $\hat{\Phi}_{n \rightarrow n+1} = \Phi_{n+1 \rightarrow n}^{-1}$, which can be expressed as follows

$$u_k^{n+1} = e^{i\tau P_{o_1}(k)} u_k^n - \sum_{T \in \hat{\mathcal{T}}_2^{r,k}(R)} \sum_{\mathbf{a} \in [0,1]^{\tilde{E}_F}} \sum_{\chi \in \{0,1\}^{L_T}} \sum_{T_0 \cdot T_1 \dots \cdot T_m \subset T} C_T$$

$$b_{\mathbf{a}, \chi, T, T_0, \dots, T_m}(\tau, i\tau \mathcal{F}_{\text{dom}}(T_j), j \in \{0, \dots, m\})$$

$$\prod_{e \in \tilde{E}_{T_j}} e^{i\tau a_e \mathcal{F}_{\text{low}}(T_j^e)} \frac{\Upsilon_\chi^p(T)(u_{k_v}^{n+\chi v}, v \in L_T), \tau}{S(T)}.$$

By using Lemma (6.4.5), we have

$$u_k^{n+1} = e^{i\tau P_{o_1}(k)} u_k^n - e^{i\tau P_{o_1}(k)} \sum_{T \in \hat{\mathcal{T}}_0^{r,k}(R)} \sum_{\mathbf{a} \in [0,1]^{\tilde{E}_F}} \sum_{\chi \in \{0,1\}^{L_T}} \sum_{T_0 \cdot T_1 \dots \cdot T_m \subset T} C_T$$

$$\left(\prod_{j=0}^m e^{i\tau \mathcal{F}_{\text{dom}}(T_j)}\right) b_{\mathbf{a}, \chi, T, T_0, \dots, T_m}(-\tau, -i\tau \mathcal{F}_{\text{dom}}(T_j), j \in \{0, \dots, m\}) \quad (6.53)$$

$$\prod_{e \in \tilde{E}_{T_j}} e^{i\tau(1-a_e) \mathcal{F}_{\text{low}}(T_j^e)} \frac{\Upsilon_\chi^p(T)(u_{k_v}^{n+1-\chi v}, v \in L_T), \tau}{S(T)} \prod_{v \in L_T} e^{-i\tau P_{o_{e_v}}(k_v)}.$$

Here we have used the fact that

$$\Upsilon_\chi^p(T)(u_{k_v}^{n+1-\chi v}, v \in L_T, \tau) \prod_{v \in L_T} e^{-i\tau P_{o_{e_v}}(k_v)} = \Upsilon_\chi^p(T)(u_{k_v}^{n+\chi v}, v \in L_T, \tau)$$

which can be proved easily by induction on T using the recursive definition of Υ_χ^p . We have also used the identity

$$P_{o_1}(k) = -P_{(t_2,0)}(k).$$

By comparing (6.45) and (6.53) we immediately obtain the conditions (6.52) for symmetry. \square

6.4.3 Examples

In this section we illustrate the general framework introduced previously on two examples: the nonlinear Schrödinger equation (see Section (6.4.3)) and the Korteweg-de Vries equation (see Section (6.4.3)).

The Nonlinear Schrödinger equation

As a first example let us consider the cubic nonlinear Schrödinger (NLS) equation

$$i\partial_t u(t, x) + \Delta u(t, x) = |u(t, x)|^2 u(t, x) \quad (t, x) \in \mathbf{R} \times \mathbb{T}^d \quad (6.54)$$

with an initial condition

$$u|_{t=0} = u_0. \quad (6.55)$$

We start with the construction of a first-order symmetric low-regularity scheme for (6.54) and illustrate how our general framework covers both the previous explicit low-regularity schemes [BS22], [ABBS22b] and the case of symmetric low-regularity schemes for NLS which was recently introduced and then studied in [AB23b] and [FMS23]. We then exhibit our new symmetric midpoint rule framework (6.43), which in particular allows for a symmetric second order scheme which is optimal in the sense of regularity.

Note that the Schrödinger equation (6.54) fits into the general framework (6.1) with

$$\mathcal{L}\left(\nabla, \frac{1}{\varepsilon}\right) = \Delta, \quad \alpha = 0 \quad \text{and} \quad p(u, \bar{u}) = u^2 \bar{u}.$$

Here $\mathcal{L} = \{t_1, t_2\}$, $P_{t_1} = -\lambda^2$ and $P_{t_2} = \lambda^2$, and the structure constant $C_T = 1$ for all $T \in \hat{\mathcal{T}}_0^{r,k}(R)$, for any $r \in \mathbf{N}$. Then, we denote by \mid an edge decorated by $(t_1, 0)$, $\dot{\mid}$ an edge denoted by $(t_1, 1)$ by \mid an edge decorated by $(t_2, 0)$ and by $\dot{\mid}$ an edge decorated by $(t_2, 1)$. The set $\hat{\mathcal{T}}_0^{0,k}(R)$ is given by:

$$\hat{\mathcal{T}}_0^{0,k}(R) = \left\{ T_0, T_1, k_i \in \mathbf{Z}^d \right\}, \quad T_0 = \mid, \quad T_1 = \begin{array}{c} \circledast k_1 \\ \circledast k_2 \\ \circledast k_3 \\ \mid \\ \bullet \end{array}, \quad (6.56)$$

and $\hat{\mathcal{T}}_0^{1,k}(R)$ is given by:

$$\hat{\mathcal{T}}_0^{1,k}(R) = \left\{ T_0, T_1, T_2, T_3, k_i \in \mathbf{Z}^d \right\}, \quad T_2 = \begin{array}{c} \circledast k_2 \\ \circledast k_1 \quad \circledast k_3 \\ \circledast k_4 \quad \circledast k_5 \\ \mid \\ \bullet \end{array}, \quad T_3 = \begin{array}{c} \circledast k_2 \\ \circledast k_1 \quad \circledast k_3 \\ \circledast k_4 \quad \circledast k_5 \\ \mid \\ \bullet \end{array}. \quad (6.57)$$

If we take all coefficients equal to zero whenever T is not given by

$$T = \begin{array}{c} \circledast k_2 \\ \circledast k_1 \quad \circledast k_3 \\ \mid \\ \bullet \end{array},$$

and we consider only the forest $F = T$, then the general formula (6.45) reduces to a single term of the form:

$$u_k^{n+1} = e^{-i\tau k^2} u_k^n + e^{-i\tau k^2} \sum_{a \in [0,1]} \sum_{\chi \in \{0,1\}^{L_T}} b_{a,\chi}(\tau, i\tau \mathcal{F}_{\text{dom}}(T)) e^{i\tau a \mathcal{F}_{\text{low}}(T)} \frac{\Upsilon_\chi^p(T)(u_{k_v}^{n+\chi_v}, v \in L_T)}{S(T)}.$$

Note here $|L_T| = 3$ so we can equivalently write the above expression in the following form in Fourier coordinates. Indeed, by noting that $\mathcal{F}_{\text{dom}}(T) = 2k_1^2$, $\mathcal{F}_{\text{low}}(T) = 2k_2 k_3 - 2k_1 k_2 - 2k_1 k_3$ we have

$$u_k^{n+1} = e^{-i\tau k^2} u_k^n + e^{-i\tau k^2} \sum_{k=-k_1+k_2+k_3} \sum_{a \in [0,1]} \sum_{\chi \in \{0,1\}^3} b_{a,\chi}(\tau, 2i\tau k_1^2) e^{i\tau a 2(k_2 k_3 - k_1 k_2 - k_1 k_3)} \overline{\hat{v}_{k_1}^{n+\chi_1}} \hat{v}_{k_2}^{n+\chi_2} \hat{v}_{k_3}^{n+\chi_3}. \quad (6.58)$$

First of all we note that the first order integrator developed in [OS18] falls in this category: Take $b_{0,(0,0,0)}(\tau, z) = -i\tau \varphi_1(z)$

and all other coefficients to zero then we find

$$u_k^{n+1} = e^{-i\tau k^2} u_k^n - i e^{-i\tau k^2} \sum_{k=-k_1+k_2+k_3} \tau \varphi_1(2i\tau k_1^2) \overline{u_{k_1}^n} u_{k_2}^n u_{k_3}^n,$$

which is exactly equal to the integrator introduced in [OS18, (4)]. In physical space the above scheme is given by

$$u^{n+1} = \Phi_{\text{NLS},1}^\tau(u^n) = e^{i\tau\Delta} u^n - i e^{i\tau\Delta} ((u^n)^2 \varphi_1(-2i\tau\Delta) \overline{u^n}), \quad (6.59)$$

where the filter function φ_1 is defined as $\varphi_1(\sigma) = \frac{e^\sigma - 1}{\sigma}$.

Let us now consider symmetric schemes. Following Proposition (6.4.7) the scheme (6.45) is symmetric if the following equality is satisfied for all $a \in [0, 1], \chi \in \{0, 1\}$ ³:

$$-e^z b_{a,\chi}(-\tau, -z) = b_{1-a,1-\chi}(\tau, z). \quad (6.60)$$

Intuitively speaking the above equations provide a sufficient condition relating the coefficients $b_{a,\chi}$ and $b_{1-a,1-\chi}$ therefore allowing us to find symmetric schemes if we specify one of the two for each value of a, χ . There are a large class of first order schemes in this form, but perhaps one of the simplest ones is the following symmetrised version of the integrator from [OS18] which was recently introduced in [AB23b]: Take $b_{0,(0,0,0)}(\tau, z) = i/2\tau\varphi_1(z/2)$, then by (6.60) we should choose $b_{1,(1,1,1)}(\tau, z) = i/2\tau\varphi_1(-z/2)$. We take all other coefficients equal to zero, which results precisely in the following integrator:

$$\begin{aligned} u^{n+1} &= \Phi_{\text{NLS},2}^\tau(u^n) = e^{i\tau\Delta} u^n - i \frac{\tau}{2} e^{i\tau\Delta} ((u^n)^2 \varphi_1(-i\tau\Delta) \overline{u^n}) \\ &\quad - i \frac{\tau}{2} ((u^{n+1})^2 \varphi_1(i\tau\Delta) \overline{u^{n+1}}). \end{aligned} \quad (6.61)$$

Note this is not the only symmetric first order integrator that can be found in this way. For example we could have taken

$$b_{0,(1,0,0)}(\tau, z) = i/2\tau\varphi_1(z/2), \quad b_{1,(0,1,1)}(\tau, z) = i/2\tau\varphi_1(-z/2),$$

and all other coefficients zero.

Next we choose the coefficients

$$b_{a,(\chi_1,\chi_2,\chi_3)}(\tau, z) = -i \frac{\tau}{16} \varphi_1(z)$$

for every $a, \chi_j \in \{0, 1\}$. The other coefficients are set to be zero which leads to the following symmetric scheme (6.54)

$$\begin{aligned} u^{n+1} &= \Phi_{\text{NLS},3}^\tau(u^n) \\ &= e^{i\tau\Delta} u^n - i \frac{\tau}{16} e^{i\tau\Delta} \left((u^n + e^{-i\tau\Delta} u^{n+1})^2 \varphi_1(-2i\tau\Delta) (\overline{u^n} + e^{i\tau\Delta} \overline{u^{n+1}}) \right) \\ &\quad - i \frac{\tau}{16} \left((e^{i\tau\Delta} u^n + u^{n+1})^2 \varphi_1(2i\tau\Delta) (e^{-i\tau\Delta} \overline{u^n} + \overline{u^{n+1}}) \right). \end{aligned} \quad (6.62)$$

The above scheme can also be recursively derived by the general framework of the midpoint rule (6.43) and therefore allows for higher order symmetric counterparts which are optimal in the sense of regularity. Our characterisation of symmetric schemes in Proposition (6.4.7) immediately confirm this method to be symmetric, since for all a, χ we have

$$-e^z b_{a,\chi}(-\tau, -z) = -i \frac{\tau}{16} e^z \varphi_1(-z) = -i \frac{\tau}{16} \frac{1 - e^z}{-z} = \varphi_1(z) b_{1-a,1-\chi}(\tau, z).$$

Proposition 6.4.8 *The scheme (6.62) can be derived from the general tree series expansion (6.43).*

Proof. At first order it follows from (6.43) that we have

$$\begin{aligned} U_k^r(\tau, u) &= \sum_{T \in \mathcal{T}_0^{0,k}(R)} \frac{\Upsilon_{\text{mid}}^p(T)(u, \tau)}{S(T)} (\Pi_{\text{mid}}^{n,r} T_0)(\tau) \\ &= \frac{\Upsilon_{\text{mid}}^p(T_0)(u, \tau)}{S(T_0)} (\Pi_{\text{mid}}^{n,r} T_0)(\tau) + \sum_{k=-k_1+k_2+k_3} \frac{\Upsilon_{\text{mid}}^p(T_1)(u, \tau)}{S(T_1)} (\Pi_{\text{mid}}^{n,r} T_1)(\tau) \end{aligned}$$

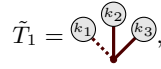
From the definition of the symmetry factor, one has

$$S(T_0) = 1, \quad S(T_1) = 2$$

for $S(T_1)$ the factor two is due to the fact that we have two solid brown edges \mid attached to the same node in T_1 . Moreover, we have:

$$\begin{aligned} \Upsilon_{\text{mid}}^p(T_0)(u, \tau) &= u_k^\ell \\ \hat{\Upsilon}_{\text{mid}}^p(T_0)(u, \tau) &= \frac{1}{2}(e^{i\tau k^2} u_k^{\ell+1} + u_k^\ell) \end{aligned}$$

where we have used ℓ instead of n such that to not create confusion with $\Pi^{n,r}$. By multiplicativity, for the following tree:



we have

$$\begin{aligned} \Upsilon_{\text{mid}}^p(T_1)(u, \tau) &= \hat{\Upsilon}_{\text{mid}}^p(\tilde{T}_1)(u, \tau) \\ &= 2 \frac{1}{2}(e^{-i\tau k_1^2} \bar{u}_{k_1}^{\ell+1} + \bar{u}_{k_1}^\ell) \frac{1}{2}(e^{i\tau k_2^2} u_{k_2}^{\ell+1} + u_{k_2}^\ell) \frac{1}{2}(e^{i\tau k_3^2} u_{k_3}^{\ell+1} + u_{k_3}^\ell) \end{aligned}$$

On the other hand, we have

$$(\Pi_{\text{mid}}^{n,r} T_0)(\tau) = e^{-i\tau k^2}, \quad (\Pi_{\text{mid}}^{n,r} \tilde{T}_1)(s, \tau) = e^{i(k_1^2 - k_2^2 - k_3^2)},$$

Then,

$$(\Pi_{\text{mid}}^{n,r} T_1)(\tau) = e^{-i\tau k^2} \mathcal{K}_{o_2}^{k,r}((\Pi_{\text{mid}}^{n,r-1} \tilde{T}_1)(\cdot, \tau), n)(\tau)$$

We compute the scheme for $n = 1$ and $r = 0$. We obtain the following term:

$$\mathcal{K}_{o_2}^{k,r}((\Pi_{\text{mid}}^{n,r-1} \tilde{T}_1)(\cdot, \tau), n)(\tau) = -i \int_0^\tau e^{is\mathcal{L}_{\text{dom}}} ds \left(\frac{1 + e^{i\tau \mathcal{L}_{\text{low}}}}{2} \right)$$

where

$$\mathcal{L}_{\text{dom}} = 2k_1^2, \quad \mathcal{L}_{\text{low}} = k^2 - k_1^2 - k_2^2 - k_3^2.$$

In the end, we have

$$(\Pi_{\text{mid}}^{n,r} T_1)(\tau) = -i\tau \varphi_1(2i\tau k_1^2) \left(\frac{e^{-i\tau k^2} + e^{-i\tau(k_1^2 + k_2^2 + k_3^2)}}{2} \right).$$

We note that

$$\varphi_1(2i\tau k_1^2) e^{-2i\tau k_1^2} = \varphi_1(-2i\tau k_1^2).$$

Therefore, we have

$$\begin{aligned} \sum_{k=-k_1+k_2+k_3} \frac{\Upsilon_{\text{mid}}^p(T_1)(u, \tau)}{S(T_1)} (\Pi_{\text{mid}}^{n,r} T_1)(\tau) &= -i \sum_{k=-k_1+k_2+k_3} \frac{e^{-i\tau k^2}}{2} \tau \varphi_1(2i\tau k_1^2) \\ &\frac{1}{2}(e^{-i\tau k_1^2} \bar{u}_{k_1}^{\ell+1} + \bar{u}_{k_1}^\ell) \frac{1}{2}(e^{i\tau k_2^2} u_{k_2}^{\ell+1} + u_{k_2}^\ell) \frac{1}{2}(e^{i\tau k_3^2} u_{k_3}^{\ell+1} + u_{k_3}^\ell) \\ &+ \tau \frac{\varphi_1(-2i\tau k_1^2)}{2} \frac{1}{2}(\bar{u}_{k_1}^{\ell+1} + e^{i\tau k_1^2} \bar{u}_{k_1}^\ell) \frac{1}{2}(u_{k_2}^{\ell+1} + e^{-i\tau k_2^2} u_{k_2}^\ell) \frac{1}{2}(u_{k_3}^{\ell+1} + e^{-i\tau k_3^2} u_{k_3}^\ell). \end{aligned}$$

In physical space this leads to the first order symmetric low regularity integrator for the NLS equation (6.62). \square

Remark 6.4.9 The derivation of the scheme (6.62) from the general midpoint Duhamel iterations exhibits an interesting

recipe for resonance based schemes that are constructed for equations of the form

$$\begin{aligned} i\partial_t u(t, x) + \mathcal{L}\left(\nabla, \frac{1}{\varepsilon}\right)u(t, x) &= |\nabla|^\alpha p(u(t, x), \bar{u}(t, x)), \\ u(0, x) &= v(x). \end{aligned}$$

Indeed, suppose we have already obtained an explicit *first-order* resonance based scheme for the above equation (cf. [OS18, HS17b] etc.) of the general form

$$u^{n+1} = \Phi_\tau(u^n),$$

where Φ_τ is a general nonlinear map representing the time step, then this can be easily converted to a second order symmetric method simply by considering instead

$$u^{n+1} = \Phi_\tau\left(\frac{e^{-i\tau\mathcal{L}\left(\nabla, \frac{1}{\varepsilon}\right)}u^{n+1} + u^n}{2}\right).$$

Remark 6.4.10 In similar vein to Proposition (6.4.8) we could derive the scheme (6.61) from a generalised tree series expansion. However, instead of using a midpoint iteration of Duhamel's formula as introduced in Section (6.3.3) we would have to iterate in the following way: By averaging (6.34) and (6.35) we find

$$\begin{aligned} u_k(t_n + s) &= \frac{e^{-isk^2}u_k(t_n) + e^{-i(s-\tau)k^2}u_k(t_n + \tau)}{2} \\ &\quad - \frac{i}{2}e^{-isk^2} \sum_{k=-k_1+k_2+k_3} \underbrace{\int_0^s e^{i\tilde{s}k^2} \overline{u_{k_1}(t_n + \tilde{s})} u_{k_2}(t_n + \tilde{s}) u_{k_3}(t_n + \tilde{s}) d\tilde{s}}_{=: \mathcal{I}_1} \\ &\quad - \frac{i}{2}e^{-isk^2} \sum_{k=-k_1+k_2+k_3} \underbrace{\int_\tau^s e^{i\tilde{s}k^2} \overline{u_{k_1}(t_n + \tilde{s})} u_{k_2}(t_n + \tilde{s}) u_{k_3}(t_n + \tilde{s}) d\tilde{s}}_{=: \mathcal{I}_2}. \end{aligned}$$

Instead of iterating this midpoint expression throughout all appearances of $u_j(t_n + \tilde{s})$ in the above expression (as we do for the Duhamel midpoint iterates) we could just as well choose to iterate the left endpoint Duhamel formula (6.34) in the terms from \mathcal{I}_1 and the right endpoint Duhamel formula (6.35) in the terms from \mathcal{I}_2 . Repeating this process can be captured with a decorated tree series in analogous manner to the midpoint iterations and truncating such an expansion again leads to symmetric low-regularity schemes, including (after one such iteration and truncation of all terms involving at least double integrals) the scheme (6.61).

Proposition 6.4.11 *The schemes (6.59), (6.61) and (6.62) have a local error of order $\mathcal{O}(\tau^2\nabla u)$.*

Proof. First, for the explicit scheme (6.59) the local error directly follows from Theorem (6.3.15) and can be computed using Definition (6.3.12) as it is performed in the proof of [BS22, Cor. 5.1]. In order to obtain the local error bounds of the implicit schemes (6.61), (6.62) one needs to apply Theorem (6.3.15) and to combine it with a fixed-point argument on the numerical flow. To go further, the first order convergence of these schemes follow by combining the local error bound with a stability argument, we refer to the works [MS22, AB23b] which perform this analysis in full detail. \square

Remark 6.4.12 The symmetric scheme (6.61) was first rigorously analysed in [AB23b]. In particular it was shown in [AB23b] that the local error of the scheme is of order $\mathcal{O}(\tau^2\nabla u)$, which is optimal in regard of the regularity assumptions. Indeed, the scheme (6.61) does not require more regularity on the solution than previously constructed asymmetric low regularity integrators such as (6.59) introduced in [OS18, BS22]. As the scheme (6.61) is symmetric it is naturally also of second order; however, not under optimal regularity assumptions (see also Remark (6.2.6)). More precisely, by exploiting the tools presented in [AB23b] one can show that the scheme (6.61) (as well as (6.62)) is of second order with a local error of order $\mathcal{O}(\tau^3\nabla\Delta u)$. This error structure imposes more regularity on the solution than asymmetric low-regularity integrators such as the ones proposed in [BS22] which only require the boundedness of two additional derivatives instead of three due to the local error of the form $\mathcal{O}(\tau^3\Delta u)$.

Our new symmetric midpoint rule framework (6.43) allows for a symmetric second order scheme which is optimal in the sense of regularity, i.e., has a local error structure of the form $\mathcal{O}(\tau^3\Delta u)$, see the scheme (6.63) below.

Proposition 6.4.13 *The second order scheme coming from (6.43) is given by:*

$$u^{n+1} = \varphi_{NLS,4}^\tau(u^n) = e^{i\tau\Delta}u^n \tag{6.63}$$

$$\begin{aligned}
& -i\frac{\tau}{8}e^{i\tau\Delta}\left((u^n + e^{-i\tau\Delta}u^{n+1})^2(\varphi_1(-2i\tau\Delta) - \varphi_2(-2i\tau\Delta))\left(\overline{u^n} + e^{i\tau\Delta}\overline{u^{n+1}}\right)\right) \\
& -i\frac{\tau}{8}\left((e^{i\tau\Delta}u^n + u^{n+1})^2\varphi_2(-2i\tau\Delta)\left(e^{i\tau\Delta}\overline{u^n} + e^{2i\tau\Delta}\overline{u^{n+1}}\right)\right)
\end{aligned}$$

with a local error structure of the form $\mathcal{O}(\tau^3\Delta u)$ and $\varphi_2(\sigma) = \frac{e^\sigma - \varphi_1(\sigma)}{\sigma}$.

Remark 6.4.14 In practice the computational effort required to compute u^{n+1} in (6.63) is not significantly larger than the solution of (6.15) or other previous symmetric low-regularity methods for the NLSE. In particular, a similar analysis to that presented in [AB23b, Section 3], [BMS22, Appendix A] and [MS23] shows that the implicit equations can be solved efficiently using fixed point iterations, and that the number of iterations required is independent of the number of spatial discretisation points.

Remark 6.4.15 One can find the coefficients b for the scheme (6.63) such that it is of the form given by (6.45).

Proof of Proposition (6.4.13). For the scheme of order two ($r = 1$) and $n = 2$, one has to consider:

$$\begin{aligned}
U_k^{n,1}(\tau, u) &= \sum_{T \in \tilde{\mathcal{T}}_0^{1,k}(R)} \frac{\Upsilon_{\text{mid}}^p(T)(u, \tau)}{S(T)} (\Pi_{\text{mid}}^{n,1}T_0)(\tau) \\
&= \frac{\Upsilon_{\text{mid}}^p(T_0)(u, \tau)}{S(T_0)} (\Pi_{\text{mid}}^{n,1}T_0)(\tau) + \sum_{k=-k_1+k_2+k_3} \frac{\Upsilon_{\text{mid}}^p(T_1)(u, \tau)}{S(T_1)} (\Pi_{\text{mid}}^{n,1}T_1)(\tau) \\
&+ \sum_{k=-k_1+k_2+k_3-k_4+k_5} \frac{\Upsilon_{\text{mid}}^p(T_2)(u, \tau)}{S(T_2)} (\Pi_{\text{mid}}^{n,1}T_2)(\tau) \\
&+ \sum_{k_1-k_2-k_3+k_4+k_5=k} \frac{\Upsilon_{\text{mid}}^p(T_3)(u, \tau)}{S(T_3)} (\Pi_{\text{mid}}^{n,1}T_3)(\tau).
\end{aligned}$$

From the definition of the symmetry factor, we have

$$S(T_2) = 1 \times 2 = 2, \quad S(T_3) = 2 \times 2 = 4,$$

for $S(T_2)$ the factor one corresponds to the fact that for the node on top of the first blue edges the symmetry factor is one. Indeed, the trees on top of the brown edges are different: a leaf decorated by k_5 is different from a tree having three leaves. Moreover, we have:

$$\Upsilon_{\text{mid}}^p(T_j)(u, \tau) = \Upsilon^p(T_j)\left(\frac{1}{2}(e^{i\tau k^2}u^{n+1} + u^n)\right), \quad j \in \{2, 3\},$$

where

$$\Upsilon^p(T_2)(u) = 4\bar{u}_{k_1}u_{k_2}u_{k_3}\bar{u}_{k_4}u_{k_5}, \quad \Upsilon^p(T_3)(u) = 4u_{k_1}\bar{u}_{k_2}\bar{u}_{k_3}u_{k_4}u_{k_5}.$$

The factor 4 in both expressions comes from the two brown edges that appear twice inside the decorated trees T_2 and T_3 . For the term $(\Pi_{\text{mid}}^{2,1}T_1)(\tau)$, we proceed with interpolation at two nodes ($a_0 = 0, a_1 = 1$):

$$p_2(s, \tau) = 1 + \frac{s}{\tau}\left(e^{is\mathcal{L}_{\text{low}}} - 1\right),$$

where

$$\mathcal{L}_{\text{dom}} = 2k_1^2, \quad \mathcal{L}_{\text{low}} = k^2 - k_1^2 - k_2^2 - k_3^2.$$

We obtain

$$\begin{aligned}
\mathcal{K}_{\mathcal{O}_2}^{k,1}((\Pi_{\text{mid}}^{2,0}\tilde{T}_1)(\cdot, \tau), 2)(\tau) &= -i\int_0^\tau e^{is\mathcal{L}_{\text{dom}}}ds - i\int_0^\tau se^{is\mathcal{L}_{\text{dom}}}ds\left(\frac{e^{i\tau\mathcal{L}_{\text{low}}} - 1}{\tau}\right) \\
&- i\tau\varphi_1(2i\tau k_1^2) - i\tau\varphi_2(2i\tau k_1^2)\left(e^{ik^2-k_1^2-k_2^2-k_3^2} - 1\right).
\end{aligned}$$

Therefore,

$$\sum_{k=-k_1+k_2+k_3} \frac{\Upsilon_{\text{mid}}^p(T_1)(u, \tau)}{S(T_1)} (\Pi_{\text{mid}}^{2,1}T_1)(\tau)$$

$$\begin{aligned}
&= \left(-i\tau\varphi_1(2i\tau k_1^2) - i\tau\varphi_2(2i\tau k_1^2) \left(e^{ik^2 - k_1^2 - k_2^2 - k_3^2} - 1 \right) \right) \\
&\times \left(e^{-i\tau k_1^2} \bar{u}_{k_1}^{n+1} + \bar{u}_{k_1}^n \right) \frac{1}{2} \left(e^{i\tau k_2^2} u_{k_2}^{n+1} + u_{k_2}^n \right) \frac{1}{2} \left(e^{i\tau k_3^2} u_{k_3}^{n+1} + u_{k_3}^n \right)
\end{aligned}$$

For the decorated tree T_2 , we have

$$(\Pi_{\text{mid}}^{2,1} T_2)(\tau) = e^{-i\tau k^2} \mathcal{K}_{o_2}^{k,1} \left((\Pi_{\text{mid}}^{2,0} F_2)(\cdot, \tau), 2 \right) (0, \tau) \quad (6.64)$$

where

$$F_2 = \mathcal{I}_{(t_1,1)}(\lambda_{k_4}) \mathcal{I}_{(t_1,0)}(\lambda_{k_5}) T_1.$$

Then,

$$(\Pi_{\text{mid}}^{2,0} \mathcal{I}_{(t_1,1)}(\lambda_{k_4}) \mathcal{I}_{(t_1,0)}(\lambda_{k_5}))(s, \tau) = e^{is(k_4^2 - k_5^2)}$$

and for $\tilde{k} = -k_1 + k_2 + k_3$

$$\begin{aligned}
(\Pi_{\text{mid}}^{2,0} T_1)(s, \tau) &= \frac{1}{2} e^{-is\tilde{k}^2} \left(\mathcal{K}_{o_2}^{\tilde{k},0} \left((\Pi_{\text{mid}}^{2,-1} \tilde{T}_1)(\cdot, \tau), 2 \right) (s, \tau) \right. \\
&\quad \left. + \mathcal{K}_{o_2}^{\tilde{k},0} \left((\Pi_{\text{mid}}^{2,-1} \tilde{T}_1)(\cdot, \tau), 2 \right) (s, 0) \right),
\end{aligned}$$

Now, because of $n = 2$, we perform a direct interpolation of the full operator which gives

$$\mathcal{K}_{o_2}^{\tilde{k},0} \left((\Pi_{\text{mid}}^{2,-1} \tilde{T}_1)(\cdot, \tau), 2 \right) (s, \tau) = -i \int_{\tau}^s ds \left(\frac{1 + e^{i\tau(\tilde{k}^2 + k_1^2 - k_2^2 - k_3^2)}}{2} \right).$$

We obtain

$$(\Pi_{\text{mid}}^{2,0} T_1)(s, \tau) = -i \frac{(2s - \tau)}{2} e^{-is\tilde{k}^2} \left(\frac{1 + e^{i\tau(\tilde{k}^2 + k_1^2 - k_2^2 - k_3^2)}}{2} \right).$$

Therefore, we find

$$(\Pi_{\text{mid}}^{2,0} F_2)(s, \tau) = -i \frac{(2s - \tau)}{2} e^{is(k_4^2 - k_5^2 - \tilde{k}^2)} \left(\frac{1 + e^{i\tau(\tilde{k}^2 + k_1^2 - k_2^2 - k_3^2)}}{2} \right)$$

and by performing again an interpolation of the full operator:

$$\begin{aligned}
(\Pi_{\text{mid}}^{2,1} T_2)(\tau) &= - \int_0^{\tau} \frac{(2s - \tau)}{2} ds \\
&\quad e^{-i\tau k^2} \left(\frac{1 + e^{i\tau(k^2 + k_4^2 - k_5^2 - \tilde{k}^2)}}{2} \right) \left(\frac{1 + e^{i\tau(\tilde{k}^2 + k_1^2 - k_2^2 - k_3^2)}}{2} \right) \\
&= 0
\end{aligned}$$

because we have

$$\int_0^{\tau} \frac{(2s - \tau)}{2} ds = 0.$$

A similar computation shows that

$$(\Pi_{\text{mid}}^{2,1} T_3)(\tau) = 0.$$

The local error analysis follows from the proof of [BS22, Cor. 5.3]. \square

Example 26 To illustrate how the general formula can be used to express more general higher order resonance based

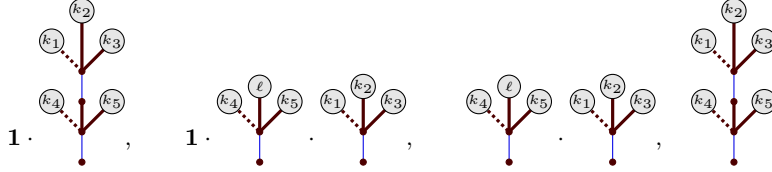
schemes, let us consider the following low-regularity integrator

$$\begin{aligned}
u^{n+1} &= e^{i\tau\Delta}u - i\frac{\tau}{2}e^{i\tau\Delta}\left((u^n)^2(\varphi_1(-i\tau\Delta) - \varphi_2(-i\tau\Delta))\overline{u^n}\right) \\
&\quad - i\frac{\tau}{2}\left((u^{n+1})^2(\varphi_1(i\tau\Delta) - \varphi_2(i\tau\Delta))\overline{u^{n+1}}\right) \\
&\quad - i\frac{\tau}{2}e^{i\frac{\tau}{2}\Delta}\left(e^{i\frac{\tau}{2}\Delta}u^n\right)^2\varphi_2(-i\tau\Delta)e^{i\frac{\tau}{2}\Delta}\overline{u^n} \\
&\quad - i\frac{\tau}{2}e^{i\frac{\tau}{2}\Delta}\left(e^{-i\frac{\tau}{2}\Delta}u^{n+1}\right)^2\varphi_2(i\tau\Delta)e^{-i\frac{\tau}{2}\Delta}\overline{u^{n+1}} \\
&\quad - \frac{\tau^2}{8}|u^n|^4e^{-i\tau\Delta}u^{n+1} + \frac{\tau^2}{8}|u^{n+1}|^4e^{i\tau\Delta}u^n
\end{aligned} \tag{6.65}$$

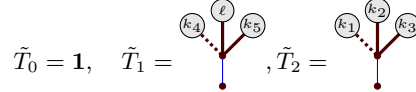
which is motivated from [BS22, (5.16)] and has a local error of the form $\mathcal{O}(\tau^3\Delta)$. We will see that this scheme is in the form of the general formula (6.45) with $r = 1$. Indeed, we already saw at the beginning of this section that

$$\hat{\mathcal{T}}_0^{1,k}(R) = \left\{T_0, T_1, T_2, T_3, k_i \in \mathbf{Z}^d\right\}$$

where $T_i, i = 0, 1, 2, 3$, were defined in (6.56) and (6.57). In the interest of brevity we will not derive all the coefficients b in the expression of (6.65) in the form (6.45). Instead let us focus on the coefficients arising from the contribution to (6.45) arising from $T = \tilde{T}_2$ where \tilde{T}_2 is obtained by removing the brown edge attached to the root. To understand this we first recall the forest splittings of this choice of T from Example (23):



Let us now consider the contribution from the second of these splittings, $\tilde{T}_0 \cdot \tilde{T}_1 \cdot \tilde{T}_2$ with



where from Kirchhoff's law we have $k = -k_4 + l + k_5$ and $l = -k_1 + k_2 + k_3$. The dominant and lower order operators arising in these splittings are given by

$$\begin{aligned}
\mathcal{F}_{\text{dom}}(\tilde{T}_0) &= 0, \mathcal{F}_{\text{low}}(\tilde{T}_0) = 0 \\
\mathcal{F}_{\text{dom}}(\tilde{T}_1) &= 2k_4^2, \mathcal{F}_{\text{low}}(\tilde{T}_1) = k^2 - k_4^2 - l^2 - k_5^2 = 2(-k_4l - k_4k_5 + lk_5) \\
\mathcal{F}_{\text{dom}}(\tilde{T}_2) &= 2k_1^2, \mathcal{F}_{\text{low}}(\tilde{T}_2) = l^2 - k_1^2 - k_2^2 - k_3^2 = 2(-k_1k_2 - k_1k_3 + k_2k_3),
\end{aligned}$$

Moreover we have $|\tilde{E}_T|$ (there are only two blue edges in T corresponding to time-integration) and $|L_T| = 5$ (T has 5 leaves), and given the above splitting, $|\tilde{E}_{\tilde{T}_0}| = 0, |\tilde{E}_{\tilde{T}_1}| = |\tilde{E}_{\tilde{T}_2}| = 1$. Thus the contribution from this term to the overall sum in (6.45) is of the form (recall that $C_T = 1$ for all T in the NLSE case)

$$\begin{aligned}
&\sum_{\mathbf{a} \in [0,1]^2} \sum_{\chi \in \{0,1\}^5} b_{\mathbf{a},\chi,T,\tilde{T}_0,\tilde{T}_1,\tilde{T}_2}(\tau, i\tau\mathcal{F}_{\text{dom}}(\tilde{T}_0), i\tau\mathcal{F}_{\text{dom}}(\tilde{T}_1), i\tau\mathcal{F}_{\text{dom}}(\tilde{T}_2)) \\
&\quad e^{i\tau a_1\mathcal{F}_{\text{low}}(\tilde{T}_1)} e^{i\tau a_2\mathcal{F}_{\text{low}}(\tilde{T}_2)} \frac{\Upsilon_\chi^p(T)(u_{k_v}^{n+\chi_v}, v \in L_T, \tau)}{S(T)}
\end{aligned}$$

From the derivation in the proof of Proposition (6.4.13) and (6.44) we have that

$$\begin{aligned}
&\frac{\Upsilon_\chi^p(T)(u_{k_v}^{n+\chi_v}, v \in L_T, \tau)}{S(T)} \\
&= 2e^{-i\tau\chi_1k_1^2}\overline{u_{k_1}^{\chi_1}}e^{i\tau\chi_2k_2^2}u_{k_2}^{\chi_2}e^{i\tau\chi_3k_3^2}u_{k_3}^{\chi_3}e^{-i\tau\chi_4k_4^2}\overline{u_{k_4}^{\chi_4}}e^{i\tau\chi_5k_5^2}u_{k_5}^{\chi_5}
\end{aligned}$$

Thus the contribution to (6.45) equals

$$\begin{aligned} & \sum_{\mathbf{a} \in [0,1]^2} \sum_{\chi \in \{0,1\}^5} b_{\mathbf{a}, \chi, T, \tilde{T}_0, \tilde{T}_1, \tilde{T}_2}(\tau, 0, 2i\tau k_4^2, 2i\tau k_1^2) \\ & e^{i\tau a_1(k^2 - k_4^2 - (-k_1 + k_2 + k_3)^2 - k_5^2)} e^{i\tau a_2((-k_1 + k_2 + k_3)^2 - k_1^2 - k_2^2 - k_3^2)} \\ & 2e^{-i\tau \chi_1 k_1^2} \bar{u}_{k_1}^{\chi_1} e^{i\tau \chi_2 k_2^2} u_{k_2}^{\chi_2} e^{i\tau \chi_3 k_3^2} u_{k_3}^{\chi_3} e^{-i\tau \chi_4 k_4^2} \bar{u}_{k_4}^{\chi_4} e^{i\tau \chi_5 k_5^2} u_{k_5}^{\chi_5} \end{aligned}$$

Let us now show that the quintic terms in (6.65) arise precisely from these contributions: Indeed suppose we choose

$$b_{\mathbf{0}, (0,0,0,0,1), T, \tilde{T}_0, \tilde{T}_1, \tilde{T}_2}(\tau, z_0, z_1, z_2) = -\frac{\tau^2}{16}, \quad (6.66)$$

$$b_{(1,1), (1,0,0,0,0), T, \tilde{T}_0, \tilde{T}_1, \tilde{T}_2}(\tau, z_0, z_1, z_2) = -e^{z_0 + z_1 + z_2} \frac{\tau^2}{16} \quad (6.67)$$

and all other coefficients b in the above expression equal to zero then we arrive precisely at the contributions of the form

$$-\frac{\tau^2}{8} |u^n|^4 e^{-i\tau \Delta} u^{n+1} + \frac{\tau^2}{8} |u^{n+1}|^4 e^{i\tau \Delta} u^n$$

in the overall scheme, corresponding to the quintic terms in (6.65). The remaining terms in the scheme can be expressed similarly from contributions from lower rank trees T_0, T_1 . Moreover, we note that the coefficients as given by (6.66) clearly satisfy (6.52) and that the same holds for the coefficients of lower order contributions, thus confirming that the scheme (6.65) is symmetric.

The Korteweg–de Vries equation

The Korteweg–de Vries (KdV) equation is given by

$$\partial_t u + \partial_x^3 u = \frac{1}{2} \partial_x u^2 \quad (6.68)$$

It fits into the general framework with

$$\mathcal{L}\left(\nabla, \frac{1}{\varepsilon}\right) = i\partial_x^3, \quad \alpha = 1 \quad \text{and} \quad p(u, \bar{u}) = p(u) = i\frac{1}{2}u^2.$$

Here $\mathcal{L} = \{t_1, t_2\}$, $P_{t_1} = -\lambda^3$ and $P_{t_2} = \lambda^3$. Moreover, in this case the structure constant C_T reflects the presence of the Burger's nonlinearity in the iterations of Duhamel's formula, which means

$$C_T = \prod_{\substack{e=(v,u) \in \tilde{E}_T \\ u \in N_T \setminus \{e_T\}}} (-1)^{\mathfrak{p}(e)} i\mathfrak{o}(u)$$

where we recall $\mathfrak{c}(e) = (t(e), \mathfrak{p}(e))$ is the edge decoration of e with $t(e) \in \mathfrak{L}$ and $\mathfrak{p}(e) \in \{0, 1\}$. Note by Kirchhoff's law the above definition is invariant under the choice of node u or v for an edge $e = (u, v)$ in the product, so long as the node is an interior one. Then, we denoted by \mathbf{l} an edge decorated by $(t_1, 0)$ and by \mathbf{l} an edge decorated by $(t_2, 0)$. Following the formalism given in [BHZ19], we can provide the rules that generate the trees obtained by iterating Duhamel's formula:

$$R(\mathbf{l}) = \{(\mathbf{l}, \mathbf{l})\}, \quad R(\mathbf{l}) = \{(\mathbf{l}), ()\}.$$

The general framework (6.42) derived in Section (6.3.3) builds the foundation of the first- and second-order resonance based schemes presented below for the KdV equation (6.68). The structure of the schemes depends on the regularity of the solution.

Corollary 6.4.16 *For the KdV equation (6.68) the general midpoint scheme (6.42) takes at first order the form*

$$\begin{aligned} u^{\ell+1} &= e^{-\tau \partial_x^3} u^\ell + \frac{1}{24} \left(e^{-\tau \partial_x^3} \partial_x^{-1} u^\ell + \partial_x^{-1} u^{\ell+1} \right)^2 \\ &\quad - \frac{1}{24} e^{-\tau \partial_x^3} \left(\partial_x^{-1} u^\ell + e^{\tau \partial_x^3} \partial_x^{-1} u^{\ell+1} \right)^2 \end{aligned} \quad (6.69)$$

with a local error of order $\mathcal{O}(\tau^2 \partial_x^2 u)$ at first-order and with a local error of order $\mathcal{O}(\tau^3 \partial_x^4 u)$ at second order.

Remark 6.4.17 Note that this schemes has been obtained in [MS23]. It was shown that this scheme is of even order for higher regularity in H^4 (see [MS22, Thm 5.2]). By embedding this scheme into our general framework, we know that it has the same local error analysis as the second-order scheme introduced in [BS22].

$$\begin{aligned} u^{\ell+1} &= e^{-\tau\partial_x^3} u^\ell + \frac{1}{6} \left(e^{-\tau\partial_x^3} \partial_x^{-1} u^\ell \right)^2 - \frac{1}{6} e^{-\tau\partial_x^3} \left(\partial_x^{-1} u^\ell \right)^2 \\ &\quad + \frac{\tau^2}{4} e^{-\tau\partial_x^3} \Psi(i\tau\partial_x^2) \left(\partial_x \left(u^\ell \partial_x (u^\ell u^\ell) \right) \right) \end{aligned} \quad (6.70)$$

with a local error of order $\mathcal{O}(\tau^3 \partial_x^4 u)$ and a suitable filter function Ψ satisfying

$$\Psi = \Psi(i\tau\partial_x^2), \quad \Psi(0) = 1, \quad \|\tau\Psi(i\tau\partial_x^2)\partial_x^2\|_r \leq 1.$$

Proof. The proof follows the line of argumentation to the analysis for the Schrödinger equation. For the first-order scheme, we have

$$\begin{aligned} U_k^{n,0}(\tau, v) &= \frac{\Upsilon_{\text{mid}}^p(T_0)(\tau, v)}{S(T_0)} \Pi_{\text{mid}}^{n,0}(T_0)(\tau) \\ &\quad + \sum_{k=k_1+k_2} \frac{\Upsilon_{\text{mid}}^p(T_1)(\tau, v)}{S(T_1)} \Pi_{\text{mid}}^{n,0}(T_1)(\tau). \end{aligned} \quad (6.71)$$

where the trees of interest are

$$\hat{\mathcal{T}}_0^{0,k}(R) = \{T_0, T_1, k_i \in \mathbf{Z}^d\}, \quad T_0 = \begin{array}{c} \textcircled{k} \\ | \\ \bullet \end{array} \quad \text{and} \quad T_1 = \begin{array}{c} \textcircled{k_1} \textcircled{k_2} \\ \diagdown \quad \diagup \\ | \\ \bullet \end{array}$$

and in symbolic notation takes the form

$$T_1 = \mathcal{I}_{(t_1,0)}(\mathcal{I}_{(t_2,0)}(\lambda_k F_1)) \quad F_1 = \mathcal{I}_{(t_1,0)}(\lambda_{k_1}) \mathcal{I}_{(t_1,0)}(\lambda_{k_2}) \quad \text{with } k = k_1 + k_2.$$

For the first term we readily obtain that

$$\frac{\Upsilon_{\text{mid}}^p(T_0)(\tau, v)}{S(T_0)} \Pi_{\text{mid}}^{n,0}(T_0)(\tau) = e^{-i\tau k^3} \hat{v}_k.$$

It remains to compute the second term. Note that thanks to (6.28) we have that

$$\begin{aligned} \Pi^{n,0}(T_1)(\tau) &= e^{-i\tau k^3} \Pi^{n,0}(\mathcal{I}_{(t_2,0)}(\lambda_k F_1))(\tau) \\ &= e^{-i\tau k^3} \mathcal{K}_{(t_2,0)}^{k,0}(\Pi^{n,-1}(F_1), n)(\tau) \\ &= e^{-i\tau k^3} \mathcal{K}_{(t_2,0)}^{k,0} \left(e^{i\xi(-k_1^3 - k_2^3)}, n \right)(\tau). \end{aligned} \quad (6.72)$$

where we have used for the third line

$$(\Pi^{n,-1} F_1)(\tau) = (\Pi^{n,-1} \mathcal{I}_{(t_1,0)}(\lambda_{k_1}))(\tau) (\Pi^{n,-1} \mathcal{I}_{(t_1,0)}(\lambda_{k_2}))(\tau) = e^{-i\tau k_1^3} e^{-i\tau k_2^3}.$$

Next we observe that

$$P_{(t_2,0)}(k) - k_1^3 - k_2^3 = k^3 - k_1^3 - k_2^3 = 3k_1 k_2 (k_1 + k_2)$$

such that

$$\frac{1}{P_{(t_2,0)}(k) - k_1^3 - k_2^3}$$

can be mapped back to physical space. Therefore, we set

$$\mathcal{L}_{\text{dom}} = P_{(t_2,0)}(k) - k_1^3 - k_2^3 = 3k_1 k_2 (k_1 + k_2)$$

and integrate all frequencies exactly. This implies


$$\begin{aligned} \Pi^{n,0}(T_1)(\tau) &= e^{-i\tau k^3} \frac{i(k_1 + k_2)}{3ik_1k_2(k_1 + k_2)} \left(e^{i\tau(k^3 - k_1^3 - k_2^3)} - 1 \right) \\ &= \frac{1}{3k_1k_2} \left(e^{-i\tau(k_1^3 + k_2^3)} - e^{-i\tau k^3} \right). \end{aligned}$$

Together with (6.71) this yields the scheme (6.69). For the second-order scheme, we first notice that

$$\Pi_{\text{mid}}^{n,0}(T_0)(\tau) = \Pi_{\text{mid}}^{n,1}(T_0)(\tau), \quad \Pi_{\text{mid}}^{n,0}(T_1)(\tau) = \Pi_{\text{mid}}^{n,1}(T_1)(\tau).$$

Indeed, for the tree T_1 , we perform an exact integration without any discretisation. Then, we need to take into account the following trees

$$\hat{\mathcal{T}}_0^{1,k}(R) = \{T_0, T_1, T_2, k_i \in \mathbf{Z}^d\}, \quad T_2 =$$



Then we can proceed as in the second-order schemes for the Schrödinger equation to show its contribution is zero that is

$$\Pi_{\text{mid}}^{4,1}(T_2)(\tau) = 0.$$

□

6.5 Numerical Experiments

We now test the practical performance of our new symmetric schemes in practical experiments evaluating both their low-regularity convergence properties and their ability to correctly preserve constants of motion in the relevant equations. In fitting with our above construction our spatial discretisation is a Fourier spectral method throughout with M modes. In order to understand the low-regularity convergence properties of our methods we follow [OS18] and consider the following types of initial data:

1. Smooth initial data,

$$u_0(x) = \frac{\cos(x)}{2 + \sin(x)}. \tag{6.73}$$

2. Low-regularity initial data $u_0 \in H^\vartheta$, for some $\vartheta > 0$, of the following form. Firstly we choose a vector sampled from a uniform distribution $U_m \sim U([0, 1] + i[0, 1])$, $m = -M/2 + 1, \dots, M/2$ and then we define

$$u_0(x) := U_0 + \sum_{\substack{m=-M/2+1 \\ m \neq 0}}^{M/2} e^{imx} |m|^{-\vartheta} U_m. \tag{6.74}$$

Both choices of initial data are rescaled such that $u_0 \mapsto u_0 / \|u_0\|_{L^2}$.

6.5.1 The Korteweg–de Vries equation

We consider the resonance based midpoint rule (6.69) introduced in [MS23] which our midpoint iterates (section (6.3.3)) are able to recover. This rule has excellent low-regularity convergence properties and at the same time is able to conserve momentum and energy of the KdV equation over long times even in the low-regularity regime. We refer to the numerical simulations made in [MS23] where the favourable properties of this method are displayed.

6.5.2 The Nonlinear Schrödinger equation

In the upcoming numerical experiments we compare the performance of our new symmetric integrators ((6.62) and (6.63)), to the following state-of-the-art reference schemes for the NLSE:

- The Strang splitting [MQ02], as an example of a classical symmetric numerical technique;

- The first and second order resonance based integrators introduced by Ostermann & Schratz [OS18] and Bruned & Schratz [BS22, Section 5.1.2] respectively, as examples of asymmetric low-regularity schemes;
- The symmetrised low-regularity integrator introduced by Alama Bronsard [AB23b], as an example of previous structure preserving low-regularity schemes.

In the following numerical experiments we focus on the 1d case, i.e. the NLSE formulated on \mathbb{T} , but our methods equally apply to higher dimensional settings where their favourable performance can also be observed.

In the first instance we consider the long-time structure preservation properties of our newly designed symmetric low-regularity integrators. For this we consider two first integrals of the cubic NLSE, the normalisation

$$I_0^{[NLSE]}[u] = \int_{\mathbb{T}} |u|^2 dx,$$

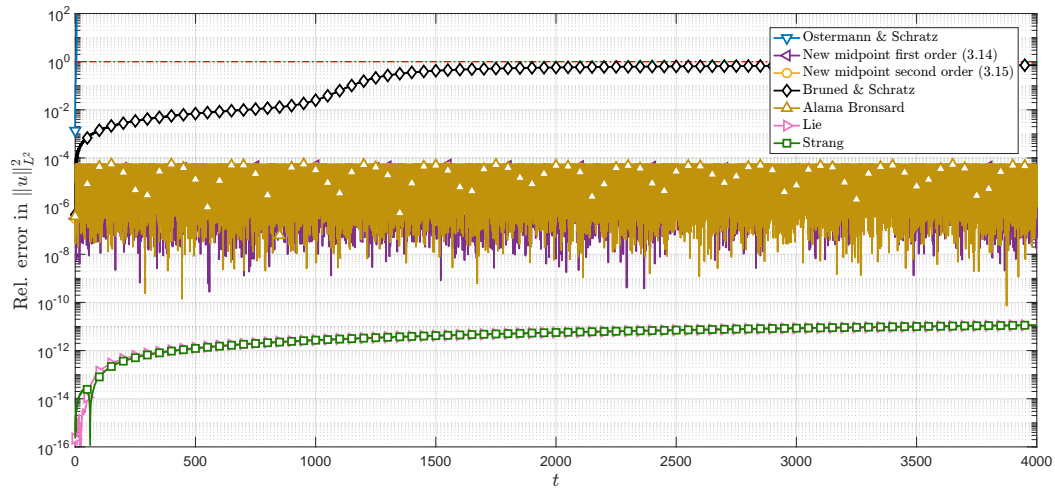
and the energy

$$I_1^{[NLSE]}[u] = \int_{\mathbb{T}} |\nabla u|^2 + \frac{1}{2}|u|^4 dx.$$

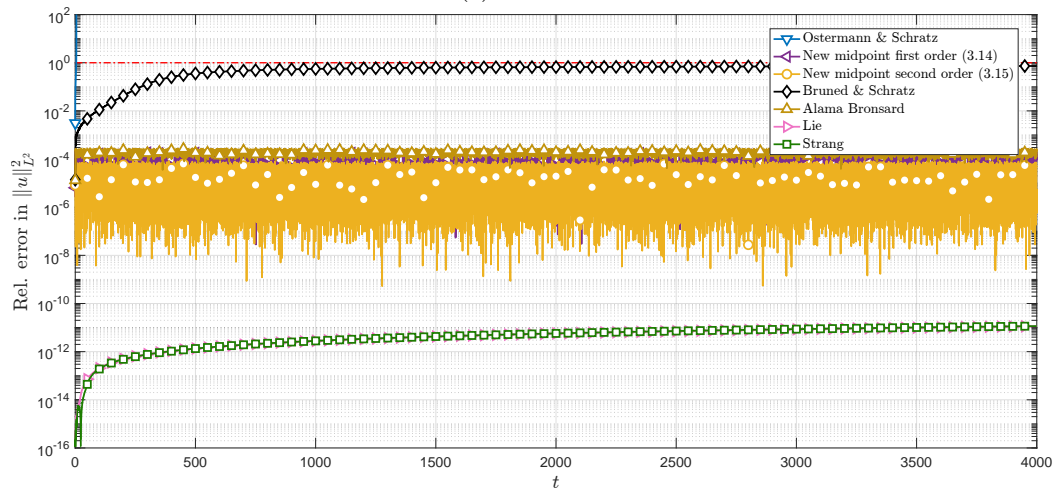
Symmetric numerical schemes are typically unable to preserve such conservation laws exactly, however it is known for the ODE case [HLW10, Chapter XI] (and also observed numerically for the PDE case, for example in [CCO08]) that symmetric methods can exhibit very good approximate long-time preservation of such first integrals. In the following numerical experiments we test this behaviour by looking at the error in these quantities for a fixed time step $\tau = 0.02$ and highest frequency $M = 1024$, over a long time interval, much larger than $\mathcal{O}(1/\tau)$. Firstly, in figure (6.4) we observe that the normalisation appears to be preserved really well, in particular (the example is representative of a host of numerical experiments for various time steps which we performed) the preservation is much better than previous asymmetric resonance based schemes. We note that the Strang splitting conserves quadratic first integrals, i.e. the normalisation, to machine accuracy and thus undoubtedly outperforms our schemes on the level of normalisation preservation.

Our next numerical result for the NLSE, presented in Figure (6.6)&(6.5), shows the error in the NLSE energy over a long time interval, for a fixed time step $\tau = 0.02$. Albeit rigorous theory exists for the ODE case [HLW10], there is again no theoretical guarantee for the long-time preservation of the energy under symmetric methods. Indeed in practical experiments it can be seen that symmetric schemes are able to clearly outperform asymmetric integrators in the long-time approximate energy preservation. For the Strang splitting this behaviour was rigorously analysed in [Fao12] where a CFL condition was necessary to guarantee long-time approximate energy preservation beyond the realms of forward error analysis. This CFL condition is indeed observed even for smooth data in our experiments. Perhaps somewhat surprisingly our new symmetric resonance based scheme do not appear to suffer from comparable CFL conditions and, as expected, perform well for both smooth and low-regularity solutions.

Finally, we performed experiments to confirm that the low-regularity convergence properties of our symmetric schemes are at least as good as in prior asymmetric methods. In the following numerical experiments our reference solutions were computed with $M = 2^{14}$ Fourier modes and a time step $\tau = 10^{-6}$ with the symmetrised method from [AB23b]. In Figures (6.7) & (6.8) we choose to measure the error in H^1 -norm, and observe the convergence properties of our methods for initial data of various levels of regularity. In all of these experiments the number of spatial discretisation modes was taken to be $M = 1024$ and the initial data chosen according to (6.74) & (6.73). In Figure (6.7) we observe that our new methods have exactly the predicted convergence properties at those levels of regularity: The integrator (6.62) is optimal for first order convergence in the sense of regularity, meaning it converges at first order in H^1 with H^2 data, while the integrator (6.63) is optimally convergent in the sense of regularity up to second order meaning it converges at $\mathcal{O}(\tau)$ in H^1 for data in H^2 and at $\mathcal{O}(\tau^2)$ in H^1 for data in H^3 . For smaller values of τ the error forms a plateau around 10^{-4} and 10^{-7} in Figures 6.7a and 6.7b respectively. This is due to the error made by the pseudo-spectral space discretisation, which decreases as the regularity of the initial data is increased. The behaviour of the splitting methods observed in these experiments matches exactly with the convergence analysis given by [Lub08, BBD02] and suffers from significant order reduction in low-regularity regimes.

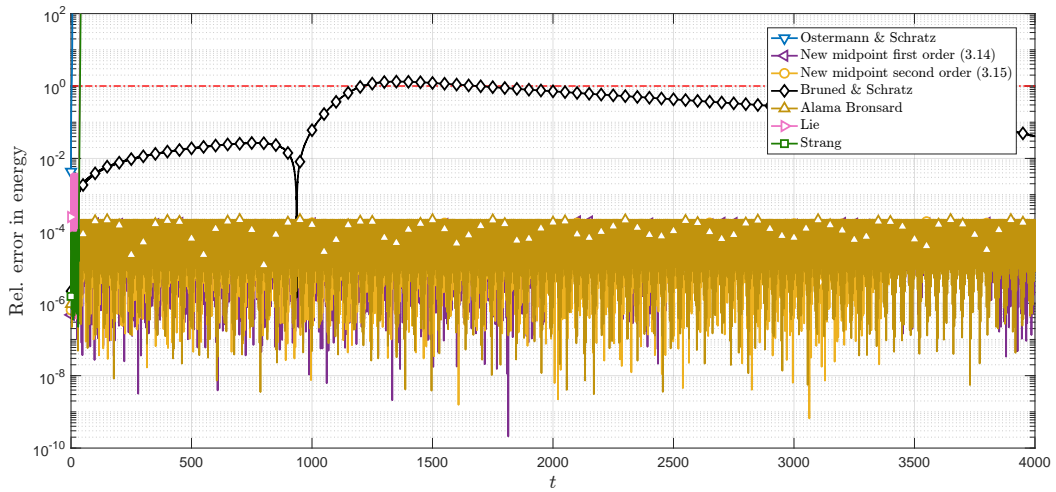


(a) C^∞ data.

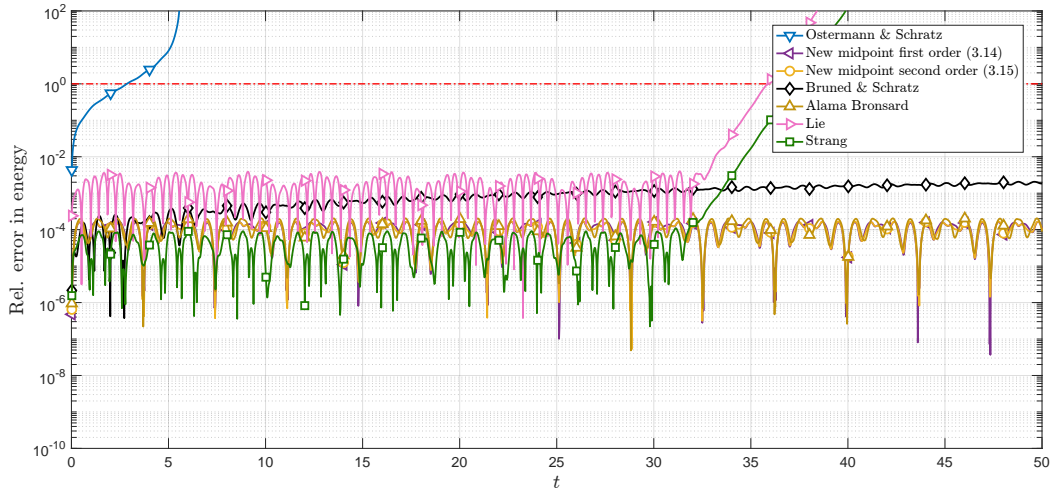


(b) H^2 data.

Figure 6.4 – Error in the normalisation $\|u^n\|_{L^2}$, for time step $\tau = 0.02$, $M = 1024$, and long-time interval $t = n\tau \in [0, 4000]$.

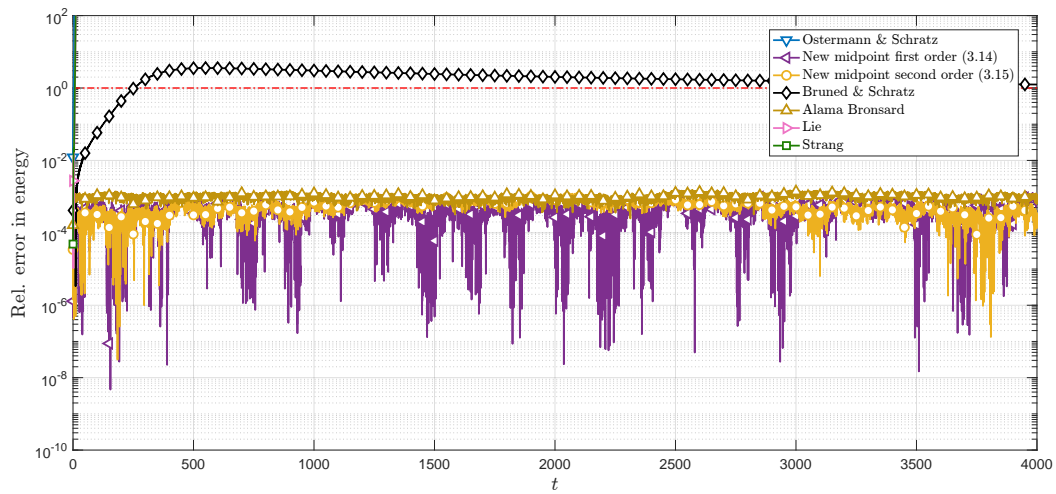


(a) Long-time interval $t = n\tau \in [0, 4000]$.

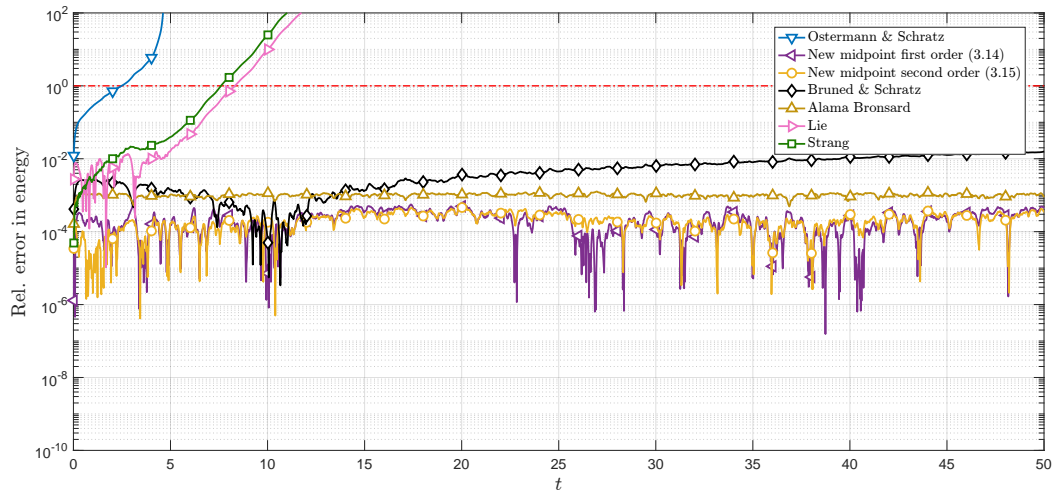


(b) Magnification of $t = n\tau \in [0, 50]$.

Figure 6.5 – Error in the Hamiltonian, for time step $\tau = 0.02$, $M = 1024$ and C^∞ data.

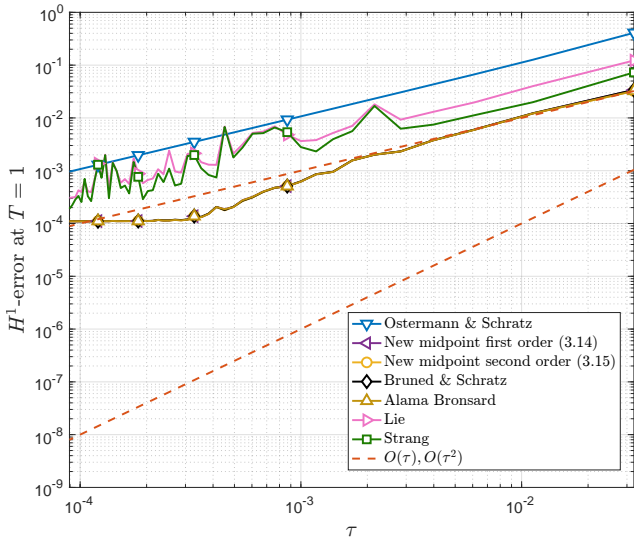


(a) Long-time interval $t = n\tau \in [0, 4000]$.

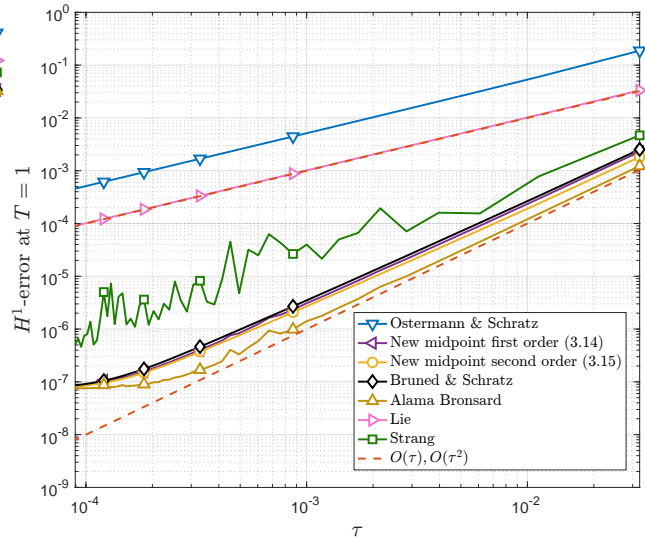


(b) Magnification of $t = n\tau \in [0, 50]$.

Figure 6.6 – Error in the Hamiltonian, for time step $\tau = 0.02$, $M = 1024$, and H^2 data.

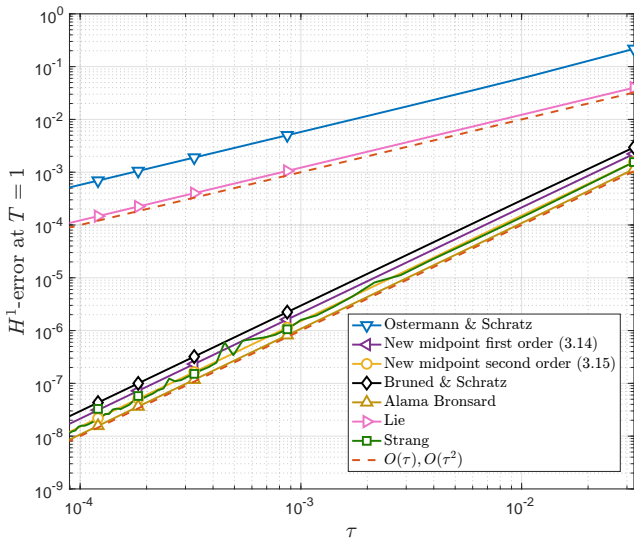


(a) H^2 -initial data, $\vartheta = 2$ in (6.74).

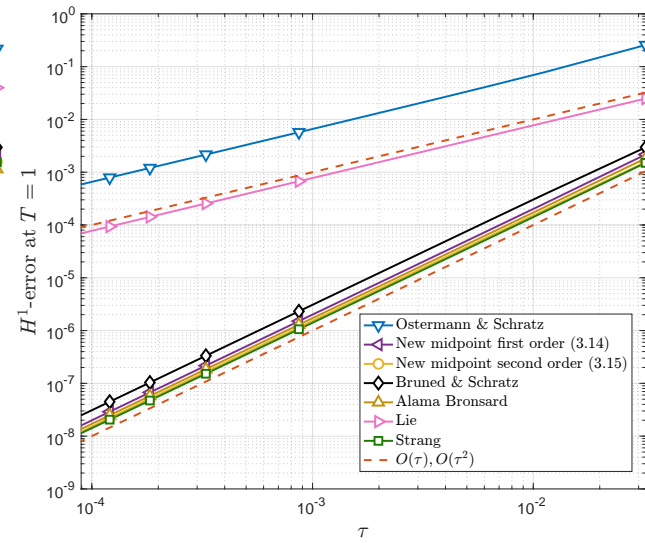


(b) H^3 -initial data, $\vartheta = 3$ in (6.74).

Figure 6.7 – H^1 -error at $T = 1$ as a function of the timestep τ for low-regularity initial data.



(a) H^4 -initial data, $\vartheta = 4$ in (6.74).



(b) C^∞ -initial data (6.73).

Figure 6.8 – H^1 -error at $T = 1$ as a function of the timestep τ for more regular initial data.

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