Time-integration methods for a dispersion-managed nonlinear Schrödinger equation

Zur Erlangung des akademischen Grades eines

Doktors der Naturwissenschaften

von der KIT-Fakultät für Mathematik des

Karlsruher Instituts für Technologie (KIT)

genehmigte

Dissertation

von

Marcel Mikl

Tag der mündlichen Prüfung: 28. Juni 2017

Referent: Prof. Dr. Tobias Jahnke

Korreferentin: Prof. Dr. Marlis Hochbruck

Contents

CHAPTER 1

Introduction

1.1. Motivation

A large part of modern civilization is based on a simple physical principle – *total internal reflection*. Total internal reflection is the phenomenon that occurs when a beam of light is entirely reflected if it strikes the boundary of a medium at specific angles. This phenomenon makes it possible, in particular, to confine light inside a medium and thus total internal reflection forms the foundation for ultrafast high-bit-rate data transfer via optical fiber cables around the whole globe, see for instance [3,4,17,32]. Maintaining and improving this worldwide communication network is a multi-billion dollar industry (cf. [32, Ch. 1]) and each progress in this technology potentially impacts our everyday lives. Apart from solving *the last mile problem*, i.e. providing cost-efficient connection services from data centers to and from end-users (cf. [42]), there are two key limiting factors of modern fiber-optic communication: *attenuation* (or total fiber loss) and *dispersion*, cf. [3, Ch. 5].

Attenuation. Attenuation characterizes the loss of power of a signal during transmission via an optical fiber cable. It is described as the quotient of output and input power $P_{\text{out}}/P_{\text{in}}$ and is typically measured in dB/km (decibels per kilometer), where

$$\text{dB(attenuation)} = -10 \log_{10} \left(\frac{P_{\text{out}}}{P_{\text{in}}} \right) ,$$

cf. [32, Ch. 2]. Therefore, low attenuation is an important quality feature of any fiber cable. Modern fabrication technology and availability of high-purity silica permit the manufacturing of fibers with attenuation below 0.3 dB/km (cf. [32, Ch. 5]), i.e. a 1 mW (milliwatt) signal reduces to 1 µW (microwatt) after the transmission over 100 km; still a power reduction by a factor of 1000. Typically, the effect of attenuation in long-haul communication systems is compensated by periodically amplifying the signal and thereby restoring its energy (cf. [32, Ch. 12]) such that attenuation is a bothersome but manageable problem.

Dispersion. In the context of nonlinear optics, dispersion is generally understood as the spreading out of a light pulse during transmission via an optical fiber cable. It is measured in terms of pulse spreading $\triangle t$ per unit distance in nanoseconds (ns) per kilometer (km)

$$\triangle t = \text{dispersion (ns/km)} \times \text{distance (km)}\,,$$

cf. [32, Ch. 5]. The broadening of light pulses over time is a major problem in long-haul data transmission through intercontinental fiber cables. High-bit-rate data transfer requires transmitting as many light pulses as possible, but at the same time, interaction between different pulses has to be avoided in order to ensure that the pulses are still well separated at the receiver. As a consequence, the transmission rate has to be adjusted according to the spreading in the fiber cable and thus dispersion is a limiting factor, cf. [32, Ch. 2]. Dispersion has several causes – starting from small irregularities during the manufacturing of the cable, up to the fact that the refractive index of any material depends on the wavelength of the traversing light resulting in different propagation speeds for various frequency components of, e.g., a laser pulse – and hence dispersion is a key issue of fiber-optic communication, cf. [3, Ch. 7]. On the other hand, it turned out that dispersion is *not only* detrimental because it suppresses other unwanted effects (cf. [3, Ch. 7]), e.g., small dispersion enhances *four-wave-mixing*, cf. [58].

The complexity of dispersion in nonlinear optics is the starting point for various *dispersion management* techniques, cf. [3, Ch. 7]. One potential remedy is to engineer fiber cables with alternating sections of opposing dispersion such that the average dispersion is mostly neutralized allowing for high local dispersion and low global dispersion. This idea was first proposed in [43] and has developed to a successful technique since then; cf. [2,27,48,49]. A common approach is alternating the sections with respect to the amplifier spacing, i.e. switching every $\approx 50-80$ km; cf. [3, Ch. 7].

From a mathematical point of view, propagation of light – as an electromagnetic wave – is described by Maxwell's equations. However, in nonlinear optics it is customary to investigate properties and features of light propagation within fiber cables by means of envelope (or effective) equations – with the benefit of a model reduction. This approach usually results in various types of one-dimensional nonlinear Schrödinger equations (NLS). Hence, NLS-type equations ubiquitously appear in various variants in nonlinear optics in order to investigate a multitude of questions concerning light propagation in fiber cables.

Clearly, this approach relies on the assumption that the considered envelope equation captures the crucial properties of the traversing pulse such that analyzing and simulating the envelope equation instead of the full Maxwell system gives valuable insights. A formal justification of this general approach can be found, e.g., in [3, Ch. 2]. For a more rigorous derivation of the NLS as an envelope equation we refer to [50], whereas a more basic approach can be found in [22, Ch. 1 and Ch. 35]. Further, we recommend [47] for a critical examination of this subject.

1.2. Scope and outline

A specific NLS-type equation arising in the field of nonlinear optics is the *dispersion-managed nonlinear Schrödinger equation* (DMNLS) modeling dispersion-managed fiber cables with alternating sections of opposing dispersion as motivated in the previous section. We consider the DMNLS in the form

$$\begin{aligned} \partial_t u(t,x) &= \tfrac{\mathrm{i}}{\varepsilon}\gamma\left(\tfrac{t}{\varepsilon}\right)\partial_x^2 u(t,x) + \mathrm{i}\left|u(t,x)\right|^2 u(t,x)\,, \\ u(0,x) &= u_0(x)\,, \end{aligned} \tag{1.1}$$

on the one-dimensional torus $\mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$. For finite $0 < T \in \mathbb{R}$ the function u maps from $[0,T]\times\mathbb{T}$ to $\mathbb{C}$; furthermore, the parameter $\varepsilon \in \mathbb{R}$ is considered to be small, i.e. $0 < \varepsilon \ll T$. The coefficient function $\gamma\colon \mathbb{R}\to\mathbb{R}$ is given by

$$\gamma(t) = \chi(t) + \varepsilon\alpha\,, \tag{1.2}$$

where $0 \le \alpha \in \mathbb{R}$ and

$$\chi(t) = \begin{cases} -\delta & \text{if} \quad t \in [n, n+1) \quad \text{for even } n \in \mathbb{N}, \\ \delta & \text{if} \quad t \in [n, n+1) \quad \text{for odd } n \in \mathbb{N} \end{cases} \tag{1.3}$$

is a periodic, piecewise constant function, with $0 < \delta \in \mathbb{R}$. We assume $\delta > \varepsilon\alpha$ such that $\gamma(t) \neq 0$ for every $t \in [0,T]$. This is an appropriate setting for modeling dispersion-managed fiber cables with symmetric dispersion maps, cf. [4,9,58].

In the context of nonlinear fiber optics, the "time variable" t in (1.1) corresponds to the distance along the fiber cable, whereas the "space variable" x represents a (retarded) time. Hence, the coefficient function γ (depending on t) models the periodically changing sections of opposing dispersion along the fiber cable introduced in

Section 1.1. The small parameter ε originates from the fact that sections with equal dispersion in the cable are very small compared to its total length (represented by T).

Remark. Taking the legs of equal dispersion of length $\approx 50-80$ km (see Section 1.1) and considering fiber-cables of length $\approx 8000-40000$ km, we observe that scaling the total length of the cable to 1 naturally leads to ε ranging from 0.01 to 0.002. Hence, the parameter ε can be considered small in the sense $\varepsilon \ll 1$ but not so small that solely considering the limit case $\varepsilon \to 0$ is not always justified.

The DMNLS (1.1) is the main object of research in this thesis. Our particular focus lies on constructing and analyzing suitable problem-adapted time-integration schemes. Time-integration methods for the DMNLS require particular attention because approximating solutions of the DMNLS poses considerable challenges: the small parameter ε and the coefficient function γ combine to produce rapid oscillations with frequency $\sim 1/\varepsilon$ for typical solutions of the DMNLS. Consequently, applying traditional time-integrators to the DMNLS yields acceptable accuracy, if at all, only for tiny step-sizes $\tau \ll \varepsilon$. Roughly speaking, this is because the global error of a traditional p-th order method typically scales like the product of the p-th power of the step-size τ and the $(p+1)$-th derivative of the right-hand side, i.e. if the solution oscillates with frequency $\sim 1/\varepsilon$ the quantity $\frac{1}{\varepsilon}\mathcal{O}\big((\tau/\varepsilon)^p\big)$ has to be small. For the DMNLS, however, in addition to the rapid oscillations, the right-hand side contains the discontinuous coefficient function γ; hence, there is no second-order derivative with respect to time of a solution u of the DMNLS. In particular, this renders higher-order Taylor expansions of u impossible and certainly contradicts vital assumptions in the error analysis of many traditional time-integrators. Finally, the nonlinear term $\mathrm{i}|u|^2u$ makes implicit schemes prohibitively costly.

Approximating highly oscillatory problems is an active field of research and the state of the art is documented in [16,19,29,34,54]. In the following, we solely address selected references concerning, in particular, highly oscillatory partial differential equations: for semilinear wave equations, trigonometric integrators are proposed and analyzed in [25,28,33]. Furthermore, a connection between trigonometric integrators and splitting methods has been studied recently in [12]. For linear Schrödinger equations in the semiclassical regime, special time-integration methods are introduced in [7,21]. For nonlinear Schrödinger equations with semiclassical scaling, the detrimental effects of oscillations on splitting methods are studied in [6]. Conversely, for the DMNLS with $\gamma \equiv 1$, and with a more general nonlinearity, it is shown in [15] that the oscillatory behavior leads to higher accuracy for splitting methods provided the step-size is chosen in a special way. Moreover, there is a vast literature on heterogeneous multiscale methods (HMMs) for equations containing coefficients typically varying rapidly in space (instead of time); see [1] for an overview. Here, we explicitly point out a variant of HMMs concerning oscillations in time – the stroboscopic averaging method; cf. [13], see also [14] for the investigation of the long-time behavior of a method based on stroboscopic averaging applied to an NLS.

It lies in the very nature of tailor-made numerical integrators for highly oscillatory differential equations that they exploit particular structures and properties of the underlying problems. Hence, it is obvious that such methods typically perform inadequately when applied to a different class of equations. In the above references the underlying equations and the corresponding assumptions differ considerably from the present situation of the DMNLS, where the (possibly) unbounded differential operator multiplied by the time-dependent, discontinuous coefficient function γ and the small parameter ε in combination with the nonlinearity pose a novel set of challenges for constructing tailored time-integration methods.

Numerical and analytical difficulties of the DMNLS have led mathematical research to consider the Gabitov-Turitsyn equation (GTE) instead. The GTE originates from the DMNLS via a transformation and averaging; cf. [23,24]. It has been intensively studied in [26,35,53,57,60] with particular focus on stationary soliton-like solutions (or dispersion-managed solitons), see also [9,58] for reviews. The averaging step in deriving the GTE eliminates the dependence on ε and thus the rapid oscillations. Hence, the GTE is more accessible particularly from a numerical point of view. However, the downside of averaging is that the GTE is only an approximation of the DMNLS and that the accuracy of this approximation depends on the parameter ε, cf. [53]. Because the parameter ε is fixed in particular applications, it cannot always be ensured that simulating the GTE instead of the DMNLS yields the desired accuracy.

The aim of this thesis. In this thesis, we aim for constructing and analyzing tailor-made time-integration schemes for the DMNLS. We require methods that allow for approximations of the DMNLS in any desired accuracy, and, in particular, are reliable in the sense that reducing the step-size τ of the method certainly increases the accuracy of the approximation. Moreover, we demand competitiveness of the methods in terms of computational work versus accuracy as a secondary objective.

In Chapter 2, we start by investigating the DMNLS. Here, we establish well-posedness of the equation in an adequate analytic setting. Then, we introduce a beneficial transformation leading to an equivalent formulation of the DMNLS denoted by transformed DMNLS – or tDMNLS for short. The tDMNLS appears to be more accessible for constructing novel numerical schemes, and hence plays an important role in the course of this thesis. Moreover, we provide a suitable analytical setting as a basis for all following examinations.

Chapter 3 is dedicated to a limit system of the tDMNLS for $\varepsilon \to 0$. It turns out that the derivation of the limit system is closely related to the derivation of the GTE, and hence that the limit system is in a sense equivalent to the GTE. We investigate the accuracy of the limit system as an approximation to the tDMNLS. Naturally, our results are closely related to similar results for the GTE (cf. [53]) but are proven with other techniques and under lower regularity assumptions.

In Chapter 4, we extent techniques from [38,39] and obtain our first numerical scheme for the tDMNLS – the adiabatic Euler method[1]. We show that the adiabatic Euler method is a first-order scheme uniformly in ε, i.e. we show that the global error of the adiabatic Euler method scales like $\mathcal{O}(\tau)$ with a constant independent of ε. Another extension of the above techniques, based on the explicit midpoint rule, leads us to the adiabatic midpoint rule in Chapter 5. Again, we show that this method is a first-order scheme uniformly in ε. In addition, however, the adiabatic midpoint rule has the following advantageous properties:

- its accuracy improves to $\mathcal{O}(\tau\varepsilon)$ for step-sizes $\tau = \varepsilon/k$ with $k \in \mathbb{N}$,
- its accuracy improves to $\mathcal{O}(\tau^2)$ for step-sizes $\tau = k\varepsilon$ with $k \in \mathbb{N}$,

in each case with a constant independent of ε. The error analysis of the adiabatic midpoint rule (Theorem 10 and Theorem 11) is the first main result in this thesis. The thorough investigation of this method points out two key aspects of the underlying construction principle: first, cancellation effects of highly oscillatory error terms provide higher accuracy for specific step-sizes. Second, approximating the tDMNLS, in some cases, complies with approximating the corresponding limit system, and hence understanding the relation of the tDMNLS and the limit system is crucial for explaining the error behavior.

In Chapter 6, we briefly address constructing a genuine second-order scheme. It turns out that such methods can be obtained with our techniques, in principle, but require exorbitant computational cost. However, the construction of the second-order scheme points out a minor improvement for our other schemes as a nice side effect.

[1] The term *adiabatic* is derived from [39] where the construction idea originates from. It has no special meaning in our context.

Chapters 7 and 8 are devoted to an extension of the previously introduced construction principles to exponential integrators. The resulting methods – the adiabatic exponential Euler method and the adiabatic exponential midpoint rule – are related to Magnus integrators [10,36], see also [34]. Once more, we show first-order convergence uniformly in ε for both methods. However, the second main result of this thesis is that the accuracy of the adiabatic exponential midpoint rule also increases for step-sizes that are integer fractions of integer multiples of ε (Theorem 19). Moreover, numerical experiments suggest that employing the exponential schemes to the tDMNLS reduces the error constants of the global error bound significantly compared to the corresponding non-exponential scheme.

Finally, we give a short summary, some final considerations and a brief outlook in Chapter 9.

Numerical experiments. In the course of this thesis, we provide several numerical examples to illustrate our results. All computations have been conducted in MATLAB (version R2015a) on a laptop with an Intel i7-4710MQ CPU (4 cores at 2.50 GHz) and 16 GB of RAM. Because we consider these computations as *proof of principle* for the introduced numerical methods, we will tacitly omit most questions concerning the implementation (and in particular all MATLAB-specific aspects of the implementation) of the numerical methods.

Prepublications. Some results of this thesis have been published in advance in a preprint with Prof. Dr. Tobias Jahnke: *Adiabatic midpoint rule for the dispersion-managed nonlinear Schrödinger equation*, see [40]. Moreover, some results of this thesis have been published in advance but in a different context in a preprint with Prof. Dr. Tobias Jahnke and Prof. Dr. Roland Schnaubelt: *Strang splitting for a semilinear Schrödinger equation with damping and forcing*, see [41]. We will point out these results at the appropriate place.

CHAPTER 2

The dispersion-managed nonlinear Schrödinger equation

In this chapter, we investigate the dispersion-managed nonlinear Schrödinger equation (1.1) denoted by DMNLS. After establishing a well-posedness result of the DMNLS in Section 2.1, we continue by formulating the DMNLS in terms of a Fourier series representation in Section 2.2. Here, we also outline the idea of the spectral collocation method in order to obtain a space discretization of the DMNLS. In Section 2.3, we illustrate the challenges to approximate solutions of the DMNLS by numerical schemes using the example of splitting methods. Following this setback, we introduce an additional transformation of the DMNLS in Section 2.4 leading us to the transformed dispersion-managed nonlinear Schrödinger equation (tDMNLS). The tDMNLS is equivalent to the DMNLS (in some sense), however, investigating the tDMNLS instead of the DMNLS turns out advantageous. For this reason, we use the tDMNLS as starting point for further analysis, and in particular for constructing novel time-integration schemes. Concluding this chapter, we introduce in Section 2.5 a suitable analytic setting for all further investigations.

2.1. The DMNLS – a well-posed problem

The DMNLS (1.1) is considered as evolution equation in the Hilbert space $L_2(\mathbb{T})$ of square integrable functions equipped with the inner product

$$\langle v, w\rangle = \int_{\mathbb{T}} v(x)\overline{w}(x)\,\mathrm{d}x\,, \qquad v, w \in L_2(\mathbb{T})$$

and the induced norm $\|v\|_{L_2(\mathbb{T})} = \sqrt{\langle v, v\rangle}$. Since any complex-valued $v \in L_2(\mathbb{T})$ can be represented in an $L_2(\mathbb{T})$-sense by its corresponding Fourier series

$$v(x) = \sum_{m\in\mathbb{Z}} v_m e^{\mathrm{i}mx}\,, \qquad \text{where} \quad v_m := \langle v, e^{\mathrm{i}m\cdot}\rangle\,,$$

it is convenient to identify v with the complex sequence $(v_m)_{m\in\mathbb{Z}}$. We define $|m|_+ := \max\{1,|m|\}$ and consider for $(z_m)_{m\in\mathbb{Z}}$ in $\mathbb{C}$ the norm

$$\|z\|_{\ell^2_s} = \left(\sum_{m\in\mathbb{Z}} |m|_+^{2s}|z_m|^2\right)^{1/2}, \qquad s \geq 0\,,$$

and the space

$$\ell^2_s := \Big\{(z_m)_{m\in\mathbb{Z}} \text{ in } \mathbb{C} \;\mid\; \|z\|_{\ell^2_s} < \infty\Big\} \cong H^s(\mathbb{T})\,,$$

where $H^s(\mathbb{T})$ is the classical Sobolev space of all functions $v\colon \mathbb{T}\to\mathbb{C}$ with partial derivatives up to order $s\in\mathbb{N}$ in $L_2(\mathbb{T})$. In particular, we identify $\ell^2_0 \cong H^0(\mathbb{T}) = L_2(\mathbb{T})$ on the basis of Parseval's equation, i.e.

$$\int_{\mathbb{T}} v(x)\overline{w}(x)\,\mathrm{d}x = \sum_{m\in\mathbb{Z}} v_m\overline{w}_m\,.$$

The natural question to ask here is whether or not the DMNLS is well-posed in this setting. We consider the DMNLS to be globally well-posed in the Sobolev space $H^k(\mathbb{T})$ if, for any choice of initial value $u_0 \in H^k(\mathbb{T})$, there exists a unique solution $u \in C\big([0,T], H^k(\mathbb{T})\big)$.

The classical NLS on the torus is exhaustively studied with respect to well-posedness for instance in [11]. However, to the best of our knowledge there are no rigorous results that directly treat the well-posedness of the DMNLS. The following corollary states the global well-posedness of the DMNLS in $H^k(\mathbb{T})$ for $k\in\mathbb{N}$. In the proof, we exploit established well-posedness results for the cubic NLS, i.e. for the DMNLS with constant $\gamma(\frac{t}{\varepsilon}) = \pm\delta+\varepsilon\alpha$. A similar idea has been used in [5] to analyze the well-posedness of the DMNLS in $L_2(\mathbb{R}^d)$ with $\varepsilon = 1$ and $u\colon (0,\infty)\times\mathbb{R}^d \to \mathbb{C}$.

Corollary 1. *Consider the DMNLS* (1.1) *with initial value* $u_0 \in H^k(\mathbb{T})$ *with* $k\in\mathbb{N}$. *Then, there exists a unique solution* $u \in C\big([0,T], H^k(\mathbb{T})\big)$.

Proof. The proof is based on the fact that the coefficient function γ is piecewise constant and switches between the two values $\pm\delta+\varepsilon\alpha \geq 0$. Therefore, we consider the two equations

$$\partial_t u_1(t,x) = -\mathrm{i}\lambda_1\partial_x^2 u_1(t,x) + \mathrm{i}\,|u_1(t,x)|^2\,u_1(t,x) \tag{2.1}$$

and

$$\partial_t u_2(t,x) = \mathrm{i}\lambda_2\partial_x^2 u_2(t,x) + \mathrm{i}\,|u_2(t,x)|^2\,u_2(t,x)\,, \tag{2.2}$$

with[1]

$$\lambda_1 = \frac{\delta-\varepsilon\alpha}{\varepsilon} > 0 \qquad\text{and}\qquad \lambda_2 = \frac{\delta+\varepsilon\alpha}{\varepsilon} > 0\,.$$

[1] Recall that $\delta > \varepsilon\alpha$, see Section 1.2

If we employ the transformation $\tilde{t} = -t\lambda_1$ in (2.1) and the transformation $\tilde{t} = t\lambda_2$ in (2.2) and, by abuse of notation, denote the new time variable $\tilde{t}$ again by t, then we arrive at the equivalent equations

$$\partial_t u_1(t,x) = \mathrm{i}\partial_x^2 u_1(t,x) - \frac{\mathrm{i}}{\lambda_1} |u_1(t,x)|^2 u_1(t,x) \tag{2.3}$$

and

$$\partial_t u_2(t,x) = \mathrm{i}\partial_x^2 u_2(t,x) + \frac{\mathrm{i}}{\lambda_2} |u_2(t,x)|^2 u_2(t,x)\,. \tag{2.4}$$

Because the global well-posedness in $H^k(\mathbb{T})$ for $k \geq 0$ for each of the equations (2.3) and (2.4) is established in [11, Theorem 2.1], we infer the global well-posedness of (2.1) and (2.2) in $H^k(\mathbb{T})$ for $k \geq 0$. Now, we can construct the desired solution of the DMNLS as follows: we write $T = N\varepsilon + t_\varepsilon$ with $N \in \mathbb{N}$ and $t_\varepsilon \in [0,\varepsilon)$, then we partition

$$[0,T] = \left\{ \bigcup_{n=0}^{N-1} [n\varepsilon, (n+1)\varepsilon] \right\} \cup [N\varepsilon, T]\,.$$

Now, we alternate between equation (2.1) and (2.2) on consecutive subintervals. In other words, we start by posing (2.1) for $t \in [0,\varepsilon]$ with initial value $u_1(0) = u_0 \in H^k(\mathbb{T})$ for $k \in \mathbb{N}$. Then, we consider (2.2) for $t \in [\varepsilon, 2\varepsilon]$ with initial value $u_2(\varepsilon) = u_1(\varepsilon)$ where $u_1(\varepsilon) \in H^k(\mathbb{T})$ is the endpoint of the solution from before. In this fashion, we obtain iteratively a solution u of the DMNLS on the whole time interval $[0,T]$. This solution conserves the regularity of the initial value $u_0 \in H^k(\mathbb{T})$ due to the global well-posedness of (2.1) and (2.2), and is continuous in time by construction. □

Remark. Considering the equations (2.3) and (2.4), we observe that the coefficient in front of the nonlinearity $\mathrm{i}|u|^2 u$ changes its sign. In the context of the NLS a positive sign characterizes the *focusing* case, whereas a negative sign denotes the *defocusing* case. Hence, one can interpret the oscillations in the DMNLS, introduced by the coefficient function γ, in terms of alternation between focusing and defocusing behavior.

2.2. The DMNLS in Fourier space

The solution u of the DMNLS can be at least formally represented by the Fourier series

$$u(t,x) = \sum_{m\in\mathbb{Z}} c_m(t) e^{\mathrm{i}mx}\,. \tag{2.5}$$

This is a well-known approach for partial differential equations, see for instance [56] or [20, Ch. III] for the "classical" cubic NLS. Differentiating (2.5) formally gives

$$\partial_t u(t,x) = \sum_{m\in\mathbb{Z}} c_m'(t) e^{\mathrm{i}mx} \tag{2.6}$$

and

$$\partial_x^2 u(t,x) = -\sum_{m\in\mathbb{Z}} c_m(t) m^2 e^{\mathrm{i}mx}\,. \tag{2.7}$$

Furthermore, the cubic nonlinearity is given by

$$\begin{aligned} \mathrm{i}\left|u(t,x)\right|^2 u(t,x) &= \mathrm{i}u(t,x)\overline{u}(t,x)u(t,x) \\ &= \mathrm{i}\sum_{j\in\mathbb{Z}}\sum_{k\in\mathbb{Z}}\sum_{l\in\mathbb{Z}} c_j(t)\overline{c}_k(t)c_l(t)e^{\mathrm{i}(j-k+l)x} \\ &= \mathrm{i}\sum_{m\in\mathbb{Z}}\sum_{j-k+l=m} c_j(t)\overline{c}_k(t)c_l(t)e^{\mathrm{i}mx}\,. \end{aligned} \tag{2.8}$$

Hence, if we define for $m \in \mathbb{Z}$ the index set

$$I_m = \left\{(j,k,l) \in \mathbb{Z}^3 : j-k+l = m\right\}\,, \tag{2.9}$$

we obtain the system with infinitely many ODEs

$$c_m'(t) = -\tfrac{\mathrm{i}}{\varepsilon}\gamma\left(\tfrac{t}{\varepsilon}\right) m^2 c_m(t) + \mathrm{i}\sum_{I_m} c_j(t)\overline{c}_k(t)c_l(t)\,, \quad m \in \mathbb{Z}\,, \tag{2.10}$$

by inserting (2.6)-(2.8) into (1.1) and equating coefficients for fixed m. Here and subsequently we write

$$\sum_{I_m} \quad \text{instead of} \quad \sum_{(j,k,l)\in I_m}$$

to simplify notation.

Because the Fourier transform (2.5) is an isomorphism from $H^s(\mathbb{T})$ onto ℓ_s^2, the ODE system (2.10) is equivalent to (1.1) in the sense that the Fourier series (2.5) allows us to translate solutions of (1.1) into solutions of (2.10) and vice versa provided the initial value is sufficiently smooth. In particular, Corollary 1 implies that for initial values $c_0 = \big(c_m(0)\big)_{m\in\mathbb{Z}}$ in ℓ_s^2 the ODE system (2.10) has a unique solution $c \in C\big([0,T],\ell_s^2\big)$. Henceforth, we write DMNLS and mean either (1.1) or (2.10) and distinguish only where necessary.

2.2.1. On space discretization

In the following, we briefly introduce the (pseudo-)spectral collocation method to obtain a space discretization of the DMNLS. The explanations are based on [20, Ch. III] and [45, Ch. III].

In this approach, we aim for an approximation of the exact solution of the DMNLS (1.1), represented (formally) by (2.5), in terms of

$$u(t,x) = \sum_{m\in\mathbb{Z}} c_m(t)e^{\mathrm{i}mx} \approx \sum_{m=-L}^{L-1} \tilde{c}_m(t)e^{\mathrm{i}mx} = \tilde{u}(t,x)\,,$$

i.e. we approximate the infinite Fourier series (2.5) by a finite sum. In order to determine the unknown coefficients $\tilde{c}_m(t)$, we choose $L \in \mathbb{N}$ and obtain $2L$ equidistant points in the interval $[-\pi,\pi]$ by defining $x_q = qh$ for $q = -L,\dots,L-1$ with step-size $h = 2\pi/2L = \pi/L$. Now, we require that the approximation $\tilde{u}$ satisfies the DMNLS at each grid point x_q for $q = -L,\dots,L-1$ for all $t \in [0,T]$. In order to obtain an ODE system for the coefficients $\tilde{c}_m(t)$, we exchange

$$\sum_{m\in\mathbb{Z}} \quad \text{by} \quad \sum_{m=-L}^{L-1}$$

in (2.6) and (2.7). Moreover, we observe that

$$e^{\mathrm{i}2Lx_q} = e^{\mathrm{i}2L\pi q/L} = e^{\mathrm{i}2\pi q} = 1\,, \qquad q \in \mathbb{Z}\,,$$

and thus

$$e^{\mathrm{i}(m+2L)x_q} = e^{\mathrm{i}mx_q}\,, \qquad q \in \mathbb{Z}\,,$$

which implies for any Fourier series

$$\sum_{m\in\mathbb{Z}} \hat{c}_m(t)e^{\mathrm{i}mx_q} = \sum_{m=-L}^{L-1}\left(\sum_{\lambda\in\mathbb{Z}} \hat{c}_{m+2L\lambda}(t)\right)e^{\mathrm{i}mx_q}\,.$$

Hence, the nonlinearity (2.8) can be represented at each grid point x_q by the trigonometric polynomial

$$\mathrm{i}|\tilde{u}(t,x_q)|^2\tilde{u}(t,x_q) = \mathrm{i}\sum_{m=-L}^{L-1}\sum_{\lambda\in\mathbb{Z}}\sum_{I_{m+2L\lambda}} \tilde{c}_j(t)\bar{\tilde{c}}_k(t)\tilde{c}_l(t)e^{\mathrm{i}mx_q}\,. \tag{2.11}$$

However, because we have $j,k,l \in \{-L\dots,L-1\}$ and hence

$$j-k+l \in \{-3L+1,\dots,3L-2\}\,,$$

we only have to consider $\lambda \in \{-1,0,1\}$ in (2.11). This phenomenon is known as aliasing, see for instance [56, Ch. 2]. For this reason, we define analogously to (2.9) for $m \in \mathbb{Z}$ the index set

$$\tilde{I}_m := \left\{(j,k,l) \in \{-L,\dots,L-1\}^3 : j-k+l = m+2L\lambda \text{ with } \lambda \in \{-1,0,1\}\right\}\,. \tag{2.12}$$

Ultimately, we obtain the (finite) system of ODEs

$$\tilde{c}_m'(t) = -\tfrac{\mathrm{i}}{\varepsilon}\gamma\left(\tfrac{t}{\varepsilon}\right) m^2 \tilde{c}_m(t) + \mathrm{i}\sum_{\tilde{I}_m} \tilde{c}_j(t)\overline{\tilde{c}}_k(t)\tilde{c}_l(t)\,, \quad m = -L, \dots, L-1 \tag{2.13}$$

for the coefficients $\tilde{c}_m(t)$, and hence a space discretization of the DMNLS.

Remark. In this thesis, we focus solely on the error analysis of the semi-discretization in time for any numerical method presented. Nevertheless, the (pseudo-)spectral collocation method introduced in this section is employed in all subsequent numerical examples. General results on the accuracy of spectral collocation methods can be found in [45,56]. Moreover, a convergence analysis of the fully discretized NLS (spectral collocation in space and Lie splitting in time) is given in [20, Ch. IV].

2.3. Numerical challenges

Splitting methods are popular for approximating solutions of NLS-type equations. This is because usually solving the linear part and the nonlinear part separately is much easier than solving the complete NLS. One seminal paper in this context is [44], the idea goes back to [55].

Despite the time-dependent coefficient function γ the DMNLS is essentially amenable to splitting methods: we consider the linear sub-problem

$$\partial_t v(t) = \tfrac{\mathrm{i}}{\varepsilon}\gamma\left(\tfrac{t}{\varepsilon}\right)\partial_x^2 v(t)\,, \quad v(0) = v_0 \tag{2.14}$$

and the nonlinear sub-problem

$$\partial_t w(t) = \mathrm{i}|w(t)|^2 w(t), \qquad w(0) = w_0 \tag{2.15}$$

of the DMNLS separately. Here, we omit the space variable x to simplify notation. For $f \in L_2(\mathbb{T})$ we denote the propagator associated with the sub-problem (2.14) by

$$\big(\mathcal{L}_\varepsilon(t,s) f\big)(x) \coloneqq \Big(e^{\mathrm{i}\Gamma_\varepsilon(t,s)\partial_x^2} f\Big)(x) = \sum_{m\in\mathbb{Z}} e^{-\mathrm{i}\Gamma_\varepsilon(t,s)m^2} f_m e^{\mathrm{i}mx}\,,$$

where

$$\Gamma_\varepsilon(t,s) \coloneqq \int_{s/\varepsilon}^{t/\varepsilon} \gamma(\sigma)\,\mathrm{d}\sigma\,,$$

cf. [5]. The mapping $t \mapsto \mathcal{L}_\varepsilon(t,0)$ defines a family of strongly continuous unitary operators on $L_2(\mathbb{T})$ and for $t \geq 0$ we obtain a solution of (2.14) via

$$v(t) = \mathcal{L}_\varepsilon(t,0)v_0\,, \tag{2.16}$$

cf. [5]. Hence, it is possible to solve (2.14) exactly in Fourier space. The nonlinear sub-problem (2.15) of the DMNLS matches the nonlinear sub-problem of the "classical" cubic NLS and thus it is well-known how to handle it, see for instance [20,40,44]. For the convenience of the reader, we recapitulate these results: we define the nonlinear mapping

$$B\colon L_2(\mathbb{T}) \to L_1(\mathbb{T}), \qquad B(w) = \mathrm{i}|w|^2 \,.$$

If $w \in H^1(\mathbb{T})$, then $B(w) \in L_\infty(\mathbb{T})$ due to the Sobolev embedding $H^1(\mathbb{T}) \hookrightarrow L_\infty(\mathbb{T})$. Hence, for fixed $w \in H^1(\mathbb{T})$, we can identify the function $x \mapsto B(w)(x) = \mathrm{i}|w(x)|^2$ with the multiplication operator

$$B(w)\colon L_2(\mathbb{T}) \to L_2(\mathbb{T}), \qquad B(w)v = \mathrm{i}|w|^2 v \,,$$

which generates a unitary group denoted by $\big(e^{tB(w)}\big)_{t\in\mathbb{R}}$ on $L_2(\mathbb{T})$. Since

$$\partial_t\big(|w(t)|^2\big) = 2\mathrm{Re}\big(\overline{w}(t)\partial_t w(t)\big) = 2\mathrm{Re}\big(\mathrm{i}|w(t)|^4\big) = 0$$

by (2.15), it follows that $|w(t)|^2$ is time invariant and therefore $|w(t)|^2 = |w(0)|^2$. Hence, the solution of (2.15) is explicitly given by

$$w(t) = e^{tB(w_0)} w_0 \,. \tag{2.17}$$

In conclusion, the sub-problem (2.14) as well as the sub-problem (2.15) can be solved exactly via (2.16) and (2.17) allowing us to approximate solutions of the full DMNLS by a splitting approach: let $t_n = n\tau$ for $n \in \mathbb{N}$ and some fixed step-size $\tau > 0$. We obtain approximations $u_n \approx u(t_n)$ of the DMNLS recursively, e.g., via

the Lie splitting

$$\begin{aligned} u_n^* &= e^{\tau B(u_n)} u_n \,, \\ u_{n+1} &= \mathcal{L}_\varepsilon(t_{n+1}, t_n) u_n^* \,, \end{aligned}$$

the Strang splitting

$$\begin{aligned} u_n^* &= e^{\tau/2 B(u_n)} u_n \,, \\ u_n^{**} &= \mathcal{L}_\varepsilon(t_{n+1}, t_n) u_n^* \,, \\ u_{n+1} &= e^{\tau/2 B(u_n^{**})} u_n^{**} \,, \end{aligned}$$

by solving the sub-problems (2.14) and (2.15) in alternating fashion.

In the following, we demonstrate the behavior of both splitting methods by a numerical example. We consider the DMNLS with $\alpha = 0.1$, $\delta = 1$, $T = 1$ with initial

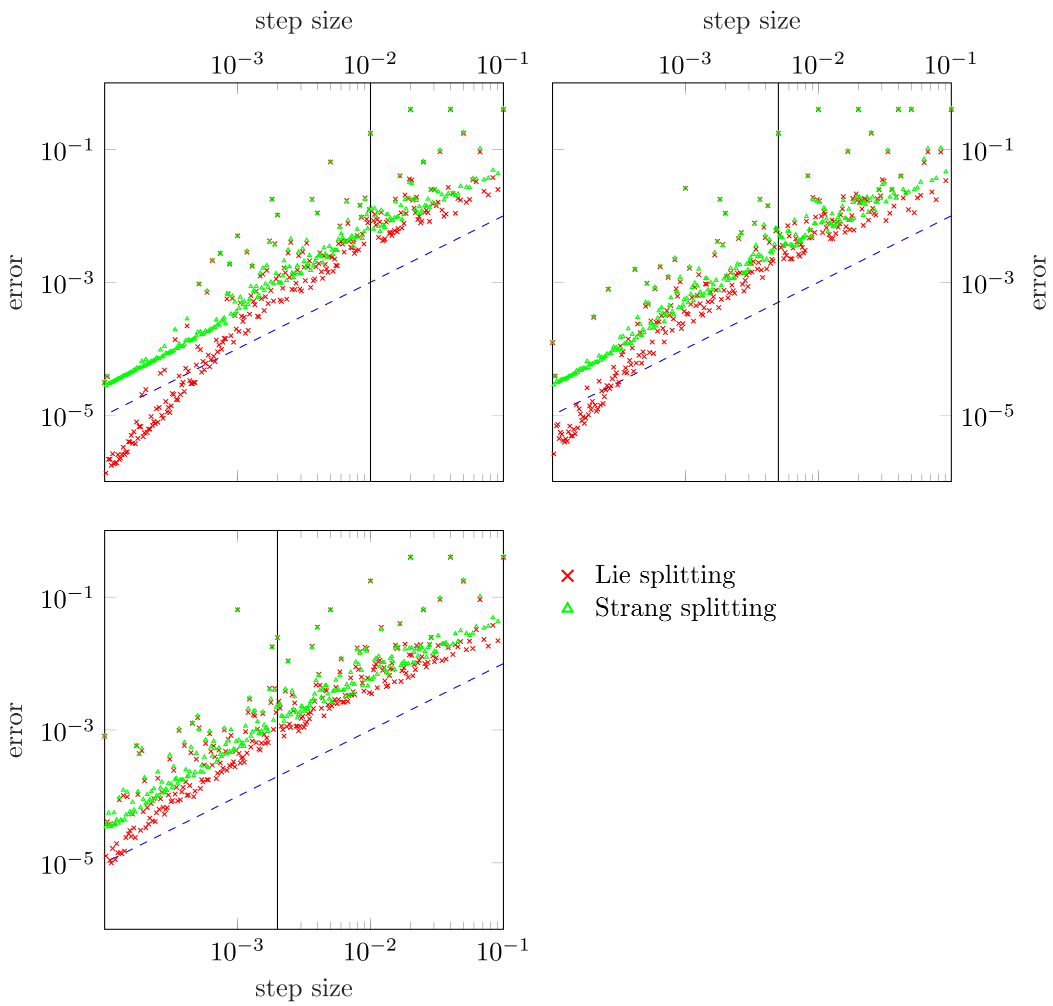

Figure 2.1: Maximal ℓ_0^2-error over time of the Lie splitting and Strang splitting for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). The dashed blue with is a reference line for order one. The black vertical line is at $\tau = \varepsilon$.

value[2] $u_0(x) = e^{-3x^2}e^{3ix}$ and 64 equidistant grid points in the interval $[-\pi, \pi]$ (cf. Section 2.2.1) for $\varepsilon = 0.01$, 0.005, 0.002. To this setting, we apply the Lie splitting and the Strang splitting method. The reference solution is also computed by the Strang splitting but with a very large number of steps ($\approx 10^6$).

The panels of Figure 2.1 show the accuracy of the splitting methods for roughly logarithmically spread step-sizes τ and $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). The dashed blue line is a reference line for order one, and the black vertical line highlights the value $\tau = \varepsilon$. The behavior of both splitting methods appears to be somewhat erratic in the sense that small changes of the step-

[2]The initial value is only approximately periodic, but this error can be neglected.

size may change the accuracy by a factor of 10 to 100. Moreover, the accuracy of the splitting methods seems to decrease for decreasing values of ε, and we observe outliers in the regime $\tau > \varepsilon$ suggesting that the accuracy does not improve at all for several choices of step-sizes τ.

Remark. It is worth mentioning that the splitting methods in this example yield particularly poor results for step-sizes that are integer multiples of ε suggesting a completely different behavior of the DMNLS compared to the highly oscillatory NLS considered in [15].

Conclusion. The above experiment indicates the challenging task to approximate solutions of the DMNLS with high accuracy. In particular, we observe that obtaining high accuracy with splitting methods heavily depends on the step-size τ and on the parameter ε, and hence these methods are not very appealing.

2.4. The tDMNLS – an equivalent problem

One challenge of the DMNLS is that the right-hand side is unbounded in the limit $\varepsilon \to 0$. This can be circumvented by an equivalent transformation of the DMNLS based on the fact that the exact solution of the linear part (2.10) is known in terms of (2.16). Defining the function

$$\widehat{\phi}(z) \coloneqq \int_0^z \gamma(\sigma)\,\mathrm{d}\sigma = \phi(z) + \alpha\varepsilon z \quad \text{with} \quad \phi(z) \coloneqq \int_0^z \chi(\sigma)\,\mathrm{d}\sigma \tag{2.18}$$

allows us to express solutions of the linear part of (2.10) in the form

$$c_k(t) = \exp\left(-\mathrm{i}k^2\widehat{\phi}\left(\tfrac{t}{\varepsilon}\right)\right) c_k(0)\,, \qquad k \in \mathbb{Z}\,. \tag{2.19}$$

Here, we recognize that the derivative of $\widehat{\phi}$ does not exist in the classical sense. It can be understood as piece-wise derivative on the open intervals $\big(n\varepsilon, (n+1)\varepsilon\big)$ for $n \in \mathbb{N}$ with left-continuous extension. However, we will write

$$\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\phi}\left(\tfrac{t}{\varepsilon}\right) = \tfrac{1}{\varepsilon}\gamma\left(\tfrac{t}{\varepsilon}\right)$$

by abuse of notation. The exact solution formula (2.19) of the linear part in (2.10) motivates the change of variables

$$y_k(t) \coloneqq \exp\left(\mathrm{i}k^2\widehat{\phi}\left(\tfrac{t}{\varepsilon}\right)\right) c_k(t)\,, \qquad k \in \mathbb{Z}\,, \tag{2.20}$$

in the ODE system (2.10). Similar transformations have been used in [39] and [38] in case of oscillatory linear Schrödinger equations. Moreover, this transformation is known as the Floquet-Lyapunov transformation in physics; cf. [46,57]. Differentiating (2.20) yields

$$c_m'(t) = -\tfrac{\mathrm{i}}{\varepsilon}\gamma\left(\tfrac{t}{\varepsilon}\right) m^2 c_m(t) + \exp\left(-\mathrm{i}m^2\widehat{\phi}\left(\tfrac{t}{\varepsilon}\right)\right) y_k'(t)\,. \tag{2.21}$$

Now, equating (2.21) with the corresponding equation in (2.10) cancels the linear part and we obtain the transformed DMNLS (tDMNLS)

$$y_m'(t) = \mathrm{i}\sum_{I_m} y_j(t)\overline{y}_k(t)y_l(t)\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{t}{\varepsilon}\right)\right), \qquad m\in\mathbb{Z}\,, \tag{2.22}$$

where we employ the abbreviation

$$\omega_{[jklm]} = j^2 - k^2 + l^2 - m^2.$$

Since we have for arbitrary $\varepsilon \neq 0$

$$\left|\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{t}{\varepsilon}\right)\right)\right| = 1\,,$$

the right-hand side of equation the tDMNLS is bounded for $\varepsilon \to 0$ provided the sequence $\big(y_m(t)\big)_{m\in\mathbb{Z}}$ decays sufficiently fast, see Lemma 2 (below).

For this reason, we henceforth study the tDMNLS instead of the DMNLS. Moreover, we simplify notation by abbreviating

$$Y_{jkl}(t) = y_j(t)\overline{y}_k(t)y_l(t)\,, \quad \widehat{Y}_{jklm}(t) = Y_{jkl}(t)\exp(-\mathrm{i}\omega_{[jklm]}t\alpha) \tag{2.23}$$

to write the tDMNLS in the form

$$y_m'(t) = \mathrm{i}\sum_{I_m} \widehat{Y}_{jklm}(t)\exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{t}{\varepsilon}\right)\right), \qquad m\in\mathbb{Z}\,. \tag{2.24}$$

Because the transformation (2.20) is an isomorphism from ℓ_s^2 onto ℓ_s^2 the DMNLS and the tDMNLS are equivalent in the sense that the transformation (2.20) allows us to convert solutions of the tDMNLS into solutions of the DMNLS (2.10) and vice versa. Hence, according to Corollary 1, the tDMNLS is well-posed in ℓ_s^2.

Clearly, replacing I_m in (2.24) by the finite set $\tilde{I}_m$ given in (2.12) yields a spatially discretized version of the tDMNLS. We will utilize this space discretization in all subsequent numerical examples without further notice.

Remark. The downside of reformulating the DMNLS in terms of the tDMNLS is the occurring multiple sum in (2.24). Without the transformation evaluations of the nonlinear part of the DMNLS could be realized in terms of point-wise multiplications, cf. Section 2.3. Now, the nested sum structure renders evaluations more costly from a numerical point of view.

2.5. Analytic setting

So far, we have performed two transformations, (2.5) and (2.20), to obtain the tDMNLS (2.24) – an equivalent formulation of the DMNLS (1.1). In order to analyze the tDMNLS and to investigate the error behavior of the numerical methods introduced in this thesis, we establish a suitable analytic setting in this section.

Because the Fourier transform as well as the transformation (2.20) are isometries on $L_2(\mathbb{T}) \to \ell_0^2$ and $\ell_0^2 \to \ell_0^2$, respectively, a natural choice appears to be the space ℓ_0^2. However, to cope with the nonlinear structure of the tDMNLS the ℓ_0^2-norm is inadequate, because the underlying space ℓ_0^2 has no Banach algebra structure, i.e.

$$\|vw\|_{\ell_0^2} < \infty \not\Leftarrow \|v\|_{\ell_0^2} < \infty \,\wedge\, \|w\|_{\ell_0^2} < \infty\,.$$

Because estimating the norm of a product by the norms of its factors is crucial in the course of this thesis, we adopt an analytic setting from [20, Ch. III.2.].

For $z = (z_m)_{m\in\mathbb{Z}}$ in $\mathbb{C}$, we define the norm

$$\|z\|_{\ell_s^1} = \sum_{m\in\mathbb{Z}} |m|_+^s \, |z_m| \,, \qquad s \geq 0\,,$$

with $|m|_+ := \max\{1, |m|\}$ as before (see Section 2.1), and the corresponding Banach space

$$\ell_s^1 := \Big\{ (z_m)_{m\in\mathbb{Z}} \text{ in } \mathbb{C} \;\mid\; \|z\|_{\ell_s^1} < \infty \Big\}\,. \tag{2.25}$$

The spaces ℓ_s^2 and ℓ_s^1 are related by the following embedding: let $r, s \in \mathbb{N}$ with $r > s$, then

$$\ell_r^2 \hookrightarrow \ell_s^1 \hookrightarrow \ell_s^2\,, \quad \text{i.e.} \quad \|z\|_{\ell_s^2} \leq \|z\|_{\ell_s^1} \leq C\,\|z\|_{\ell_r^2}\,, \tag{2.26}$$

see [20, Proposition III.2.]. The embedding (2.26) allows us to prove error bounds in ℓ_0^1 in order to obtain error bounds in ℓ_0^2. Moreover, starting from the original DMNLS (1.1), the summability of the initial value y_0 in ℓ_s^1 for the tDMNLS can be ensured, e.g., by supposing that the initial value u_0 of the DMNLS is in $H^{s+1}(\mathbb{T})$. In this case the initial value y_0 is in particular in ℓ_{s+1}^2, and thus Corollary 1 implies that $y \in C\big([0,T], \ell_{s+1}^2\big)$. This motivates the definition

$$M_s^y := \max_{t\in[0,T]} \|y(t)\|_{\ell_s^1}\,. \tag{2.27}$$

Throughout this thesis, we pose regularity assumptions on the initial value y_0 of the tDMNLS in the space ℓ_{s+1}^2 in order to ensure that $M_s^y \leq \infty$.

The sequence spaces ℓ_s^1 are much more convenient for estimates concerning the tDMNLS. In particular, the space ℓ_0^1 – the space of absolutely convergent sequences

– is a Banach algebra, cf. [59, Ch. IX]. In this setting, we will now prove a tangible bound for the right-hand side of the tDMNLS as announced in Section 2.4.

Henceforth, we will write ℓ^1 instead of ℓ^1_0 to simplify notation. Moreover, $C > 0$ and $C(\cdot) > 0$ denote universal constants, possibly taking different values at various appearances. The notation $C(\cdot)$ means that the constant depends only on the values specified in the brackets.

Lemma 2. *Let y be the solution of* (2.22) *with initial value $y_0 \in \ell^2_1$. Then, we have*

$$\left\|y'(t)\right\|_{\ell^1} \leq C(M_0^y)\,.$$

Proof. Substituting (2.22) yields

$$\begin{aligned}
\left\|y'(t)\right\|_{\ell^1} = \sum_{m\in\mathbb{Z}} \left|y'_m(t)\right| &= \sum_{m\in\mathbb{Z}} \left| \mathrm{i} \sum_{I_m} y_j(t)\overline{y}_k(t)y_l(t) \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{t}{\varepsilon}\right)\right)\right| \\
&\leq \sum_{m\in\mathbb{Z}} \sum_{I_m} |y_j(t)|\,|\overline{y}_k(t)|\,|y_l(t)| \\
&\leq \left(\sum_{j\in\mathbb{Z}} |y_j(t)|\right)\left(\sum_{k\in\mathbb{Z}} |\overline{y}_k(t)|\right)\left(\sum_{l\in\mathbb{Z}} |y_l(t)|\right) \\
&= \|y(t)\|^3_{\ell^1}\ .
\end{aligned}$$

□

Remark. Estimating products of infinite sequences plays an important role in this thesis. In these estimates, we frequently employ the Banach algebra structure of ℓ^1 as pointed out in the proof of Lemma 2.

2.5.1. Miscellaneous analytical tools

Throughout the proofs in this thesis we commonly employ three well-known (but easily forgotten) analytical tools without further notice. For the convenience of the reader, we state these estimates in this section (without proof).

The continuous Gronwall lemma.
Let $u\colon [t_0, t_1] \to \mathbb{R}$ be a continuous and non-negative function, and suppose that u satisfies the integral inequality

$$u(t) \leq K + C\int_{t_0}^{t} u(s)\,\mathrm{d}s\,, \qquad t \in [t_0, t_1]\,,$$

for two constants $K, C \geq 0$. Then, we have the estimate

$$u(t) \leq Ke^{C(t-t_0)}\,, \qquad t \in [t_0, t_1]\,.$$

The discrete Gronwall lemma.

Let $(u_n)_{n\in\mathbb{N}}$ in $\mathbb{R}$ be a non-negative sequence, and suppose that $(u_n)_{n\in\mathbb{N}}$ satisfies the inequality

$$u_N \le K + \tau C \sum_{n=0}^{N-1} u_n\,, \qquad N \in \mathbb{N}\,,$$

for constants $K \ge 0$ and $\tau C \ge 0$. Then, we have the estimate

$$u_N \le K e^{N\tau C}\,, \qquad N \in \mathbb{N}\,.$$

The summation by parts formula.

Let $(a_n)_{n\in\mathbb{N}}$ and $(b_n)_{n\in\mathbb{N}}$ in $\mathbb{C}$ be two sequences. Then, the following equality holds.

$$\sum_{n=1}^{N} a_n b_n = a_N \sum_{n=1}^{N} b_n - \sum_{n=1}^{N-1} (a_{n+1} - a_n) \sum_{j=1}^{n} b_j\,, \qquad N \in \mathbb{N}\,.$$

CHAPTER 3

The limit system

In Chapter 2, we have transformed the DMNLS into the tDMNLS and observed that the right-hand side of the tDMNLS is bounded in the limit $\varepsilon \to 0$, cf. Lemma 2. However, the tDMNLS is not a universal remedy because it still contains rapidly oscillating phases. This chapter is devoted to an analytic approach to this problem; the main idea is to apply an additional averaging step to the tDMNLS. This averaging results in an equation that is independent of the parameter ε and of the coefficient function γ – the limit system. We start by motivating the averaging idea in Section 3.1. Following this formal derivation of the limit system, we state a rigorous theorem in Section 3.2 concerning the accuracy of the limit system as an approximation to the tDMNLS. Moreover, we illustrate our analytical results by various numerical experiments. The proof is postponed to Section 3.3.

Remark. The results of this chapter (in particular Theorem 3) have been published to some extend with Prof. Dr. Tobias Jahnke in the preprint [40].

3.1. Derivation

The aim of this section is to derive an equation which captures the asymptotic behavior of the tDMNLS in the limit $\varepsilon \to 0$. One way to obtain such an equation is the method of multiple scales, a formal calculation technique, which is quite popular in engineering, physics, and applied mathematics, cf. [51].

In the following, we briefly demonstrate this method using the example of the tDMNLS: we introduce a fast time scale $\sigma = t/\varepsilon$ and make the ansatz

$$y_m(t) = \sum_{n=0}^{\infty} \varepsilon^n z_m^{(n)}(t, \sigma)\,, \tag{3.1}$$

where we suppose that the functions $z_m^{(n)}(t,\sigma)$ are 2-periodic in the second argument, i.e. that we have

$$z_m^{(n)}(t,\sigma) = z_m^{(n)}(t,\sigma+2)\,. \tag{3.2}$$

Differentiating (3.1) yields

$$\frac{\mathrm{d}}{\mathrm{d}t} y_m(t) = \sum_{n=0}^{\infty} \left(\varepsilon^n \partial_1 z_m^{(n)}(t,\sigma) + \varepsilon^{n-1} \partial_2 z_m^{(n)}(t,\sigma) \right)\,, \tag{3.3}$$

where ∂_1 and ∂_2 denote the partial derivative with respect to the first and second variable, respectively. If we substitute the ansatz (3.1) into (2.24) and equate coefficients of equal powers of ε, we obtain for ε^{-1}

$$\partial_2 z_m^{(0)}(t,\sigma) = 0 \tag{3.4}$$

and for ε^n with $n \geq 0$

$$\partial_1 z_m^{(n)} + \partial_2 z_m^{(n+1)} = \mathrm{i} \sum_{I_m} \sum_{p+q+r=n} z_j^{(p)} \overline{z}_k^{(q)} z_l^{(r)} \exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha t + \phi(\sigma))\right). \tag{3.5}$$

Here and subsequently, we usually omit the time-dependence of $z_m^{(\cdot)}$ for readability. Clearly, the time parameter σ depends on t, however, we treat σ and t henceforth as independent variables. According to (3.4), the function $z_m^{(0)}$ is independent of σ, and hence

$$z_m^{(0)}(t,\sigma) = z_m^{(0)}(t)\,. \tag{3.6}$$

Moreover, considering (3.5) for $n = 0$ and integrating from 0 to 2 with respect to the second variable yields

$$\int_0^2 \partial_1 z_m^{(0)} + \partial_2 z_m^{(1)} \,\mathrm{d}\sigma = \mathrm{i} \sum_{I_m} \int_0^2 z_j^{(0)} \overline{z}_k^{(0)} z_l^{(0)} \exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha t + \phi(\sigma))\right) \mathrm{d}\sigma\,.$$

Thanks to (3.2) and (3.6), we arrive at

$$2\partial_1 z_m^{(0)} = \mathrm{i} \sum_{I_m} z_j^{(0)} \overline{z}_k^{(0)} z_l^{(0)} \exp\left(-\mathrm{i}\omega_{[jklm]}\alpha t\right) \int_0^2 \exp\left(-\mathrm{i}\omega_{[jklm]}\phi(\sigma)\right) \mathrm{d}\sigma\,.$$

Since

$$\phi(z) = \int_0^z \chi(\sigma)\,\mathrm{d}\sigma = \begin{cases} -\delta z & \text{if} \quad z \in [0,1)\,, \\ -\delta(2-z) & \text{if} \quad z \in [1,2)\,, \end{cases} \tag{3.7}$$

by definition (1.3), a small computation gives

$$\int_0^2 \exp\left(-\mathrm{i}\omega\phi(\sigma)\right) \mathrm{d}\sigma = 2\int_0^1 \exp(\mathrm{i}\omega\delta\xi)\,\mathrm{d}\xi\,,$$

and thus we obtain the leading order equation

$$\partial_1 z_m^{(0)} = \mathrm{i} \sum_{I_m} z_j^{(0)} \overline{z}_k^{(0)} z_l^{(0)} \exp\left(-\mathrm{i}\omega_{[jklm]}\alpha t\right) \int_0^1 \exp\left(\mathrm{i}\omega_{[jklm]}\delta\xi\right) \mathrm{d}\xi \,. \tag{3.8}$$

With the abbreviation $v_m(t) = z_m^{(0)}(t)$, we write (3.8) in the form

$$v_m'(t) = \mathrm{i} \sum_{I_m} \widehat{V}_{jklm}(t) \int_0^1 \exp\left(\mathrm{i}\omega_{[jklm]}\delta\xi\right) \mathrm{d}\xi \,, \qquad m \in \mathbb{Z} \,, \tag{3.9}$$

where

$$V_{jkl}(t) = v_j(t)\overline{v}_k(t)v_l(t) \quad \text{and} \quad \widehat{V}_{jklm}(t) = V_{jkl}(t) \exp\left(-\mathrm{i}\omega_{[jklm]}t\alpha\right) \tag{3.10}$$

in the spirit of (2.23). In contrast to the tDMNLS (2.24), the right-hand side of (3.9) is independent of ε and no longer contains the discontinuous coefficient function γ.

Moreover, the formal calculation with the method of multiple scales suggests that solutions of (3.9) yield approximations of order ε to solutions of the tDMNLS. However, the derivation of (3.9) is only formal and it requires further investigation to analyze rigorously in which sense the ODE system (3.9) is related to the tDMNLS. In fact, we will prove in the following sections that solutions of the tDMNLS actually converge to solutions of (3.9) in the limit $\varepsilon \to 0$ in ℓ^1. For this reason, we denote the ODE system (3.9) as the limit system.

Remark. The derivation of the limit system (3.9), i.e. the derivation of the leading order equation of (3.5), can be interpreted in terms of averaging where the highly oscillatory part of the exponential function in the tDMNLS is replaced by its averaged value over one period, i.e.

$$\exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{t}{\varepsilon}\right)\right) \approx \frac{1}{2\varepsilon} \int_0^{2\varepsilon} \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s = \int_0^1 \exp(\mathrm{i}\omega\delta\xi) \,\mathrm{d}\xi \,. \tag{3.11}$$

3.1.1. Relation to the Gabitov-Turitsyn equation

The Gabitov-Turitsyn equation (GTE) follows also from the DMNLS via a transformation and averaging (cf. [23,24]), and hence the derivation of the limit system (3.9) is closely related to the derivation of the GTE. Here, the phase $\widehat{\phi}(t/\varepsilon) = \phi(t/\varepsilon) + \alpha t$ is replaced by $\phi(t/\varepsilon)$ in the transformation (2.20). Then, substituting the oscillating phase by its mean as in (3.11) yields the discrete counterpart of the GTE

$$q_m'(t) = -\mathrm{i}m^2\alpha q_m(t) + \mathrm{i} \sum_{I_m} q_j(t)\overline{q}_k(t)q_l(t) \int_0^1 \exp(\mathrm{i}\omega_{[jklm]}\delta\xi) \,\mathrm{d}\xi \,, \quad m \in \mathbb{Z} \,. \tag{3.12}$$

Each of these equations still contains a linear term, whereas the linear part is completely eliminated in (3.9). The ODE systems (3.12) and (3.9) are equivalent in the sense that a sequence $\big(q_m(t)\big)_{m\in\mathbb{Z}}$ is a solution of (3.12) if and only if $\big(v_m(t)\big)_{m\in\mathbb{Z}}$ with

$$v_m(t) = \exp(\mathrm{i}m^2\alpha t)q_m(t)\,, \quad m \in \mathbb{Z}$$

is a solution of (3.9).

The original GTE proposed in [23,24] is obtained analogously if the DMNLS is considered on $\mathbb{R}$ instead of $\mathbb{T}$, the Fourier series (2.5) is replaced by the Fourier transform, and the double sum in the nonlinear term is exchanged for a double integral.

3.1.2. Higher order limit systems

Because solutions of the limit system presumably yield approximations to solutions of the tDMNLS in some sense, it is natural to consider higher order approximations. Formally, the method of multiple scales allows for deriving additional correction terms. In this manner, higher order GTE equations are constructed in [8], see also [9]. The derived equations give some insight into the structure and properties of the DMNLS, however, these equations contain four-fold integrals and thus are, on the downside, inconvenient for numerical computations, cf. [9, p. 137].

Equally, it is possible to derive higher order terms for the limit system with the method of multiple scales introduced in Section 3.1 by considering (3.5) for $n > 0$. These terms, however, contain nested multiple sums, which renders them also impractical for numerical approximations due to exorbitant computational costs. For this reason, we do not consider higher order limit systems in this thesis.

3.2. Relation to the tDMNLS

In this section, we underpin the formal calculations with the method of multiple scales from Section 3.1 by rigorous estimates concerning the accuracy of solutions of the limit system (3.9) considered as approximations for the tDMNLS. In particular, the results of this investigation justify the term "limit system" for the ODE system (3.9). To the best of our knowledge, there are no rigorous analytical results concerning the well-posedness of the GTE and thus of the limit system (3.9). Therefore, we make the following assumption.

Assumption 1. *We suppose that for $s = 0, 1, \dots, 5$ the limit system* (3.9) *with initial value $v_0 \in \ell^2_s$ has a unique solution $v \in C\big([0,T], \ell^2_s\big)$.*

We employ the abbreviation

$$M_s^v := \max_{t\in[0,T]} \|v(t)\|_{\ell_s^1} \tag{3.13}$$

for solutions v of (3.9). Assumption 1 particularly implies that $M_s^v < \infty$ for initial values $v_0 \in \ell_{s+1}^2$, cf. Section 2.5. For simplicity, we also abbreviate

$$M_s := \max\{M_s^y, M_s^v\} . \tag{3.14}$$

The following theorem is closely related to similar results for the GTE, cf. [53].

Theorem 3. *Let y and v be solutions of the tDMNLS* (2.24) *and the limit system* (3.9)*, respectively. Under Assumption 1 the following estimates hold.*

(i) If $y(0) = v(0) \in \ell_1^2$, then we have

$$\|y(t) - v(t)\|_{\ell^1} \le \varepsilon \left(1 + \tfrac{1+\alpha}{\delta} t\right) C(M_0) e^{tC(M_0)} , \quad t \in [0,T] .$$

(ii) If $y(0) = v(0) \in \ell_3^2$, then we have for $t_k = \varepsilon k$ with $k \in \mathbb{N}$

$$\|y(t_k) - v(t_k)\|_{\ell^1} \le \frac{\varepsilon^2}{\delta} t_k C(\alpha, M_0, M_2) e^{t_k C(M_0)} , \quad t_k \in [0,T] .$$

In case of $\alpha = 0$ the first constant depends only on M_0.

Theorem 3 is proven in Section 3.3.

In the following, we illustrate Theorem 3 with two numerical example. For the first example, we consider the DMNLS with $\alpha = 0.1$, $\delta = 0.1$ and $T = 1$ with initial value[1] $u_0(x) = e^{-3x^2} e^{3ix}$ and 128 equidistant grid points in the interval $[-\pi, \pi]$ for $\varepsilon = 0.1, 0.05, 0.01$.

Figure 3.1 shows the evolution in time of the real part (left) and imaginary part (right) of the coefficient $y_m(t)$ of the tDMNLS for $m = -5$. We observe that for decreasing values of ε the frequency of the small scale oscillations increases but their amplitude decreases. In fact, we observe the convergence for $\varepsilon \to 0$ to the corresponding coefficient of the limit system (3.9) as stated in Theorem 3. Moreover, we observe intersections with the limit equation close to multiples of ε.

Figure 3.2 illustrates the real part (left) and imaginary part (right) of the difference $y_m(t) - v_m(t)$ over time for fixed $\varepsilon = 0.1$ and $-4 \le m \le 10$. The black vertical lines are at 3ε and 7ε, respectively. We observe that at multiples of ε the difference does not vanish, but, is much smaller for all coefficients, in accordance with the improved error bound of part (ii) of Theorem 3.

[1] The initial value is only approximately periodic, but this error can be neglected.

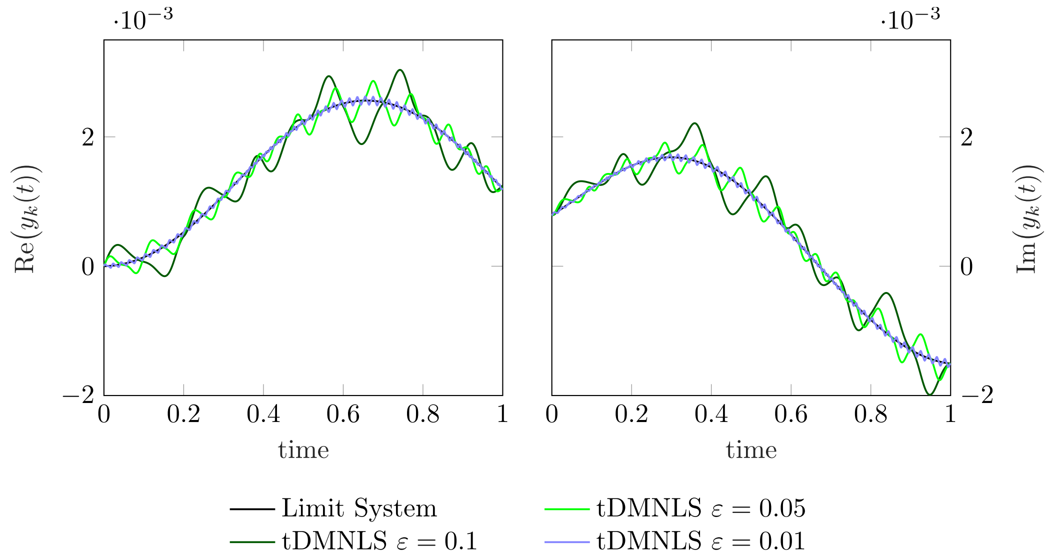

Figure 3.1: Evolution over time of the real part (left) and imaginary part (right) of one coefficient of the limit system (3.9) and the corresponding coefficient of the tDMNLS computed with $\varepsilon = 0.1,\, 0.05,\, 0.01$.

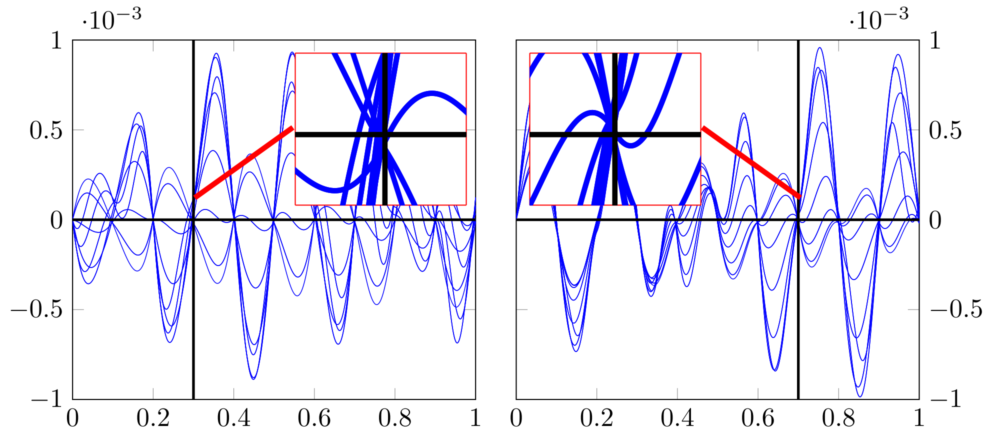

Figure 3.2: Evolution over time of the real part (left) and imaginary part (right) of the difference between various coefficients of the tDMNLS with $\varepsilon = 0.1$ and the corresponding coefficients of the limit system (3.9) computed with the same initial value.

For the second example, we again consider solutions of the limit system (3.9) as approximation to solutions of the tDMNLS (2.24). In the same setting as before, but with 64 equidistant grid points in space, we approximate solutions of the limit system with Runge-Kutta methods (RKMs) of order one, two, and three, namely with the explicit Euler method, Heun's method, and the Bogacki-Shampine method.

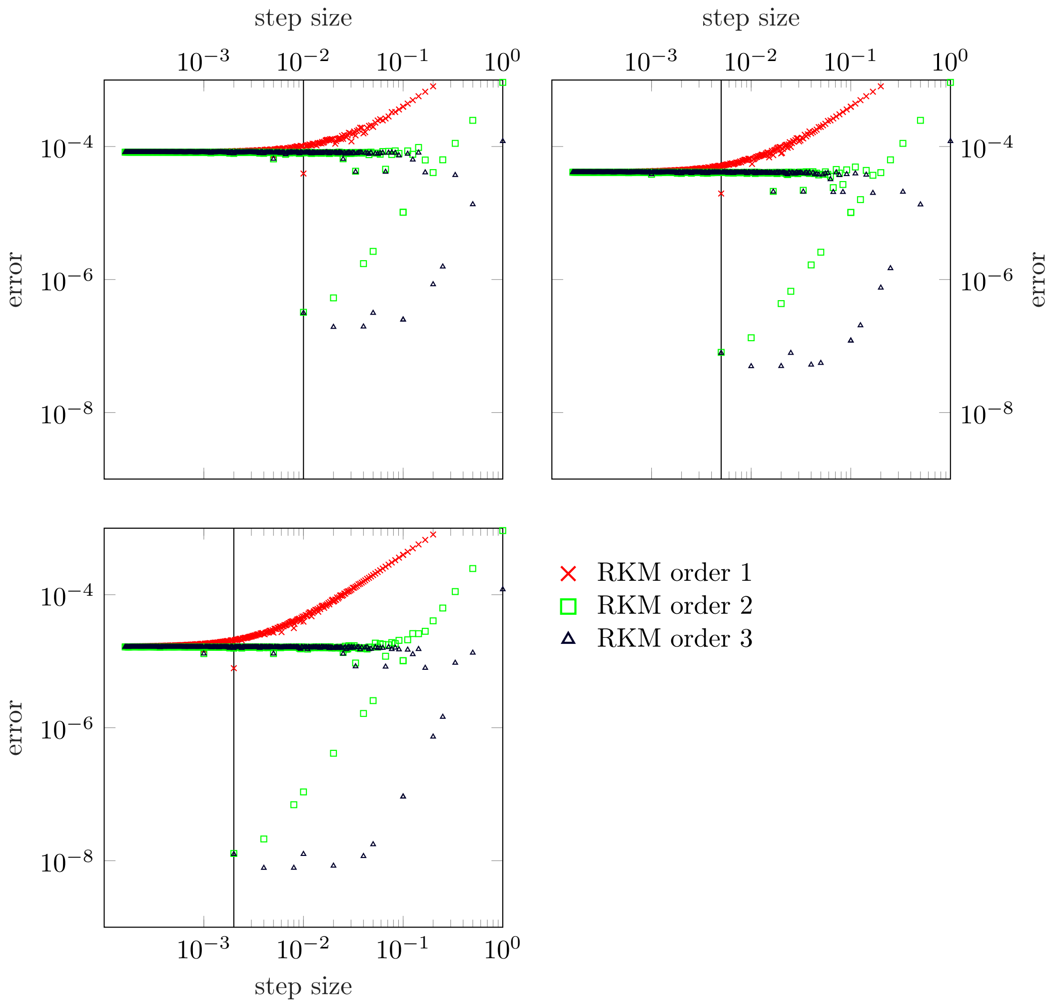

Figure 3.3: Maximal ℓ_0^2-error over time of Runge-Kutta methods of order one, two and three applied to the limit system (3.9) considered as approximations to the tDMNLS (2.24) for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). The black vertical line is at $\tau = \varepsilon$

The panels of Figure 3.3 show the accuracy of the RKMs applied to the limit system compared to the tDMNLS considered with $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). The solutions of the tDMNLS are approximated by the Strang splitting method with a large number of steps ($\approx 10^6$). The black vertical line indicates the value $\tau = \varepsilon$. We observe that the accuracy of the RKM approximations to the tDMNLS is fixed to a maximum level. In the regime $\tau < \varepsilon$ (left of the black line), this level decreases linearly for decreasing values of ε as stated in part (i) of Theorem 3. In the regime $\tau > \varepsilon$ (right of the black line), we observe the same fixed level of accuracy as before. However, if the step-sizes τ are multiples of ε, then the maximum level of accuracy increases particularly for the approximations with the

RKM of order two and order three. Here, we observe that for these step-sizes the maximum level of accuracy improves quadratically in accordance with part (ii) of Theorem 3. The first order method does not benefit as much from the improved error bound of the limit system because the approximation error is too large for these step-sizes.

Conclusion. The limit system can be used to approximate solutions of the tDMNLS (2.24). According to Theorem 3, these approximations can obtain an accuracy up to $\mathcal{O}(\varepsilon^2)$ at integer multiples of ε. Depending on the order of the time-integrator, this level of accuracy is reached for different step-sizes. For a method of order p the accuracy is in $\mathcal{O}(\max\{\varepsilon^2, \tau^p\})$ for step-sizes τ chosen as integer multiple of ε. For $p > 2$, however, often more than one evaluation of the right-hand side of (3.9) is necessary, e.g., for RKMs. Thus, higher order methods will typically not pay in terms of work versus accuracy. If the step-size τ is an integer multiple of ε, then each time discretization point t_n is also an integer multiple of ε. Typically, approximations at other times $t \in (t_n, t_{n+1})$ can be easily obtained by using a time-integrator on the small interval $[t_n, t]$ of length $\mathcal{O}(\tau)$. This principle is used, e.g., in numerical stroboscopic averaging, cf. [13]. Because we are interested in approximations of the tDMNLS, one has to solve the tDMNLS instead of the limit system on these small time intervals.

3.3. Proof of Theorem 3

Before we start with the proof of Theorem 3, we make a few preparations. Since the limit system (3.9) emerges from the tDMNLS (2.24) via replacing the periodic exponential by its averaged value (see Section 3.1), it is essential to control this replacement in the differential equations. Therefore, we describe the difference between the exponential and its average in terms of the function

$$g_\omega(\sigma) = \exp\big(-\mathrm{i}\omega\phi(\sigma)\big) - \frac{\exp(\mathrm{i}\omega\delta) - 1}{\mathrm{i}\omega\delta}\,, \qquad \omega \neq 0\,, \tag{3.15}$$

and prove the following lemma containing estimates for integrals involving the product of g_ω with sufficiently smooth functions.

Lemma 4. *Let $\varepsilon > 0$, $\omega \neq 0$ and g_ω as in (3.15). If $f \in C^1(\mathbb{R})$, then*

$$(i) \qquad \left| \int_0^1 f(\varepsilon\sigma) g_\omega(\sigma)\,\mathrm{d}\sigma \right| \leq \frac{\varepsilon}{\delta} C \max_{\sigma\in[0,1]} \left|\omega^{-1} f'(\varepsilon\sigma)\right|$$

and

$$(ii) \qquad \left| \int_1^2 f(\varepsilon\sigma) g_\omega(\sigma)\,\mathrm{d}\sigma \right| \leq \frac{\varepsilon}{\delta} C \max_{\sigma\in[1,2]} \left|\omega^{-1} f'(\varepsilon\sigma)\right| .$$

If $f \in C^2(\mathbb{R})$, then

$$(iii) \qquad \left| \int_0^2 f(\varepsilon\sigma) g_\omega(\sigma)\,\mathrm{d}\sigma \right| \le \frac{\varepsilon^2}{\delta} C \max_{\sigma\in[0,2]} \left|\omega^{-1} f''(\varepsilon\sigma)\right|$$

and

$$(iv) \qquad \left| \int_1^3 f(\varepsilon\sigma) g_\omega(\sigma)\,\mathrm{d}\sigma \right| \le \frac{\varepsilon^2}{\delta} C \max_{\sigma\in[1,3]} \left|\omega^{-1} f''(\varepsilon\sigma)\right|$$

Proof. Equation (3.7) allows us to partition

$$g_\omega(\sigma) = \begin{cases} g_{\omega,1}(\sigma) & \text{if} \quad \sigma \in [0,1)\,, \\ g_{\omega,2}(\sigma) & \text{if} \quad \sigma \in [1,2)\,, \end{cases}$$

with

$$g_{\omega,1}(\sigma) = \exp(\mathrm{i}\omega\delta\sigma) - \frac{\exp(\mathrm{i}\omega\delta) - 1}{\mathrm{i}\omega\delta}$$

and

$$g_{\omega,2}(\sigma) = \exp(\mathrm{i}\omega\delta(2-\sigma)) - \frac{\exp(\mathrm{i}\omega\delta) - 1}{\mathrm{i}\omega\delta}\,.$$

In order to prove assertions (i) and (ii), we use integration by parts. Differentiating shows that the functions

$$G_{\omega,1}(\sigma) = \frac{\exp(\mathrm{i}\omega\delta\sigma) - 1}{\mathrm{i}\omega\delta} - \sigma \frac{\exp(\mathrm{i}\omega\delta) - 1}{\mathrm{i}\omega\delta}$$

and

$$G_{\omega,2}(\sigma) = \frac{\exp(\mathrm{i}\omega\delta(2-\sigma)) - \exp(\mathrm{i}\omega\delta)}{-\mathrm{i}\omega\delta} - (\sigma - 1)\frac{\exp(\mathrm{i}\omega\delta) - 1}{\mathrm{i}\omega\delta}$$

are anti-derivatives of $g_{\omega,1}$ and $g_{\omega,2}$, respectively. In addition, we have

$$G_{\omega,1}(0) = G_{\omega,1}(1) = 0 \quad \text{and} \quad G_{\omega,2}(1) = G_{\omega,2}(2) = 0 \tag{3.16}$$

and the estimates

$$\max_{\sigma\in[0,1]} |\omega G_{\omega,1}(\sigma)| \le \frac{1}{\delta} \max_{\sigma\in[0,1]} \big\{2 + 2\sigma\big\} \le \frac{4}{\delta}\,, \tag{3.17}$$

$$\max_{\sigma\in[1,2]} |\omega G_{\omega,2}(\sigma)| \le \frac{1}{\delta} \max_{\sigma\in[1,2]} \big\{2 + 2(\sigma-1)\big\} \le \frac{4}{\delta}\,, \tag{3.18}$$

such that integration by parts yields

$$\left| \int_0^1 f(\varepsilon\sigma) g_\omega(\sigma)\,\mathrm{d}\sigma \right| = \varepsilon \left| \int_0^1 f'(\varepsilon\sigma) G_{\omega,1}(\sigma)\,\mathrm{d}\sigma \right| \le \frac{\varepsilon}{\delta} C \max_{\sigma\in[0,1]} \left|\omega^{-1} f'(\varepsilon\sigma)\right|$$

as well as

$$\left| \int_1^2 f(\varepsilon\sigma) g_\omega(\sigma)\,\mathrm{d}\sigma \right| = \varepsilon \left| \int_1^2 f'(\varepsilon\sigma) G_{\omega,2}(\sigma)\,\mathrm{d}\sigma \right| \le \frac{\varepsilon}{\delta} C \max_{\sigma\in[1,2]} \left|\omega^{-1} f'(\varepsilon\sigma)\right|\,.$$

For inequality (iii), we employ integration by parts twice. Again, differentiating shows that the functions

$$\widetilde{G}_{\omega,1}(\sigma) = \frac{1}{\mathrm{i}\omega\delta}\left(\frac{\exp(\mathrm{i}\omega\delta\sigma)-1}{\mathrm{i}\omega\delta} - \sigma - \frac{\sigma^2}{2}\big(\exp(\mathrm{i}\omega\delta)-1\big)\right)$$

and

$$\begin{aligned}\widetilde{G}_{\omega,2}(\sigma) = \frac{1}{-\mathrm{i}\omega\delta}\Bigg(&\frac{\exp(\mathrm{i}\omega\delta(2-\sigma))-1}{-\mathrm{i}\omega\delta}\\ &- (\sigma-2)\exp(\mathrm{i}\omega\delta) + \frac{\sigma^2-2\sigma}{2}\big(\exp(\mathrm{i}\omega\delta)-1\big)\Bigg)\end{aligned}$$

are anti-derivatives of $G_{\omega,1}$ and $G_{\omega,2}$, respectively. Furthermore, we have

$$\widetilde{G}_{\omega,1}(0) = \widetilde{G}_{\omega,2}(2) = 0 \quad \text{and} \quad \widetilde{G}_{\omega,1}(1) = \widetilde{G}_{\omega,2}(1)\,.$$

Because

$$\left|\frac{\exp(\mathrm{i}\omega\delta\theta)-1}{\mathrm{i}\omega\delta}\right| = \left|\int_0^\theta \exp(\mathrm{i}\omega\delta\xi)\,\mathrm{d}\xi\right| \le |\theta|\ , \tag{3.19}$$

we obtain the estimates

$$\max_{\sigma\in[0,1]}\left|\omega\widetilde{G}_{\omega,1}(\sigma)\right| \le \frac{3}{\delta} \quad \text{and} \quad \max_{\sigma\in[1,2]}\left|\omega\widetilde{G}_{\omega,2}(\sigma)\right| \le \frac{3}{\delta}\,.$$

Then, splitting the integral and applying integration by parts twice yields

$$\begin{aligned}\left|\int_0^2 f(\varepsilon\sigma)g_\omega(\sigma)\ \mathrm{d}\sigma\right| &= \left|\int_0^1 f(\varepsilon\sigma)g_{\omega,1}(\sigma)\,\mathrm{d}\sigma + \int_1^2 f(\varepsilon\sigma)g_{\omega,2}(\sigma)\,\mathrm{d}\sigma\right|\\ &= \varepsilon\left|\int_0^1 f'(\varepsilon\sigma)G_{\omega,1}(\sigma)\,\mathrm{d}\sigma + \int_1^2 f'(\varepsilon\sigma)G_{\omega,2}(\sigma)\,\mathrm{d}\sigma\right|\\ &= \varepsilon^2\left|\int_0^1 f''(\varepsilon\sigma)\widetilde{G}_{\omega,1}(\sigma)\,\mathrm{d}\sigma + \int_1^2 f''(\varepsilon\sigma)\widetilde{G}_{\omega,2}(\sigma)\,\mathrm{d}\sigma\right|\\ &\le \frac{\varepsilon^2}{\delta}C\max_{\sigma\in[0,2]}\left|\omega^{-1}f''(\varepsilon\sigma)\right|\ .\end{aligned}$$

By definition (2.18) the function ϕ is 2-periodic, and hence we obtain

$$\left|\int_1^3 f(\varepsilon\sigma)g_\omega(\sigma)\ \mathrm{d}\sigma\right| = \left|\int_1^2 f(\varepsilon\sigma)g_{\omega,2}(\sigma)\,\mathrm{d}\sigma + \int_0^1 f\big(\varepsilon(\sigma+2)\big)g_{\omega,1}(\sigma)\,\mathrm{d}\sigma\right|\ .$$

Now, the inequality (iv) follows analogously via integration by parts and the anti-derivatives

$$\widehat{G}_{\omega,1}(\sigma) = \frac{1}{\mathrm{i}\omega\delta}\left(\frac{\exp(\mathrm{i}\omega\delta\sigma)-\exp(\mathrm{i}\omega\delta)}{\mathrm{i}\omega\delta} - (\sigma-1) - \frac{\sigma^2-1}{2}\big(\exp(\mathrm{i}\omega\delta)-1\big)\right)$$

and

$$\begin{aligned}\widehat{G}_{\omega,2}(\sigma) = \frac{1}{-\mathrm{i}\omega\delta}\Bigg(&\frac{\exp(\mathrm{i}\omega\delta(2-\sigma))-\exp(\mathrm{i}\omega\delta)}{-\mathrm{i}\omega\delta}\\ &- (\sigma-1)\exp(\mathrm{i}\omega\delta) + \frac{(\sigma-1)^2}{2}\big(\exp(\mathrm{i}\omega\delta)-1\big)\Bigg)\end{aligned}$$

of $G_{\omega,1}$ and $G_{\omega,2}$, respectively, with the properties

$$\widehat{G}_{\omega,1}(1) = \widehat{G}_{\omega,2}(1) = 0 \quad \text{and} \quad \widehat{G}_{\omega,1}(0) = \widetilde{G}_{\omega,2}(2)\,.$$

$\square$

Equipped with Lemma 4 we are now in a position to prove Theorem 3.

Proof of Theorem 3. Because we have

$$\int_0^1 \exp\big(\mathrm{i}\omega\delta\xi\big)\,\mathrm{d}\xi = \begin{cases} \frac{\exp(\mathrm{i}\omega\delta)-1}{\mathrm{i}\omega\delta} & \text{if} \quad \omega \neq 0\,, \\ 1 & \text{if} \quad \omega = 0\,, \end{cases} \tag{3.20}$$

for the integral in the limit system (3.9), it is convenient to distinguish $\omega = 0$ and $\omega \neq 0$, and thus to split the index set I_m into a "zero set" Z_m and a "non-zero set" N_m given by

$$Z_m = \big\{(j,k,l) \in I_m \mid \omega_{[jklm]} = 0\big\} \quad \text{and} \quad N_m = \big\{(j,k,l) \in I_m \mid \omega_{[jklm]} \neq 0\big\}\;.$$

Now, integrating (3.9) gives

$$v_m(t) = v_m(0) + \mathrm{i}\sum_{Z_m}\int_0^t V_{jkl}(s)\,\mathrm{d}s + \mathrm{i}\sum_{N_m}\frac{\exp(\mathrm{i}\omega_{[jklm]}\delta)-1}{\mathrm{i}\omega_{[jklm]}\delta}\int_0^t \widehat{V}_{jklm}(s)\,\mathrm{d}s\,. \tag{3.21}$$

Likewise, we obtain with (2.24)

$$y_m(t) = y_m(0) + \mathrm{i}\sum_{Z_m}\int_0^t Y_{jkl}(s)\,\mathrm{d}s + \mathrm{i}\sum_{N_m}\int_0^t \widehat{Y}_{jklm}(s)\exp\big(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\big)\,\mathrm{d}s\,. \tag{3.22}$$

If we now subtract (3.21) from (3.22), we arrive at

$$\begin{aligned} \|y(t)-v(t)\|_{\ell^1} \le \sum_{m\in\mathbb{Z}}\sum_{Z_m}\int_0^t |Y_{jkl}(s)-V_{jkl}(s)|\,\mathrm{d}s \\ + \sum_{m\in\mathbb{Z}}\sum_{N_m}\int_0^t \Big|\widehat{Y}_{jklm}(s)-\widehat{V}_{jklm}(s)\Big|\,\mathrm{d}s \\ + \sum_{m\in\mathbb{Z}}\sum_{N_m}\left|\int_0^t \widehat{V}_{jklm}(s) g_{\omega_{[jklm]}}\left(\tfrac{s}{\varepsilon}\right)\mathrm{d}s\right|\,, \end{aligned}$$

with $g_{\omega_{[jklm]}}$ defined in (3.15). Since

$$\begin{aligned} \Big|\widehat{Y}_{jklm}(s)-\widehat{V}_{jklm}(s)\Big| &= |Y_{jkl}(s)-V_{jkl}(s)| \\ &\le |y_j(s)-v_j(s)|\cdot|\bar{y}_k(s)|\cdot|y_l(s)| \\ &\quad + |v_j(s)|\cdot|\bar{y}_k(s)-\bar{v}_k(s)|\cdot|y_l(s)| \\ &\quad + |v_j(s)|\cdot|\bar{v}_k(s)|\cdot|y_l(s)-v_l(s)|\,, \end{aligned}$$

we obtain

$$\|y(t) - v(t)\|_{\ell^1} \leq C(M_0) \int_0^t \|y(s) - v(s)\|_{\ell^1} \, \mathrm{d}s + \sum_{m \in \mathbb{Z}} \sum_{N_m} \left| \int_0^t \widehat{V}_{jklm}(s) g_{\omega_{[jklm]}}\left(\tfrac{s}{\varepsilon}\right) \mathrm{d}s \right| . \tag{3.23}$$

In order to complete the proof of Theorem 3, we now deduce estimates for the second term in (3.23) under the assumptions of the settings (i) and (ii), respectively. Then, the two assertions follow from Gronwall's lemma.

First, we fix $t \in [0, T]$ and use the partition $t = (L + \theta)\varepsilon + t_\varepsilon$ with $L \in \mathbb{N}$ even, $\theta \in \{0, 1\}$ and $t_\varepsilon \in [0, \varepsilon)$ obtaining the decomposition

$$\int_0^t \widehat{V}_{jklm}(s) g_{\omega_{[jklm]}}\left(\tfrac{s}{\varepsilon}\right) \mathrm{d}s = T^{(1)}_{jklm} + T^{(2)}_{jklm} + T^{(3)}_{jklm} ,$$

with

$$T^{(1)}_{jklm} = \sum_{p=0}^{\frac{L}{2}-1} \int_{2\varepsilon p}^{2\varepsilon(p+1)} \widehat{V}_{jklm}(s) g_{\omega_{[jklm]}}\left(\tfrac{s}{\varepsilon}\right) \mathrm{d}s , \tag{3.24}$$

$$T^{(2)}_{jklm} = \int_{\varepsilon L}^{\varepsilon(L+\theta)} \widehat{V}_{jklm}(s) g_{\omega_{[jklm]}}\left(\tfrac{s}{\varepsilon}\right) \mathrm{d}s \tag{3.25}$$

and

$$T^{(3)}_{jklm} = \int_{\varepsilon(L+\theta)}^{\varepsilon(L+\theta)+t_\varepsilon} \widehat{V}_{jklm}(s) g_{\omega_{[jklm]}}\left(\tfrac{s}{\varepsilon}\right) \mathrm{d}s .$$

We conclude from (3.19) that $\left| g_{\omega_{[jklm]}}\left(\tfrac{s}{\varepsilon}\right) \right| \leq 2$ and because $\left| \widehat{V}_{jklm}(s) \right| = |V_{jkl}(s)|$, we immediately obtain

$$\sum_{m \in \mathbb{Z}} \sum_{N_m} \left| T^{(2)}_{jklm} \right| \leq \varepsilon C(M_0) \quad \text{and} \quad \sum_{m \in \mathbb{Z}} \sum_{N_m} \left| T^{(3)}_{jklm} \right| \leq \varepsilon C(M_0) .$$

Moreover, if we substitute $\sigma = s/\varepsilon$ in each summand of (3.24) and apply part (i) and (ii) of Lemma 4, we get the estimate

$$\sum_{m \in \mathbb{Z}} \sum_{N_m} \left| T^{(1)}_{jklm} \right| \leq \frac{\varepsilon}{\delta} t C \max_{s \in [0,t]} \sum_{m \in \mathbb{Z}} \sum_{N_m} \left| \omega^{-1}_{[jklm]} \widehat{V}'_{jklm}(s) \right| .$$

Since $0 \leq |\omega^{-1}_{[jklm]}| \leq 1$ for $m \in \mathbb{Z}$ and $(j, k, l) \in N_m$, we have

$$\left| \omega^{-1}_{[jklm]} \widehat{V}'_{jklm}(s) \right| \leq \left| V'_{jkl}(s) \right| + \alpha \left| V_{jkl}(s) \right| , \tag{3.26}$$

and hence Lemma 21 (Appendix A) implies

$$\sum_{m \in \mathbb{Z}} \sum_{N_m} \left| \int_0^t \widehat{V}_{jklm}(s) g_{\omega_{[jklm]}}\left(\tfrac{s}{\varepsilon}\right) \mathrm{d}s \right| \leq \varepsilon \left(1 + \tfrac{1+\alpha}{\delta} t\right) C(M_0) . \tag{3.27}$$

Now, combining (3.23) with (3.27) results in

$$\|y(t)-v(t)\|_{\ell^1} \leq C(M_0)\int_0^t \|y(s)-v(s)\|_{\ell^1}\,\mathrm{d}s + \varepsilon\left(1+\tfrac{1+\alpha}{\delta}t\right)C(M_0)$$

and Gronwall's lemma yields part (i) of Theorem 3.

We attain part (ii) by improving the estimate (3.27). Since now t_k is a multiple of ε, we have $t_k = (L+\theta)\varepsilon$ with $L \in \mathbb{N}$ even, $\theta \in \{0,1\}$, and hence

$$\int_0^{t_k} \widehat{V}_{jklm}(s) g_{\omega_{[jklm]}}\left(\tfrac{s}{\varepsilon}\right)\mathrm{d}s = T^{(1)}_{jklm} + T^{(2)}_{jklm}\,,$$

with $T^{(1)}_{jklm}$ and $T^{(2)}_{jklm}$ given in (3.24) and (3.25). After substituting $\sigma = s/\varepsilon$, part (iii) of Lemma 4 yields the estimate

$$\sum_{m\in\mathbb{Z}}\sum_{N_m}\left|T^{(1)}_{jklm}\right| \leq \frac{\varepsilon^2}{\delta}t_k C \max_{s\in[0,t_k]}\sum_{m\in\mathbb{Z}}\sum_{N_m}\left|\omega^{-1}_{[jklm]}\widehat{V}''_{jklm}(s)\right|$$

and part (i) of Lemma 4 yields

$$\sum_{m\in\mathbb{Z}}\sum_{N_m}\left|T^{(2)}_{jklm}\right| \leq \frac{\varepsilon^2}{\delta}t_k C \max_{s\in[0,t_k]}\sum_{m\in\mathbb{Z}}\sum_{N_m}\left|\omega^{-1}_{[jklm]}\widehat{V}'_{jklm}(s)\right|\,.$$

Combining (3.26) and

$$\left|\omega^{-1}_{[jklm]}\widehat{V}''_{jklm}(s)\right| \leq \left|V''_{jkl}(s)\right| + 2\alpha\left|V'_{jkl}(s)\right| + \alpha^2\left|\omega_{[jklm]}V_{jkl}(s)\right|$$

with Lemma 21 (Appendix A) leads to the improved estimate

$$\sum_{m\in\mathbb{Z}}\sum_{N_m}\left|\int_0^{t_k}\widehat{V}_{jklm}(s) g_{\omega_{[jklm]}}\left(\tfrac{s}{\varepsilon}\right)\mathrm{d}s\right| \leq \frac{\varepsilon^2}{\delta}t_k\Big((1+\alpha)C(M_0)+(\alpha+\alpha^2)C(M_2)\Big)\,. \tag{3.28}$$

Now, part (ii) of Theorem 3 follows by inserting (3.28) into (3.23) and applying Gronwall's lemma. In particular, we observe that for $\alpha = 0$ the estimate improves as specified.

□

CHAPTER 4

The adiabatic Euler method

In this chapter, we commence constructing novel numerical methods for the DMNLS whose accuracy is not fixed by the value ε and whose accuracy improves reliably if the step-size is decreased, cf. Section 2.3. One essential idea is not to approximate solutions of the DMNLS directly; instead, we use the tDMNLS as an equivalent formulation of the problem. Our approach extends techniques from [38,39] and is introduced in Section 4.1 to obtain a first-order method – the adiabatic Euler method. First-order methods are certainly not satisfactory to approximate solutions of the DMNLS, however, studying first-order methods permits valuable insight for the construction and the analysis of more elaborate methods. We state our results regarding the analysis of the adiabatic Euler method and illustrate the behavior of the method by numerical examples in Section 4.2. The proof of the error bound is postponed to Section 4.3.

4.1. Construction

Let $t_n = n\tau$ with $n \in \mathbb{N}$ and step-size $\tau > 0$. Taking the integral from t_n to t_{n+1} of the tDMNLS (2.24) yields

$$y_m(t_{n+1}) = y_m(t_n) + \mathrm{i} \sum_{I_m} \int_{t_n}^{t_{n+1}} \widehat{Y}_{jklm}(s) \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,, \quad m \in \mathbb{Z}\,. \quad (4.1)$$

The integral in (4.1) is highly oscillatory such that it is essential not to approximate it naively by a quadrature formula. The key idea of our approach is to retain the integral over the highly oscillatory phases and solely fix non-oscillatory terms at $s = t_n$. However, we can choose either to fix the term $\exp(-\mathrm{i}\omega_{[jklm]}\alpha s)$ along with the term $Y_{jkl}(s)$ or to retain the term inside the integral. This results in two different variants of the adiabatic Euler method which both yield approximations $y_m^{(n)} \approx y_m(t_n)$ to solutions of the tDMNLS:

the ϕ-variant

$$y_m^{(n+1)} = y_m^{(n)} + \mathrm{i} \sum_{I_m} \widehat{Y}_{jklm}^{(n)} \int_{t_n}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,, \tag{4.2}$$

the $\widehat{\phi}$-variant

$$y_m^{(n+1)} = y_m^{(n)} + \mathrm{i} \sum_{I_m} Y_{jkl}^{(n)} \int_{t_n}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,. \tag{4.3}$$

Here, we abbreviate

$$Y_{jkl}^{(n)} = y_j^{(n)} \overline{y}_k^{(n)} y_l^{(n)} \quad \text{and} \quad \widehat{Y}_{jklm}^{(n)} = Y_{jkl}^{(n)} \exp(-\mathrm{i}\omega_{[jklm]} t_n \alpha)\,. \tag{4.4}$$

In the ϕ-variant the entire term $\widehat{Y}_{jklm}(s)$ is fixed at $s = t_n$, whereas the term $\exp(-\mathrm{i}\omega_{[jklm]}\alpha s)$ is kept inside the integral in the $\widehat{\phi}$-variant. The remaining integral in both methods can be computed exactly in each time-step by suitably decomposing the integral at multiples of ε.

In the following, we show how to compute the integral of the $\widehat{\phi}$-variant because the integral of the ϕ-variant can be treated alike with $\alpha = 0$. The computation follows a recurring principle: because there is no explicit formula for the integrand due to the piecewise defined function χ, given in (1.3), we split the integration interval at integer multiples of ε obtaining sub-intervals of length ε and two smaller remainder intervals. If we distinguish odd and even multiples of ε, the definition (2.18) yields an explicit formula for the integrand on each sub-interval. Hence, we can compute all sub-integrals exactly and then obtain the entire integral by adding up.

We choose $\kappa_1, \kappa_2 \in \mathbb{N}$ with $\kappa_2 \geq \kappa_1$ such that $(\varepsilon\kappa_1 - t_n) \in [0, \varepsilon)$ and $(t_{n+1} - \varepsilon\kappa_2) \in [0, \varepsilon)$. Then, we partition

$$\int_{t_n}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s = T_1 + T_2 + T_3\,, \tag{4.5}$$

with

$$\begin{aligned}
T_1 &= \int_{t_n}^{\varepsilon\kappa_1} \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,, \\
T_2 &= \sum_{p=\kappa_1}^{\kappa_2-1} \int_{p\varepsilon}^{(p+1)\varepsilon} \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,, \\
T_3 &= \int_{\varepsilon\kappa_2}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,.
\end{aligned}$$

Now, we can compute all sub-integrals by substituting $\sigma = s/\varepsilon$ and using the following lemma. For convenience, we employ the abbreviation

$$E_\theta(z) \coloneqq \exp(-\mathrm{i}\omega\theta z) \quad \text{for} \quad \theta \in \{\alpha, \delta\}.$$

Lemma 5. *Let $\omega \neq 0$ and $a \in [\kappa, \kappa+1]$, $b \in [\kappa, \kappa+1]$ for some $\kappa \in \mathbb{N}$.*

(i) If κ is even, then

$$\int_a^b \exp\Big(-\mathrm{i}\omega\widehat{\phi}(\sigma)\Big)\,\mathrm{d}\sigma = \frac{E_\alpha(\varepsilon b)E_\delta(\kappa - b) - E_\alpha(\varepsilon a)E_\delta(\kappa - a)}{-\mathrm{i}\omega(\alpha\varepsilon - \delta)}\,.$$

(ii) If κ is odd, then

$$\int_a^b \exp\Big(-\mathrm{i}\omega\widehat{\phi}(\sigma)\Big)\,\mathrm{d}\sigma = \frac{E_\alpha(\varepsilon b)E_\delta(b - \kappa - 1) - E_\alpha(\varepsilon a)E_\delta(a - \kappa - 1)}{-\mathrm{i}\omega(\alpha\varepsilon + \delta)}\,.$$

Proof. By definition (2.18), we have

$$\widehat{\phi}(z) = \begin{cases} -\delta(z-\kappa) + \alpha\varepsilon z & \text{if} \quad z \in [\kappa, \kappa+1)\,, \quad \kappa \text{ even}\,, \\ \delta\big(z - (\kappa+1)\big) + \alpha\varepsilon z & \text{if} \quad z \in [\kappa, \kappa+1)\,, \quad \kappa \text{ odd}\,. \end{cases}$$

Hence, we obtain for even κ

$$\int_a^b \exp\Big(-\mathrm{i}\omega\widehat{\phi}(\sigma)\Big)\,\mathrm{d}\sigma = \int_{a-\kappa}^{b-\kappa} E_\alpha\big(\varepsilon(\sigma+\kappa)\big)E_\delta(-\sigma)\,\mathrm{d}\sigma\,.$$

Applying the integration by parts formula gives

$$\begin{aligned}\int_{a-\kappa}^{b-\kappa} E_\alpha\big(\varepsilon(\sigma+\kappa)\big)E_\delta(-\sigma)\,\mathrm{d}\sigma &= (\mathrm{i}\omega\delta)^{-1}\big(E_\alpha(\varepsilon b)E_\delta(\kappa - b) - E_\alpha(\varepsilon a)E_\delta(\kappa - a)\big) \\ &\quad + \frac{\alpha\varepsilon}{\delta}\int_{a-\kappa}^{b-\kappa} E_\alpha\big(\varepsilon(\sigma+\kappa)\big)E_\delta(-\sigma)\,\mathrm{d}\sigma\,. \end{aligned} \tag{4.6}$$

Now, the desired integral stands on both sides of the equation (4.6), and hence rearranging the terms combined with the relation

$$\Big(1 - \frac{\alpha\varepsilon}{\delta}\Big)^{-1}(\mathrm{i}\omega\delta)^{-1} = \big(-\mathrm{i}\omega(\alpha\varepsilon - \delta)\big)^{-1}$$

yields the assertion (i). Equation (ii) follows analogously. □

Clearly, the decomposition (4.5) combined with repeated application of Lemma 5 allows us to compute the integrals appearing in both variants, (4.2) and (4.3), of the adiabatic Euler method exactly. However, there is a considerable difference between both methods in implementing this computation due to the fact that the integrand in the ϕ-variant is periodic: if $\alpha = 0$, then Lemma 5 yields

$$\int_p^{p+1} \exp\left(-\mathrm{i}\omega\phi(\sigma)\right) \mathrm{d}\sigma = \frac{\exp(\mathrm{i}\omega\delta) - 1}{\mathrm{i}\omega\delta} \quad \text{for} \quad p \in \mathbb{N}\,, \tag{4.7}$$

and hence

$$T_2 = \varepsilon \sum_{p=\kappa_1}^{\kappa_2 - 1} \int_p^{p+1} \exp\left(-\mathrm{i}\omega\phi(\sigma)\right) \mathrm{d}\sigma = \varepsilon(\kappa_2 - \kappa_1) \frac{\exp(\mathrm{i}\omega\delta) - 1}{\mathrm{i}\omega\delta}\,.$$

Thus, the periodicity of the integrand in (4.2) allows us to compute the integral with constant complexity. In contrast, the value of each sub-integral in method (4.3) changes on each sub-interval. Since the number of sub-integrals grows for increasing step-sizes τ, this implies additional computational costs if τ is large compared to ε. We investigate this observation in the course of numerical experiments presented in Section 4.2.1.

4.2. Properties: accuracy and relation to the limit system

In the next theorem, we state first-order convergence of the adiabatic Euler method with a constant independent of ε.

Theorem 6. *The global error of the adiabatic Euler method applied to the tDMNLS* (2.24) *satisfies the following bounds.*

(i) If $y_0 \in \ell^2_3$, then the global error of the ϕ-variant (4.2) *is bounded by*

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \leq \tau\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,, \quad \tau n \leq T\,,$$

for sufficiently small step-sizes τ.

(ii) If $y_0 \in \ell^2_1$, then the global error of the $\widehat{\phi}$-variant (4.3) *is bounded by*

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \leq \tau C(T, M_0^y)\,, \quad \tau n \leq T\,,$$

for sufficiently small step-sizes τ.

Theorem 6 is proven in Section 4.3.

Remark. We require "sufficiently small step-sizes" in Theorem 6 and in all subsequent theorems concerning the accuracy of our numerical methods because we rely on a standard bootstrap-type argument (cf. [15,18,20,25,31]) in order to ensure the boundedness of the numerical solution in ℓ^1. This argument is given in detail in Appendix B and we will point out where it enters our respective error analysis at the appropriate place. We emphasize that step-size restrictions in this vein are not a characteristic property of the DMNLS nor specific for the introduced methods in this thesis. Moreover, we report that we did not encounter any stability problems with "large" step-sizes in our numerical experiments.

Theorem 6 states first-order convergence independently of ε for both variants of the adiabatic Euler method. However, we require different levels of regularity for the initial value y_0. In summary, we observe that fixing the term $\exp(-\mathrm{i}\omega_{[jklm]}\alpha s)$ in the ϕ-variant yields, on the one hand, a periodic integrand allowing us to compute the arising integrals efficiently, see (4.7). On the downside, we require higher regularity for the initial value compared to the $\widehat{\phi}$-variant for first-order convergence. We illustrate the behavior of the adiabatic Euler method in the numerical experiments presented in Section 4.2.1.

Because the tDMNLS (2.24) converges to the limit system (3.9) for $\varepsilon \to 0$ (see Theorem 3) it is natural to investigate the behavior of the adiabatic Euler method in the same limit. The next lemma connects the adiabatic Euler method applied to the tDMNLS and the standard explicit Euler method applied to the limit system.

Lemma 7. *Let $a, b \in \mathbb{R}$ with $b > a$. We have*

$$\lim_{\varepsilon \to 0} \int_a^b \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s = (b-a) \int_0^1 \exp\left(\mathrm{i}\omega\delta\xi\right) \mathrm{d}\xi \,.$$

Proof. Considering the partition $a = \kappa_1\varepsilon - r_1^*$ and $b = \kappa_2\varepsilon + r_2^*$ with $\kappa_1, \kappa_2 \in \mathbb{N}$ and $r_1^*, r_2^* \in [0, \varepsilon)$ yields the decomposition

$$\lim_{\varepsilon \to 0} \int_a^b \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s = T_1 + T_2 + T_3 \,,$$

with

$$T_1 = \int_{\kappa_1\varepsilon - r_1^*}^{\kappa_1\varepsilon} \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \,, \qquad T_2 = \int_{\kappa_1\varepsilon}^{\kappa_2\varepsilon} \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \,,$$

$$T_3 = \int_{\kappa_2\varepsilon}^{\kappa_2\varepsilon + r_2^*} \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \,.$$

Because $|T_1| \leq \varepsilon$ and $|T_3| \leq \varepsilon$, we have $\lim_{\varepsilon\to 0} T_1 = 0$ and $\lim_{\varepsilon \to 0} T_3 = 0$, respectively. Moreover, the relation (4.7) implies

$$T_2 = \varepsilon(\kappa_2 - \kappa_1) \int_0^1 \exp\left(\mathrm{i}\omega\delta\xi\right) \mathrm{d}\xi = (b - r_2^* - a + r_1^*) \int_0^1 \exp\left(\mathrm{i}\omega\delta\xi\right) \mathrm{d}\xi$$

and passing to the limit $\varepsilon \to 0$ completes the proof. □

Consequently, we infer from Lemma 7 that for fixed τ the ϕ-variant (4.2) of the adiabatic Euler method applied to the tDMNLS reduces in the limit $\varepsilon \to 0$ to the standard explicit Euler method

$$v_m^{(n+1)} = v_m^{(n)} + \tau \mathrm{i} \sum_{I_m} \widehat{V}_{jklm}^{(n)} \int_0^1 \exp\left(\mathrm{i}\omega_{[jklm]}\delta\xi\right) \mathrm{d}\xi$$

for the limit system.

Remark. One can show similarly to Lemma 7 that

$$\lim_{\varepsilon\to 0} \int_a^b \exp\left(-\mathrm{i}\omega\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s = \int_a^b \exp\left(-\mathrm{i}\omega\alpha s\right) \mathrm{d}s \int_0^1 \exp\left(\mathrm{i}\omega\delta\xi\right) \mathrm{d}\xi\,,$$

and hence the $\widehat{\phi}$-variant (4.3) of the adiabatic Euler method reduces in the limit $\varepsilon \to 0$ to the method

$$v_m^{(n+1)} = v_m^{(n)} + \mathrm{i} \sum_{I_m} V_{jkl}^{(n)} \int_{t_n}^{t_{n+1}} \exp\left(-\mathrm{i}\omega\alpha s\right) \mathrm{d}s \int_0^1 \exp\left(\mathrm{i}\omega_{[jklm]}\delta\xi\right) \mathrm{d}\xi$$

for the limit system.

4.2.1. Numerical experiments

In the following, we illustrate the behavior of the adiabatic Euler method by numerical examples. We consider the tDMNLS with $\alpha = 0.1$, $\delta = 1$ and $T = 1$ with initial value[1] $u_0(x) = e^{-3x^2} e^{3\mathrm{i}x}$ and 64 equidistant grid points in the interval $[-\pi, \pi]$ for $\varepsilon = 0.01, 0.005, 0.002$. To this setting we apply both variants, (4.2) and (4.3), of the adiabatic Euler method. The reference solution is computed by the Strang splitting method with a large number of steps ($\approx 10^6$).

Figure 4.1 shows the accuracy of the ϕ-variant (4.2) and the $\widehat{\phi}$-variant (4.3) of the adiabatic Euler method for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). In addition, the accuracy of the Strang splitting method is shown for comparison. The dashed blue line is a reference line for order one, and the black vertical line highlights the value $\tau = \varepsilon$. First, we observe the familiar erratic behavior of the Strang splitting method, see Section 2.3. In addition, we observe first-order convergence of the adiabatic Euler method in both variants in each panel of Figure 4.1, i.e. convergence independently of ε as stated in Theorem 6.

Figure 4.2 shows the corresponding computation times of the ϕ-variant and the $\widehat{\phi}$-variant of the adiabatic Euler method. Again, the black vertical line highlights the value $\tau = \varepsilon$. We observe that the computation time of the ϕ-variant is independent

[1]The initial value is only approximately periodic, but this error can be neglected.

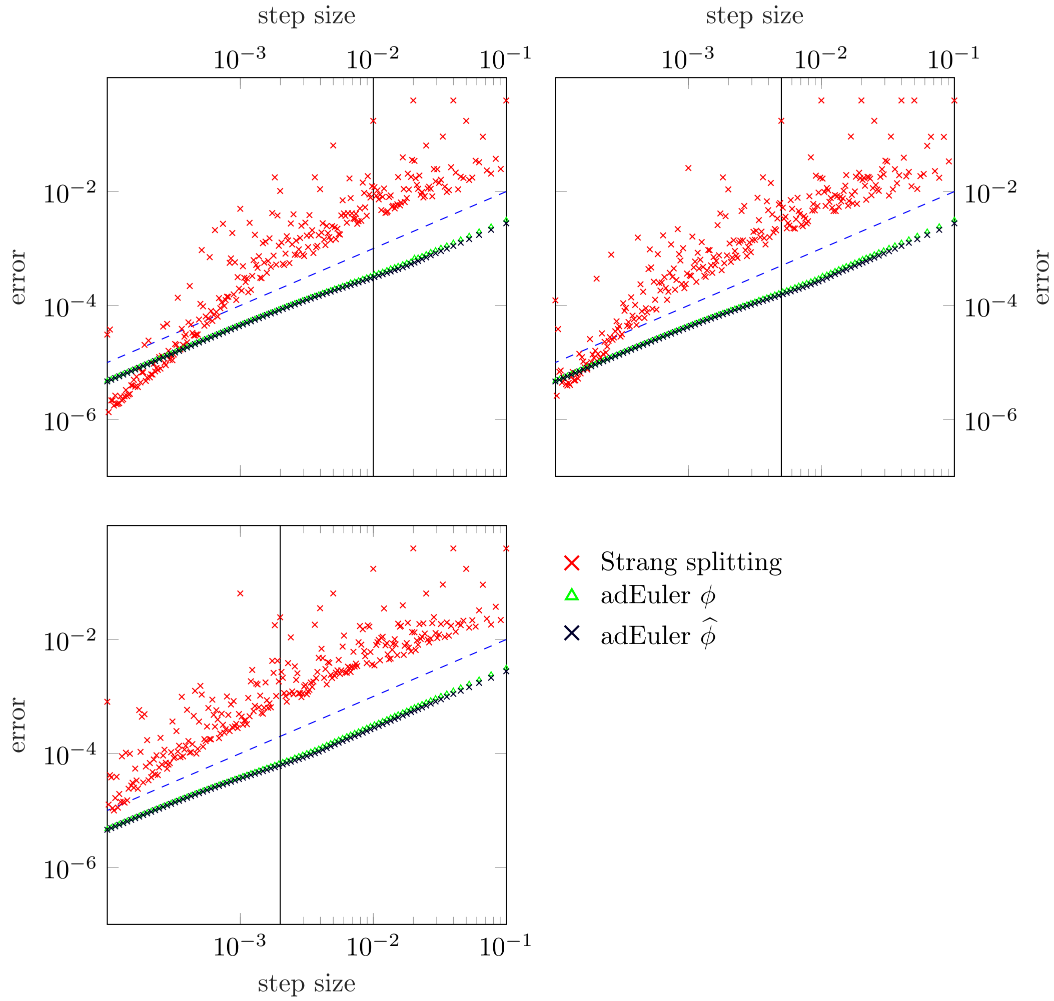

Figure 4.1: Maximal ℓ_0^2-error over time of both variants of the adiabatic Euler method for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). For comparison, the ℓ_0^2-error of the Strang splitting is shown. The dashed blue line is a reference line for order one and the black vertical line is at $\tau = \varepsilon$.

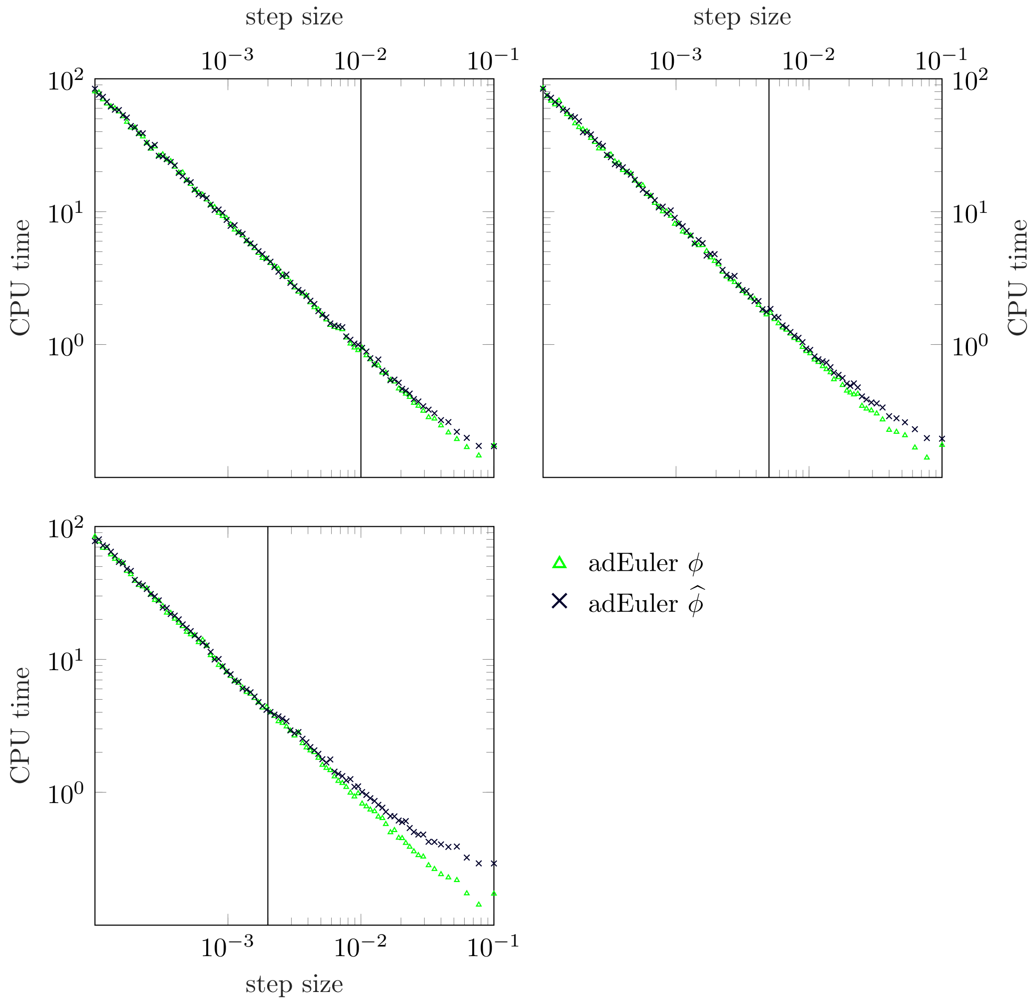

Figure 4.2: Computational time of the ϕ-variant and the $\widehat{\phi}$-variant of the adiabatic Euler method for various step-sizes and for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left).

of the value ε, whereas the computation time of the $\widehat{\phi}$-variant behaves differently. In the regime $\tau > \varepsilon$ (right of the black line), the computational time of the $\widehat{\phi}$-variant is larger than the computation time of the ϕ-variant in each panel. In the regime $\tau < \varepsilon$ (left of the black line), the computational times of the methods are almost identical. Moreover, we observe that decreasing the value of ε results in higher computational costs for the $\widehat{\phi}$-variant. This is because for large step-sizes τ (compared to the value of ε) the number of summands in T_2 in the decomposition (4.5) increases. This effect, in turn, increases the computation cost for the $\widehat{\phi}$-variant, whereas we can exploit the periodicity of the function ϕ in the ϕ-variant, see (4.7).

4.3. Proof of Theorem 6

In order to prove first-order convergence uniformly in ε for both variants, (4.2) and (4.3), of the adiabatic Euler method, we follow the classical concept of "stability and consistency yields convergence". Before we start with the proof, we make a few preparations. First, let

$$\Psi_\theta^n(z) = \big(\psi_{\theta,m}^n(z)\big)_{m\in\mathbb{Z}} \tag{4.8}$$

denote $n \in \mathbb{N}$ steps of the ϕ-variant of the adiabatic Euler method with step-size τ starting at time θ with initial data $z = (z_m)_{m\in\mathbb{Z}}$. If $n = 1$, we simply write $\Psi_\theta(z)$ instead of $\Psi_\theta^1(z)$. Moreover, for $k, n \in \mathbb{N}$ the relations

$$\Psi_\theta^0(z) = z \quad \text{and} \quad \Psi_{t_k}^n(z) = \Psi_{t_{n+k-1}}\Big(\Psi_{t_k}^{n-1}(z)\Big)$$

follow directly from the definition. Analogously, we define

$$\widehat{\Psi}_\theta^n(z) = \big(\widehat{\psi}_{\theta,m}^n(z)\big)_{m\in\mathbb{Z}}$$

for the $\widehat{\phi}$-variant.

Next, we state and prove two lemmas concerning the local error (consistency) and the stability of the adiabatic Euler method, respectively.

Lemma 8. *The local error the adiabatic Euler method applied to the tDMNLS* (2.24) *satisfies the following bounds.*

(i) If $y_0 \in \ell_3^2$, then the local error of the ϕ-variant (4.2) *is bounded by*

$$\big\|y(t_{n+1}) - \Psi_{t_n}\big(y(t_n)\big)\big\|_{\ell^1} \le \tau^2\big(C(M_0^y) + \alpha C(M_2^y)\big)\,, \quad n\tau \le T\,.$$

(ii) If $y_0 \in \ell_1^2$, then the local error of the $\widehat{\phi}$-variant (4.3) *is bounded by*

$$\Big\|y(t_{n+1}) - \widehat{\Psi}_{t_n}\big(y(t_n)\big)\Big\|_{\ell^1} \le \tau^2 C(M_0^y)\,, \quad n\tau \le T\,.$$

Proof. Expanding the exact solution of the tDMNLS (4.1) yields

$$\begin{aligned} y_m(t_{n+1}) = y_m(t_n) + \mathrm{i}\sum_{I_m} \widehat{Y}_{jklm}(t_n) \int_{t_n}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \\ + \mathrm{i}\sum_{I_m} \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \widehat{Y}'_{jklm}(\sigma)\, \mathrm{d}\sigma \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,. \end{aligned} \tag{4.9}$$

Moreover, one step with method (4.2) starting at the exact value $y(t_n)$ reads

$$\Psi_{t_n}\big(y(t_n)\big) = y_m(t_n) + \mathrm{i}\sum_{I_m} \widehat{Y}_{jklm}(t_n) \int_{t_n}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,. \tag{4.10}$$

Hence, subtracting (4.10) from (4.9) yields

$$\left\|y(t_{n+1}) - \Psi_{t_n}\big(y(t_n)\big)\right\|_{\ell^1} \le \sum_{m\in\mathbb{Z}} \sum_{I_m} \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \left|\widehat{Y}'_{jklm}(\sigma)\right| \mathrm{d}\sigma\,.$$

Because of the estimate

$$\begin{aligned} \left|\widehat{Y}'_{jklm}(\sigma)\right| &= \left|\big(Y'_{jkl}(\sigma) - \mathrm{i}\omega_{[jklm]}\alpha Y_{jkl}(\sigma)\big) \exp(-\mathrm{i}\omega_{[jklm]}\sigma\alpha)\right| \\ &\le \left|Y'_{jkl}(\sigma)\right| + \alpha\left|\omega_{[jklm]}Y_{jkl}(\sigma)\right|\,, \end{aligned} \tag{4.11}$$

the bound (i) follows with Lemma 22 (Appendix A).

The estimate (ii) follows analogously if we subtract one step of method (4.3) with initial value $y(t_n)$ from the alternative expansion

$$\begin{aligned} y_m(t_{n+1}) = y_m(t_n) + \mathrm{i}\sum_{I_m} Y_{jkl}(t_n) \int_{t_n}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \\ + \mathrm{i}\sum_{I_m} \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} Y'_{jkl}(\sigma)\, \mathrm{d}\sigma \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \end{aligned}$$

of the exact solution. This yields

$$\left\|y(t_{n+1}) - \widehat{\Psi}_{t_n}\big(y(t_n)\big)\right\|_{\ell^1} \le \sum_{m\in\mathbb{Z}} \sum_{I_m} \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \left|Y'_{jkl}(\sigma)\right| \mathrm{d}\sigma$$

and the estimate (ii) follows with Lemma 22 (Appendix A). □

Remark. The different levels of regularity for the initial value y_0 required in the proof for both variants of the adiabatic Euler method originate from the fact that differentiating the function $\widehat{Y}_{jklm}(s)$ yields a summand with the factor $\omega_{[jklm]}$, see (4.11). This factor does not appear if we differentiate the function $Y_{jkl}(s)$.

The second lemma concerns the stability of the adiabatic Euler method.

Lemma 9. *For $\mu, \nu \in \ell^1$ with $M := \max\{\|\mu\|_{\ell^1}, \|\nu\|_{\ell^1}\}$ we have*

$$\|\Psi_{t_n}(\mu) - \Psi_{t_n}(\nu)\|_{\ell^1} \leq e^{\tau C(M)} \|\mu - \nu\|_{\ell^1}$$

and

$$\left\|\widehat{\Psi}_{t_n}(\mu) - \widehat{\Psi}_{t_n}(\nu)\right\|_{\ell^1} \leq e^{\tau C(M)} \|\mu - \nu\|_{\ell^1} .$$

Proof. Inserting μ and ν in method (4.2) yields

$$\begin{aligned}\|\Psi_{t_n}(\mu) - \Psi_{t_n}(\nu)\|_{\ell^1} &\leq \sum_{m\in\mathbb{Z}} |\psi_{t_n,m}(\mu) - \psi_{t_n,m}(\nu)| \\ &\leq \sum_{m\in\mathbb{Z}} |\mu_m - \nu_m| + \tau \sum_{m\in\mathbb{Z}} \sum_{I_m} |\mu_j \overline{\mu}_k \mu_l - \nu_j \overline{\nu}_k \nu_l| .\end{aligned}$$

Because of the relation

$$\begin{aligned}|\mu_j \overline{\mu}_k \mu_l - \nu_j \overline{\nu}_k \nu_l| \leq{}& |\mu_j - \nu_j| \cdot |\overline{\mu}_k| \cdot |\mu_l| + |\nu_j| \cdot |\overline{\nu}_k - \overline{\nu}_k| \cdot |\mu_l| \\ &+ |\nu_j| \cdot |\overline{\nu}_k| \cdot |\mu_l - \nu_l| ,\end{aligned}$$

we obtain

$$\|\Psi_{t_n}(\mu) - \Psi_{t_n}(\nu)\|_{\ell^1} \leq \|\mu - \nu\|_{\ell^1} + 3\tau M^2 \|\mu - \nu\|_{\ell^1}$$

and with $(1 + x) \leq e^x$ the first estimate follows. Moreover, we have

$$\left|\widehat{\psi}_{t_n,m}(\mu) - \widehat{\psi}_{t_n,m}(\nu)\right| = |\psi_{t_n,m}(\mu) - \psi_{t_n,m}(\nu)| ,$$

and hence the second estimate follows analogously. □

With these preparations, we are now in a position to prove Theorem 6 by combining Lemma 9 and Lemma 8 with the classical telescoping sum argument of Lady Windermere's fan, see [30].

Proof of Theorem 6. We start by proving the first-order convergence of the ϕ-variant (4.2) of the adiabatic Euler method.

First, we establish the boundedness of the numerical scheme in ℓ^1. On the basis of Lemma 9 and Lemma 8 the ϕ-variant of the adiabatic Euler method fulfills the assumptions of Proposition 23 (Appendix B). Hence, we can choose, e.g., the constant $M_0^\star = 2M_0^y$ in order to obtain a step-size $\tau_0 = C(T, M_0^y, C_{loc})$, where C_{loc} is the constant from the local error bound in Lemma 8, such that for step-sizes $\tau \leq \tau_0$ we have

$$\left\|\Psi_{t_p}^n\big(y(t_p)\big)\right\|_{\ell^1} \leq M_0^\star = C(M_0^y) \quad \text{for all} \quad p \in \mathbb{N} , \quad t_{p+n} \leq T . \tag{4.12}$$

Now, the first-order convergence follows with the telescoping sum

$$\left\| y(t_n) - \Psi_0^n\big(y^{(0)}\big) \right\|_{\ell^1} \leq \sum_{k=0}^{n-1} \left\| \Psi_{t_{n-k}}^k\big(y(t_{n-k})\big) - \Psi_{t_{n-k-1}}^{k+1}\big(y(t_{n-k-1})\big) \right\|_{\ell^1} . \tag{4.13}$$

Thanks to the boundedness of the numerical solution (4.12), applying Lemma 9 repeatedly gives

$$\left\| y(t_n) - \Psi_0^n\big(y^{(0)}\big) \right\|_{\ell^1} \leq e^{TC(M_0^y)} \sum_{k=0}^{n-1} \left\| y(t_{n-k}) - \Psi_{t_{n-k-1}}\big(y(t_{n-k-1})\big) \right\|_{\ell^1} . \tag{4.14}$$

Finally, we obtain with Lemma 8 the estimate

$$\left\| y(t_n) - \Psi_0^n\big(y^{(0)}\big) \right\|_{\ell^1} \leq T e^{TC(M_0^y)} \big(C(M_0^y) + \alpha C(M_2^y) \big) \tau \, .$$

Analogously, we get

$$\left\| y(t_n) - \widehat{\Psi}_0^n\big(y^{(0)}\big) \right\|_{\ell^1} \leq T e^{TC(M_0^y)} C(M_0^y) \tau$$

for the $\widehat{\phi}$-variant of the adiabatic Euler method.

□

Remark. The boundedness of the numerical solution (4.12) is crucial for obtaining an uniform bound with respect to n in the estimate (4.14) with Lemma 9. Otherwise the constant from Lemma 9 changes in each application.

CHAPTER 5

The adiabatic midpoint rule

In Chapter 4, we have laid the foundation to construct numerical methods for the tDMNLS. Now, we aim for higher order methods using the same construction principles. Because evaluating the right-hand side of the tDMNLS is rather expensive due to the multiple sum structure, we restrict ourselves to one evaluation in each time-step. If we additionally require an explicit scheme, these specifications naturally lead us towards a two-step method based on the explicit midpoint rule. The resulting adiabatic midpoint rule is introduced in Section 5.1. Following the construction, we state and illustrate the results of our error analysis of the adiabatic midpoint rule in Section 5.2. This error analysis (Theorem 10 and Theorem 11) is the first main result in this thesis. It turns out that our approach does not give a "classical" second-order method. Instead, the error behavior is rather unique in the sense that we obtain various levels of accuracy for different choices of step-sizes. For a full understanding and a proof of this behavior, we deviate from the classical concept "stability and consistency yields convergence" and thoroughly investigate the highly oscillatory error terms of the method in Section 5.3 and Section 5.4.

Remark. The results of this chapter (in particular Theorem 10) have been published to some extend with Prof. Dr. Tobias Jahnke in the preprint [40].

5.1. Construction

Integrating the tDMNLS from t_{n-1} to t_{n+1} gives

$$y_m(t_{n+1}) = y_m(t_{n-1}) + \mathrm{i} \sum_{I_m} \int_{t_{n-1}}^{t_{n+1}} \widehat{Y}_{jklm}(s) \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \,, \quad m \in \mathbb{Z} \,.$$

Similar to the construction of the adiabatic Euler method (cf. Section 4.1), we consider two options for approximating the remaining integral which gives rise to two different variants of the adiabatic midpoint rule:

the ϕ-variant

$$y_m^{(n+1)} = y_m^{(n-1)} + \mathrm{i} \sum_{I_m} \widehat{Y}_{jklm}^{(n)} \int_{t_{n-1}}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,, \tag{5.1}$$

the $\widehat{\phi}$-variant

$$y_m^{(n+1)} = y_m^{(n-1)} + \mathrm{i} \sum_{I_m} Y_{jkl}^{(n)} \int_{t_{n-1}}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,, \tag{5.2}$$

with $\widehat{Y}_{jklm}^{(n)}$ and $Y_{jkl}^{(n)}$ defined in (4.4).

The adiabatic midpoint rule is an explicit two-step scheme. As a starting step, we propose the $\widehat{\phi}$-variant of the adiabatic Euler method, i.e.

$$y_m^{(1)} = y_m^{(0)} + \mathrm{i} \sum_{I_m} Y_{jkl}^{(0)} \int_0^{\tau} \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,, \tag{5.3}$$

because it has lower regularity requirements than the ϕ-variant, see Theorem 6.

Similar to the adiabatic Euler method, one can compute the remaining integrals in the methods (5.1) and (5.2) exactly by Lemma 5 via a suitable decomposition of the integrals at multiples of ε, cf. (4.5). Again, the periodic integrand in the ϕ-variant allows us to compute the integral with constant complexity with respect to ε, cf. Section 4.1.

5.2. Properties: relation to the limit system and accuracy

As a first property of the adiabatic midpoint rule, we observe that by Lemma 7 the ϕ-variant (5.1) reduces in the limit $\varepsilon \to 0$ to the standard explicit midpoint rule

$$v_m^{(n+1)} = v_m^{(n-1)} + 2\tau\mathrm{i} \sum_{I_m} \widehat{V}_{jklm}^{(n)} \int_0^1 \exp(\mathrm{i}\omega_{[jklm]}\delta\xi)\, \mathrm{d}\xi$$

for the limit system. Furthermore, there is an additional relation to the limit system for *fixed* ε. If we choose step-sizes $\tau = k\varepsilon$ for some $k \in \mathbb{N}$, then the integral in (5.1) simplifies to

$$\int_{t_{n-1}}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s = 2\tau \int_0^1 \exp\left(\mathrm{i}\omega_{[jklm]}\delta\xi\right) \mathrm{d}\xi\,,$$

cf. Lemma 5 (with $\alpha = 0$), see also (4.7). In this case the ϕ-variant of the adiabatic midpoint rule (5.1) reads

$$y_m^{(n+1)} = y_m^{(n-1)} + 2\tau\mathrm{i} \sum_{I_m} \widehat{Y}_{jklm}^{(n)} \int_0^1 \exp\left(\mathrm{i}\omega_{[jklm]}\delta\xi\right) \mathrm{d}\xi\,. \tag{5.4}$$

Hence, the method can be interpreted as the classical explicit midpoint rule applied to the limit system (3.9), i.e. $y_m^{(n)} \approx v_m(t_n)$. This results in an advantageous error behavior for these specific step-sizes.

Remark. Similarly, the adiabatic Euler method (4.2) reduces to the standard explicit Euler method for fixed ε and step-sizes $\tau = k\varepsilon$ for $k \in \mathbb{N}$. However, in this case there is no particular advantage concerning the error behavior.

As a whole, the error behavior of the adiabatic midpoint rule is rather complex. In contrast to the "classical" error behavior of the explicit midpoint rule, we do not obtain second-order convergence for arbitrary step-sizes. Instead, we get first-order convergence, although with a constant independent of ε. Moreover, in addition to the beneficial connection to the limit system there is another special feature of the adiabatic midpoint rule: the accuracy of the method improves by a factor of ε for step-sizes τ that are integer fractions of ε.

The following two theorems contain the results of our error analysis of the adiabatic midpoint rule, they constitute the first main result in this thesis. In the first theorem, we state the error behavior of the ϕ-variant (5.1).

Theorem 10. *Let $y^{(n)}$ be the approximations of the tDMNLS* (2.24) *with the ϕ-variant of the adiabatic midpoint rule* (5.1). *Then, the global error satisfies the following bounds.*

(i) If $y_0 \in \ell^2_3$, then we have

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \le \tau \big(C(T, M_0^y) + \alpha C(T, M_2^y) \big) , \quad \tau n \le T,$$

for sufficiently small step-sizes τ.

(ii) If $y_0 \in \ell^2_5$ and if we choose step-sizes $\tau = \varepsilon / k$ for some $k \in \mathbb{N}$, then we have

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \le \varepsilon\tau \big(C(T, M_0^y) + \alpha C(T, M_2^y) + \alpha^2 C(T, M_4^y) \big) , \quad \tau n \le T,$$

for sufficiently small step-sizes τ.

(iii) Suppose that Assumption 1 holds. If $y_0 \in \ell^2_5$ and if we choose step-sizes $\tau = \varepsilon k$ for some $k \in \mathbb{N}$, then we have

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \le \big(\tfrac{\varepsilon^2}{\delta} + \tau^2 \big) C(T, \alpha, M_0, M_2, M_4) , \quad \tau n \le T,$$

for sufficiently small step-sizes τ. In case of $\alpha = 0$ the constant depends only on T and M_0.

Theorem 10 is proven in Section 5.3.

For the $\widehat{\phi}$-variant (5.2) of the adiabatic midpoint rule, we obtain a corresponding theorem for the accuracy of the method. It turns out that the special step-sizes – integer multiples and integer fractions of ε – again lead to an improved accuracy. As for the adiabatic Euler method, the $\widehat{\phi}$-variant of the adiabatic midpoint rule requires lower regularity for the initial value y_0, cf. Theorem 6. This benefit is again accompanied by higher computational costs due to the more expansive evaluations of the remaining integral in the scheme, cf. Section 4.1.

Theorem 11. *Let $y^{(n)}$ be the approximations of the tDMNLS* (2.24) *with the $\widehat{\phi}$-variant of the adiabatic midpoint rule* (5.2)*. Then, the global error satisfies the following bounds.*

(i) If $y_0 \in \ell^2_1$, then we have

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \leq \tau C(T, M_0^y)\,, \quad \tau n \leq T,$$

for sufficiently small step-sizes τ.

(ii) If $y_0 \in \ell^2_3$ and if we choose step-sizes $\tau = \varepsilon/k$ for some $k \in \mathbb{N}$, then we have

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \leq \varepsilon\tau\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,, \quad \tau n \leq T,$$

for sufficiently small step-sizes τ.

(iii) Suppose that Assumption 1 holds. If $y_0 \in \ell^2_3$ and if we choose step-sizes $\tau = \varepsilon k$ for some $k \in \mathbb{N}$, then we have

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \leq \big(\tfrac{\varepsilon^2}{\delta} + \tau^2\big) C(T, \alpha, M_0, M_2)\,, \quad \tau n \leq T,$$

for sufficiently small step-sizes τ. In case of $\alpha = 0$ the constant depends only on T and M_0.

Theorem 11 is proven in Section 5.4.

In the following, we demonstrate the assertions of Theorem 10 and Theorem 11 by a numerical example. We consider the tDMNLS with $\alpha = 0.1$, $T = 1$, $\delta = 1$, the initial value $u_0(x) = e^{-3x^2}e^{3ix}$ with 64 equidistant grid points in the interval $[-\pi, \pi]$ for $\varepsilon = 0.01$ and $\varepsilon = 0.002$. To either setting, we apply both variants, (5.1) and (5.2), of the adiabatic midpoint rule. The reference solution is computed by the Strang splitting method with a large number of steps ($> 10^6$).

The left panels of Figure 5.1 show the accuracy of the adiabatic midpoint rule for roughly logarithmically spread step-sizes τ. The dashed blue lines are reference lines

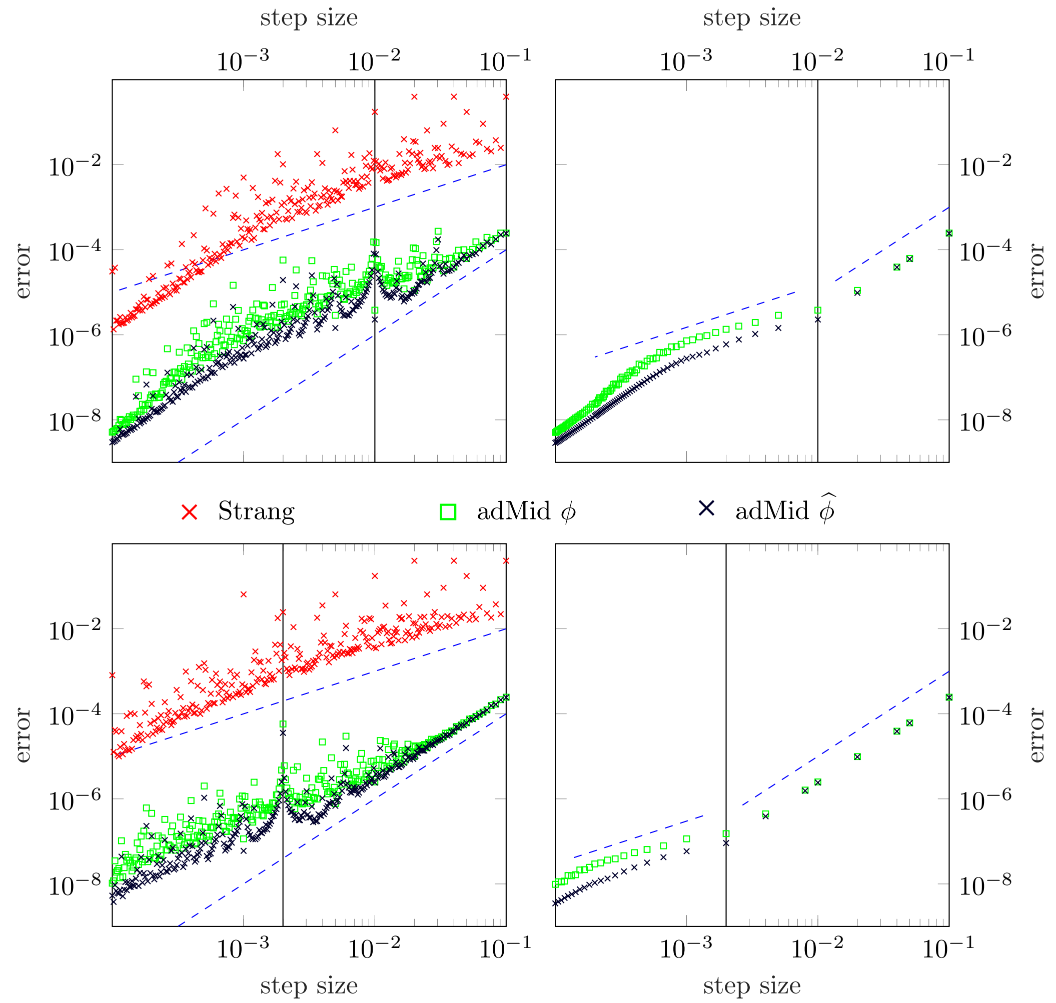

Figure 5.1: Maximal ℓ_0^2-error over time of the adiabatic midpoint rule in variants (5.1) and (5.2) for $\varepsilon = 0.01$ (top) and $\varepsilon = 0.002$ (bottom). In the left panels, the accuracy is shown for many different step-sizes τ, additionally, the accuracy of the Strang splitting is displayed as a reference. In the right panels only step-sizes that are integer multiples and integer fractions of ε are shown. The black vertical line is at $\tau = \varepsilon$

for order one and order two. The black vertical line highlights the value $\tau = \varepsilon$. Moreover, the accuracy of the Strang splitting method is shown. In this setting, the behavior of the adiabatic midpoint rule appears to be as erratic as the behavior of the Strang splitting method, i.e. small changes of the step-size can change the error by a factor of 10 to 100. Even though the adiabatic midpoint rule appears to be "better than order one for many step-sizes" several outliers stipulate first-order convergence as claimed in Theorem 10 and 11 part (i).

The right panels of Figure 5.1 display solely the error of the adiabatic midpoint rule for step-sizes chosen according to part (ii) and (iii) of Theorem 10 and 11, i.e. step-sizes that are integer multiples and integer fractions of ε. Here, the dashed blue lines are references for $\mathcal{O}(\tau^2)$ and $\mathcal{O}(\tau\varepsilon)$. We observe second-order accuracy in the regime $\tau > \varepsilon$ (right of the black line) and an accuracy in $\mathcal{O}(\tau\varepsilon)$ for $\tau < \varepsilon$ (left of the black line) as stated in part (ii) and (iii) of Theorem 10 and Theorem 11, respectively. Moreover, the numerical experiment suggests that the constant of the global error bound for the $\widehat{\phi}$-variant of the adiabatic midpoint rule is smaller than the corresponding constant of the ϕ-variant. Hence, the periodic integral in the ϕ-variant of the adiabatic midpoint rule, and thus the reduced computational time, appears to come at a cost of a slightly larger error constant in the global error bound.

Remark. In the top right panel of Figure 5.1, we even observe second-order accuracy for very small step-sizes τ suggesting that at some point the step-size τ is small enough such that the method resolves the oscillations produced by $\phi\left(\frac{s}{\varepsilon}\right)$ and $\widehat{\phi}\left(\frac{s}{\varepsilon}\right)$, respectively, and the "classical" second-order of the standard explicit midpoint rule is reflected. Although this behavior is somewhat expected, it is unclear[1] how to prove that the accuracy of the method increases after a certain threshold for the step-size. This is because higher order time derivatives of the solution y of the tDMNLS do not exist due to the discontinuous coefficient function γ.

Conclusion. The previous theorems and observations show that approximating solutions of the tDMNLS by the adiabatic midpoint rule with step-sizes $\tau = k\varepsilon$ provides an accuracy of $\mathcal{O}(\tau^2)$. This is the same level of accuracy that one can obtain by the standard explicit midpoint rule applied to the limit system, see Chapter 3. However, if a better accuracy than $\mathcal{O}(\varepsilon^2)$ is desired, one can use the adiabatic midpoint rule with the special step-size $\tau = \varepsilon/k$ for some $k \in \mathbb{N}$. This gives an accuracy of $\mathcal{O}(\tau\varepsilon) = \mathcal{O}(\varepsilon^2/k)$, whereas such step-sizes only lead to an accuracy of $\mathcal{O}(\varepsilon)$ in the case of the standard explicit midpoint rule applied to the limit system. In this sense,

[1] In this context, the term "unclear" as usual stands for "unknown to the author".

the adiabatic midpoint rule provides reliable approximations of the tDMNLS in any desired accuracy.

Approximations of the tDMNLS with the adiabatic midpoint rule are usually limited to discretization points t_n that are integer multiples or integer fractions of ε. However, this is not a severe restriction because approximations at other times $t \in (t_n, t_{n+1})$ can be obtained by subsequent time integration in the small time interval (t_n, t) as, e.g., in the case of the stroboscopic averaging method, cf. [13], or simply by interpolation. A final appraisal of the method requires further investigations in terms of computational cost versus accuracy. We will address this issue to some extend in Section 9.2.

5.3. Proof of Theorem 10

In order to proof Theorem 10, we reformulate the two-step method (5.1) as a one-step method. First, we define

$$\left\{A\left(t, \tfrac{s}{\varepsilon}, \mu\right) z\right\}_m = \mathrm{i} \sum_{I_m} \mu_j \bar{\mu}_k z_l \exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha t + \phi\left(\tfrac{s}{\varepsilon}\right))\right) \tag{5.5}$$

for two sequences $\mu = (\mu_m)_{m\in\mathbb{Z}}$ and $z = (z_m)_{m\in\mathbb{Z}}$ in $\mathbb{C}$. Then, the two-step method (5.1) reads

$$y^{(n+1)} = y^{(n-1)} + \int_{t_{n-1}}^{t_{n+1}} A\left(t_n, \tfrac{s}{\varepsilon}, y^{(n)}\right) y^{(n)} \,\mathrm{d}s\,.$$

With the abbreviations

$$\mathbf{y}_{n+1} = \begin{pmatrix} y^{(n+1)} \\ y^{(n)} \end{pmatrix}, \quad \mathcal{J} = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \mathcal{M}_n = \begin{pmatrix} \int_{t_{n-1}}^{t_{n+1}} A\left(t_n, \tfrac{s}{\varepsilon}, y^{(n)}\right) \mathrm{d}s & 0 \\ 0 & 0 \end{pmatrix}, \tag{5.6}$$

we obtain the one-step formulation

$$\mathbf{y}_{n+1} = (\mathcal{J} + \mathcal{M}_n)\,\mathbf{y}_n \tag{5.7}$$

of the adiabatic midpoint rule (5.1).

One can use the one-step formulation (5.7) to show that the assumptions of Proposition 23 (Appendix B) are fulfilled. This implies that there is a constant $\tau_0 > 0$, depending only on T and on the exact solution y of the tDMNLS, such that for step-sizes $\tau \leq \tau_0$ the numerical solution $\mathbf{y}_n$ is bounded in ℓ_1 for all $\tau n \leq T$ with a constant depending only M_0^y. We omit the details of this assertion, because in contrast to the proof of Theorem 6 in Section 4.3, combining the assumptions of Proposition 23

(Appendix B) – stability and consistency – with a telescoping sum argument is not sufficient to prove Theorem 10. Hence, we solely state that for sufficiently small step-sizes, i.e. $\tau \leq \tau_0$, we have the bound

$$\left\| y^{(n)} \right\|_{\ell^1} \leq C(M_0^y) \quad \text{for all} \quad \tau n \leq T\,, \tag{5.8}$$

cf. (4.12). Estimate (5.8) is used frequently throughout the proof.

The foundation for the proof of Theorem 10 is an error recursion formula for the explicit midpoint rule from [37], which we adopt for the one-step formulation of the adiabatic midpoint rule (5.7). We define the error term

$$\mathbf{d}_{n+1} = \big(\mathcal{J} + \mathcal{M}_n\big)\mathbf{y}(t_n) - \mathbf{y}(t_{n+1})\,, \quad \text{with} \quad \mathbf{y}(t_{n+1}) = \begin{pmatrix} y(t_{n+1}) \\ y(t_n) \end{pmatrix}. \tag{5.9}$$

Then, the global error $\mathbf{e}_N = \mathbf{y}_N - \mathbf{y}(t_N)$ satisfies the following recursion formula; cf. [37].

Lemma 12. *With the abbreviations* (5.6) *and* (5.9) *the global error of method* (5.7) *is given by*

$$\mathbf{e}_{N+1} = \mathcal{J}^N \mathbf{e}_1 + \sum_{n=1}^{N} \mathcal{J}^{N-n} \mathcal{M}_n \mathbf{e}_n + \sum_{n=1}^{N} \mathcal{J}^{N-n} \mathbf{d}_{n+1}\,, \qquad N \geq 1\,.$$

Proof. The error recursion formula is proven by induction, see [37]. For $N = 1$ we have

$$\begin{aligned}
\mathcal{J}\mathbf{e}_1 + \mathcal{M}_1\mathbf{e}_1 + \mathbf{d}_2 &= (\mathcal{J} + \mathcal{M}_1)\mathbf{e}_1 + (\mathcal{J} + \mathcal{M}_1)\mathbf{y}(t_1) - \mathbf{y}(t_2) \\
&= (\mathcal{J} + \mathcal{M}_1)\big(\mathbf{y}_1 - \mathbf{y}(t_1)\big) + (\mathcal{J} + \mathcal{M}_1)\mathbf{y}(t_1) - \mathbf{y}(t_2) \\
&= (\mathcal{J} + \mathcal{M}_1)\mathbf{y}_1 - \mathbf{y}(t_2) \\
&= \mathbf{y}_2 - \mathbf{y}(t_2) \\
&= \mathbf{e}_2\,.
\end{aligned}$$

Now, we assume that

$$\mathbf{e}_N = \mathcal{J}^{N-1}\mathbf{e}_1 + \sum_{n=1}^{N-1} \mathcal{J}^{N-1-n}\mathcal{M}_n\mathbf{e}_n + \sum_{n=1}^{N-1} \mathcal{J}^{N-1-n}\mathbf{d}_{n+1} \tag{5.10}$$

holds for arbitrary but fixed $N \in \mathbb{N}$. Then, we conclude

$$\begin{aligned}
\mathbf{e}_{N+1} &= \mathbf{y}_{N+1} - \mathbf{y}(t_{N+1}) \\
&= (\mathcal{J} + \mathcal{M}_N)\mathbf{y}_N - \mathbf{y}(t_{N+1}) \\
&= \mathcal{J}\mathbf{e}_N + \mathcal{M}_N\mathbf{e}_N + \mathbf{d}_{N+1}\,.
\end{aligned}$$

Substituting (5.10) into $\mathcal{J}\mathbf{e}_N$ yields

$$\begin{aligned}
\mathbf{e}_{N+1} &= \mathcal{J}\Big(\mathcal{J}^{N-1}\mathbf{e}_1 + \sum_{n=1}^{N-1} \mathcal{J}^{N-1-n}\mathcal{M}_n\mathbf{e}_n + \sum_{n=1}^{N-1} \mathcal{J}^{N-1-n}\mathbf{d}_{n+1}\Big) + \mathcal{M}_N\mathbf{e}_N + \mathbf{d}_{N+1} \\
&= \mathcal{J}^N\mathbf{e}_1 + \sum_{n=1}^{N-1} \mathcal{J}^{N-n}\mathcal{M}_n\mathbf{e}_n + \sum_{n=1}^{N-1} \mathcal{J}^{N-n}\mathbf{d}_{n+1} + \mathcal{M}_N\mathbf{e}_N + \mathbf{d}_{N+1} \\
&= \mathcal{J}^N\mathbf{e}_1 + \sum_{n=1}^{N} \mathcal{J}^{N-n}\mathcal{M}_n\mathbf{e}_n + \sum_{n=1}^{N} \mathcal{J}^{N-n}\mathbf{d}_{n+1}\,,
\end{aligned}$$

which completes the proof. □

The error recursion formula in Lemma 12 lays out the strategy for the error analysis of the adiabatic midpoint rule (5.1): we continue by estimating each part of the recursion formula and, finally, apply the discrete Gronwall lemma.

For the first summand, we recall that the starting step is conducted by the $\widehat{\phi}$-variant of the adiabatic Euler method (5.3). Hence, for arbitrary $y_0 \in \ell^1$ Lemma 8 yields the estimate

$$\left\|\mathcal{J}^N\mathbf{e}_1\right\|_{\ell^1} \le \|\mathbf{e}_1\|_{\ell^1} \le \left\|y^{(1)} - y(t_1)\right\|_{\ell^1} \le \tau^2 C(M_0^y)\,. \tag{5.11}$$

Moreover, let $\{\mathcal{M}_n\mathbf{e}_n\}_m$ denote the m-th entry of $\mathcal{M}_n\mathbf{e}_n$. By (5.6), all non-zero entries of $\mathcal{M}_n\mathbf{e}_n$ are of the form

$$\{\mathcal{M}_n\mathbf{e}_n\}_m = \mathrm{i}\sum_{I_m} y_j^{(n)}\overline{y}_k^{(n)}\big(y_l^{(n)} - y_l(t_n)\big)\int_{t_{n-1}}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha t_n + \phi\left(\tfrac{s}{\varepsilon}\right))\right)\mathrm{d}s\,.$$

Hence, the estimate

$$\left\|\sum_{n=1}^{N} \mathcal{J}^{N-n}\mathcal{M}_n\mathbf{e}_n\right\|_{\ell^1} \le \tau C(M_0^y)\sum_{n=1}^{N}\|\mathbf{e}_n\|_{\ell^1} \tag{5.12}$$

follows with the bound for the numerical solution (5.8).

Estimate (5.11) and the estimate (5.12) are used in order to prove each of the error bounds stated in Theorem 10. The different levels of accuracy in part (i)-(iii) are solely based on different estimates of the remaining term

$$\left\|\sum_{n=1}^{N} \mathcal{J}^{N-n}\mathbf{d}_{n+1}\right\|_{\ell^1} \tag{5.13}$$

of the recursion formula in Lemma 12. In the following, we deduce suitable estimates for (5.13) in each setting of Theorem 10.

For the remaining proof, we denote the m-entry of a sequence $\mathbf{z} := (\mathbf{z}_m)_{m\in\mathbb{Z}}$ by $\{z\}_m$.

5.3.1. Proof of part (i)

We prove the linear convergence of the ϕ-variant of the adiabatic midpoint rule (5.1) with a constant that does not depend on ε. By (5.9), all non-zero entries of $\mathbf{d}_{n+1}$ are of the form

$$\{d_{n+1}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}} y_j^{(n)}\overline{y}_k^{(n)} y_l(t_n)\exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha t_n + \phi\left(\tfrac{s}{\varepsilon}\right))\right)\mathrm{d}s \\ + y_m(t_{n-1}) - y_m(t_{n+1})\,. \tag{5.14}$$

Hence, if we substitute

$$y_m(t_{n+1}) = y_m(t_{n-1}) + \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}} \widehat{Y}_{jklm}(t_n)\exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s \\ + \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s}\widehat{Y}'_{jklm}(\sigma)\,\mathrm{d}\sigma\exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s$$

into (5.14), then the partition

$$\{d_{n+1}\}_m = \{d_{n+1}^{(1)}\}_m - \{d_{n+1}^{(2)}\}_m\,, \tag{5.15}$$

with

$$\{d_{n+1}^{(1)}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\left(y_j^{(n)}\overline{y}_k^{(n)} - y_j(t_n)\overline{y}_k(t_n)\right)y_l(t_n) \\ \exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha t_n + \phi\left(\tfrac{s}{\varepsilon}\right))\right)\mathrm{d}s$$

and

$$\{d_{n+1}^{(2)}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s}\widehat{Y}'_{jklm}(\sigma)\,\mathrm{d}\sigma\exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s \tag{5.16}$$

follows. Because of the estimate

$$\left|\left(y_j^{(n)}\overline{y}_k^{(n)} - y_j(t_n)\overline{y}_k(t_n)\right)y_l(t_n)\exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha t_n + \phi\left(\tfrac{s}{\varepsilon}\right))\right)\right| \\ \leq \left(|y_j^{(n)} - y_j(t_n)||\overline{y}_k^{(n)}| + |\overline{y}_k^{(n)} - \overline{y}_k(t_n)|\,|y_j(t_n)|\right)|y_l(t_n)|\ ,$$

we can conclude from (5.8) that

$$\left\|\mathbf{d}_{n+1}^{(1)}\right\|_{\ell^1} \leq \tau C(M_0^y)\left\|y^{(n)} - y(t_n)\right\|_{\ell^1} \leq \tau C(M_0^y)\left\|\mathbf{e}_n\right\|_{\ell^1}\ . \tag{5.17}$$

Furthermore, differentiating (2.23) gives

$$\left|\widehat{Y}'_{jklm}(\sigma)\right| \leq \left|Y'_{jkl}(\sigma)\right| + \alpha\left|\omega_{[jklm]}Y_{jkl}(\sigma)\right|\ . \tag{5.18}$$

Hence, applying Lemma 22 (Appendix A) results in

$$\left\|\mathbf{d}_{n+1}^{(2)}\right\|_{\ell^1} \leq \tau^2\big(C(M_0^y) + \alpha C(M_2^y)\big)\,. \tag{5.19}$$

By estimating

$$\left\|\sum_{n=1}^{N} \mathcal{J}^{N-n}\mathbf{d}_{n+1}\right\|_{\ell^1} \leq \sum_{n=1}^{N} \|\mathbf{d}_{n+1}\|_{\ell^1} \leq \sum_{n=1}^{N} \left\|\mathbf{d}_{n+1}^{(1)}\right\|_{\ell^1} + \sum_{n=1}^{N} \left\|\mathbf{d}_{n+1}^{(2)}\right\|_{\ell^1}\,, \tag{5.20}$$

we finally arrive at

$$\left\|\sum_{n=1}^{N} \mathcal{J}^{N-n}\mathbf{d}_{n+1}\right\|_{\ell^1} \leq \tau C(M_0^y)\sum_{n=1}^{N} \|\mathbf{e}_n\|_{\ell^1} + \tau\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,. \tag{5.21}$$

Now, combining (5.11), (5.12) and (5.21) with Lemma 12 gives the estimate

$$\|\mathbf{e}_{N+1}\|_{\ell^1} \leq \tau C(M_0^y)\sum_{n=1}^{N} \|\mathbf{e}_n\|_{\ell^1} + \tau\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,,$$

and hence applying the discrete Gronwall yields

$$\|\mathbf{e}_{N+1}\|_{\ell^1} \leq \tau\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)e^{TC(M_0^y)}$$

completing the proof of part (i).

5.3.2. Proof of part (ii)

Considering step-sizes $\tau = \varepsilon/k$ for some $k \in \mathbb{N}$ allows us to improve the estimate (5.21). For this purpose, we revisit the estimate (5.20) and, in particular, the estimates (5.17) and (5.19), respectively. We observe that the crucial estimate for the accuracy of the method is the bound (5.19) for $\mathbf{d}_{n+1}^{(2)}$, whereas the bound (5.17) for $\mathbf{d}_{n+1}^{(1)}$ is not critical. Hence, we start by estimating

$$\left\|\sum_{n=1}^{N} \mathcal{J}^{N-n}\mathbf{d}_{n+1}\right\|_{\ell^1} \leq \tau C(M_0^y)\sum_{n=1}^{N} \|\mathbf{e}_n\|_{\ell^1} + \left\|\sum_{n=1}^{N} \mathcal{J}^{N-n}\mathbf{d}_{n+1}^{(2)}\right\|_{\ell^1}\,. \tag{5.22}$$

The cornerstone for improving the estimate (5.21) is now to exploit cancellation effects in the summation of double integrals of the form

$$\mathcal{I}_n = \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{\sigma}{\varepsilon}\right)\right) \mathrm{d}\sigma \exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,. \tag{5.23}$$

These cancellations take place during time intervals of the length 2ε. Hence, if T is not an integer multiple of 2ε, we have to account for summands in a possible smaller time frame at the end of the time interval $[0,T]$: we subdivide $N = 2kL + n^*$ with $L \in \mathbb{N}$, $k = \varepsilon/\tau$ and $n^* \in \{0,\dots,2k-1\}$ and partition

$$\left\| \sum_{n=1}^{N} \mathcal{J}^{N-n} \mathbf{d}_{n+1}^{(2)} \right\|_{\ell^1} \leq \left\| \sum_{n=1}^{2kL-1} \mathcal{J}^{N-n} \mathbf{d}_{n+1}^{(2)} \right\|_{\ell^1} + \left\| \sum_{n=2kL}^{2kL+n^*} \mathcal{J}^{N-n} \mathbf{d}_{n+1}^{(2)} \right\|_{\ell^1} . \tag{5.24}$$

Because $n^*\tau^2 \leq 2k\tau^2 = 2\tau\varepsilon$, the excessive summands can be estimated by (5.19) via

$$\left\| \sum_{n=2kL}^{2kL+n^*} \mathcal{J}^{N-n} \mathbf{d}_{n+1}^{(2)} \right\|_{\ell^1} \leq \varepsilon\tau\big(C(M_0^y) + \alpha C(M_2^y)\big) . \tag{5.25}$$

In order to take advantage of the cancellation effects for estimating the remaining sum in (5.24), it is now crucial to avoid the triangle inequality. To cope with the row-switching matrix $\mathcal{J}$, we partition the sum into

$$\left\| \sum_{n=1}^{2kL-1} \mathcal{J}^{N-n} \mathbf{d}_{n+1}^{(2)} \right\|_{\ell^1} \leq \left\| \sum_{\substack{n=1 \\ n \text{ odd}}}^{2kL-1} \mathbf{d}_{n+1}^{(2)} \right\|_{\ell^1} + \left\| \sum_{\substack{n=1 \\ n \text{ even}}}^{2kL-1} \mathbf{d}_{n+1}^{(2)} \right\|_{\ell^1} , \tag{5.26}$$

i.e. we consider the summation of odd and even n separately. In order to estimate (5.26) further, we specify the cancellation effects of the double integrals (5.23) in the following lemma.

Lemma 13. *Let $k, L \in \mathbb{N}$ and suppose that $\tau = \varepsilon/k$ for $k \in \mathbb{N}$. Then, we have for a sequence $(a_n)_{n\in\mathbb{N}}$ and $\mathcal{I}_n$ given in (5.23) the estimates*

$$(i) \qquad \left| \sum_{\substack{n=1 \\ n \text{ even}}}^{2kL-1} a_n \mathcal{I}_n \right| \leq 2\varepsilon\tau \sum_{n=1}^{kL-2} \left| a_{2(n+1)} - a_{2n} \right|$$

and

$$(ii) \qquad \left| \sum_{\substack{n=1 \\ n \text{ odd}}}^{2kL-1} a_n \mathcal{I}_n \right| \leq 2\varepsilon\tau \sum_{n=1}^{kL-2} \left| a_{2n+1} - a_{2n-1} \right| .$$

Proof. Applying the summation by parts formula gives

$$\begin{aligned} \sum_{\substack{n=1 \\ n \text{ even}}}^{2kL-1} a_n \mathcal{I}_n &= \sum_{n=1}^{kL-1} a_{2n} \mathcal{I}_{2n} \\ &= \left(\sum_{n=1}^{kL-1} \mathcal{I}_{2n} \right) a_{2(kL-1)} - \sum_{n=1}^{kL-2} \left(\sum_{j=1}^{n} \mathcal{I}_{2j} \right) \left(a_{2(n+1)} - a_{2n} \right) . \end{aligned} \tag{5.27}$$

With the partition $n = (kl-1) + n^*$ for $l \in \mathbb{N}$ and $n^* \in \{0,\dots,k\}$, we subdivide

$$\sum_{j=1}^{n} \mathcal{I}_{2j} = \sum_{j=1}^{lk-1} \mathcal{I}_{2j} + \sum_{j=lk}^{lk+n^*} \mathcal{I}_{2j} , \tag{5.28}$$

and hence if we prove that

$$\sum_{n=1}^{lk-1} \mathcal{I}_{2n} = 0 \quad \text{for} \quad l \in \mathbb{N}\,, \tag{5.29}$$

then we obtain with

$$\left| \sum_{j=lk}^{lk+n^*} \mathcal{I}_{2j} \right| \leq 2\tau^2 n^*$$

the estimate (i) via

$$\left| \sum_{\substack{n=1 \\ n \text{ even}}}^{2kL-1} a_n \mathcal{I}_n \right| \leq \sum_{n=1}^{kL-2} 2\tau^2 n^* \left| a_{2(n+1)} - a_{2n} \right| \leq 2\varepsilon\tau \sum_{n=1}^{kL-2} \left| a_{2(n+1)} - a_{2n} \right| .$$

It remains to prove (5.29). By definition (2.18), ϕ is symmetric and periodic, i.e.

$$\phi(1+s) = \phi(1-s)\,, \qquad \phi(2+s) = \phi(2-s) \tag{5.30}$$

and

$$\phi(s) = \phi(2+s)\,. \tag{5.31}$$

Since $t_{2k} = 2\varepsilon$ and $t_1 = \varepsilon/k$, it follows with (5.31) and (5.30) that

$$\begin{aligned}
&\int_{t_{2k}}^{t_{2k+1}} \int_{t_{2k}}^{s} \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{\sigma}{\varepsilon}\right)\right) \mathrm{d}\sigma \exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \\
&\qquad = \varepsilon^2 \int_{2}^{2+1/k} \int_{2}^{s} \exp\big(-\mathrm{i}\omega\phi(\sigma)\big) \mathrm{d}\sigma \exp\big(-\mathrm{i}\tilde{\omega}\phi(s)\big) \mathrm{d}s \\
&\qquad = \varepsilon^2 \int_{0}^{1/k} \int_{0}^{s} \exp\big(-\mathrm{i}\omega\phi(2+\sigma)\big) \mathrm{d}\sigma \exp\big(-\mathrm{i}\tilde{\omega}\phi(2+s)\big) \mathrm{d}s \\
&\qquad = \varepsilon^2 \int_{0}^{1/k} \int_{0}^{s} \exp\big(-\mathrm{i}\omega\phi(2-\sigma)\big) \mathrm{d}\sigma \exp\big(-\mathrm{i}\tilde{\omega}\phi(2-s)\big) \mathrm{d}s \\
&\qquad = \varepsilon^2 \int_{0}^{-1/k} \int_{0}^{s} \exp\big(-\mathrm{i}\omega\phi(2+\sigma)\big) \mathrm{d}\sigma \exp\big(-\mathrm{i}\tilde{\omega}\phi(2+s)\big) \mathrm{d}s \\
&\qquad = -\varepsilon^2 \int_{-1/k}^{0} \int_{0}^{s} \exp\big(-\mathrm{i}\omega\phi(2+\sigma)\big) \mathrm{d}\sigma \exp\big(-\mathrm{i}\tilde{\omega}\phi(2+s)\big) \mathrm{d}s \\
&\qquad = -\varepsilon^2 \int_{2-1/k}^{2} \int_{2}^{s} \exp\big(-\mathrm{i}\omega\phi(\sigma)\big) \mathrm{d}\sigma \exp\big(-\mathrm{i}\tilde{\omega}\phi(s)\big) \mathrm{d}s \\
&\qquad = -\int_{t_{2k-1}}^{t_{2k}} \int_{t_{2k}}^{s} \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{\sigma}{\varepsilon}\right)\right) \mathrm{d}\sigma \exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,,
\end{aligned}$$

and therefore

$$\mathcal{I}_{2k} = 0\,. \tag{5.32}$$

Thanks to (5.31), we have in addition

$$\mathcal{I}_n = \mathcal{I}_{n+2k}\,. \tag{5.33}$$

Henceforth, we assume that k is even; the case k is odd follows with minor modifications. Because of (5.32) and (5.33), we can write

$$\sum_{n=1}^{kl-1} \mathcal{I}_{2n} = \sum_{j=1}^{l} \sum_{n=(j-1)k+1}^{kj-1} \mathcal{I}_{2n} = l \sum_{n=1}^{k-1} \mathcal{I}_{2n} \,.$$

Then, rearranging the summands symmetrically with respect to ε results in

$$\sum_{n=1}^{kl-1} \mathcal{I}_{2n} = l \left(\mathcal{I}_k + \sum_{n=1}^{k/2-1} \left(\mathcal{I}_{2n} + \mathcal{I}_{2(k-n)} \right) \right) \,.$$

One can show, analogously to (5.32), with (5.31) and (5.30) that

$$\mathcal{I}_k = 0, \quad \mathcal{I}_{2n} + \mathcal{I}_{2(k-n)} = 0 \quad \text{for} \quad n = 1, \ldots, k/2-1 \tag{5.34}$$

completing the proof of (5.29), and thus of the estimate (i).

Estimate (ii) follows in the same way with

$$\sum_{n=1}^{kl} \mathcal{I}_{2n-1} = l \sum_{n=1}^{k/2} \left(\mathcal{I}_{2n-1} + \mathcal{I}_{2(k-n)+1} \right) \,, \quad \text{for} \quad l \in \mathbb{N}$$

and by showing that

$$\mathcal{I}_{2n-1} + \mathcal{I}_{2(k-n)+1} = 0 \quad \text{for} \quad n = 1, \ldots, k/2 \,. \tag{5.35}$$

□

Equipped with Lemma 13 we continue estimating (5.26). Because we have

$$\widehat{Y}'_{jklm}(\sigma) = \left(Y'_{jkl}(\sigma) - \mathrm{i}\omega_{[jklm]} \alpha Y_{jkl}(\sigma) \right) \exp\left(-\mathrm{i}\omega_{[jklm]} \alpha\sigma \right) \,, \tag{5.36}$$

by (2.23), we can partition $\{d^{(2)}_{n+1}\}_m$, given in (5.16), into

$$\{d^{(2)}_{n+1}\}_m = \{S^{(1)}_{n+1}\}_m + \{S^{(2)}_{n+1}\}_m \,,$$

with

$$\{S^{(1)}_{n+1}\}_m = \mathrm{i} \sum_{I_m} \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} Y'_{jkl}(\sigma) \exp\left(-\mathrm{i}\omega_{[jklm]} \left(\alpha\sigma + \phi\left(\tfrac{s}{\varepsilon}\right) \right) \right) \mathrm{d}\sigma \, \mathrm{d}s$$

and

$$\{S^{(2)}_{n+1}\}_m = \alpha \sum_{I_m} \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \omega_{[jklm]} \widehat{Y}_{jklm}(\sigma) \exp\left(-\mathrm{i}\omega_{[jklm]} \phi\left(\tfrac{s}{\varepsilon}\right) \right) \mathrm{d}\sigma \, \mathrm{d}s \,.$$

The aim for the next two steps is separating suitable parts of $\{S^{(1)}_{n+1}\}_m$ and $\{S^{(2)}_{n+1}\}_m$, respectively, for which we then employ Lemma 13. As a final step, we use the discrete Gronwall lemma.

Step 1. By definition (2.23) we have

$$Y'_{jkl}(\sigma) = y'_j(\sigma)\overline{y}_k(\sigma)y_l(\sigma) + y_j(\sigma)\overline{y}'_k(\sigma)y_l(\sigma) + y_j(\sigma)\overline{y}_k(\sigma)y'_l(\sigma)\,,$$

and hence we obtain the partition

$$\{S^{(1)}_{n+1}\}_m = \{T^{(1)}_{n+1}\}_m + \{T^{(2)}_{n+1}\}_m + \{T^{(3)}_{n+1}\}_m\,,$$

with

$$\{T^{(1)}_{n+1}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} y'_j(\sigma)\overline{y}_k(\sigma)y_l(\sigma)\exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha\sigma+\phi\left(\tfrac{s}{\varepsilon}\right))\right)\mathrm{d}\sigma\,\mathrm{d}s\,, \tag{5.37}$$

$$\{T^{(2)}_{n+1}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} y_j(\sigma)\overline{y}'_k(\sigma)y_l(\sigma)\exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha\sigma+\phi\left(\tfrac{s}{\varepsilon}\right))\right)\mathrm{d}\sigma\,\mathrm{d}s\,, \tag{5.38}$$

$$\{T^{(3)}_{n+1}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} y_j(\sigma)\overline{y}_k(\sigma)y'_l(\sigma)\exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha\sigma+\phi\left(\tfrac{s}{\varepsilon}\right))\right)\mathrm{d}\sigma\,\mathrm{d}s\,. \tag{5.39}$$

Observing that the terms (5.37)-(5.39) are structured similarly, we solely derive an estimate for the term (5.37) to demonstrate the procedure. Analogously, one can prove similar estimates for (5.38) and (5.39).

Inserting the tDMNLS (2.24) for the derivative $y'_j(\sigma)$ yields

$$\begin{aligned}\{T^{(1)}_{n+1}\}_m = -\sum_{I_m}\sum_{I_j}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} & Y_{pqrkl}(\sigma)\exp\left(-\mathrm{i}(\omega_{[pqrj]}+\omega_{[jklm]})\alpha\sigma\right)\\ & \exp\left(-\mathrm{i}\omega_{[pqrj]}\phi\left(\tfrac{\sigma}{\varepsilon}\right)\right)\mathrm{d}\sigma\exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s\,,\end{aligned} \tag{5.40}$$

where we abbreviate

$$Y_{pqrkl}(\sigma) = y_p(\sigma)\overline{y}_q(\sigma)y_r(\sigma)\overline{y}_k(\sigma)y_l(\sigma) \tag{5.41}$$

in the spirit of (2.23) and (3.10), and use the shorthand notation

$$\sum_{I_j} \quad \text{instead of} \quad \sum_{(p,q,r)\in I_j}\,.$$

For simplicity, we fix $m \in \mathbb{Z}$, $(j,k,l) \in I_m$ and $(p,q,r) \in I_j$. Moreover, we write $\tilde{\omega} = \omega_{[jklm]}$ and $\omega = \omega_{[pqrj]}$ for short, and particularly define

$$F(\sigma) = Y_{pqrkl}(\sigma) \exp\big(-\mathrm{i}(\omega_{[pqrj]} + \omega_{[jklm]})\alpha\sigma\big) \ . \tag{5.42}$$

Hence, we obtain for any summand of (5.40) the partition

$$\int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} F(\sigma) \exp\big(-\mathrm{i}\omega\phi\left(\tfrac{\sigma}{\varepsilon}\right)\big)\, \mathrm{d}\sigma \exp\big(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{s}{\varepsilon}\right)\big)\, \mathrm{d}s = F(t_n)\mathcal{I}_n + R_{n+1}^{(1)} \,,$$

with $\mathcal{I}_n$ from (5.23) and

$$R_{n+1}^{(1)} = \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{\sigma_1} F'(\sigma_2)\, \mathrm{d}\sigma_2 \exp\big(-\mathrm{i}\omega\phi\left(\tfrac{\sigma_1}{\varepsilon}\right)\big)\, \mathrm{d}\sigma_1 \exp\big(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{s}{\varepsilon}\right)\big)\, \mathrm{d}s \,.$$

It is clear that

$$\left|\sum_{n=1}^{2kL-1} R_{n+1}^{(1)}\right| \le \tau^2 C(T) \max_{\sigma\in[0,T]} \left|F'(\sigma)\right| \,. \tag{5.43}$$

Moreover, we infer

$$|F(t_{2n+2}) - F(t_{2n})| = \left|\int_{t_{2n}}^{t_{2n+2}} F'(\sigma)\, \mathrm{d}\sigma\right| \le \tau C \max_{\sigma\in[t_{2n},t_{2n+2}]} \left|F'(\sigma)\right| \tag{5.44}$$

and likewise

$$|F(t_{2n+1}) - F(t_{2n-1})| \le \tau C \max_{\sigma\in[t_{2n-1},t_{2n+1}]} \left|F'(\sigma)\right| \,. \tag{5.45}$$

According to Lemma 13 the estimates

$$\left|\sum_{\substack{n=1\\ n \text{ even}}}^{2kL-1} F(t_n)\mathcal{I}_n\right| \le \varepsilon\tau C(T) \max_{\sigma\in[0,T]} \left|F'(\sigma)\right| \tag{5.46}$$

and

$$\left|\sum_{\substack{n=1\\ n \text{ odd}}}^{2kL-1} F(t_n)\mathcal{I}_n\right| \le \varepsilon\tau C(T) \max_{\sigma\in[0,T]} \left|F'(\sigma)\right| \tag{5.47}$$

follow, and because

$$\left|F'(\sigma)\right| \le \left|Y'_{pqrkl}(\sigma)\right| + \alpha \left|(\omega_{[jklm]} + \omega_{[pqrj]})Y_{pqrkl}(\sigma)\right| \,,$$

combining (5.43)-(5.47) with Lemma 22 (Appendix A) results in

$$\left\|\sum_{n=1}^{2kL-1} \mathcal{J}^{N-n}\mathbf{S}_{n+1}^{(1)}\right\|_{\ell^1} \le \varepsilon\tau\big(C(T,M_0^y) + \alpha C(T,M_2^y)\big) \,. \tag{5.48}$$

Step 2. We fix $m \in \mathbb{Z}$ and $(j,k,l) \in I_m$. In addition, we write $\tilde{\omega} = \omega_{[jklm]}$ for short and define

$$\widehat{F}(\sigma) = \omega_{[jklm]} \widehat{Y}_{jklm}(\sigma)\,.$$

Then, we have for any summand of $\{S^{(2)}_{n+1}\}_m$ the partition

$$\alpha \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \widehat{F}(\sigma) \exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}\sigma\, \mathrm{d}s = \alpha\Big(\widehat{F}(t_n)\mathcal{I}_n + R^{(2)}_{n+1}\Big)\,,$$

where $\mathcal{I}_n$ is given in (5.23) with $\omega = 0$, and

$$R^{(2)}_{n+1} = \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{\sigma_1} \widehat{F}'(\sigma_2)\, \mathrm{d}\sigma_2 \exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}\sigma_1\, \mathrm{d}s\,.$$

It is clear that

$$\left|\sum_{n=1}^{2kL-1} R^{(2)}_{n+1}\right| \le \tau^2 C(T) \max_{\sigma\in[0,T]} \left|\widehat{F}'(\sigma)\right|\,. \tag{5.49}$$

As in step 1, Lemma 13 (with $\omega = 0$) yields

$$\left|\sum_{\substack{n=1\\ n \text{ even}}}^{2kL-1} \widehat{F}(t_n)\mathcal{I}_n\right| \le \varepsilon\tau C(T) \max_{\sigma\in[0,T]} \left|\widehat{F}'(\sigma)\right| \tag{5.50}$$

and

$$\left|\sum_{\substack{n=1\\ n \text{ odd}}}^{2kL-1} \widehat{F}(t_n)\mathcal{I}_n\right| \le \varepsilon\tau C(T) \max_{\sigma\in[0,T]} \left|\widehat{F}'(\sigma)\right|\,, \tag{5.51}$$

and because

$$\left|\widehat{F}'(\sigma)\right| \le \left|\omega_{[jklm]} Y'_{jkl}(\sigma)\right| + \alpha \left|\omega^2_{[jklm]} Y_{jkl}(\sigma)\right|\,,$$

combining (5.49)-(5.51) with Lemma 22 (Appendix A) results in

$$\left\|\sum_{n=1}^{2kL-1} \mathcal{J}^{N-n} \mathbf{S}^{(2)}_{n+1}\right\|_{\ell^1} \le \varepsilon\tau\big(\alpha C(T, M_2^y) + \alpha^2 C(T, M_4^y)\big)\,. \tag{5.52}$$

Step 3. Finally, we substitute (5.48) and (5.52) into (5.22) obtaining

$$\begin{aligned}\left\|\sum_{n=1}^{N} \mathcal{J}^{N-n} \mathbf{d}_{n+1}\right\|_{\ell^1} &\le \tau C(M_0^y) \sum_{n=1}^{N} \|\mathbf{e}_n\|_{\ell^1} \\ &\quad + \varepsilon\tau\big(C(T, M_0^y) + \alpha C(T, M_2^y) + \alpha^2 C(T, M_4^y)\big)\,. \end{aligned} \tag{5.53}$$

Now, combining (5.11), (5.12) and (5.53) with the recursion formula in Lemma 12 gives the estimate

$$\|\mathbf{e}_{N+1}\|_{\ell^1} \le \tau C(M_0^y) \sum_{n=1}^{N} \|\mathbf{e}_n\|_{\ell^1} + \varepsilon\tau\big(C(T, M_0^y) + \alpha C(T, M_2^y) + \alpha^2 C(T, M_4^y)\big)$$

and applying the discrete Gronwall lemma completes the proof of part (ii).

5.3.3. Proof of part (iii)

We recall that for step-sizes $\tau = \varepsilon k$ for $k \in \mathbb{N}$ the ϕ-variant of the adiabatic midpoint rule coincides with the classical explicit midpoint rule applied to the limit system, see (5.4). Thanks to Theorem 3 the estimate

$$\begin{aligned}\left\|y(t_n) - y^{(n)}\right\|_{\ell^1} &\leq \|y(t_n) - v(t_n)\|_{\ell^1} + \left\|v(t_n) - y^{(n)}\right\|_{\ell^1} \\ &\leq \frac{\varepsilon^2}{\delta} C(t_n, \alpha, M_0, M_2) + \left\|v(t_n) - y^{(n)}\right\|_{\ell^1}\end{aligned} \tag{5.54}$$

follows, with M_s given in (3.14). Thus, it remains to show that the explicit midpoint rule applied to the limit system (3.9) is of order two. We define

$$\mathbf{v}(t_{n+1}) = \begin{pmatrix} v(t_{n+1}) \\ v(t_n) \end{pmatrix} \quad \text{and} \quad \tilde{\mathbf{d}}_{n+1} = \big(\mathcal{J} + \mathcal{M}_n\big)\mathbf{v}(t_n) - \mathbf{v}(t_{n+1})\,. \tag{5.55}$$

Then, one can show (cf. Lemma 12) that the global error $\mathbf{e}_n = \mathbf{v}_n - \mathbf{v}(t_n)$ satisfies the recursion formula

$$\mathbf{e}_{N+1} = \mathcal{J}^N \mathbf{e}_1 + \sum_{n=1}^{N} \mathcal{J}^{N-n} \mathcal{M}_n \mathbf{e}_n + \sum_{n=1}^{N} \mathcal{J}^{N-n} \tilde{\mathbf{d}}_{n+1}\,, \qquad N \geq 1\,. \tag{5.56}$$

In order to estimate the first two terms of the recursion formula (5.56) the estimates (5.11) and (5.12) are still available. Hence, it remains to derive an estimate for the third term. Definition (5.55) implies that all non-zero entries of $\tilde{\mathbf{d}}_{n+1}$ are of the form

$$\begin{aligned}\{\tilde{d}_{n+1}\}_m = 2\tau \mathrm{i} \sum_{I_m} y_j^{(n)} \overline{y}_k^{(n)} v_l(t_n) \exp\left(-\mathrm{i}\omega_{[jklm]}\alpha t_n\right) \int_0^1 \exp\left(\mathrm{i}\omega_{[jklm]}\delta\xi\right) \mathrm{d}\xi \\ + v_m(t_{n-1}) - v_m(t_{n+1})\,.\end{aligned} \tag{5.57}$$

Moreover, the fundamental theorem of calculus applied to (3.9) gives

$$v_m(t_{n+1}) = v_m(t_{n-1}) + \mathrm{i} \sum_{I_m} \int_{t_{n-1}}^{t_{n+1}} \widehat{V}_{jklm}(s)\,\mathrm{d}s \int_0^1 \exp\left(\mathrm{i}\omega_{[jklm]}\delta\xi\right) \mathrm{d}\xi\,. \tag{5.58}$$

In contrast to $\widehat{Y}_{jklm}(s)$, the product $\widehat{V}_{jklm}(s)$ is independent of ε. Therefore, employing the Taylor expansion

$$\widehat{V}_{jklm}(s) = \widehat{V}_{jklm}(t_n) + (s - t_n)\widehat{V}'_{jklm}(t_n) + \int_{t_n}^{s} \int_{t_n}^{\sigma_1} \widehat{V}''_{jklm}(\sigma_2)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1 \tag{5.59}$$

does not produce any factors of $1/\varepsilon$. Now, combining (5.59) with (5.58) and substituting into (5.57) yields the partition

$$\{\tilde{d}_{n+1}\}_m = \{\tilde{d}^{(1)}_{n+1}\}_m - \{\tilde{d}^{(2)}_{n+1}\}_m\,,$$

with

$$\{\tilde{d}_{n+1}^{(1)}\}_m = 2\tau\mathrm{i}\sum_{I_m}\big(y_j^{(n)}\overline{y}_k^{(n)} - v_j(t_n)\overline{v}_k(t_n)\big)v_l(t_n)$$
$$\exp\big(-\mathrm{i}\omega_{[jklm]}\alpha t_n\big)\int_0^1 \exp\big(\mathrm{i}\omega_{[jklm]}\delta\xi\big)\,\mathrm{d}\xi$$

and

$$\{\tilde{d}_{n+1}^{(2)}\}_m = \mathrm{i}\sum_{I_m}\int_0^1 \exp\big(\mathrm{i}\omega_{[jklm]}\delta\xi\big)\,\mathrm{d}\xi\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s}\int_{t_n}^{\sigma_1}\widehat{V}''_{jklm}(\sigma_2)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,\mathrm{d}s\,.$$

Here, the second summand from (5.59) vanishes due to the symmetry of the integral. According to (5.8) the numerical solution is bounded, and hence we obtain

$$\left\|\tilde{\mathbf{d}}_{n+1}^{(1)}\right\|_{\ell^1} \le \tau C(M_0)\,\|\mathbf{e}_n\|_{\ell^1}\ .$$

Because we have

$$\left|\widehat{V}''_{jklm}(s)\right| \le \left|V''_{jkl}(s)\right| + 2\alpha\left|\omega_{[jklm]}V'_{jkl}(s)\right| + \alpha^2\left|\omega^2_{[jklm]}V_{jkl}(s)\right|\ ,$$

Lemma 21 (Appendix A) implies

$$\left\|\tilde{\mathbf{d}}_{n+1}^{(2)}\right\|_{\ell^1} \le \tau^3\big(C(M_0^v) + \alpha C(M_2^v) + \alpha^2 C(M_4^v)\big)\,.$$

Finally, we arrive at

$$\left\|\sum_{n=1}^{N}\mathcal{J}^{N-n}\tilde{\mathbf{d}}_{n+1}\right\|_{\ell^1} \le \tau C(M_0)\sum_{n=1}^{N}\|\mathbf{e}_n\|_{\ell^1} + \tau^2\big(C(M_0^v) + \alpha C(M_2^v) + \alpha^2 C(M_4^v)\big)\,. \tag{5.60}$$

Now, substituting (5.11), (5.12) and (5.60) into the recursion formula (5.56) and applying the discrete Gronwall lemma yields

$$\|\mathbf{e}_{n+1}\|_{\ell^1} \le \tau^2\big(C(M_0^v) + \alpha C(M_2^v) + \alpha^2 C(M_4^v)\big)e^{TC(M_0)}\,. \tag{5.61}$$

In combination with (5.54) this estimate completes the proof of part (iii). Here, we recall that for $\alpha = 0$ the constant from Theorem 3 depends only on M_0 and observe that the constant in (5.61) improves accordingly.

□

5.4. Proof of Theorem 11

Clearly, the $\widehat{\phi}$-variant (5.2) and the ϕ-variant (5.1) of the adiabatic midpoint rule are closely related. Therefore, we follow the basic framework of the proof of Theorem 10 in Section 5.3. However, there are several deviations leading, in particular, to lower regularity requirements.

With A given in (5.5), we define

$$\widehat{\mathcal{M}}_n = \begin{pmatrix} \int_{t_{n-1}}^{t_{n+1}} A\left(s, \frac{s}{\varepsilon}, y^{(n)}\right) \mathrm{d}s & 0 \\ 0 & 0 \end{pmatrix}$$

obtaining the one-step formulation

$$\mathbf{y}_{n+1} = (\mathcal{J} + \widehat{\mathcal{M}}_n)\mathbf{y}_n$$

for the $\widehat{\phi}$-variant (5.2) of the adiabatic midpoint rule, where $\mathcal{J}$ and $\mathbf{y}_n$ are given in (5.6). One can show with Proposition 23 (Appendix B) that the estimate

$$\left\| y^{(n)} \right\|_{\ell^1} \le C(M_0^y) \quad \text{for all} \quad \tau n \le T \tag{5.62}$$

holds for sufficiently small the step-sizes τ, cf. (5.8). Again, we omit the corresponding computation.

Moreover, one can show that the global error $\mathbf{e}_N = \mathbf{y}_N - \mathbf{y}(t_N)$ of method (5.2) satisfies the error recursion formula

$$\mathbf{e}_{N+1} = \mathcal{J}^N \mathbf{e}_1 + \sum_{n=1}^{N} \mathcal{J}^{N-n} \widehat{\mathcal{M}}_n \mathbf{e}_n + \sum_{n=1}^{N} \mathcal{J}^{N-n} \hat{\mathbf{d}}_{n+1}\,, \qquad N \ge 1\,, \tag{5.63}$$

with the error terms

$$\hat{\mathbf{d}}_{n+1} = \big(\mathcal{J} + \widehat{\mathcal{M}}_n\big)\mathbf{y}(t_n) - \mathbf{y}(t_{n+1})\,, \tag{5.64}$$

cf. Lemma 12.

Because the starting step of the $\widehat{\phi}$-variant of the adiabatic midpoint rule is also conducted by the adiabatic Euler method (5.3) the estimate (5.11) holds for the first summand in (5.63). In addition, we obtain with (5.62) the estimate

$$\left\| \sum_{n=1}^{N} \mathcal{J}^{N-n} \widehat{\mathcal{M}}_n \mathbf{e}_n \right\|_{\ell^1} \le \tau C(M_0^y) \sum_{n=1}^{N} \|\mathbf{e}_n\|_{\ell^1} \tag{5.65}$$

analogously to (5.12). Hence, it remains to derive estimates for the third term of the recursion formula (5.63) in each setting of Theorem 11.

Again, we denote the m-entry of a sequence $\mathbf{z} \coloneqq (\mathbf{z}_m)_{m\in\mathbb{Z}}$ by $\{z\}_m$.

5.4.1. Proof of part (i)

Proving the linear convergence of the $\widehat{\phi}$-variant of the adiabatic midpoint rule with a constant independent of ε is straightforward. According to (5.64) all non-zero entries of $\hat{\mathbf{d}}_{n+1}$ are of the form

$$\begin{aligned}\{\hat{d}_{n+1}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}} y_j^{(n)}\overline{y}_k^{(n)} y_l(t_n)\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s \\ + y_m(t_{n-1}) - y_m(t_{n+1})\,. \end{aligned} \tag{5.66}$$

Substituting the expansion

$$\begin{aligned} y_m(t_{n+1}) = y_m(t_{n-1}) + \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}} Y_{jkl}(t_n)\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s \\ + \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} Y'_{jkl}(\sigma)\,\mathrm{d}\sigma\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s \end{aligned}$$

yields the partition

$$\{\hat{d}_{n+1}\}_m = \{\hat{d}_{n+1}^{(1)}\}_m - \{\hat{d}_{n+1}^{(2)}\}_m\,, \tag{5.67}$$

with

$$\{\hat{d}_{n+1}^{(1)}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\left(y_j^{(n)}\overline{y}_k^{(n)} - y_j(t_n)\overline{y}_k(t_n)\right)y_l(t_n)\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s$$

and

$$\{\hat{d}_{n+1}^{(2)}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} Y'_{jkl}(\sigma)\,\mathrm{d}\sigma\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s\,. \tag{5.68}$$

As in (5.17), we obtain with the boundedness of the numerical solution (5.62) the estimate

$$\left\|\hat{\mathbf{d}}_{n+1}^{(1)}\right\|_{\ell^1} \le \tau C(M_0^y)\left\|\mathbf{e}_n\right\|_{\ell^1}\,. \tag{5.69}$$

Moreover, Lemma 22 (Appendix A) implies the bound

$$\left\|\hat{\mathbf{d}}_{n+1}^{(2)}\right\|_{\ell^1} \le \tau^2 C(M_0^y)\,, \tag{5.70}$$

and hence we arrive at

$$\left\|\sum_{n=1}^{N}\mathcal{J}^{N-n}\hat{\mathbf{d}}_{n+1}\right\|_{\ell^1} \le \tau C(M_0^y)\sum_{n=1}^{N}\left\|\mathbf{e}_n\right\|_{\ell^1} + \tau C(M_0^y)\,. \tag{5.71}$$

Now, combining (5.11), (5.69) and (5.71) with the recursion formula (5.63), and applying the discrete Gronwall lemma yields

$$\left\|\mathbf{e}_{N+1}\right\|_{\ell^1} \le \tau C(T, M_0^y)e^{TC(M_0^y)}$$

completing the proof of part (i).

5.4.2. Proof of part (ii)

Let $\tau = \varepsilon/k$ for $k \in \mathbb{N}$. Similar to the proof of part (ii) of Theorem 10 in Section 5.3.2, we now aim for improving the estimate (5.71) by exploiting cancellation effects of highly oscillatory double integrals in the error terms. In the $\widehat{\phi}$-variant of the adiabatic midpoint rule these double integrals are of the form

$$\widehat{\mathcal{I}}_n = \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \exp\Big(-\mathrm{i}\omega\widehat{\phi}\left(\tfrac{\sigma}{\varepsilon}\right)\Big)\,\mathrm{d}\sigma \exp\Big(-\mathrm{i}\tilde{\omega}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\Big)\,\mathrm{d}s\,. \tag{5.72}$$

The following lemma contains a suitable adaptation of Lemma 13.

Lemma 14. *Let $k, L \in \mathbb{N}$ and suppose that $\tau = \varepsilon/k$. Further, we consider the double integral $\widehat{\mathcal{I}}_n$ given in* (5.72) *and a sequence $(a_n)_{n\in\mathbb{N}}$. Then, with the sequence $(\hat{a}_n)_{n\in\mathbb{N}}$ given by*

$$\hat{a}_n = \exp\big(-\mathrm{i}(\omega+\tilde{\omega})\alpha t_n\big)a_n\,,$$

we have the estimates

$$(i)\qquad \left|\sum_{\substack{n=1\\ n\ \text{even}}}^{2kL-1} a_n\widehat{\mathcal{I}}_n\right| \le 2\varepsilon\tau\sum_{n=1}^{kL-2}\left|\hat{a}_{2(n+1)}-\hat{a}_{2n}\right| + \alpha\tau^3 C\sum_{\substack{n=1\\ n\ \text{even}}}^{2kL-1}\Big(|\omega a_n| + |\tilde{\omega}a_n|\Big)$$

and

$$(ii)\qquad \left|\sum_{\substack{n=1\\ n\ \text{odd}}}^{2kL-1} a_n\widehat{\mathcal{I}}_n\right| \le 2\varepsilon\tau\sum_{n=1}^{kL-2}\left|\hat{a}_{2n+1}-\hat{a}_{2n-1}\right| + \alpha\tau^3 C\sum_{\substack{n=1\\ n\ \text{odd}}}^{2kL-1}\Big(|\omega a_n| + |\tilde{\omega}a_n|\Big)\,.$$

Proof. By the definition (2.18), we obtain for each ω the expansion

$$\exp\left(-\mathrm{i}\omega\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) = \Big(\exp\left(-\mathrm{i}\omega\alpha t_n\right) - \mathrm{i}\omega\alpha\int_{t_n}^{s}\exp\left(-\mathrm{i}\omega\alpha\xi\right)\mathrm{d}\xi\Big)\exp\left(-\mathrm{i}\omega\phi\left(\tfrac{s}{\varepsilon}\right)\right) \tag{5.73}$$

allowing us to partition (5.72) into

$$\widehat{\mathcal{I}}_n = \exp\left(-\mathrm{i}(\omega+\tilde{\omega})\alpha t_n\right)\mathcal{I}_n - \mathrm{i}\alpha(\omega R^{(1)} + \tilde{\omega}R^{(2)})\,,$$

with

$$R^{(1)} = \int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s}\int_{t_n}^{\sigma}\exp\left(-\mathrm{i}\omega\alpha\xi\right)\mathrm{d}\xi\exp\left(-\mathrm{i}\omega\phi\left(\tfrac{\sigma}{\varepsilon}\right)\right)\mathrm{d}\sigma\exp\Big(-\mathrm{i}\tilde{\omega}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\Big)\,\mathrm{d}s$$

and

$$R^{(2)} = \exp\left(-\mathrm{i}\omega\alpha t_n\right)\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s}\exp\left(-\mathrm{i}\omega\phi\left(\tfrac{\sigma}{\varepsilon}\right)\right)\mathrm{d}\sigma$$
$$\int_{t_n}^{s}\exp\left(-\mathrm{i}\tilde{\omega}\alpha\xi\right)\mathrm{d}\xi\exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s\,.$$

Because

$$\left|R^{(1)}\right| \leq \tau^3 C \quad \text{and} \quad \left|R^{(2)}\right| \leq \tau^3 C\,,$$

we obtain inequality (i) by estimating

$$\left|\sum_{\substack{n=1\\ n \text{ even}}}^{2kL-1} a_n \widehat{\mathcal{I}}_n\right| \leq \left|\sum_{\substack{n=1\\ n \text{ even}}}^{2kL-1} \hat{a}_n \mathcal{I}_n\right| + \alpha\tau^3 C \sum_{\substack{n=1\\ n \text{ even}}}^{2kL-1} \Big(|\omega a_n| + |\tilde{\omega} a_n| \Big)\,,$$

and then applying Lemma 13 to the first sum. Inequality (ii) follows analogously. □

We are now in a position to improve the estimate (5.71). According to (5.69), the estimate

$$\left\|\sum_{n=1}^{N} \mathcal{J}^{N-n} \hat{\mathbf{d}}_{n+1}\right\|_{\ell^1} \leq \tau C(M_0^y) \sum_{n=1}^{N} \|\mathbf{e}_n\|_{\ell^1} + \left\|\sum_{n=1}^{N} \mathcal{J}^{N-n} \hat{\mathbf{d}}^{(2)}_{n+1}\right\|_{\ell^1} \tag{5.74}$$

follows. As in (5.24), we continue by splitting off possible summands outside the 2ε time frames: subdividing $N = 2kL + n^*$ with $L \in \mathbb{N}$ and $n^* \in \{0, \ldots, 2k-1\}$ gives

$$\left\|\sum_{n=1}^{N} \mathcal{J}^{N-n} \hat{\mathbf{d}}^{(2)}_{n+1}\right\|_{\ell^1} \leq \left\|\sum_{n=1}^{2kL-1} \mathcal{J}^{N-n} \hat{\mathbf{d}}^{(2)}_{n+1}\right\|_{\ell^1} + \left\|\sum_{n=2kL}^{2kL+n^*} \mathcal{J}^{N-n} \hat{\mathbf{d}}^{(2)}_{n+1}\right\|_{\ell^1}.$$

By (5.70) and with $n^*\tau^2 \leq 2\tau\varepsilon$, we have

$$\left\|\sum_{n=2kL}^{2kL+n^*} \mathcal{J}^{N-n} \hat{\mathbf{d}}^{(2)}_{n+1}\right\|_{\ell^1} \leq \varepsilon\tau C(M_0^y)\,. \tag{5.75}$$

In order to estimate the remaining sum, we subdivide summands with odd and even indices due to the row-switching matrix $\mathcal{J}$, cf. (5.26). However, we will only consider the sum

$$\left\|\sum_{\substack{n=1\\ n \text{ odd}}}^{2kL-1} \hat{\mathbf{d}}^{(2)}_{n+1}\right\|_{\ell^1}$$

because an estimate for the sum over even indices follows analogously.

Definition (2.23) yields

$$Y'_{jkl}(\sigma) = y'_j(\sigma)\overline{y}_k(\sigma)y_l(\sigma) + y_j(\sigma)\overline{y}'_k(\sigma)y_l(\sigma) + y_j(\sigma)\overline{y}_k(\sigma)y'_l(\sigma)\,,$$

and thus we obtain the partition

$$\{\hat{d}^{(2)}_{n+1}\}_m = \{\widehat{T}^{(1)}_{n+1}\}_m + \{\widehat{T}^{(2)}_{n+1}\}_m + \{\widehat{T}^{(3)}_{n+1}\}_m\,,$$

with

$$\{\widehat{T}^{(1)}_{n+1}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} y_j'(\sigma)\overline{y}_k(\sigma)y_l(\sigma)\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}\sigma\,\mathrm{d}s\,, \tag{5.76}$$

$$\{\widehat{T}^{(2)}_{n+1}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} y_j(\sigma)\overline{y}_k'(\sigma)y_l(\sigma)\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}\sigma\,\mathrm{d}s\,, \tag{5.77}$$

$$\{\widehat{T}^{(3)}_{n+1}\}_m = \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} y_j(\sigma)\overline{y}_k(\sigma)y_l'(\sigma)\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}\sigma\,\mathrm{d}s\,. \tag{5.78}$$

Henceforth, we solely estimate the term (5.76) because one can show similar bounds for the terms (5.77) and (5.78) analogously. Replacing $y_j'(\sigma)$ by the tDMNLS gives

$$\{\widehat{T}^{(1)}_{n+1}\}_m = -\sum_{I_m}\sum_{I_j}\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} Y_{pqrkl}(\sigma) \exp\left(-\mathrm{i}\omega_{[pqrj]}\widehat{\phi}\left(\tfrac{\sigma}{\varepsilon}\right)\right)\mathrm{d}\sigma\exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s\,, \tag{5.79}$$

with $Y_{pqrkl}(\sigma)$ defined in (5.41).

Now, we aim to apply Lemma 14. For fixed $m\in\mathbb{Z}$, $(j,k,l)\in I_m$ and $(p,q,r)\in I_j$, we write $\omega=\omega_{[pqrj]}$, $\tilde{\omega}=\omega_{[jklm]}$ and $Y(\sigma)=Y_{pqrkl}(\sigma)$ for short. Then, any summand of (5.79) reads

$$\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} Y(\sigma)\exp\left(-\mathrm{i}\omega\widehat{\phi}\left(\tfrac{\sigma}{\varepsilon}\right)\right)\mathrm{d}\sigma\exp\left(-\mathrm{i}\tilde{\omega}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s = Y(t_n)\widehat{\mathcal{I}}_n+\widehat{R}_n\,,$$

with $\widehat{\mathcal{I}}_n$ given in (5.72) and

$$\widehat{R}_n = \int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s}\int_{t_n}^{\sigma_1} Y'(\sigma_2)\,\mathrm{d}\sigma_2\exp\left(-\mathrm{i}\omega\widehat{\phi}\left(\tfrac{\sigma_1}{\varepsilon}\right)\right)\mathrm{d}\sigma_1\exp\left(-\mathrm{i}\tilde{\omega}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s\,.$$

It is clear that the estimate

$$\left|\widehat{R}_n\right|\le\tau^3C(M_0^y) \tag{5.80}$$

holds. Moreover, with the abbreviation

$$F(\sigma)=\exp\bigl(-\mathrm{i}(\omega+\tilde{\omega})\alpha\sigma\bigr)Y(\sigma)\,,$$

Lemma 14 implies the estimate

$$\left|\sum_{\substack{n=1\\ n\text{ odd}}}^{2kL-1} Y(t_n)\widehat{\mathcal{I}}_n\right|\le C(T)\max_{\sigma\in[0,T]}\left\{\varepsilon\tau\left|F'(\sigma)\right|+\tau^2\alpha\bigl(\,|\omega Y(\sigma)|+|\tilde{\omega}Y(\sigma)|\,\bigr)\right\},$$

cf. (5.46), and hence we conclude from Lemma 22 (Appendix A) that

$$\left\|\sum_{\substack{n=1\\ n\text{ odd}}}^{2kL-1}\widehat{\mathbf{T}}^{(1)}_{n+1}\right\|_{\ell^1}\le\varepsilon\tau\Bigl(C(T,M_0^y)+\alpha C(T,M_2^y)\Bigr)\,. \tag{5.81}$$

Ultimately, we obtain the estimate

$$\left\| \sum_{n=1}^{N} \mathcal{J}^{N-n} \hat{\mathbf{d}}_{n+1} \right\|_{\ell^1} \leq \tau C(M_0^y) \sum_{n=1}^{N} \|\mathbf{e}_n\|_{\ell^1} + \varepsilon\tau \Big(C(T, M_0^y) + \alpha C(T, M_2^y) \Big) . \quad (5.82)$$

Now, combining (5.11), (5.65), and (5.82) with the recursion formula (5.63), and applying the discrete Gronwall lemma yields part (ii).

5.4.3. Proof of part (iii)

We consider step-sizes $\tau = k\varepsilon$ with $k \in \mathbb{N}$. As in the proof of part (iii) of Theorem 10 in Section 5.3.3, the estimate

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \leq \frac{\varepsilon^2}{\delta} C(t_n, \alpha, M_0, M_2) + \left\| v(t_n) - y^{(n)} \right\|_{\ell^1} \quad (5.83)$$

follows from Theorem 3. Therefore, we treat the approximations of the tDMNLS by the $\widehat{\phi}$-variant of the adiabatic midpoint rule (5.2) as approximations of the limit system (3.9) and derive subsequently a suitable bound for this approach. We define

$$\tilde{\mathbf{d}}_{n+1} = \big(\mathcal{J} + \widehat{\mathcal{M}}_n\big)\mathbf{v}(t_n) - \mathbf{v}(t_{n+1}) \quad (5.84)$$

with $\mathbf{v}(t_n)$ given in (5.55).

One can show (cf. Lemma 12) that the global error $\mathbf{e}_n = \mathbf{v}_n - \mathbf{v}(t_n)$ satisfies the recursion formula

$$\mathbf{e}_{N+1} = \mathcal{J}^N \mathbf{e}_1 + \sum_{n=1}^{N} \mathcal{J}^{N-n} \widehat{\mathcal{M}}_n \mathbf{e}_n + \sum_{n=1}^{N} \mathcal{J}^{N-n} \tilde{\mathbf{d}}_{n+1} , \qquad N \geq 1 . \quad (5.85)$$

Because the bounds (5.11) and (5.65) are already at our disposal, it remains to estimate the third term in the recursion formula. By definition (5.84), any non-zero entry of $\tilde{\mathbf{d}}_{n+1}$ is of the form

$$\begin{aligned} \{\tilde{d}_{n+1}\}_m = \mathrm{i} \sum_{I_m} y_j^{(n)} \overline{y}_k^{(n)} v_l(t_n) \int_{t_{n-1}}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]} \widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \\ + v_m(t_{n-1}) - v_m(t_{n+1}) . \end{aligned} \quad (5.86)$$

Employing the Taylor expansion

$$V_{jkl}(s) = V_{jkl}(t_n) + (s - t_n) V'_{jkl}(t_n) + \int_{t_n}^{s} \int_{t_n}^{\sigma_1} V''_{jkl}(\sigma_2) \,\mathrm{d}\sigma_2 \,\mathrm{d}\sigma_1$$

in order to expand the exact solution

$$v_m(t_{n+1}) = v_m(t_{n-1}) + \mathrm{i} \sum_{I_m} \int_{t_{n-1}}^{t_{n+1}} V_{jkl}(s) \exp\big(-\mathrm{i}\omega_{[jklm]}\alpha s\big) \,\mathrm{d}s \int_0^1 \exp\big(\mathrm{i}\omega_{[jklm]}\delta\xi\big) \,\mathrm{d}\xi$$

of the limit system gives us the partition

$$\{\tilde{d}_{n+1}\}_m = \{\tilde{d}^{(1)}_{n+1}\}_m + \{\tilde{d}^{(2)}_{n+1}\}_m - \{\tilde{d}^{(3)}_{n+1}\}_m - \{\tilde{d}^{(4)}_{n+1}\}_m\,,$$

with

$$\begin{aligned}
\{\tilde{d}^{(1)}_{n+1}\}_m &= \mathrm{i}\sum_{I_m}\big(y_j^{(n)}\overline{y}_k^{(n)} - v_j(t_n)\overline{v}_k(t_n)\big)v_l(t_n)\int_{t_{n-1}}^{t_{n+1}}\exp\Big(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\Big)\,\mathrm{d}s\,,\\
\{\tilde{d}^{(2)}_{n+1}\}_m &= \mathrm{i}\sum_{I_m}V_{jkl}(t_n)\int_{t_{n-1}}^{t_{n+1}}\exp\left(-\mathrm{i}\omega_{[jklm]}\alpha s\right)\\
&\qquad\Big(\exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) - \int_0^1\exp\big(\mathrm{i}\omega_{[jklm]}\delta\xi\big)\,\mathrm{d}\xi\Big)\,\mathrm{d}s\,, \qquad (5.87)\\
\{\tilde{d}^{(3)}_{n+1}\}_m &= \mathrm{i}\sum_{I_m}V'_{jkl}(t_n)\int_0^1\exp\big(\mathrm{i}\omega_{[jklm]}\delta\xi\big)\,\mathrm{d}\xi\int_{t_{n-1}}^{t_{n+1}}(s-t_n)\exp\big(-\mathrm{i}\omega_{[jklm]}\alpha s\big)\,\mathrm{d}s\,,\\
\{\tilde{d}^{(4)}_{n+1}\}_m &= \mathrm{i}\sum_{I_m}\int_0^1\exp\big(\mathrm{i}\omega_{[jklm]}\delta\xi\big)\,\mathrm{d}\xi\\
&\qquad\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s}\int_{t_n}^{\sigma_1}V''_{jkl}(\sigma_2)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\exp\big(-\mathrm{i}\omega_{[jklm]}\alpha s\big)\,\mathrm{d}s\,.
\end{aligned}$$

On account of (5.62), we obtain the estimate

$$\left\|\tilde{\mathbf{d}}^{(1)}_{n+1}\right\|_{\ell^1} \le \tau C(M_0)\left\|\mathbf{e}_n\right\|_{\ell^1}\,. \qquad (5.88)$$

Moreover, Lemma 21 (Appendix A) implies

$$\left\|\tilde{\mathbf{d}}^{(4)}_{n+1}\right\|_{\ell^1} \le \tau^3\big(C(M_0^v) + \alpha C(M_2^v)\big)\,. \qquad (5.89)$$

Thanks to the expansion

$$\exp\left(-\mathrm{i}\omega\alpha s\right) = \exp\left(-\mathrm{i}\omega\alpha t_n\right) - \mathrm{i}\omega\alpha\int_{t_n}^{s}\exp\left(-\mathrm{i}\omega\alpha\sigma\right)\mathrm{d}\sigma\,,$$

we obtain

$$\begin{aligned}
\{\tilde{d}^{(3)}_{n+1}\}_m = \alpha\sum_{I_m}&\omega_{[jklm]}V'_{jkl}(t_n)\int_0^1\exp\big(\mathrm{i}\omega_{[jklm]}\delta\xi\big)\,\mathrm{d}\xi\\
&\int_{t_{n-1}}^{t_{n+1}}(s-t_n)\int_{t_n}^{s}\exp\big(-\mathrm{i}\omega_{[jklm]}\alpha\sigma\big)\,\mathrm{d}\sigma\,\mathrm{d}s\,,
\end{aligned}$$

where the leading order term vanishes due to the symmetry of the integral. Hence, the bound

$$\left\|\tilde{\mathbf{d}}^{(3)}_{n+1}\right\|_{\ell^1} \le \alpha\tau^3 C(M_2^v) \qquad (5.90)$$

follows with Lemma 21 (Appendix A). Combining (5.88)-(5.90) yields the bound

$$\begin{aligned}
\left\|\sum_{n=1}^{N}\mathcal{J}^{N-n}\tilde{\mathbf{d}}_{n+1}\right\|_{\ell^1} \le \tau C(M_0)\sum_{n=1}^{N}\left\|\mathbf{e}_n\right\|_{\ell^1} + \sum_{n=1}^{N}\left\|\tilde{\mathbf{d}}^{(2)}_{n+1}\right\|_{\ell^1}&\\
+ \tau^2\big(C(T,M_0^v) + \alpha C(T,M_2^v)\big)\,.& \qquad (5.91)
\end{aligned}$$

Acquiring a suitable estimate for the remaining sum over $\tilde{\mathbf{d}}_{n+1}^{(2)}$ requires special care. Here, the restriction to step-sizes $\tau = k\varepsilon$ for $k \in \mathbb{N}$ is crucial. We start by subdividing the sum into odd and even indices

$$\sum_{n=1}^{N} \left\| \tilde{\mathbf{d}}_{n+1}^{(2)} \right\|_{\ell^1} = \sum_{\substack{n=1 \\ n \text{ odd}}}^{N} \left\| \tilde{\mathbf{d}}_{n+1}^{(2)} \right\|_{\ell^1} + \sum_{\substack{n=1 \\ n \text{ even}}}^{N} \left\| \tilde{\mathbf{d}}_{n+1}^{(2)} \right\|_{\ell^1} . \tag{5.92}$$

First, we consider the sum over odd indices n. Because $\{\tilde{d}_{n+1}^{(2)}\}_m = 0$ if $\omega_{[jklm]} = 0$, we subsequently assume that $\omega_{[jklm]} \neq 0$ with no loss of generality. Now, we aim to apply part (iii) of Lemma 4 (Section 3.3) in order to estimate the difference in (5.87). For fixed $m \in \mathbb{Z}$ and $(j,k,l) \in I_m$ we write $\omega = \omega_{[jklm]}$ and $V(s) = V_{jkl}(s)$. Moreover, we define

$$f_\omega(s) \coloneqq \exp\left(-\mathrm{i}\omega\alpha s\right) .$$

By (5.87) any summand of $\tilde{\mathbf{d}}_{n+1}^{(2)}$ reads

$$\begin{aligned}
V(t_n) \int_{t_{n-1}}^{t_{n+1}} & f_\omega(s) \left(\exp\left(-\mathrm{i}\omega\phi\left(\tfrac{s}{\varepsilon}\right)\right) - \int_0^1 \exp\left(\mathrm{i}\omega\delta\xi\right) \mathrm{d}\xi \right) \mathrm{d}s \\
&= V(t_n) \int_{t_{n-1}}^{t_{n+1}} f_\omega(s) g_\omega\left(\tfrac{s}{\varepsilon}\right) \mathrm{d}s \\
&= \varepsilon V(t_n) \int_0^{2k} f_\omega(\varepsilon\sigma + t_{n-1}) g_\omega(\sigma)\, \mathrm{d}\sigma \\
&= \varepsilon V(t_n) \sum_{\kappa=1}^{k} \int_0^2 f_\omega\big(\varepsilon(\sigma + 2(\kappa-1)) + t_{n-1}\big) g_\omega(\sigma)\, \mathrm{d}\sigma \,,
\end{aligned}$$

where g_ω is the function from Lemma 4, given in (3.15). In particular, we used that g_ω is 2-periodic. Because $\left|\omega^{-1} f_\omega''(s)\right| = \alpha^2 |\omega|$, part (iii) of Lemma 4 implies

$$\left| \varepsilon V(t_n) \sum_{\kappa=1}^{k} \int_0^2 f_\omega\big(\varepsilon(\sigma + 2(\kappa-1)) + t_{n-1}\big) g_\omega(\sigma)\, \mathrm{d}\sigma \right| \leq \tau\alpha^2 \frac{\varepsilon^2}{\delta} C \left|\omega V(t_n)\right| \,,$$

and hence we obtain with Lemma 21 (Appendix A) the estimate

$$\sum_{\substack{n=1 \\ n \text{ odd}}}^{N} \left\| \tilde{\mathbf{d}}_{n+1}^{(2)} \right\|_{\ell^1} \leq \alpha^2 \frac{\varepsilon^2}{\delta} C(T, M_2^v) \,. \tag{5.93}$$

For the sum over even indices n, the estimate

$$\sum_{\substack{n=1 \\ n \text{ even}}}^{N} \left\| \tilde{\mathbf{d}}_{n+1}^{(2)} \right\|_{\ell^1} \leq \alpha^2 \frac{\varepsilon^2}{\delta} C(T, M_2^v) \tag{5.94}$$

follows analogously with part (iv) of Lemma 4 and minor modifications.

Ultimately, we obtain the estimate

$$\left\| \sum_{n=1}^{N} \mathcal{J}^{N-n} \tilde{\mathbf{d}}_{n+1} \right\|_{\ell^1} \leq \tau C(M_0) \sum_{n=1}^{N} \|\mathbf{e}_n\|_{\ell^1} + \big(\tfrac{\varepsilon^2}{\delta} + \tau^2\big)\big(C(T, M_0^v) + (\alpha + \alpha^2) C(T, M_2^v)\big) . \tag{5.95}$$

Now, substituting (5.11), (5.65) and (5.95) into the recursion formula (5.85) and applying Gronwall's lemma yields the desired bound for the approximations of the $\widehat{\phi}$-variant of the adiabatic midpoint rule considered as approximations of the limit system. In particular, we observe that for $\alpha = 0$ the constant improves as specified.

□

Remark. Again, we require different levels of regularity for the initial value y_0 in the proofs for both variants of the adiabatic midpoint rule because differentiating $\widehat{Y}_{jklm}$ instead of Y_{jkl} yields an additional factor $\omega_{[jklm]}$. Comparing part (i) of both proofs, the key difference is the estimate (5.70) in contrast to the corresponding estimate (5.19) resulting in higher regularity requirements. In part (ii) of the proof of Theorem 10 the term $\widehat{Y}_{jklm}$ leads to an additional term in (5.36). Ultimately, this results in the higher regularity requirements compared to part (ii) of the proof of Theorem 11 where the term does not appear. In particular, the absence of this term simplifies the proof of part (ii) of Theorem 11. In contrast, part (iii) of the proof of Theorem 10 is more straightforward than part (iii) of the proof of Theorem 11 due to the fact that we can exploit the symmetry of the integral in (5.58), and hence the second term in the expansion (5.59) vanishes. Conversely, we obtain additional terms in the proof of Theorem 11, here particularly the term (5.87) requires extra care.

CHAPTER 6

On second-order methods

As we have observed in the previous chapter, the adiabatic midpoint rule is not a genuine second-order method. It is possible to extend the construction ideas from Chapter 4 and 5 to construct second-order methods in principle. We introduce such a second-order method by refining the adiabatic Euler method (Chapter 4) in Section 6.1 and illustrate the convergence behavior by numerical examples. However, it turns out that second-order methods based on this construction idea are of little practical relevance due to fact that each time-step requires the computation of nested multiple sums implying exorbitant computational costs. Hence, we stop at the construction of the scheme and omit any rigorous error analysis in this chapter. As a secondary observation, constructing the second-order method points out an improvement of the ϕ-variant of the adiabatic Euler method and the adiabatic midpoint rule, respectively, by including an additional correction term into the numerical scheme – the α-correction, which we address in Section 6.2.

6.1. Construction

Our starting point is the equation (4.1). We use the fundamental theorem of calculus to expand the exact solution of the tDMNLS further via

$$\begin{aligned} y_m(t_{n+1}) = y_m(t_n) + \mathrm{i} \sum_{I_m} \widehat{Y}_{jklm}(t_n) \int_{t_n}^{t_{n+1}} \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \\ + \mathrm{i} \sum_{I_m} \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \widehat{Y}'_{jklm}(\sigma)\, \mathrm{d}\sigma \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s\,. \end{aligned} \tag{6.1}$$

Remark. Suitably expanding the exact solution y of the tDMNLS underlies several limitations: first, we recall that higher order derivatives of y do not exist due to the discontinuous coefficient function γ, see (1.2). Moreover, differentiating the exponential term $\exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\frac{s}{\varepsilon}\right)\right)$ with respect to s yields the factor $1/\varepsilon$, and thus should be avoided in order to obtain estimates that are independent of ε. We circumvent these limitations in the expansion (6.1) by solely fixing the term $\widehat{Y}_{jklm}(s)$ at $s = t_n$ and keeping the exponential phase term untouched.

In order to construct the second-order method, we aim to include a suitable approximation of the double integral term into the numerical scheme. By (5.36) we have

$$\begin{aligned}\widehat{Y}'_{jklm}(\sigma) = \Big(&y'_j(\sigma)\overline{y}_k(\sigma)y_l(\sigma) + y_j(\sigma)\overline{y}'_k(\sigma)y_l(\sigma)\\ &+ y_j(\sigma)\overline{y}_k(\sigma)y'_l(\sigma)\Big)\exp\left(-\mathrm{i}\omega_{[jklm]}\alpha\sigma\right) - \mathrm{i}\omega_{[jklm]}\alpha\widehat{Y}_{jklm}(\sigma)\,. \qquad (6.2)\end{aligned}$$

The double integral can now be approximated by substituting the derivatives of y by the tDMNLS and fixing the non-oscillating terms at $\sigma = t_n$ while retaining the double integral over the remaining oscillatory phase terms – the construction idea of the adiabatic Euler method. Moreover, we observe that the summation indices j and l are symmetric, i.e. we have

$$\sum_{I_m} y'_j(\sigma)\overline{y}_k(\sigma)y_l(\sigma)\exp\left(-\mathrm{i}\omega_{[jklm]}\alpha\sigma\right) = \sum_{I_m} y_j(\sigma)\overline{y}_k(\sigma)y'_l(\sigma)\exp\left(-\mathrm{i}\omega_{[jklm]}\alpha\sigma\right)\,,$$

and hence there are only three different summands (not four) in (6.2). With this approach we obtain the one-step method

$$\begin{aligned}y^{(n+1)} = y^{(n)} + \mathrm{i}\sum_{I_m}\widehat{Y}^{(n)}_{jklm}\int_{t_n}^{t_{n+1}}&\left(1 - \mathrm{i}\omega_{[jklm]}\alpha(s-t_n)\right)\exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s\\ &-2\sum_{I_m}\sum_{I_j}\widehat{F}^{(n)}_{jklpqr}\tilde{I}_n(\omega_{[pqrj]},\omega_{[jklm]})\\ &+\sum_{I_m}\sum_{I_k}\widehat{G}^{(n)}_{jklpqr}\tilde{I}_n(-\omega_{[pqrk]},\omega_{[jklm]})\,, \qquad (6.3)\end{aligned}$$

where we use the abbreviations

$$\begin{aligned}\widehat{F}^{(n)}_{jklpqr} &= \overline{y}^{(n)}_k y^{(n)}_l y^{(n)}_p \overline{y}^{(n)}_q y^{(n)}_r \exp\left(-\mathrm{i}(\omega_{[jklm]} + \omega_{[pqrj]})\alpha t_n\right)\,,\\ \widehat{G}^{(n)}_{jklpqr} &= y^{(n)}_j y^{(n)}_l \overline{y}^{(n)}_p y^{(n)}_q \overline{y}^{(n)}_r \exp\left(-\mathrm{i}(\omega_{[jklm]} - \omega_{[pqrk]})\alpha t_n\right)\end{aligned}$$

and

$$\tilde{I}_n(\tilde{\omega},\omega) = \int_{t_n}^{t_{n+1}}\int_{t_n}^{s}\exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{\sigma}{\varepsilon}\right)\right)\exp\left(-\mathrm{i}\omega\phi\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}\sigma\,\mathrm{d}s. \qquad (6.4)$$

Remark. One can show that fixing the non-oscillating terms at $\sigma = t_n$ in (6.2) yields remainder terms in $\mathcal{O}(\tau^3)$ with a constant that is independent of ε, and hence (after establishing stability) employ Lady Windermere's fan in order to prove that the method (6.3) is a second-order method uniformly in ε, cf. Section 4.3.

Method (6.3) is one example of a genuine second-order scheme for the tDMNLS. Here, all exponential terms containing α are fixed at t_n. Naturally, one can keep these terms inside the integral in order to obtain additional variants of the method, cf. Section 4.1 and Section 5.1. Moreover, one can use the adiabatic midpoint rule (Chapter 5) instead of the adiabatic Euler method as a basis for a second-order two-step method. However, all these approaches lead to a similar structure of nested multiple sums implying exorbitant computational costs already for moderately many points for the space-discretization.

In addition to computing the already known integral from the adiabatic Euler method (Chapter 4), each time-step of method 6.3 requires evaluating the integral

$$\int_{t_n}^{t_{n+1}} (s - t_n) \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s \tag{6.5}$$

and the double integral (6.4). However, we observe that the integral (6.5) is the special case $\tilde{\omega} = 0$ of (6.4). Moreover, the double integral (6.4) can be computed exactly by a suitable decomposition of the integration interval at multiples of ε. Although we have fixed all exponentials containing α at t_n (i.e. despite we have periodic integrands) this computation is rather tedious and shifted into Appendix C.

We conclude this section by a numerical example illustrating the accuracy of the scheme (6.3): we consider the tDMNLS with[1] $\alpha = 0.1$, $\delta = 0.1$ and $T = 1$ with the initial value $u_0(x) = e^{-3x^2}e^{3\mathrm{i}x}$ for $\varepsilon = 0.01, 0.005, 0.002$. For this experiment, we reduce the number of grid points in the interval $[-\pi, \pi]$ to 16 equidistant points due to the increase in computational time owed to the nested multiple sum structure.

Figure 6.1 shows the accuracy of the method (6.3) for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). In addition, the accuracy of the Strang splitting method is shown for comparison. The dashed blue line is a reference line for order two, and the black vertical line highlights the value $\tau = \varepsilon$. We observe second-order accuracy of the method (6.3) in all three panels suggesting second-order convergence of the method uniformly in ε.

Remark. There are some irregularities in the accuracy especially for small step-sizes τ in the top right panel of Figure 6.1, which we tacitly blame on round-off errors in the computation of the highly oscillatory double integral after excessively testing our implementation.

[1] In order to ensure that the accuracy of the reference solution is precise enough to be considered exact, we use $\delta = 0.1$ instead of $\delta = 1$ for this experiment. Otherwise, the second-order method achieves an accuracy higher than 10^{-9} for very small steps. In this regime, the reference solution reaches its accuracy limit leading to nonsensical results for the numerical experiments.

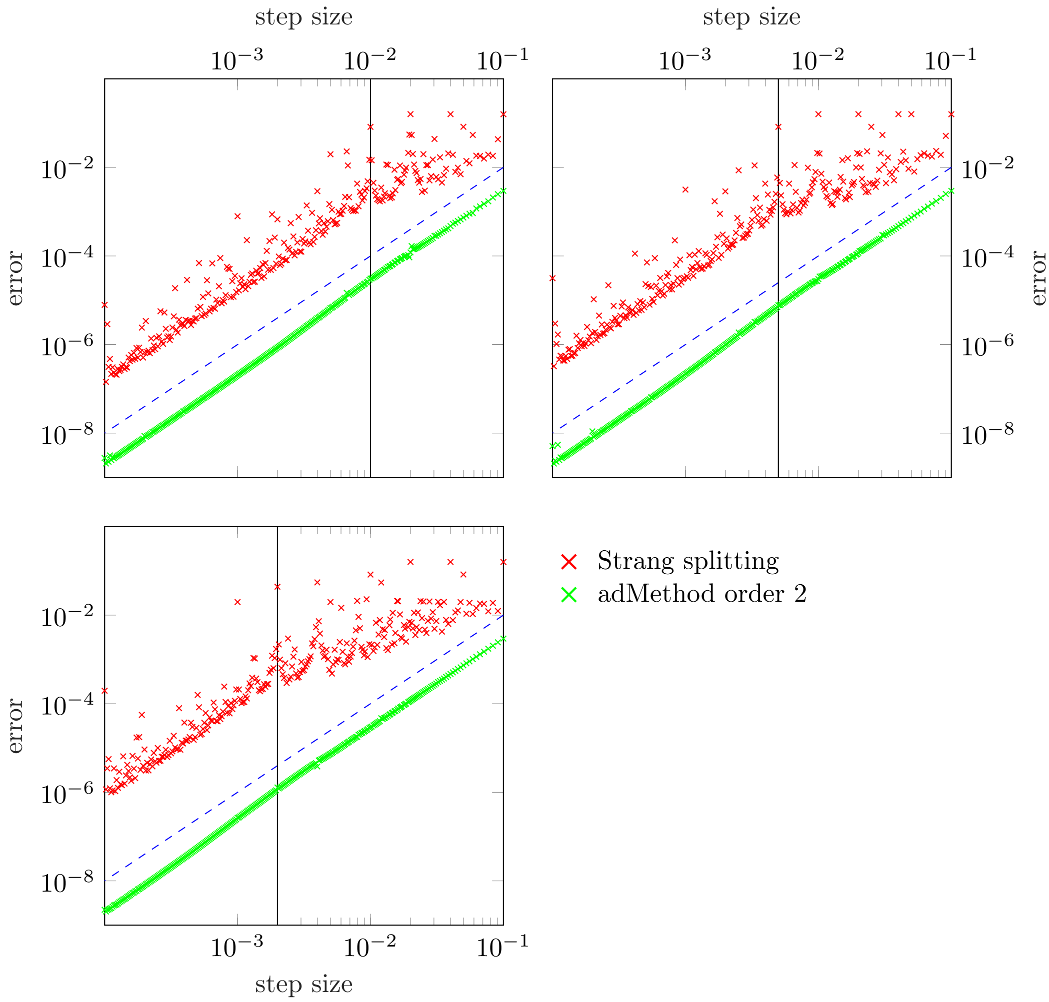

Figure 6.1: Maximal ℓ_0^2-error over time of the second-order method (6.3) for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). The dashed blue line is a reference line for order two. The black vertical line is at $\tau = \varepsilon$.

6.2. The α-correction

Despite the minor setback of the previous section, the construction of the method (6.3) points out a natural way to improve the numerical scheme of the ϕ-variants of the adiabatic Euler method (4.3) and of the adiabatic midpoint rule (5.2): we include the uncritical term (the term without any derivatives of y) of the double integral (6.1) into the respective numerical scheme. This idea gives rise to another variant for each method:

the adiabatic Euler method with α-correction

$$y^{(n+1)} = y^{(n)} + \mathrm{i} \sum_{I_m} \widehat{Y}^{(n)}_{jklm} \int_{t_n}^{t_{n+1}} \big(1 - \mathrm{i}\omega_{[jklm]}\alpha(s - t_n)\big) \exp\big(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\big)\, \mathrm{d}s\,, \tag{6.6}$$

the adiabatic midpoint rule with α-correction

$$y^{(n+1)} = y^{(n-1)} + \mathrm{i} \sum_{I_m} \widehat{Y}^{(n)}_{jklm} \int_{t_{n-1}}^{t_{n+1}} \big(1 - \mathrm{i}\omega_{[jklm]}\alpha(s - t_n)\big) \exp\big(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\big)\, \mathrm{d}s\,. \tag{6.7}$$

Clearly, including the α-correction in the scheme does not improve the order of the method. One can show that the methods (6.6) and (6.7) fulfill the same error bounds (with the same regularity requirements) as the corresponding ϕ-variants of the method (see Theorem 6 and Theorem 10) by minor modifications of the respective proofs. However, approximating an additional term from the double integral (6.1) suggests a smaller error constant of the global error bound.

Moreover, the computation of the double integral in Lemma 24 (Appendix C) implies that we have

$$\int_{2L}^{2L+2} \sigma \exp\left(-\mathrm{i}\omega\phi(\sigma)\right) \mathrm{d}\sigma = (4L+2)\frac{\exp(\mathrm{i}\omega\delta) - 1}{\mathrm{i}\omega\delta} \quad \text{for} \quad L \in \mathbb{N}\,,$$

and hence, the periodic integrand still allows us to implement the additional integral from the α-correction with constant complexity with respect to ε, cf. Section 4.1. Here, it is useful to decompose the integral at multiples of 2ε instead of multiples of ε, i.e. to employ the relation (4.7) with $p = 2L$.

Remark. We recall that the $\widehat{\phi}$-variant and the ϕ-variant of the adiabatic Euler method yield almost the same accuracy in our numerical examples, cf. Section 4.2.1. Likewise, there is no visible advantage (or disadvantage) of the adiabatic Euler method with α-correction in our experiments. For this reason, we omit numerical examples for this additional variant.

In the following, we investigate the behavior of the α-correction for the adiabatic midpoint rule. We revisit the numerical example from Section 5.2. Therefore, we consider the tDMNLS with $\alpha = 0.1$, $T = 1$, $\delta = 1$, the initial value $u_0(x) = e^{-3x^2}e^{3ix}$ with 64 equidistant grid points in the interval $[-\pi, \pi]$ and $\varepsilon = 0.01, 0.005, 0.002$. To this setting we apply all three variants, (5.1), (5.2) and (6.7), of the adiabatic midpoint rule. The step-sizes τ are chosen exclusively as integer multiples and integer fractions of ε in accordance with part (ii) and (iii) of Theorem 10 and 11. The reference solution is computed by the Strang splitting method with a large number of steps ($\approx 10^6$).

Figure 6.2 shows the accuracy of the three variants of the adiabatic midpoint rule for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). The black vertical line highlights the value $\tau = \varepsilon$. Whereas all methods yield almost the same accuracy in the regime $\tau > \varepsilon$ (right of the black line), the accuracy of the ϕ-variant of the adiabatic midpoint rule is smaller than the accuracy of the $\widehat{\phi}$-variant and of the variant with α-correction in the regime $\tau < \varepsilon$ (left of the black line). Here, we observe that the adiabatic midpoint rule with α-correction yields almost the same accuracy than the $\widehat{\phi}$-variant of the method.

Figure 6.3 shows the corresponding computational times for the previous experiment. We observe that the α-correction entails only a negligible increase in computational cost compared to the ϕ-variant but has significantly lower computational costs than the ϕ-variant in the regime $\tau > \varepsilon$, cf. Section 4.2.1.

Conclusion. The α-correction potentially lowers the constant of the global error bound, whereas it hardly increases the computational cost in relation to the ϕ-variant. In our example it yields almost the same accuracy as the $\widehat{\phi}$-variant of the adiabatic method with the lower computational costs from the ϕ-variant. Therefore, one should prefer the ϕ-variant with α-correction over the corresponding $\widehat{\phi}$-variant of the method provided the higher regularity requirements are not crucial.

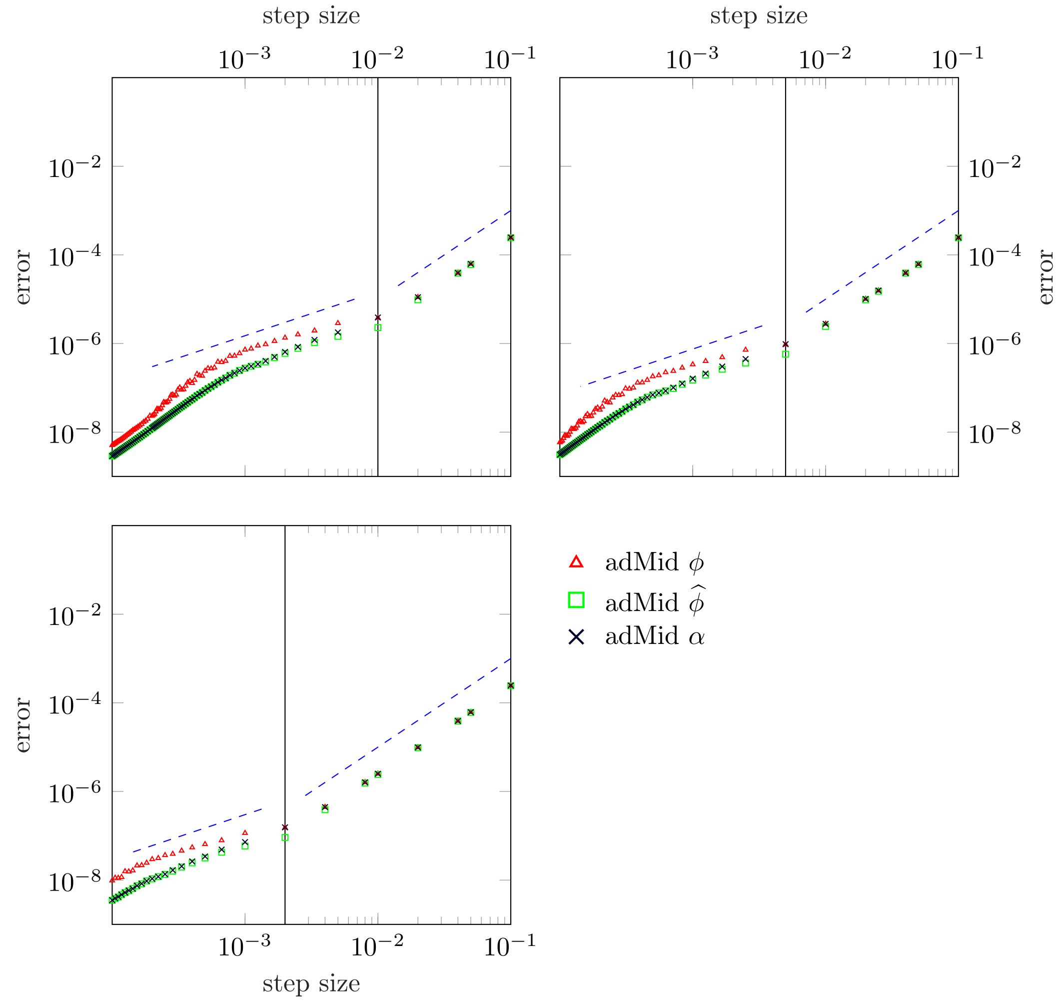

Figure 6.2: Maximal ℓ_0^2-error over time of the adiabatic midpoint rule in variant (5.1), (5.2) and (6.7) for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). The black vertical line is at $\tau = \varepsilon$. The step sizes τ are integer multiples and integer fractions of ε.

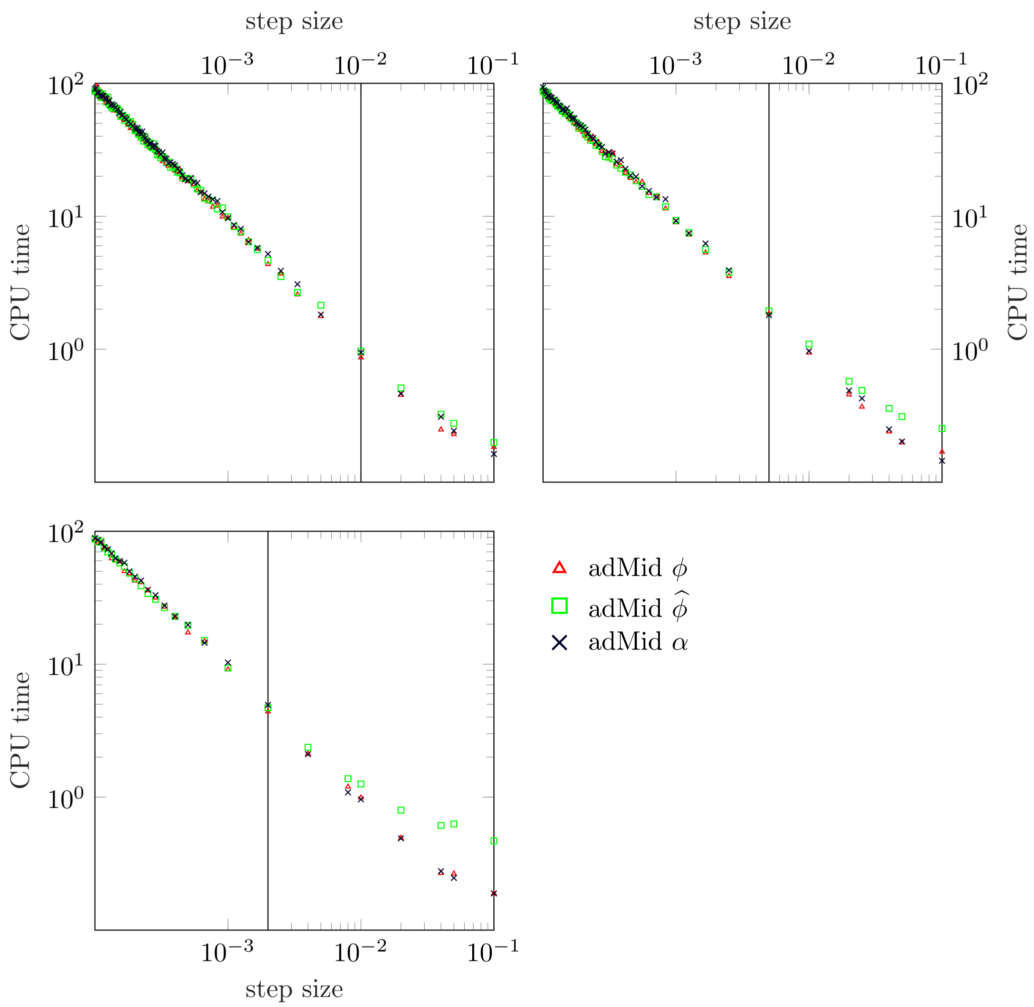

Figure 6.3: Computational time of the adiabatic midpoint rule in the variants (5.1), (5.2) and (6.7) for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). The black vertical line is at $\tau = \varepsilon$.

CHAPTER 7

The adiabatic exponential Euler method

In Chapters 4 and 5, we have constructed first novel numerical methods for the tDMNLS and identified key features of the equation allowing us to exploit the highly oscillatory behavior of the error terms. This chapter is devoted to an alternative approach for constructing numerical methods to approximate solutions of the tDMNLS leading us to exponential integrators. These exponential integrators appear to posses significantly smaller error constants in the global error bound in ℓ^1 and, in addition, preserve the ℓ^2_0-norm of the initial value over time. The price for this benefit is, however, the computation of one matrix exponential in each time step. Again, we start by constructing a first-order scheme (Section 7.1) to gain insight into the construction idea and, in particular, in the error analysis of this new class of methods. We state and discuss the result of our error analysis in Section 7.2, whereas the proof is postponed to Section 7.3.

7.1. Construction

Our exponential methods make use of a reformulation of the tDMNLS based on (5.5), i.e. on the definition

$$\left\{A\left(t, \tfrac{s}{\varepsilon}, \mu\right) z\right\}_m = \mathrm{i} \sum_{I_m} \mu_j \bar{\mu}_k z_l \exp\left(-\mathrm{i}\omega_{[jklm]}(\alpha t + \phi\left(\tfrac{s}{\varepsilon}\right))\right)$$

for two sequences $\mu = (\mu_m)_{m\in\mathbb{Z}}$ and $z = (z_m)_{m\in\mathbb{Z}}$ in $\mathbb{C}$. If we define

$$\widehat{A}(s,\mu)z \coloneqq A\left(s, \tfrac{s}{\varepsilon}, \mu\right) z\,, \tag{7.1}$$

then the tDMNLS reads

$$y'(t) = \widehat{A}\big(t, y(t)\big)y(t)\,. \tag{7.2}$$

This formulation of the tDMNLS is the starting point for constructing all subsequent exponential methods.

For a better understanding of the construction idea of the adiabatic exponential Euler method it is useful to briefly recapitulate the basic idea of *Magnus integrators*, cf. [10,36]. For this purpose, we follow the explanations from [34]. We consider for a moment the linear differential equation

$$\psi'(t) = A(t)\psi(t)\,, \qquad \psi(0) = \psi_0\,, \tag{7.3}$$

where $A(t)$ is a time-dependent, skew-Hermitian matrix. The idea of Magnus consists of deriving suitable matrices $\Omega_n[\tau]$ such that the solution of (7.3) can be written in terms of

$$\psi(t_n+\tau) = \exp\big(\Omega_n[\tau]\big)\psi(t_n)\,, \qquad n = 0,1,\dots\,. \tag{7.4}$$

It turns out that these matrices $\Omega_n[\tau]$ are given by the *Magnus expansion*

$$\begin{aligned}\Omega_n[\tau] = \int_0^\tau A(t_n+s)\,\mathrm{d}s - \frac{1}{2}\bigg(&\int_0^\tau \int_0^s A(t_n+\sigma)\,\mathrm{d}\sigma A(t_n+s)\,\mathrm{d}s \\ &- \int_0^\tau A(t_n+s)\int_0^s A(t_n+\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s\bigg) + \cdots\,.\end{aligned}$$

Now, numerical methods for (7.3) can be constructed by truncating the series and approximating the integrals via quadrature formulas. This approach results in (interpolatory) Magnus integrators.

In the following, we adapt the basic idea of Magnus integrators for the tDMNLS (7.2). As a first step, we formally linearize the equation in terms of

$$y'(t) \approx \widehat{A}\big(t, y(t_n)\big)y(t)\,, \qquad t \in [t_n, t_{n+1}] \tag{7.5}$$

by fixing the two entries of y contained in $\widehat{A}$ at $t = t_n$. Now, we aim for a suitable counterpart for the matrices $\Omega_n[\tau]$ allowing us to express the solution of (7.5) by means of an exponential, cf. (7.4). However, there are additional aspects of the tDMNLS that require special care. First, the tDMNLS is an ODE system with infinitely many equations, and hence simply considering $\widehat{A}\big(t, y(t_n)\big)$ as a matrix is inadequate[1]. Next, the term $\widehat{A}\big(t, y(t_n)\big)$ still contains highly oscillatory phases. In order to obtain estimates with constants that are independent of ε the involved integrals cannot simply be approximated by quadrature formulas.

Therefore, we establish a suitable framework for our approach and start by investigating properties of (7.1) in the next lemma.

[1] In particular, we require estimates that are independent of the space discretization.

Lemma 15. *For fixed $\mu \in \ell^1$ with $M := \|\mu\|_{\ell^1}$, it holds that*

(i) the operator $\widehat{A}(t,\mu)\colon \ell^1 \to \ell^1$ is bounded and

$$\left\|\widehat{A}(t,\mu)z\right\|_{\ell^1} \leq C(M)\,\|z\|_{\ell^1}\ , \quad \textit{for} \quad z \in \ell^1 \quad \textit{and} \quad t \in [0,T]\,.$$

(ii) the operator $\widehat{A}(t,\mu)\colon \ell^2 \to \ell^2$ is bounded and

$$\left\|\widehat{A}(t,\mu)z\right\|_{\ell^2_0} \leq C(M)\|z\|_{\ell^2_0}\,, \quad \textit{for} \quad z \in \ell^2_0 \quad \textit{and} \quad t \in [0,T]\,.$$

(iii) the operator $\widehat{A}(t,\mu)\colon \ell^2 \to \ell^2$ is skew adjoint.

Proof. Assertion (i) follows from

$$\left\|\widehat{A}(t,\mu)z\right\|_{\ell^1} \leq \sum_{m\in\mathbb{Z}}\sum_{I_m} |\mu_j\overline{\mu}_k z_l| \leq C(M)\,\|z\|_{\ell^1}\ ,$$

cf. Lemma 2. In order to prove the assertions (ii) and (iii), we define

$$\hat{a}_{m,l}(t) := \sum_{\substack{(j,k)\in\mathbb{Z}^2\\ j-k=m-l}} \mu_j\overline{\mu}_k \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{t}{\varepsilon}\right)\right) \quad \text{for} \quad m,l \in \mathbb{Z}\,.$$

This allows us to write

$$\{\widehat{A}(t,\mu)z\}_m = \sum_{l\in\mathbb{Z}} \hat{a}_{m,l}(t)z_l\,.$$

Because we have the estimate

$$\sum_{m\in\mathbb{Z}}\sum_{l\in\mathbb{Z}} |\hat{a}_{m,l}(t)| \leq M^2\,,$$

the assertion (ii) follows from the Cauchy-Schwarz inequality via

$$\begin{aligned}
\|\widehat{A}(t,\mu)z\|^2_{\ell^2_0} &\leq \sum_{m\in\mathbb{Z}}\left(\sum_{l\in\mathbb{Z}}|\hat{a}_{m,l}(t)z_l|\right)^2 \\
&= \sum_{m\in\mathbb{Z}}\left(\sum_{l\in\mathbb{Z}}\sqrt{|\hat{a}_{m,l}(t)|}\sqrt{|\hat{a}_{m,l}(t)|}\,|z_l|\right)^2 \\
&\leq \sum_{m\in\mathbb{Z}}\left(\sum_{l\in\mathbb{Z}}|\hat{a}_{m,l}(t)|\right)\left(\sum_{l\in\mathbb{Z}}|\hat{a}_{m,l}(t)|\,|z_l|^2\right) \\
&\leq M^4\|z\|^2_{\ell^2_0}\,.
\end{aligned}$$

Furthermore, we have the relation

$$
\begin{aligned}
-\overline{\hat{a}}_{l,m}(t) &= \mathrm{i} \sum_{\substack{(j,k)\in\mathbb{Z}^2\\ j-k=l-m}} \overline{\mu}_j \mu_k \exp\left(\mathrm{i}(j^2-k^2-m^2+l^2)\widehat{\phi}\left(\tfrac{t}{\varepsilon}\right)\right)\\
&= \mathrm{i} \sum_{\substack{(j,k)\in\mathbb{Z}^2\\ k-j=m-l}} \overline{\mu}_j \mu_k \exp\left(-\mathrm{i}(k^2-j^2+m^2-l^2)\widehat{\phi}\left(\tfrac{t}{\varepsilon}\right)\right) ,
\end{aligned}
$$

and hence interchanging the summation indices j and k shows that

$$
-\overline{\hat{a}}_{l,m}(t) = \hat{a}_{m,l}(t) \,. \tag{7.6}
$$

Finally, the assertion (iii) follows via

$$
\begin{aligned}
\langle \widehat{A}(t,\mu)z, x\rangle = \sum_{m\in\mathbb{Z}}\sum_{l\in\mathbb{Z}} \hat{a}_{m,l}(t) z_l \overline{x}_m &= -\sum_{m\in\mathbb{Z}}\sum_{l\in\mathbb{Z}} \overline{\hat{a}}_{l,m}(t) z_l \overline{x}_m\\
&= -\sum_{l\in\mathbb{Z}}\sum_{m\in\mathbb{Z}} z_l \overline{\hat{a}}_{l,m}(t) \overline{x}_m = -\langle z, \widehat{A}(t,\mu)x\rangle \,.
\end{aligned}
$$

□

On account of Lemma 15, the operator $\widehat{A}(t,\mu)\colon \ell^1 \to \ell^1$ is linear, non-autonomous and bounded for fixed $\mu \in \ell^1$. If we consider times $t_n = n\tau$ with $\tau > 0$ and $n \in \mathbb{N}$ and define for *fixed* n, τ and $\mu \in \ell^1$ with $M := \|\mu\|_{\ell^1}$ the linear operator

$$
\widehat{\mathcal{E}}_n[\tau,\mu] := \int_0^1 \widehat{A}(t_n + \tau\sigma, \mu)\,\mathrm{d}\sigma \,, \tag{7.7}
$$

then $\widehat{\mathcal{E}}_n[\tau,\mu]\colon \ell^1 \to \ell^1$ is again bounded with

$$
\left\|\widehat{\mathcal{E}}_n[\tau,\mu]z\right\|_{\ell^1} \le \left\|\widehat{A}(t,\mu)z\right\|_{\ell^1} \le C(M)\,\|z\|_{\ell^1} \,, \quad z\in\ell^1 \,,\ t\in[0,T] \,, \tag{7.8}
$$

see Lemma 15. Additionally, the operator $\widehat{\mathcal{E}}_n[\tau,\mu]$ is autonomous, and thus generates a uniformly continuous semigroup of bounded linear operators in ℓ^1 given by

$$
\exp\left(\sigma\widehat{\mathcal{E}}_n[\tau,\mu]\right) := \sum_{k=0}^{\infty} \frac{\left(\sigma\widehat{\mathcal{E}}_n[\tau,\mu]\right)^k}{k!} \,, \tag{7.9}
$$

cf. [52]. In the spirit of (7.4), we we can now approximate solutions of the tDMNLS by means of (7.9) via

the adiabatic exponential Euler method

$$
y^{(n+1)} = \exp\left(\tau\widehat{\mathcal{E}}_n\left[\tau, y^{(n)}\right]\right) y^{(n)} \,. \tag{7.10}
$$

Clearly, the operator in (7.10) depends on the numerical solution $y^{(n)}$, and thus changes in each time-step. In order ensure that the scheme is well-defined in terms of (7.9), we have to show that $y^{(n)} \in \ell^1$ for all $n \in \mathbb{N}$. This boundedness of the numerical solution is established in Section 7.3 (below).

The adiabatic Euler method (Chapter 4) and the method (7.10) are closely related: if we truncate the exponential series in (7.10) after the second summand, then we obtain

$$y^{(n+1)} = y^{(n)} + \tau \widehat{\mathcal{E}}_n[\tau, y^{(n)}] y^{(n)} \,. \tag{7.11}$$

Moreover, according to (7.7), we have

$$\tau \widehat{\mathcal{E}}_n\big[\tau, y^{(n)}\big] = \int_0^\tau \widehat{A}\big(t_n + \sigma, y^{(n)}\big)\, \mathrm{d}\sigma = \int_{t_n}^{t_{n+1}} \widehat{A}\big(\sigma, y^{(n)}\big)\, \mathrm{d}\sigma \,, \tag{7.12}$$

and hence we observe that the truncation (7.11) of the adiabatic exponential Euler method (7.10) is in fact the $\widehat{\phi}$-variant of the adiabatic Euler method (4.3). Furthermore, the relation (7.12) points out that the exponent in (7.10) coincides with the first term of the nonlinear Magnus expansion, cf. [10, Section 3.3]. Lastly, the equation (7.12) shows that the exponent in (7.10) can be computed exactly by Lemma 5.

Technically, the method (7.10) is the $\widehat{\phi}$-variant of the adiabatic exponential Euler method. Likewise, we can define the ϕ-variant via

$$\mathcal{E}_n[\tau, \mu] := \int_0^1 A\left(t_n, \tfrac{t_n + \tau\sigma}{\varepsilon}, \mu\right) \mathrm{d}\sigma \,.$$

Here, the term $\exp(-\mathrm{i}\omega_{[jklm]}\alpha t)$ is also fixed at $t = t_n$, which leads to a periodic integrand in the exponent of the method, cf. Section 4.1. However, one can observe in numerical experiments that the ϕ-variant does typically not improve the corresponding ϕ-variant of the adiabatic Euler method (4.2) significantly. Therefore, we omit a rigorous investigation of this method.

Moreover, we can construct an adiabatic exponential Euler method with α-correction by

$$\begin{aligned} \big\{\mathcal{E}_n^\alpha[\tau, \mu] z\big\}_m &:= \big\{\mathcal{E}_n[\tau, \mu] z\big\}_m \\ &\qquad - \mathrm{i}\alpha \sum_{I_m} \omega_{[jklm]} \mu_j \bar{\mu}_k z_l \int_0^1 \tau\sigma \exp\left(-\mathrm{i}\omega_{[jklm]} \phi\left(\tfrac{t_n + \tau\sigma}{\varepsilon}\right)\right) \mathrm{d}\sigma \,, \end{aligned}$$

where we include an additional correction term in the scheme, see Section 6.2. Since the α-correction does not improve the order of the method, we also omit a rigorous investigation of this variant of the adiabatic exponential Euler method.

Nevertheless, we include all three introduced variants of the adiabatic exponential Euler method in the numerical examples provided in the following section.

7.2. Properties: norm preservation and accuracy

One main difference between method (7.10) and the adiabatic Euler method is that the exponential method preserves the ℓ_0^2-norm of the initial value $y^{(0)}$. Provided $y^{(n)} \in \ell^1$ the operator $\exp\left(\tau\widehat{\mathcal{E}}_n[\tau, y^{(n)}]\right)$ is well-defined in terms of (7.9). In addition, Lemma 15 implies that $\widehat{\mathcal{E}}_n[\tau, y^{(n)}] \colon \ell_0^2 \to \ell_0^2$ is skew-adjoint and thus the semigroup $\Big(\exp\left(t\widehat{\mathcal{E}}_n[\tau, y^{(n)}]\right)\Big)_{t\in\mathbb{R}}$ is unitary in ℓ_0^2 by Stone's theorem. Hence, we have

$$\|y^{(n+1)}\|_{\ell_0^2} = \left\| \prod_{k=0}^{n} \exp\left(\tau\mathcal{E}_k[\tau, y^{(k)}]\right) y^{(0)} \right\|_{\ell_0^2} = \|y^{(0)}\|_{\ell_0^2}\,, \tag{7.13}$$

i.e. the ℓ_0^2-norm of the initial value $y^{(0)}$ is preserved. Analogously, one can establish the ℓ_0^2-invariance of the ϕ-variant and of the adiabatic exponential Euler method with α-correction.

The result of our error analysis of the method (7.10) is first-order convergence independently of ε.

Theorem 16. *If $y_0 \in \ell_1^2$, then the global error of the adiabatic exponential Euler method* (7.10) *applied to the tDMNLS* (7.2) *is bounded by*

$$\left\| y^{(n)} - y(t_n) \right\|_{\ell^1} \le \tau C(M_0^y)\,, \qquad \tau n \le T\,,$$

for sufficiently small step-sizes τ.

Theorem 16 is proven in Section 7.3.

Remark. One can show first-order convergence of the ϕ-variant and of the adiabatic exponential Euler method with α-correction using the same techniques as in the proof of Theorem 16 in Section 7.3. Here, the constant of the the global error bound depends additionally on M_2^y, cf. Theorem 6.

We conclude this section with a numerical experiment to compare the adiabatic exponential Euler method to the adiabatic Euler method (Chapter 4). Again, we consider the DMNLS with $\alpha = 0.1$, $\delta = 1$ and $T = 1$ with initial value $u_0(x) = e^{-3x^2}e^{3ix}$ and 64 equidistant grid points in the interval $[-\pi, \pi]$ for $\varepsilon = 0.01$, 0.005, 0.002. To this setting we apply all three variants of the adiabatic exponential Euler method. The reference solution is computed by the Strang splitting method with a very small step-size ($\approx 10^{-6}$).

Figure 7.1 depicts the accuracy of the adiabatic exponential Euler method for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). In addition, the

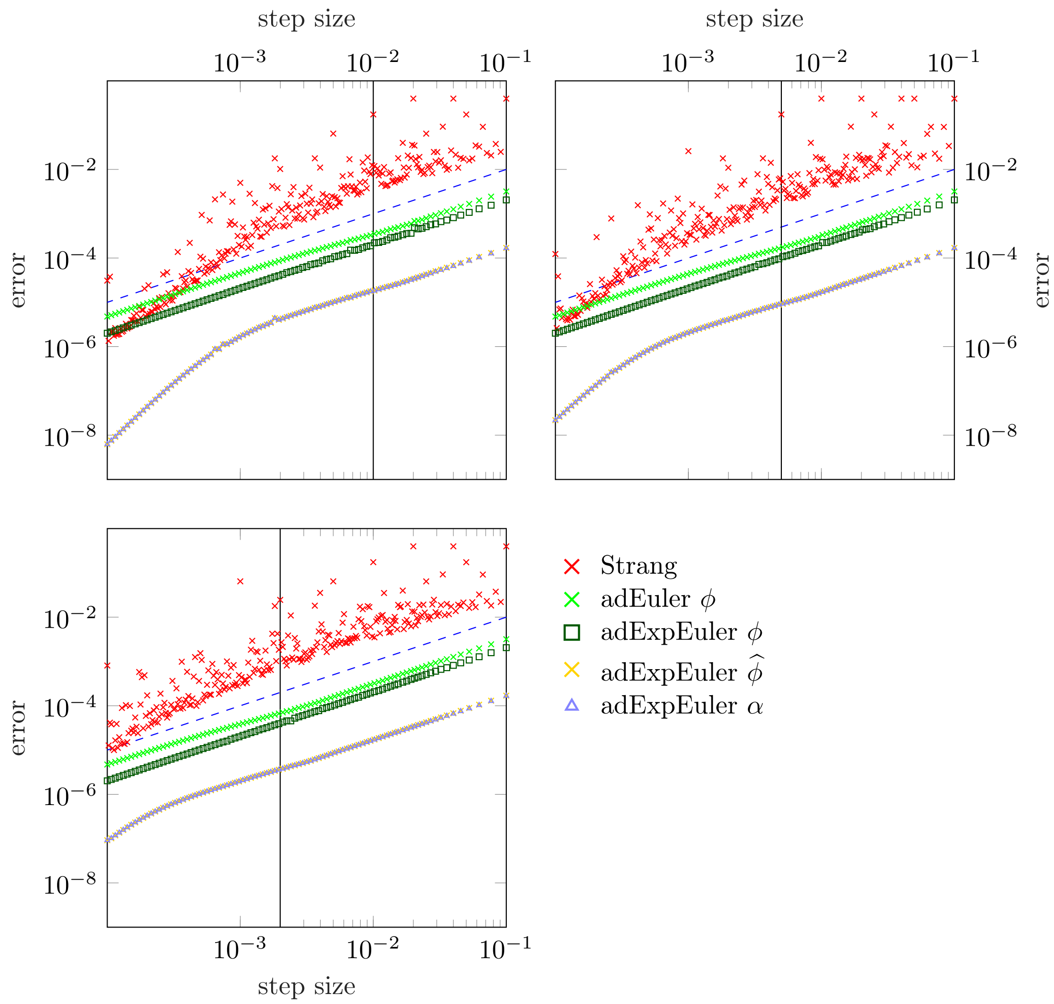

Figure 7.1: Maximal ℓ_0^2-error over time of the adiabatic exponential Euler method for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). For comparison, the ℓ_0^2-error of the adiabatic Euler method ($\widehat{\phi}$-variant) and the Strang splitting is shown. The dashed blue is a reference line for order one and the black vertical line is at $\tau = \varepsilon$.

accuracy of the $\widehat{\phi}$-variant of the adiabatic Euler method, (4.2), and of the Strang splitting method is shown for comparison. The dashed blue line is a reference line for order one, and the black vertical line highlights the value $\tau = \varepsilon$. The panels of Figure 7.1 indicate first-order convergence of the ϕ-variant of the adiabatic exponential Euler method independently of ε in accordance with Theorem 16. In addition, we observe that the error constant of this method is only slightly smaller than the error constant of the adiabatic Euler method suggesting that the exponential method has no clear advantage over the non-exponential counterpart. The values of the adiabatic exponential Euler method with α-correction lie on top of the values of the $\widehat{\phi}$-variant. We observe that the error constant of those methods is almost of two orders of magnitude smaller compared to the other methods. This observation suggests an advantage of the $\widehat{\phi}$-variant of the adiabatic exponential Euler method (and of the variant with α-correction) over the ϕ-variant and, in particular, over the adiabatic Euler method.

7.3. Proof of Theorem 16

The proof of Theorem 16 is essentially an application of the telescoping sum argument of Lady Windermere's fan, cf. Section 4.3. Therefore, we state and prove subsequently two lemmas concerning the stability and the local error of method (7.10), respectively.

In contrast to the error analysis of the adiabatic Euler method in Section 4.3, the error analysis of the adiabatic exponential Euler method requires estimates and expansions of semigroups. In the following, we provide some fundamental bounds for the operator (7.9). Let $\mu \in \ell^1$ and $M := \|\mu\|_{\ell^1}$. By definition (7.9), (7.8) and Lemma 15, we have the estimate

$$\left\| \exp\left(\sigma \widehat{\mathcal{E}}_n[\tau, \mu]\right) z \right\|_{\ell^1} \leq e^{\sigma C(M)} \|z\|_{\ell^1} \,. \tag{7.14}$$

Moreover, we make use of the (possibly) operator-valued functions

$$\varphi_k(z) = \int_0^1 e^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!} \, \mathrm{d}\theta \,, \quad k \geq 1 \,, \tag{7.15}$$

cf. [34]. These function satisfy the recurrence relation

$$\varphi_{k+1}(z) = \frac{\varphi_k(z) - \frac{1}{k!}}{z} \quad \text{with} \quad \varphi_0(z) = e^z \,,$$

which allows us, in particular, to expand (7.9) in terms of

$$\exp\left(\sigma \widehat{\mathcal{E}}_n\right) = \varphi_0\left(\sigma \widehat{\mathcal{E}}_n\right) = \sum_{k=0}^{m-1} \frac{\sigma^k}{k!} \widehat{\mathcal{E}}_n^k + (\sigma \widehat{\mathcal{E}}_n)^m \varphi_m\left(\sigma \widehat{\mathcal{E}}_n\right) , \tag{7.16}$$

where we use the abbreviation $\widehat{\mathcal{E}}_n = \widehat{\mathcal{E}}_n[\tau,\mu]$ for readability. The main feature of this expansion is that the operator $\varphi_m\big(\sigma\widehat{\mathcal{E}}_n[\tau,\mu]\big)\colon \ell_1 \to \ell_1$ in the remainder term is bounded, in fact

$$\left\|\varphi_m\big(\sigma\widehat{\mathcal{E}}_n[\tau,\mu]\big)z\right\|_{\ell^1} \le C(M)\,\|z\|_{\ell^1}\ . \tag{7.17}$$

Now, we reemploy the notation from (4.8) and denote $n \in \mathbb{N}$ steps of the adiabatic exponential Euler method (7.10) with step-size τ starting at time θ with initial data $z = (z_m)_{m\in\mathbb{Z}}$ by $\Psi_\theta^n(z)$.

Lemma 17. *Let $y_0 \in \ell_1^2$. Then, the local error of the adiabatic exponential Euler method* (7.10) *applied to the tDMNLS* (7.2) *is bounded by*

$$\big\|y(t_{n+1}) - \Psi_{t_n}\big(y(t_n)\big)\big\|_{\ell^1} \le \tau^2 C(M_0^y)\,.$$

Proof. For convenience we abbreviate $\widehat{\mathcal{E}}_n = \widehat{\mathcal{E}}_n[\tau, y(t_n)]$. Inserting the exact solution value $y(t_n)$ into the numerical scheme yields the local error

$$d_n \coloneqq y(t_{n+1}) - \exp\big(\tau\widehat{\mathcal{E}}_n\big)y(t_n)\,. \tag{7.18}$$

In order to estimate (7.18), we adapt an idea from [33], see also [34], to obtain a suitable expression for the exact solution $y(t_{n+1})$ of the tDMNLS. By definition (7.2) we have

$$y'(t) = \widehat{\mathcal{E}}_n y(t) + \Big(\widehat{A}(t, y(t)) - \widehat{\mathcal{E}}_n\Big)y(t)\,,$$

and hence applying the variation of constants formula gives

$$y(t_{n+1}) = \exp\big(\tau\widehat{\mathcal{E}}_n\big)y(t_n) + \int_{t_n}^{t_{n+1}} \exp\big((\tau-s)\widehat{\mathcal{E}}_n\big)\big(\widehat{A}(s) - \widehat{\mathcal{E}}_n\big)y(s)\,\mathrm{d}s\,, \tag{7.19}$$

where we use the abbreviation $\widehat{A}(s) = \widehat{A}\big(s, y(s)\big)$. Substituting (7.19) into (7.18) and applying (7.16) with $m = 1$ yields the partition $d_n = T_n + R_n$, with

$$T_n = \int_{t_n}^{t_{n+1}} \big(\widehat{A}(s) - \widehat{\mathcal{E}}_n\big)y(s)\,\mathrm{d}s$$

and

$$R_n = \int_{t_n}^{t_{n+1}} (\tau-s)\widehat{\mathcal{E}}_n\varphi_1\big((\tau-s)\widehat{\mathcal{E}}_n\big)\big(\widehat{A}(s) - \widehat{\mathcal{E}}_n\big)y(s)\,\mathrm{d}s\,.$$

If we combine (7.17), (7.8) and Lemma 15, we obtain the estimate

$$\|R_n\|_{\ell^1} \le \tau^2 C(M_0^y)\,. \tag{7.20}$$

Furthermore, we split $T_n = T_n^{(1)} + T_n^{(2)}$, with

$$T_n^{(1)} = \int_{t_n}^{t_{n+1}} \big(\widehat{A}(s) - \widehat{\mathcal{E}}_n\big)y(t_n)\,\mathrm{d}s$$

and

$$T_n^{(2)} = \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} \big(\widehat{A}(s) - \widehat{\mathcal{E}}_n\big) y'(\sigma) \,\mathrm{d}\sigma \,\mathrm{d}s \,.$$

Thanks to (7.8), Lemma 15 and Lemma 2, we get

$$\left\| T_n^{(2)} \right\|_{\ell^1} \le \tau^2 C(M_0^y) \,. \tag{7.21}$$

By (7.12), we have

$$\begin{aligned} \left\| T_n^{(1)} \right\|_{\ell^1} &= \left\| \int_{t_n}^{t_{n+1}} \Big(\widehat{A}\big(s, y(s)\big) - \widehat{A}\big(s, y(t_n)\big) \Big) y(t_n) \,\mathrm{d}s \right\|_{\ell^1} \\ &\le \sum_{m\in\mathbb{Z}} \sum_{I_m} \int_{t_n}^{t_{n+1}} \left| y_j(s)\overline{y}_k(s) - y_j(t_n)\overline{y}_k(t_n) \right| \left| y_l(t_n) \right| \mathrm{d}s \,. \end{aligned}$$

Because of the relation

$$\begin{aligned} y_j(s)\overline{y}_k(s) - y_j(t_n)\overline{y}_k(t_n) &= \big(y_j(s) - y_j(t_n)\big)\overline{y}_k(s) + y_j(t_n)\big(\overline{y}_k(s) - \overline{y}_k(t_n)\big) \\ &= \overline{y}_k(s) \int_{t_n}^{s} y_j'(\sigma) \,\mathrm{d}\sigma + y_j(t_n) \int_{t_n}^{s} \overline{y}_k'(\sigma) \,\mathrm{d}\sigma \,, \end{aligned} \tag{7.22}$$

the estimate

$$\left\| T_n^{(1)} \right\|_{\ell^1} \le \tau^2 C(M_0^y) \,. \tag{7.23}$$

follows from Lemma 2. Finally, we combine (7.20), (7.21) and (7.23) obtaining the desired result. □

The second lemma concerns the stability of (7.10). It has been published in a different context with Prof. Dr. Tobias Jahnke and Prof. Dr. Roland Schnaubelt in the preprint [41].

Lemma 18. *Let $\nu, \mu \in \ell^1$ and $M := \max\{\|\mu\|_{\ell^1}, \ \|\nu\|_{\ell^1}\}$. Then, we have*

$$\left\| \Psi_{t_n}(\mu) - \Psi_{t_n}(\nu) \right\|_{\ell^1} \le e^{\tau C(M)} \left\| \mu - \nu \right\|_{\ell^1} \,.$$

Proof. In order to prove the stability of method (7.10), we adapt an idea from [44]. The following argument holds for arbitrary starting time t_n, we thus assume $t_n = 0$ with no loss of generality.

We start by observing that $x(t) = \exp\big(t\widehat{\mathcal{E}}_n[\tau,\mu]\big)\mu$ and $z(t) = \exp\big(t\widehat{\mathcal{E}}_n[\tau,\nu]\big)\nu$ are solutions of the linear initial value problems

$$x'(t) = \widehat{\mathcal{E}}_n[\tau,\mu] x(t) \,, \quad x(0) = \mu \,, \quad t \ge 0,$$

and

$$z'(t) = \widehat{\mathcal{E}}_n[\tau,\nu] z(t) \,, \quad z(0) = \nu \,, \quad t \ge 0,$$

respectively. According to (7.14), both $x(t)$ and $z(t)$ are in ℓ^1 for every $t \in [0,\tau]$. Hence, (7.8) yields the estimate

$$\|x(\tau)\|_{\ell^1} \leq \|x(0)\|_{\ell^1} + \int_0^\tau \left\|\widehat{\mathcal{E}}_n[\tau,\mu]x(s)\right\|_{\ell^1} \mathrm{d}s \leq M + M^2 \int_0^\tau \|x(s)\|_{\ell^1} \mathrm{d}s\,,$$

and thus we obtain by Gronwall's lemma

$$\|x(\tau)\|_{\ell^1} \leq M e^{M^2\tau}\,. \tag{7.24}$$

Since the relation

$$\begin{aligned}\mu_j\overline{\mu}_k x_l(t) - \nu_k\overline{\nu}_k z_l(t) = \big(\mu_j - \nu_j\big)\overline{\mu}_k x_l(t) + \nu_j\big(\overline{\mu}_k - \overline{\nu}_k\big)x_l(t)\\ + \nu_j\overline{\nu}_k\big(x_l(t) - z_l(t)\big)\end{aligned}$$

holds, we can use (7.24) to estimate the difference of the right-hand sides of the initial value problems as follows

$$\begin{aligned}\left\|\widehat{\mathcal{E}}_n[\tau,\mu]x(t) - \widehat{\mathcal{E}}_n[\tau,\nu]z(t)\right\|_{\ell^1} &\leq \sum_{m\in\mathbb{Z}}\sum_{I_m} |\mu_j\overline{\mu}_k x_l(t) - \nu_j\overline{\nu}_k z_l(t)|\\ &\leq 2M\,\|x(t)\|_{\ell^1}\,\|\mu-\nu\|_{\ell^1} + M^2\,\|x(t)-z(t)\|_{\ell^1}\\ &\leq 2M^2 e^{M^2 t}\,\|\mu-\nu\|_{\ell^1} + M^2\,\|x(t)-z(t)\|_{\ell^1}\;.\end{aligned}$$

Hence, we obtain

$$\begin{aligned}\|x(\tau)-z(\tau)\|_{\ell^1} &\leq \|\mu-\nu\|_{\ell^1} + \int_0^\tau \left\|\widehat{\mathcal{E}}_n[\tau,\mu]x(s) - \widehat{\mathcal{E}}_n[\tau,\nu]z(s)\right\|_{\ell^1} \mathrm{d}s\\ &\leq \left(1 + 2M^2\int_0^\tau e^{sM^2}\,\mathrm{d}s\right)\|\mu-\nu\|_{\ell^1}\\ &\qquad + M^2\int_0^\tau \|x(s)-z(s)\|_{\ell^1}\,\mathrm{d}s\\ &\leq e^{\tau 2M^2}\,\|\mu-\nu\|_{\ell^1} + M^2\int_0^\tau \|x(s)-z(s)\|_{\ell^1}\,\mathrm{d}s\,.\end{aligned}$$

Then, applying Gronwall's lemma results in

$$\|x(\tau)-z(\tau)\|_{\ell^1} \leq e^{\tau 3M^2}\,\|\mu-\nu\|_{\ell^1}\;.$$

□

Equipped with Lemma 17 and Lemma 18, we can now prove Theorem 16.

Proof of Theorem 16. As in the proof of Theorem 6 in Section 4.3, we start by establishing the boundedness of the adiabatic exponential Euler method (7.10). On the basis of Lemma 18 and Lemma 17, we apply Proposition 23 (Appendix B) and choose the constant $M_0^\star = 2M_0^y$ to obtain a step-size $\tau_0 = C(T, M_0^y)$ such that for step-sizes $\tau \leq \tau_0$ the numerical solution is bounded in ℓ^1, i.e.

$$\left\| \Psi_{t_p}^n \big(y(t_p) \big) \right\|_{\ell^1} \leq M_0^\star \leq C(M_0^y) \quad \text{for all} \quad p \in \mathbb{N}\,, \quad t_{p+n} \leq T\,. \tag{7.25}$$

In particular, the estimate (7.25) ensures that the numerical scheme (7.10) is well-defined because it implies that the expression $\exp\big(\sigma \widehat{\mathcal{E}}_n[\tau, y^{(n)}]\big)$ exists in terms of (7.9) for all $y^{(n)}$.

Furthermore, Lemma 18 and Lemma 17 allow us to conduct the desired estimate for the global error via the telescoping sum argument of Lady Windermere's fan. Because this argument has already been presented in detail in the proof of Theorem 6 in Section 4.3, we omit the details at this point.

□

CHAPTER 8

The adiabatic exponential midpoint rule

Similar to the construction of the adiabatic midpoint rule in Section 5.1, we use the construction principles of the first-order exponential integrator (7.10) to obtain a corresponding two-step method based on the explicit midpoint rule. The resulting adiabatic exponential midpoint rule is introduced in Section 8.1. Subsequently, we state and discuss the results of our error analysis for this method in Section 8.2. It turns out that – as in the case of the adiabatic midpoint rule (Chapter 5) – we do not obtain a genuine second-order method. However, once more, the accuracy of the method improves for step-sizes that are integer multiples or integer fractions of ε due to cancellation effects in the summation of highly oscillatory error terms. The result of our error analysis is stated in Theorem 19 in Section 8.2. This theorem is the second main result of this thesis. Section 8.3 is then devoted to the proof of Theorem 19. Here, we extend techniques from Section 7.3 and suitably adapt the proofs from Section 5.3 and 5.4 to analyze the error behavior of the adiabatic exponential midpoint rule.

8.1. Construction

The starting point for constructing the adiabatic exponential midpoint rule is the tDMNLS in the form (7.2). For *fixed* $\mu \in \ell^1$ with $M := \|\mu\|_{\ell^1}$ and times $t_n = n\tau$ with $n \in \mathbb{N}$ and $\tau > 0$, we define

$$\widehat{\mathcal{M}}_n[\tau,\mu] := \frac{1}{2}\int_{-1}^{1} \widehat{A}(t_n + \tau\sigma, \mu)\,\mathrm{d}\sigma$$

obtaining a bounded, linear and autonomous operator $\widehat{\mathcal{M}}_n[\tau,\mu] \colon \ell^1 \to \ell^1$ with

$$\left\|\widehat{\mathcal{M}}_n[\tau,\mu]z\right\|_{\ell^1} \leq \left\|\widehat{A}(t,\mu)z\right\|_{\ell^1} \leq C(M)\,\|z\|_{\ell^1}\,, \quad t \in [0,T]\,, \tag{8.1}$$

see Lemma 15. The operator $\widehat{\mathcal{M}}_n[\tau,\mu]\colon \ell^1 \to \ell^1$ generates a uniformly continuous semigroup of bounded operators in ℓ^1 given by

$$\exp\big(s\widehat{\mathcal{M}}_n[\tau,\mu]\big) := \sum_{k=0}^{\infty} \frac{\big(s\widehat{\mathcal{M}}_n[\tau,\mu]\big)^k}{k!}\,, \tag{8.2}$$

cf. [52]. As in (7.14), we have the estimate

$$\Big\|\exp\big(\sigma\widehat{\mathcal{M}}_n[\tau,\mu]\big)z\Big\|_{\ell^1} \le e^{\sigma C(M)}\,\|z\|_{\ell^1} \tag{8.3}$$

and, with the abbreviation $\widehat{\mathcal{M}}_n = \widehat{\mathcal{M}}_n[\tau,\mu]$, the expansion

$$\exp\big(\sigma\widehat{\mathcal{M}}_n\big) = \varphi_0\big(\sigma\widehat{\mathcal{M}}_n\big) = \sum_{k=0}^{m-1}\frac{\sigma^k}{k!}\widehat{\mathcal{M}}_n^k + \big(\sigma\widehat{\mathcal{M}}_n\big)^m\varphi_m\big(\sigma\widehat{\mathcal{M}}_n\big) \tag{8.4}$$

by means of the φ-functions defined in (7.15) is still available, cf. (7.16). Here, the operators $\varphi_m\big(\sigma\widehat{\mathcal{M}}_n\big)\colon \ell^1 \to \ell^1$ are bounded by

$$\Big\|\varphi_m\big(\sigma\widehat{\mathcal{M}}_n\big)z\Big\|_{\ell^1} \le C(M)\,\|z\|_{\ell^1}\,. \tag{8.5}$$

The operators given in (8.2) allow us to define approximations $y^{(n)} \approx y(t_n)$ of the tDMNLS via

the adiabatic exponential midpoint rule

$$y^{(n+1)} = \exp\big(2\tau\widehat{\mathcal{M}}_n[\tau,y^{(n)}]\big)y^{(n-1)}\,. \tag{8.6}$$

The adiabatic exponential midpoint rule is a two-step scheme. As starting step we propose the adiabatic exponential Euler method (7.10), i.e.

$$y^{(1)} = \exp\big(\tau\widehat{\mathcal{E}}_n[\tau,y^{(0)}]\big)y^{(0)}\,. \tag{8.7}$$

To ensure that the scheme (8.6) is well-defined in terms of (8.2) we require $y^{(n)} \in \ell^1$ for all $n \in \mathbb{N}$. This boundedness of the numerical solution is addressed in Section 8.3 (below). Moreover, we observe that

$$2\tau\widehat{\mathcal{M}}_n[\tau,y^{(n)}] = \tau\int_{-1}^{1}\widehat{A}\big(t_n+\tau\sigma,y^{(n)}\big)\,\mathrm{d}\sigma = \int_{t_{n-1}}^{t_{n+1}}\widehat{A}\big(s,y^{(n)}\big)\,\mathrm{d}s\,, \tag{8.8}$$

which relates the exponent in (8.6) to the nonlinear Magnus expansion, cf. [10, Sec. 3.3]. In addition, the relation (8.8) implies that the exponent in (8.6) can be evaluated exactly in each time-step, cf. Section 5.1. If we consider only the first two summands of the exponential series in (8.6), we obtain the method

$$y^{(n+1)} = y^{(n-1)} + 2\tau\widehat{\mathcal{M}}_n[\tau,y^{(n)}]y^{(n-1)}\,,$$

which is almost the ϕ-variant of the adiabatic midpoint rule; the difference being that we have $y^{(n-1)}$ instead of $y^{(n)}$ in the second summand.

In addition to the $\widehat{\phi}$-variant (8.6), we can define a ϕ-variant of the adiabatic exponential midpoint rule by

$$\mathcal{M}_n[\tau,\mu] \coloneqq \frac{1}{2}\int_{-1}^{1} A\left(t_n, \tfrac{t_n+\tau\sigma}{\varepsilon}, \mu\right) \mathrm{d}\sigma$$

and a variant with α-correction via

$$\begin{aligned}\left\{\mathcal{M}_n^{\alpha}[\tau,\mu]z\right\}_m &\coloneqq \left\{\mathcal{M}[\tau,\mu]z\right\}_m \\ &\quad -\frac{\mathrm{i}\alpha}{2}\sum_{I_m}\omega_{[jklm]}\mu_j\bar{\mu}_k z_l \int_{-1}^{1} \tau\sigma \exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{t_n+\tau\sigma}{\varepsilon}\right)\right)\mathrm{d}\sigma\,.\end{aligned}$$

As for the adiabatic exponential Euler method, we omit a rigorous error analysis of these additional variants and focus solely on the $\widehat{\phi}$-variant (8.6) of the adiabatic exponential midpoint rule because it shows the most promising results in the numerical experiments given at the end of the following section.

8.2. Properties: norm preservation and accuracy

Provided $y^{(n)} \in \ell^1$ it follows from Lemma 15 that the operator $\widehat{\mathcal{M}}_n[\tau, y^{(n)}]\colon \ell_0^2 \to \ell_0^2$ is skew-adjoint. Hence, as in (7.13), we have

$$\|y^{(n)}\|_{\ell_0^2} = \|y^{(0)}\|_{\ell_0^2}\,,$$

i.e. the adiabatic exponential midpoint rule (8.6) preserves the ℓ_0^2-norm of the initial value $y^{(0)}$.

As for the adiabatic midpoint rule (see Theorem 10 and 11), the error behavior of the adiabatic exponential midpoint rule is rather complex: the method is a first-order scheme uniformly in ε, however, its accuracy improves for step-sizes that are integer fractions or integer multiples of ε. In the following theorem, we state our error analysis of the adiabatic exponential midpoint rule. It is the second main result of this thesis.

Theorem 19. *Let $y^{(n)}$ be the approximation of the tDMNLS* (2.24) *with the adiabatic exponential midpoint rule* (8.6)*. Then, the global error satisfies the following bounds.*

(i) If $y^{(0)} \in \ell_1^2$, then we have

$$\left\|y(t_n) - y^{(n)}\right\|_{\ell^1} \le \tau C(T, M_0^y)\,, \quad \tau n \le T,$$

for sufficiently small step-sizes τ.

(ii) If $y^{(0)} \in \ell_3^2$ and if we choose step-sizes $\tau = \varepsilon/k$ for some $k \in \mathbb{N}$, then we have

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \leq \varepsilon\tau\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,, \quad \tau n \leq T,$$

for sufficiently small step-sizes τ.

(iii) Suppose that Assumption 1 holds. If $y^{(0)} \in \ell_3^2$ and if we choose step-sizes $\tau = \varepsilon k$ for some $k \in \mathbb{N}$, then we have

$$\left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \leq \big(\tfrac{\varepsilon^2}{\delta} + \tau^2\big) C(T, \alpha, M_0, M_2)\,, \quad \tau n \leq T,$$

for sufficiently small step-sizes τ. In case of $\alpha = 0$ the constant depends only on T and M_0.

Theorem 19 is proven in Section 8.3.

In the following numerical example, we illustrate the behavior of the adiabatic exponential midpoint rule and compare it to the adiabatic midpoint rule (5.2). We consider the tDMNLS with $\alpha = 0.1$, $T = 1$, $\delta = 1$, the initial value $u_0(x) = e^{-3x^2} e^{3\mathrm{i}x}$ with 64 equidistant grid points in the interval $[-\pi, \pi]$ and $\varepsilon = 0.01$, 0.005, 0.002. To this setting, we apply all three variants of the adiabatic exponential midpoint rule but exclusively with step-sizes τ chosen according to part (ii) and (iii) of Theorem 19, i.e. we choose step-sizes that are integer multiples and integer fractions of ε. The reference solution is computed by the Strang splitting method with a large number of steps ($> 10^6$).

Figure 8.1 depicts the accuracy of the adiabatic exponential midpoint rule for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). In addition, the accuracy of the adiabatic midpoint rule (5.2) is shown. The black vertical line highlights the value $\tau = \varepsilon$. The dashed blue lines are reference lines for $\mathcal{O}(\tau^2)$ and $\mathcal{O}(\varepsilon\tau)$. In the regime $\tau > \varepsilon$ (right of the black line), we observe second-order accuracy in accordance to Theorem 19. Moreover, the error constants of the exponential methods are smaller than the constant of the adiabatic midpoint rule. In fact, the ϕ-variant and the adiabatic exponential midpoint rule with α-correction have only a moderately smaller error constant, whereas the error constant of the $\widehat{\phi}$-variant is significantly smaller leading to an improved accuracy of almost one order of magnitude. In the regime $\tau < \varepsilon$ (left of the black line), we observe accuracy in $\mathcal{O}(\tau\varepsilon)$. Here, the accuracy of the ϕ-variant of the exponential method almost coincides with the accuracy of the adiabatic midpoint rule. However, the accuracy of the $\widehat{\phi}$-variant suggests again an advantageous behavior of the exponential method. Lastly, the variant with α-correction closes up to the accuracy of the $\widehat{\phi}$-variant provided the step-size is sufficiently small.

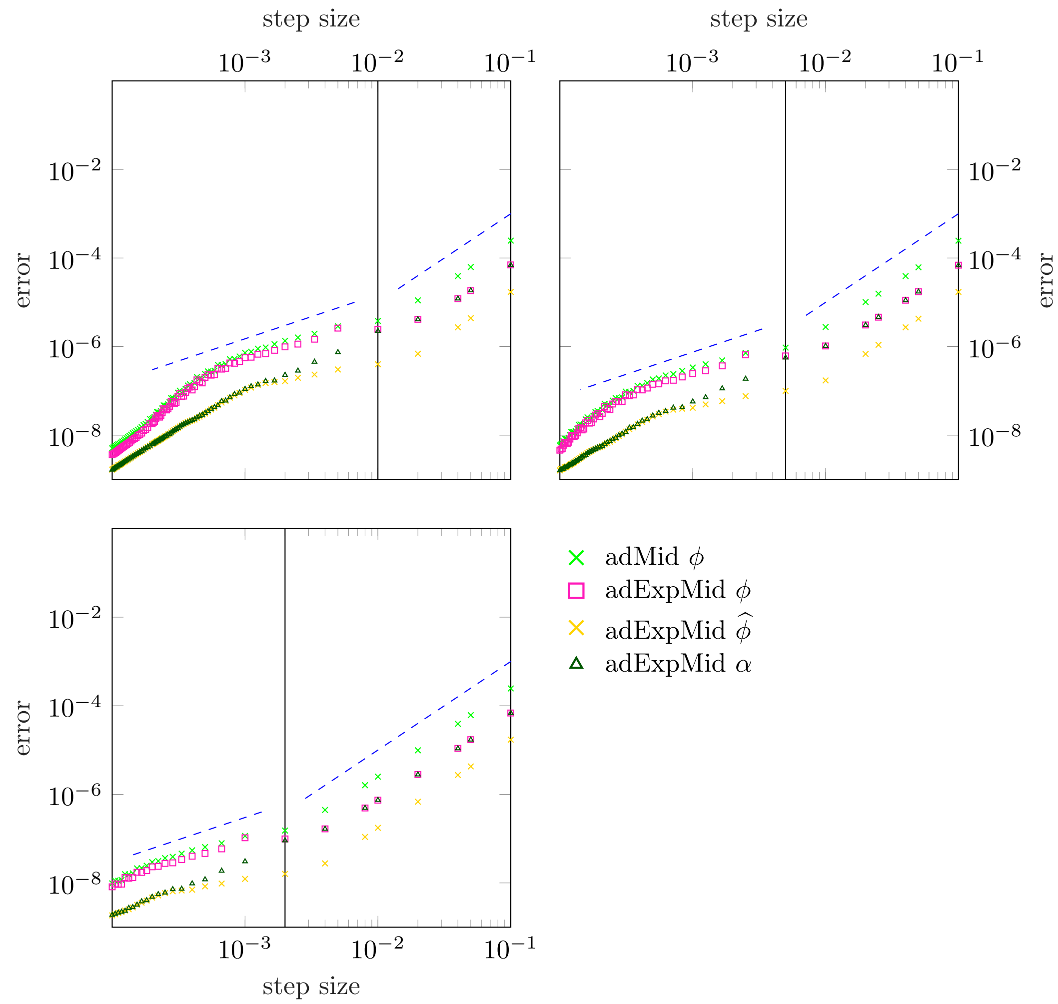

Figure 8.1: Maximal ℓ_0^2-error over time of the adiabatic exponential midpoint rule for $\varepsilon = 0.01$ (top left), $\varepsilon = 0.005$ (top right) and $\varepsilon = 0.002$ (bottom left). In addition, the accuracy of the adiabatic midpoint rule (5.2) is shown as a reference. The black vertical line is at $\tau = \varepsilon$. In all panels the step-sizes are chosen as integer multiples or integer fractions of ε.

Conclusion. Comparing the global error bounds of the adiabatic exponential midpoint rule (Theorem 19) and the adiabatic midpoint rule (Theorem 11), there is no clear advantage for either method. However, the previous numerical experiment suggests that the exponential scheme has a smaller error constant and thus indicates a higher accuracy. In particular, the $\widehat{\phi}$-variant of the adiabatic exponential midpoint rule appears to improve the accuracy significantly. Additionally, the exponential methods possess the advantage that they preserve the ℓ_0^2-norm of the initial value. Nevertheless, further investigation in terms of computational time versus accuracy is required for a final appraisal of the methods. We will address these additional considerations to some extent in Section 9.2.

8.3. Proof of Theorem 19

In order to simplify the notation throughout the proof, we use the abbreviations

$$\widehat{\mathcal{M}}_n := \widehat{\mathcal{M}}_n[\tau, y^{(n)}] \quad \text{and} \quad \widehat{\mathcal{M}}_n^* := \widehat{\mathcal{M}}_n[\tau, y(t_n)]\,.$$

The starting point to analyze the two-step method (8.6) is a recursion formula for the global error of the corresponding one-step formulation; cf. Section 5.3 and 5.4. Therefore, we define

$$\mathbf{y}_{n+1} = \begin{pmatrix} y^{(n+1)} \\ y^{(n)} \end{pmatrix} \quad \text{and} \quad \mathbf{M}_n = \begin{pmatrix} 0 & \exp\left(2\tau\widehat{\mathcal{M}}_n\right) \\ I & 0 \end{pmatrix} \tag{8.9}$$

in order to write the adiabatic exponential midpoint rule (8.6) in terms of

$$\mathbf{y}_{n+1} = \mathbf{M}_n \mathbf{y}_n\,. \tag{8.10}$$

If we define the error terms

$$\mathbf{d}_{n+1} = \mathbf{M}_n \mathbf{y}(t_n) - \mathbf{y}(t_{n+1}) \quad \text{with} \quad \mathbf{y}(t_{n+1}) = \begin{pmatrix} y(t_{n+1}) \\ y(t_n) \end{pmatrix}, \tag{8.11}$$

then we can express the global error $\mathbf{e}_N = \mathbf{y}_N - \mathbf{y}(t_N)$ via

$$\mathbf{e}_{N+1} = \mathbf{M}_N \mathbf{e}_N + \mathbf{d}_{N+1}\,.$$

Solving this recursion formula and using $\mathbf{e}_0 = 0$ gives

$$\mathbf{e}_N = \sum_{n=1}^{N} \mathbb{M}_n \mathbf{d}_n\,, \quad \text{with} \quad \mathbb{M}_n = \prod_{k=n}^{N-1} \mathbf{M}_k\,, \tag{8.12}$$

where the factors of $\mathbb{M}_n$ are considered in descending order from left to right. The error representation (8.12) is the center piece of the proof of Theorem 19.

At this point, one can use the one-step formulation (8.10) to verify that the assumptions of Proposition 23 (Appendix B), i.e. stability and consistency, are fulfilled; cf. (7.25), see also (4.12). However, in contrast to the proof of Theorem 16 combining the stability and the consistency of the method (8.6) with a telescoping sum argument is not sufficient to prove Theorem 19. Hence, we omit these additional computations. Nevertheless, we use henceforth that the bound

$$\left\| y^{(n)} \right\|_{\ell^1} \leq C(M_0^y) \quad \text{for all} \quad n\tau \leq T\,, \tag{8.13}$$

for approximations $y^{(n)}$ of the tDMNLS with method (8.6) exists for sufficiently small step-sizes τ. In particular, the estimate (8.13) ensures that the numerical scheme (8.6) is well defined.

8.3.1. Proof of part (i)

In order to prove first-order convergence it is sufficient to apply the triangle inequality to the recursion formula (8.12). Then, by definition (8.9) the bounds (8.3) and (8.13) allow us to estimate

$$\|\mathbf{e}_N\|_{\ell^1} \leq \sum_{n=1}^{N} \|\mathbb{M}_n \mathbf{d}_n\|_{\ell^1} \leq e^{C(T,M_0^y)} \sum_{n=1}^{N} \|\mathbf{d}_n\|_{\ell^1}\ , \tag{8.14}$$

and thus it remains to deduce a suitable bound for $\|\mathbf{d}_n\|_{\ell^1}$. With the abbreviation

$$d_{n+1} \coloneqq \exp\big(2\tau\widehat{\mathcal{M}}_n\big) y(t_{n-1}) - y(t_{n+1})\,, \tag{8.15}$$

we obtain

$$\mathbf{d}_{n+1} = \begin{pmatrix} d_{n+1} \\ 0 \end{pmatrix} \tag{8.16}$$

by (8.11), and hence it suffices to consider the non-zero part d_{n+1} of $\mathbf{d}_{n+1}$. As in (7.19), we obtain the representation

$$\begin{aligned} y(t_{n+1}) &= \exp\big(2\tau\widehat{\mathcal{M}}_n\big) y(t_{n-1}) \\ &\quad + \int_{t_{n-1}}^{t_{n+1}} \exp\big(2(\tau - s)\widehat{\mathcal{M}}_n\big) \Big(\widehat{A}\big(s, y(s)\big) - \widehat{\mathcal{M}}_n\Big)\, y(s)\, \mathrm{d}s \end{aligned} \tag{8.17}$$

for the exact solution of the tDMNLS by the variation of constants formula. Inserting (8.17) into (8.15) results in

$$d_{n+1} = -\int_{t_{n-1}}^{t_{n+1}} \exp\big(2(\tau - s)\widehat{\mathcal{M}}_n\big) \Big(\widehat{A}\big(s, y(s)\big) - \widehat{\mathcal{M}}_n\Big)\, y(s)\, \mathrm{d}s\,. \tag{8.18}$$

Hence, with (8.4) and the fundamental theorem of calculus, we get the partition

$$d_{n+1} = -\big(d_{n+1}^{(1)} + d_{n+1}^{(2)} + R_{n+1}^{(1)}\big)\,, \tag{8.19}$$

where

$$d_{n+1}^{(1)} = \int_{t_{n-1}}^{t_{n+1}} \exp\big(2(\tau-s)\widehat{\mathcal{M}}_n\big)\Big(\widehat{\mathcal{M}}_n^* - \widehat{\mathcal{M}}_n\Big) y(s)\,\mathrm{d}s\,, \tag{8.20}$$

$$d_{n+1}^{(2)} = \int_{t_{n-1}}^{t_{n+1}} \Big(\widehat{A}\big(s,y(s)\big) - \widehat{\mathcal{M}}_n^*\Big) y(t_n)\,\mathrm{d}s\,, \tag{8.21}$$

$$\begin{aligned} R_{n+1}^{(1)} = &\int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \Big(\widehat{A}\big(s,y(s)\big) - \widehat{\mathcal{M}}_n^*\Big) y'(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s \\ &+ 2\widehat{\mathcal{M}}_n \int_{t_{n-1}}^{t_{n+1}} (\tau-s)\varphi_1\big(2(\tau-s)\widehat{\mathcal{M}}_n\big)\Big(\widehat{A}\big(s,y(s)\big) - \widehat{\mathcal{M}}_n^*\Big) y(s)\,\mathrm{d}s\,. \end{aligned}$$

Thanks to Lemma 15, (8.1), (8.5) and Lemma 2, we get the bound

$$\left\| R_{n+1}^{(1)} \right\|_{\ell^1} \le \tau^2 C(M_0^y)\,. \tag{8.22}$$

Because of the estimate

$$\left| y_j(t_n)\overline{y}_k(t_n) - y_j^{(n)}\overline{y}_k^{(n)} \right| \le \left| y_j(t_n) - y_j^{(n)} \right| \cdot |\overline{y}_k(t_n)| + |y_j(t_n)| \cdot \left| \overline{y}_k(t_n) - \overline{y}_k^{(n)} \right|\,,$$

the bound

$$\left\| \Big(\widehat{\mathcal{M}}_n^* - \widehat{\mathcal{M}}_n\Big) z \right\|_{\ell^1} \le C(M_0^y) \left\| y(t_n) - y^{(n)} \right\|_{\ell^1} \|z\|_{\ell^1} \le C(M_0^y)\, \|\mathbf{e}_n\|_{\ell^1} \|z\|_{\ell^1} \tag{8.23}$$

follows for $z \in \ell^1$, and hence we obtain

$$\left\| d_{n+1}^{(1)} \right\|_{\ell^1} \le \tau C(M_0^y)\, \|\mathbf{e}_n\|_{\ell^1}\,, \tag{8.24}$$

by (8.3) and (8.13). According to (8.8), we have

$$d_{n+1}^{(2)} = \int_{t_{n-1}}^{t_{n+1}} \Big(\widehat{A}\big(s,y(s)\big) - \widehat{A}\big(s,y(t_n)\big)\Big) y(t_n)\,\mathrm{d}s\,.$$

Now, let $\{d_{n+1}^{(2)}\}_m$ denote the m-th entry of $d_{n+1}^{(2)}$. As in (7.22), we partition

$$\{d_{n+1}^{(2)}\}_m = \{S_{n+1}^{(1)}\}_m + \{S_{n+1}^{(2)}\}_m \tag{8.25}$$

with

$$\{S_{n+1}^{(1)}\}_m = \mathrm{i} \sum_{I_m} \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} y_j(t_n)\overline{y}_k'(\sigma) y_l(t_n) \exp\Big(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\Big)\,\mathrm{d}\sigma\,\mathrm{d}s\,, \tag{8.26}$$

$$\{S_{n+1}^{(2)}\}_m = \mathrm{i} \sum_{I_m} \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} y_j'(\sigma)\overline{y}_k(s) y_l(t_n) \exp\Big(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\Big)\,\mathrm{d}\sigma\,\mathrm{d}s\,. \tag{8.27}$$

Then, Lemma 2 implies the bounds

$$\left\| S_{n+1}^{(1)} \right\|_{\ell^1} \le \tau^2 C(M_0^y) \quad \text{and} \quad \left\| S_{n+1}^{(2)} \right\|_{\ell^1} \le \tau^2 C(M_0^y)\,. \tag{8.28}$$

Finally, we acquire the estimate

$$\|d_{n+1}\|_{\ell^1} \leq \tau C(M_0^y)\,\|\mathbf{e}_n\|_{\ell^1} + \tau^2 C(M_0^y)\,. \tag{8.29}$$

Substituting into (8.14) yields

$$\|\mathbf{e}_N\|_{\ell^1} = \tau e^{C(T,M_0^y)} \sum_{n=0}^{N-1} \|\mathbf{e}_n\|_{\ell^1} + \tau C(T, M_0^y)\,,$$

and we infer part (i) from the discrete Gronwall lemma.

8.3.2. Proof of part (ii)

In the proof of part (ii), we exploit cancellation effects in the error terms for $\tau = \varepsilon/k$ to improve the estimate (8.29). In order to utilize these cancellation effects, we avoid the triangle inequality and use a different approach to estimate the ℓ^1-norm of the global error (8.12), cf. Section 5.3.2. We start as in (5.24) and decompose $N = 2kL + n^*$ with $n^* \in \{0, \dots, 2k-1\}$ obtaining

$$\|\mathbf{e}_N\|_{\ell^1} \leq \left\| \sum_{n=1}^{2kL-1} \mathbb{M}_n \mathbf{d}_n \right\|_{\ell^1} + \left\| \sum_{n=2kL}^{2kL+n^*} \mathbb{M}_n \mathbf{d}_n \right\|_{\ell^1}. \tag{8.30}$$

Because $n^*\tau^2 \leq 2k\tau^2 = 2\tau\varepsilon$, we conclude from (8.29) that

$$\left\| \sum_{n=2kL}^{2kL+n^*} \mathbb{M}_n \mathbf{d}_n \right\|_{\ell^1} \leq \tau C(T, M_0^y) \sum_{n=2kL}^{2kL+n^*} \|\mathbf{e}_n\|_{\ell^1} + \tau\varepsilon C(M_0^y)\,. \tag{8.31}$$

In contrast to (5.26), we have now the additional term $\mathbb{M}_n$ instead of the row-switching matrix $\mathcal{J}$ in the remaining sum, and hence it is not sufficient to subdivide into summands with odd and even indices to eliminate this extra factor. Therefore, we use an additional summation by parts argument given in the following lemma.

Lemma 20. *Let $k, L \in \mathbb{N}$. Then, we have*

$$(i) \quad \left\| \sum_{\substack{n=1 \\ n \text{ even}}}^{2kL-1} \mathbb{M}_n \mathbf{d}_n \right\|_{\ell^1} \leq e^{C(T,M_0^y)} \left\| \sum_{n=1}^{kL-1} \mathbf{d}_{2n} \right\|_{\ell^1} + \tau C(M_0^y) \sum_{n=1}^{kL-2} \left\| \sum_{j=1}^{n} \mathbf{d}_{2j} \right\|_{\ell^1}$$

and

$$(ii) \quad \left\| \sum_{\substack{n=1 \\ n \text{ odd}}}^{2kL-1} \mathbb{M}_n \mathbf{d}_n \right\|_{\ell^1} \leq e^{C(T,M_0^y)} \left\| \sum_{n=1}^{kL-1} \mathbf{d}_{2n-1} \right\|_{\ell^1} + \tau C(M_0^y) \sum_{n=1}^{kL-2} \left\| \sum_{j=1}^{n} \mathbf{d}_{2j-1} \right\|_{\ell^1}.$$

Proof. First, we apply the summation by parts formula and obtain

$$\sum_{n=1}^{kL-1} \mathbb{M}_{2n} \mathbf{d}_{2n} = \mathbb{M}_{2(kL-1)} \sum_{n=1}^{kL-1} \mathbf{d}_{2n} + \sum_{n=1}^{kL-2} \big(\mathbb{M}_{2n+2} - \mathbb{M}_{2n}\big) \Big(\sum_{j=1}^{n} \mathbf{d}_{2j} \Big).$$

Then, we derive with (8.12) the factorization

$$\begin{aligned}\mathbb{M}_{2n+2} - \mathbb{M}_{2n} &= \mathbb{M}_{2n+2} - \mathbb{M}_{2n+2}\mathbf{M}_{2n+1}\mathbf{M}_{2n} \\ &= \mathbb{M}_{2n+2}\left(\begin{pmatrix} I & 0 \\ 0 & I\end{pmatrix} - \begin{pmatrix}\exp\left(2\tau\widehat{\mathcal{M}}_{2n+1}\right) & 0 \\ 0 & \exp\left(2\tau\widehat{\mathcal{M}}_{2n}\right)\end{pmatrix}\right).\end{aligned}$$

Thanks to (8.4), we get

$$\mathbb{M}_{2n+2} - \mathbb{M}_{2n} = 2\tau\mathbb{M}_{2n+2}\begin{pmatrix}\widehat{\mathcal{M}}_{2n+1}\varphi_1\left(2\tau\widehat{\mathcal{M}}_{2n+1}\right) & 0 \\ 0 & \widehat{\mathcal{M}}_{2n}\varphi_1\left(2\tau\widehat{\mathcal{M}}_{2n}\right)\end{pmatrix},$$

and hence the bound

$$\left\|\left(\mathbb{M}_{2n+2} - \mathbb{M}_{2n}\right)z\right\|_{\ell^1} \leq \tau C(M_0^y)\,\|z\|_{\ell^1} \quad \text{for} \quad z \in \ell^1$$

follows from (8.1), (8.3) and (8.5) implying the first estimate. The second estimate follows analogously with

$$\sum_{n=1}^{kL-1}\mathbb{M}_{2n-1}\mathbf{d}_{2n-1} = \mathbb{M}_{2kL-1}\sum_{n=1}^{kL-1}\mathbf{d}_{2n-1} + \sum_{n=1}^{kL-2}\left(\mathbb{M}_{2n+1} - \mathbb{M}_{2n-1}\right)\left(\sum_{j=1}^{n}\mathbf{d}_{2j-1}\right)$$

and the factorization

$$\mathbb{M}_{2n+1} - \mathbb{M}_{2n-1} = \mathbb{M}_{2n+1}\left(\begin{pmatrix} I & 0 \\ 0 & I\end{pmatrix} - \begin{pmatrix}\exp\left(2\tau\widehat{\mathcal{M}}_{2n}\right) & 0 \\ 0 & \exp\left(2\tau\widehat{\mathcal{M}}_{2n-1}\right)\end{pmatrix}\right).$$

□

Lemma 20 particularly implies that it is sufficient to conduct suitable estimates for

$$\left\|\sum_{\substack{n=1 \\ n \text{ odd}}}^{2kL-1}\mathbf{d}_n\right\|_{\ell^1} \quad \text{and} \quad \left\|\sum_{\substack{n=1 \\ n \text{ even}}}^{2kL-1}\mathbf{d}_n\right\|_{\ell^1} \quad \text{with} \quad k, L \in \mathbb{N}. \tag{8.32}$$

This is because the occurring double sums pose no additional problems: we can separate excessive summands in the inner sum as in (8.30) and apply the already available estimate (8.29) in order to obtain a suitable bound for these terms. More specifically, we partition $n = (lk + n^*)$ with $l \in \mathbb{N}$ and $n^* \in \{0, \dots, k\}$. Now, we can subdivide, e.g., the inner sum from part (i) of Lemma 20 into

$$\sum_{j=1}^{n}\mathbf{d}_{2j} = \sum_{j=1}^{lk-1}\mathbf{d}_{2j} + \sum_{j=lk}^{lk+n^*}\mathbf{d}_{2j}.$$

Then, the first sum can be estimated by the (yet to be derived) estimate for (8.32), whereas the second sum can be directly bounded by (8.29) because $n^*\tau^2 \leq 2\tau\varepsilon$.

In what follows, we derive solely an estimate for the first sum in (8.32) because a corresponding estimate for the second sum follows analogously. Moreover, we shift the summation index and consider henceforth the sum

$$\Bigg\| \sum_{\substack{n=0 \\ n \text{ even}}}^{2kL-2} \mathbf{d}_{n+1} \Bigg\|_{\ell^1}$$

for aesthetic reasons. As in part (i) of the proof, it is sufficient to consider the non-zero part d_{n+1} of $\mathbf{d}_{n+1}$, see (8.16). We start by expanding (8.15) but to a higher order. This leads us to the partition

$$d_{n+1} = -\big(d_{n+1}^{(1)} + d_{n+1}^{(2)} + d_{n+1}^{(3)} + d_{n+1}^{(4)} + R_{n+1}^{(2)}\big)\,, \tag{8.33}$$

with $d_{n+1}^{(1)}$ and $d_{n+1}^{(2)}$ defined in (8.20) and (8.21), respectively, and

$$\begin{aligned}
d_{n+1}^{(3)} &= \int_{t_{n+1}}^{t_{n+1}} \int_{t_n}^{s} \Big(\widehat{A}\big(s, y(s)\big) - \widehat{\mathcal{M}}_n^*\Big) y'(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s\,, \\
d_{n+1}^{(4)} &= \int_{t_{n-1}}^{t_{n+1}} 2(\tau - s)\widehat{\mathcal{M}}_n \Big(\widehat{A}\big(s, y(s)\big) - \widehat{\mathcal{M}}_n^*\Big) y(t_n)\,\mathrm{d}s\,, \\
R_{n+1}^{(2)} &= \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} 2(\tau - s)\widehat{\mathcal{M}}_n \Big(\widehat{A}\big(s, y(s)\big) - \widehat{\mathcal{M}}_n^*\Big) y'(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s \\
&\quad + \int_{t_{n-1}}^{t_{n+1}} \big(2(\tau - s)\widehat{\mathcal{M}}_n\big)^2 \varphi_2\big(2(\tau - s)\widehat{\mathcal{M}}_n\big) \Big(\widehat{A}\big(s, y(s)\big) - \widehat{\mathcal{M}}_n^*\Big) y(s)\,\mathrm{d}s\,.
\end{aligned}$$

Thanks to (8.1), (8.5), Lemma 15 and Lemma 2 the bound

$$\Big\| R_{n+1}^{(2)} \Big\|_{\ell^1} \le \tau^3 C(M_0^y) \tag{8.34}$$

follows. We continue by acquiring suitable estimates for $d_{n+1}^{(2)}$, $d_{n+1}^{(3)}$, and $d_{n+1}^{(4)}$ in the following three steps.

Step 1. According to the partition (8.25), we have to improve the estimate (8.28) to refine the estimate for $d_{n+1}^{(2)}$. We observe that the terms $S_{n+1}^{(1)}$ and $S_{n+1}^{(2)}$, given in (8.26) and (8.27), have the same structure as the terms (5.76)-(5.78) in the proof of Theorem 11. Therefore, we use the same principle to improve these estimates. First, we insert the tDMNLS for the derivative. Then, we fix all entries of y at t_n obtaining a leading order term that can be estimated by Lemma 14, and a remainder term bounded in $\mathcal{O}(\tau^3)$ with a constant depending only on T and M_2^y. Since this procedure has already been demonstrated in Section 5.4, we omit the details of these computations. Ultimately, we obtain the estimate

$$\Bigg\| \sum_{\substack{n=0 \\ n \text{ even}}}^{2kL-2} d_{n+1}^{(2)} \Bigg\|_{\ell^1} \le \varepsilon\tau\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,. \tag{8.35}$$

Step 2. For the bound of $d_{n+1}^{(3)}$, we partition $d_{n+1}^{(3)} = S_{n+1}^{(3)} - S_{n+1}^{(4)}$ with

$$\begin{aligned} S_{n+1}^{(3)} &= \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \widehat{A}\big(s, y(s)\big) y'(\sigma)\, \mathrm{d}\sigma\, \mathrm{d}s\,, \\ S_{n+1}^{(4)} &= \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \widehat{\mathcal{M}}_n^*\, y'(\sigma)\, \mathrm{d}\sigma\, \mathrm{d}s\,. \end{aligned} \tag{8.36}$$

If we consider the m-th entry of $S_{n+1}^{(3)}$

$$\{S_{n+1}^{(3)}\}_m = \mathrm{i} \sum_{I_m} \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} y_j(s) \overline{y}_k(s) y_l'(\sigma) \exp\left(-\mathrm{i}\omega_{[jklm]} \widehat{\phi}\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}\sigma\, \mathrm{d}s\,,$$

we can identify again the structure of the terms (5.76)-(5.78). As in the previous step, we obtain the estimate

$$\left\| \sum_{\substack{n=0 \\ n \text{ even}}}^{2kL-2} S_{n+1}^{(3)} \right\|_{\ell^1} \leq \varepsilon\tau\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,. \tag{8.37}$$

The term (8.36) can be estimated similarly, however, there is a mid-sized[1] modification, and thus we carry out the details of this computation. If we substitute the tDMNLS (2.24) for $y'(\sigma)$ the m-th entry of $S_{n+1}^{(4)}$ reads

$$\begin{aligned} \{S_{n+1}^{(4)}\}_m = -\frac{1}{2} \sum_{I_m} \sum_{I_l} y_j(t_n) \overline{y}_k(t_n) \int_{-1}^{1} \exp\left(-\mathrm{i}\omega_{[jklm]} \widehat{\phi}\left(\tfrac{t_n+\tau\xi}{\varepsilon}\right)\right) \mathrm{d}\xi \\ \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \widehat{Y}_{pqrl}(\sigma) \exp\left(-\mathrm{i}\omega_{[pqrl]} \phi\left(\tfrac{\sigma}{\varepsilon}\right)\right) \mathrm{d}\sigma\, \mathrm{d}s\,, \end{aligned} \tag{8.38}$$

with

$$Y_{pqr}(\sigma) = y_p(\sigma) \overline{y}_q(\sigma) y_r(\sigma) \quad \text{and} \quad \widehat{Y}_{pqrl}(\sigma) = Y_{pqr}(\sigma) \exp(-\mathrm{i}\omega_{[pqrl]}\sigma\alpha)\,.$$

Now, we aim to exploit the cancellation effects by summing up the double integrals. For simplification, we consider one summand of (8.38). We fix $m \in \mathbb{Z}$ as well as $(j,k,l) \in I_m$ and $(p,q,r) \in I_l$. Then, we write $\omega = \omega_{[pqrl]}$, $\tilde{\omega} = \omega_{[jklm]}$ and $\widehat{Y}(s) = \widehat{Y}_{pqrl}(s)$ for short. Moreover, we employ the abbreviations

$$f(s) = y_j(s) \overline{y}_k(s) \quad \text{and} \quad \widehat{K}_n = \int_{-1}^{1} \exp\left(-\mathrm{i}\tilde{\omega} \widehat{\phi}\left(\tfrac{t_n+\tau\xi}{\varepsilon}\right)\right) \mathrm{d}\xi\,. \tag{8.39}$$

This allows us to decompose any summand of (8.38) into

$$f(t_n) \widehat{K}_n \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \widehat{Y}(\sigma) \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{\sigma}{\varepsilon}\right)\right) \mathrm{d}\sigma\, \mathrm{d}s = f(t_n) \widehat{Y}(t_n) \widehat{K}_n \mathcal{I}_n + \mathcal{R}_n^{(1)}\,,$$

[1] The severity of the modification depends on the point of view. The author deliberately chose the classification *mid-sized* instead of *minor*.

where $\mathcal{I}_n$ is given in (5.23), with $\tilde{\omega} = 0$, and

$$\mathcal{R}_n^{(1)} = f(t_n)\widehat{K}_n \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} \int_{t_n}^{\sigma_1} \widehat{Y}'(\sigma_2)\,\mathrm{d}\sigma_2 \exp\left(-\mathrm{i}\omega\phi\left(\tfrac{\sigma_1}{\varepsilon}\right)\right)\mathrm{d}\sigma_1\,\mathrm{d}s\,. \tag{8.40}$$

In addition, we have the expansion

$$\widehat{K}_n = K_n \exp\left(-\mathrm{i}\tilde{\omega}\alpha t_n\right) - \tau\mathrm{i}\tilde{\omega}\alpha \int_{-1}^{1} \exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{t_n+\tau\xi}{\varepsilon}\right)\right) \int_0^{\xi} \exp\left(-\mathrm{i}\tilde{\omega}\alpha(t_n+\tau\theta)\right)\mathrm{d}\theta\,\mathrm{d}\xi\,,$$

where

$$K_n := \int_{-1}^{1} \exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{t_n+\tau\xi}{\varepsilon}\right)\right)\mathrm{d}\xi\,. \tag{8.41}$$

Hence, if we define

$$\widehat{f}(s) = f(s)\exp\left(-\mathrm{i}\tilde{\omega}\alpha s\right) \quad \text{and} \quad \widehat{F}(s) = \widehat{f}(s)\widehat{Y}(s)\,, \tag{8.42}$$

we can write any summand of (8.38) as

$$f(t_n)\widehat{Y}(t_n)\widehat{K}_n\mathcal{I}_n + \mathcal{R}_n^{(1)} = \widehat{F}(t_n)K_n\mathcal{I}_n + \mathcal{R}_n^{(1)} - \mathcal{R}_n^{(2)}\,,$$

where $\mathcal{R}_n^{(1)}$ is given in (8.40) and

$$\mathcal{R}_n^{(2)} = \mathrm{i}\tau\alpha\tilde{\omega} f(t_n)\widehat{Y}(t_n)\mathcal{I}_n \int_{-1}^{1} \exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{t_n+\tau\xi}{\varepsilon}\right)\right) \int_0^{\xi} \exp\left(-\mathrm{i}\tilde{\omega}\alpha(t_n+\tau\theta)\right)\mathrm{d}\theta\,\mathrm{d}\xi\,. \tag{8.43}$$

It is clear that

$$\left|\sum_{n=0}^{2kL-2} \mathcal{R}_n^{(1)}\right| \le \tau^2 C(T) \max_{\sigma\in[0,T]} \left|f(\sigma)\widehat{Y}'(\sigma)\right| \tag{8.44}$$

and

$$\left|\sum_{n=0}^{2kL-2} \mathcal{R}_n^{(2)}\right| \le \tau^2 \alpha C(T) \max_{\sigma\in[0,T]} \left|\tilde{\omega} f(\sigma)\widehat{Y}(\sigma)\right|\,. \tag{8.45}$$

In order to estimate the remaining sum

$$\left|\sum_{\substack{n=0\\ n \text{ even}}}^{2kL-2} \widehat{F}(t_n)K_n\mathcal{I}_n\right|\,,$$

we aim for the summation by parts argument from Lemma 13. However, the extra factor K_n requires additional care: if we use Lemma 13 with $a_n = \widehat{F}(t_n)K_n$ and write the difference $a_{2(n+1)} - a_{2n}$ as an integral over a derivative to obtain a factor τ as in (5.44), then differentiating yields an additional factor $1/\varepsilon$ due to the term K_n. Therefore, we use a slightly different approach and consider Lemma 13 with

$$a_n = \widehat{F}(t_n) \quad \text{and} \quad K_n\mathcal{I}_n \quad \text{instead of} \quad \mathcal{I}_n\,.$$

According to (5.34) and (5.35), Lemma 13 still holds if K_n fulfills the properties

$$K_{2n} = K_{2(k-n)}, \quad \text{for} \quad n = 1, \dots, k/2 - 1 \tag{8.46}$$

and

$$K_{2n-1} = K_{2(k-n)+1}, \quad \text{for} \quad n = 1, \dots, k/2\,. \tag{8.47}$$

Because $\tau = \varepsilon/k$ for $k \in \mathbb{N}$, we obtain on account of the symmetry and periodicity of ϕ, (5.30) and (5.31), the relation

$$\begin{aligned}
K_{2(k-n)} &= \int_{-1}^{1} \exp\left(-\mathrm{i}\tilde{\omega}\phi\left(\tfrac{t_{2(k-n)}+\tau\xi}{\varepsilon}\right)\right) \mathrm{d}\xi \\
&= \frac{\varepsilon}{\tau} \int_{2-(2n+1)/k}^{2-(2n-1)/k} \exp\big(-\mathrm{i}\tilde{\omega}\phi(\sigma)\big)\, \mathrm{d}\sigma \\
&= \frac{\varepsilon}{\tau} \int_{-(2n+1)/k}^{-(2n-1)/k} \exp\big(-\mathrm{i}\tilde{\omega}\phi(2+\sigma)\big)\, \mathrm{d}\sigma \\
&= \frac{\varepsilon}{\tau} \int_{-(2n+1)/k}^{-(2n-1)/k} \exp\big(-\mathrm{i}\tilde{\omega}\phi(2-\sigma)\big)\, \mathrm{d}\sigma \\
&= -\frac{\varepsilon}{\tau} \int_{(2n+1)/k}^{(2n-1)/k} \exp\big(-\mathrm{i}\tilde{\omega}\phi(2+\sigma)\big)\, \mathrm{d}\sigma \\
&= \frac{\varepsilon}{\tau} \int_{(2n-1)/k}^{(2n+1)/k} \exp\big(-\mathrm{i}\tilde{\omega}\phi(\sigma)\big)\, \mathrm{d}\sigma \\
&= K_{2n}\,.
\end{aligned}$$

In addition, one can show the equality (8.47) in the same way. Ultimately, Lemma 13 implies the estimate

$$\left| \sum_{\substack{n=0 \\ n \text{ even}}}^{2kL-2} \widehat{F}(t_n) K_n \mathcal{I}_n \right| \le \varepsilon\tau \max_{\sigma\in[0,T]} \left| \widehat{F}'(\sigma) \right| . \tag{8.48}$$

Because Lemma 22 (Appendix A) implies suitable bounds for the terms

$$\max_{\sigma\in[0,T]} \left| f(\sigma)\widehat{Y}'(\sigma) \right| , \quad \max_{\sigma\in[0,T]} \left| \tilde{\omega} f(\sigma)\widehat{Y}(\sigma) \right| \quad \text{and} \quad \max_{\sigma\in[0,T]} \left| \widehat{F}'(\sigma) \right| ,$$

we can combine (8.44), (8.45) and (8.48) to obtain

$$\left\| \sum_{\substack{n=0 \\ n \text{ even}}}^{2kL-2} S_{n+1}^{(4)} \right\|_{\ell^1} \le \tau\varepsilon\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,. \tag{8.49}$$

Finally, it follows from (8.37) and (8.49) that

$$\left\| \sum_{\substack{n=0 \\ n \text{ even}}}^{2kL-2} d_{n+1}^{(3)} \right\|_{\ell^1} \le \tau\varepsilon\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,. \tag{8.50}$$

Step 3. A short computation gives

$$\int_{t_{n-1}}^{t_{n+1}} 2(\tau - s)\,\mathrm{d}s = 4(\tau - t_n)\tau\,, \tag{8.51}$$

and thus we obtain with (8.8) the partition $d_{n+1}^{(4)} = S_{n+1}^{(5)} + S_{n+1}^{(6)}$, where

$$S_{n+1}^{(5)} = \int_{t_{n-1}}^{t_{n+1}} 2(t_n - s)\widehat{\mathcal{M}}_n \widehat{A}\big(s, y(s)\big) y(t_n)\,\mathrm{d}s\,, \tag{8.52}$$

$$S_{n+1}^{(6)} = \int_{t_{n-1}}^{t_{n+1}} 2(\tau - t_n)\widehat{\mathcal{M}}_n \Big(\widehat{A}\big(s, y(s)\big) - \widehat{A}\big(s, y(t_n)\big)\Big) y(t_n)\,\mathrm{d}s\,. \tag{8.53}$$

Because of the relation

$$y_j(s)\overline{y}_k(s) - y_j(t_n)\overline{y}_k(t_n) = \overline{y}_k(s)\int_{t_n}^{s} y_j'(\sigma)\,\mathrm{d}\sigma + y_j(t_n)\int_{t_n}^{s} \overline{y}_k'(\sigma)\,\mathrm{d}\sigma\,,$$

see (7.22), the estimate

$$\Big\| \Big(\widehat{A}\big(s, y(s)\big) - \widehat{A}\big(s, y(t_n)\big)\Big) y(t_n) \Big\|_{\ell^1} \le \tau C(M_0^y)$$

follows from Lemma 2, and hence we obtain the bound

$$\left\| \sum_{n=0}^{2kL-2} S_{n+1}^{(6)} \right\|_{\ell^1} \le \tau^2 C(T, M_0^y) \tag{8.54}$$

by (8.1). Similar to the estimate of the term (8.38) in the previous step, the term (8.52) requires additional care. First, we expand $S_{n+1}^{(5)} = T_{n+1}^{(1)} + T_{n+1}^{(2)}$ with

$$T_{n+1}^{(1)} = \int_{t_{n-1}}^{t_{n+1}} 2(t_n - s)\Big(\widehat{\mathcal{M}}_n - \widehat{\mathcal{M}}_n^*\Big)\widehat{A}\big(s, y(s)\big) y(t_n)\,\mathrm{d}s\,,$$

$$T_{n+1}^{(2)} = \widehat{\mathcal{M}}_n^* \int_{t_{n-1}}^{t_{n+1}} 2(t_n - s)\widehat{A}\big(s, y(s)\big) y(t_n)\,\mathrm{d}s\,.$$

By (8.23) and Lemma 15, we obtain

$$\left\| \sum_{n=0}^{2kL-2} T_{n+1}^{(1)} \right\|_{\ell^1} \le \tau^2 C(M_0^y) \sum_{n=0}^{2kL-2} \|\mathbf{e}_n\|_{\ell^1}\,. \tag{8.55}$$

Moreover, let $\{T_{n+1}^{(2)}\}_m$ denote the m-th entry of $T_{n+1}^{(2)}$. Then, we have

$$\{T_{n+1}^{(2)}\}_m = \sum_{I_m}\sum_{I_l} y_j(t_n)\overline{y}_k(t_n) \int_{-1}^{1} \exp\left(-\mathrm{i}\omega_{[jklm]}\widehat{\phi}\left(\tfrac{t_n+\tau\xi}{\varepsilon}\right)\right)\mathrm{d}\xi$$
$$\int_{t_{n-1}}^{t_{n+1}} (s - t_n)\widehat{Y}_{pqrl}(s)\exp\left(-\mathrm{i}\omega_{[pqrl]}\phi\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}s\,. \tag{8.56}$$

With the abbreviations given in (8.39) and (8.42) any fixed summand of (8.56) reads

$$f(t_n)\widehat{K}_n \int_{t_{n-1}}^{t_{n+1}} (s-t_n)\widehat{Y}(s) \exp\left(-\mathrm{i}\omega_{[pqrl]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}s = \widehat{F}(t_n)K_n\mathcal{I}_n + \tilde{\mathcal{R}}_n^{(1)} - \mathcal{R}_n^{(2)},$$

where $\mathcal{I}_n$ is given in (5.23) (with $\tilde{\omega}=0$), $\mathcal{R}_n^{(2)}$ is given in (8.43) and

$$\tilde{\mathcal{R}}_n^{(1)} = f(t_n)\widehat{K}_n \int_{t_{n-1}}^{t_{n+1}} \int_{t_n}^{s} (s-t_n)\widehat{Y}'(\sigma) \exp\left(-\mathrm{i}\omega_{[pqrl]}\phi\left(\tfrac{s}{\varepsilon}\right)\right) \mathrm{d}\sigma\, \mathrm{d}s\,.$$

Because we have

$$\left|\sum_{n=0}^{2kL-2} \tilde{\mathcal{R}}_n^{(1)}\right| \leq \tau^2 C(T, M_0^y) \max_{\sigma\in[0,T]} \left|\widehat{Y}'(\sigma)\right|,$$

we obtain analogously to (8.49) the estimate

$$\left|\sum_{\substack{n=0\\ n \text{ even}}}^{2kL-2} T_{n+1}^{(2)}\right| \leq \varepsilon\tau\big(C(T, M_0^y + \alpha C(T, M_2^y)\big)\,. \tag{8.57}$$

Then, combining (8.55) and (8.57) gives

$$\left\|\sum_{\substack{n=0\\ n \text{ even}}}^{2kL-2} S_{n+1}^{(5)}\right\|_{\ell^1} \leq \tau^2 C(M_0^y) \sum_{\substack{n=0\\ n \text{ even}}}^{2kL-2} \|\mathbf{e}_n\|_{\ell^1} + \tau\varepsilon\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,, \tag{8.58}$$

and hence (8.54) and (8.58) lead us to

$$\left\|\sum_{\substack{n=0\\ n \text{ even}}}^{2kL-2} d_{n+1}^{(4)}\right\|_{\ell^1} \leq \tau^2 C(M_0^y) \sum_{\substack{n=0\\ n \text{ even}}}^{2kL-2} \|\mathbf{e}_n\|_{\ell^1} + \tau\varepsilon\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,. \tag{8.59}$$

Finally, with the estimates (8.24), (8.34), (8.35), (8.50), and (8.59), we obtain the bound

$$\left\|\sum_{\substack{n=0\\ n \text{ even}}}^{2kL-2} \mathbf{d}_{n+1}\right\|_{\ell^1} \leq \tau C(M_0^y) \sum_{\substack{n=0\\ n \text{ even}}}^{2kL-2} \|\mathbf{e}_n\|_{\ell^1} + \tau\varepsilon\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,. \tag{8.60}$$

Analogously, one can show the bound

$$\left\|\sum_{\substack{n=0\\ n \text{ odd}}}^{2kL-2} \mathbf{d}_{n+1}\right\|_{\ell^1} \leq \tau C(M_0^y) \sum_{\substack{n=0\\ n \text{ odd}}}^{2kL-2} \|\mathbf{e}_n\|_{\ell^1} + \tau\varepsilon\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,. \tag{8.61}$$

Now, the first sum in (8.30) can be estimated by combining Lemma 20 with (8.60) and (8.61), and we finally obtain the estimate

$$\|\mathbf{e}_N\|_{\ell^1} \leq \tau C(M_0^y) \sum_{n=0}^{N-1} \|\mathbf{e}_n\|_{\ell^1} + \tau\varepsilon\big(C(T, M_0^y) + \alpha C(T, M_2^y)\big)\,.$$

Applying the discrete Gronwall lemma yields the desired result.

8.3.3. Proof of part (iii)

On the basis of Theorem 3, we consider approximations of the tDMNLS by the adiabatic exponential midpoint rule (8.6) with step-size $\tau = k\varepsilon$ as approximations of the limit system (3.9), cf. Section 5.4. It remains to show that these approximations can be suitably bounded, cf. (5.83). First, we define

$$\big\{\tilde{A}(t,\mu)z\big\}_m := \mathrm{i}\sum_{I_m} \mu_j \bar{\mu}_k z_l \exp(-\mathrm{i}\omega_{[jklm]}\alpha t) \int_0^1 \exp(\mathrm{i}\omega_{[jklm]}\delta\xi)\,\mathrm{d}\xi \tag{8.62}$$

for two sequences $\mu = (\mu_m)_{m\in\mathbb{Z}}$ and $z = (z_m)_{m\in\mathbb{Z}}$ in $\mathbb{C}$, cf. (5.5). This allows us to write the limit system (3.9) in terms of

$$v'(t) = \tilde{A}\big(t, v(t)\big)v(t)\,.$$

Clearly, for $\mu \in \ell^1$ with $M := \|\mu\|_{\ell^1}$ the operator $\tilde{A}\big(t,\mu\big)\colon \ell^1 \to \ell^1$ is bounded by

$$\left\|\tilde{A}\big(t,\mu\big)z\right\|_{\ell^1} \le C(M)\,\|z\|_{\ell^1}\ , \tag{8.63}$$

cf. Lemma 15. Next, we define the error terms

$$\tilde{\mathbf{d}}_{n+1} = \mathbf{M}_n\mathbf{v}(t_n) - \mathbf{v}(t_{n+1}) \quad \text{with} \quad \mathbf{v}(t_{n+1}) = \begin{pmatrix} v(t_{n+1}) \\ v(t_n) \end{pmatrix}, \tag{8.64}$$

in order to obtain the recursion formula

$$\mathbf{e}_N = \sum_{n=1}^{N} \mathbb{M}_n \tilde{\mathbf{d}}_n \tag{8.65}$$

for the global error $\mathbf{e}_N = \mathbf{y}_N - \mathbf{v}(t_N)$, cf. (8.12). As in (8.14), we have

$$\|\mathbf{e}_N\|_{\ell^1} \le \sum_{n=1}^{N} \left\|\mathbb{M}_n\tilde{\mathbf{d}}_n\right\|_{\ell^1} \le e^{C(T,M_0^y)} \sum_{n=1}^{N} \left\|\tilde{\mathbf{d}}_n\right\|_{\ell^1}\,. \tag{8.66}$$

By (8.64), we have

$$\tilde{\mathbf{d}}_{n+1} = \begin{pmatrix} \tilde{d}_{n+1} \\ 0 \end{pmatrix}, \quad \text{with} \quad \tilde{d}_{n+1} := \exp\big(2\tau\widehat{\mathcal{M}}_n\big)v(t_{n-1}) - v(t_{n+1})\,, \tag{8.67}$$

and thus it is sufficient to consider the non-zero part $\tilde{d}_{n+1}$ of $\tilde{\mathbf{d}}_{n+1}$.

Thanks to the variation of constant formula, we obtain

$$\begin{aligned} v(t_{n+1}) &= \exp\big(2\tau\widehat{\mathcal{M}}_n\big)v(t_{n-1}) \\ &\qquad + \int_{t_{n-1}}^{t_{n+1}} \exp\big(2(\tau-s)\widehat{\mathcal{M}}_n\big)\Big(\tilde{A}\big(s,v(s)\big) - \widehat{\mathcal{M}}_n\Big)v(s)\,\mathrm{d}s\,. \end{aligned} \tag{8.68}$$

Henceforth, we abbreviate

$$\widehat{\mathcal{M}}_n^\bullet := \widehat{\mathcal{M}}_n[\tau, v(t_n)]$$

to simplify notation. Substituting (8.68) into (8.67) and employing the expansion (8.4) gives the decomposition

$$\tilde{d}_{n+1} = -\big(\tilde{d}_{n+1}^{(1)} + \tilde{d}_{n+1}^{(2)} + \tilde{d}_{n+1}^{(3)} + \tilde{d}_{n+1}^{(4)} + \tilde{R}_{n+1}\big)\,, \tag{8.69}$$

where

$$\tilde{d}_{n+1}^{(1)} = \int_{t_{n-1}}^{t_{n+1}} \exp\big(2(\tau-s)\widehat{\mathcal{M}}_n\big)\Big(\widehat{\mathcal{M}}_n^\bullet - \widehat{\mathcal{M}}_n\Big)v(s)\,\mathrm{d}s\,, \tag{8.70}$$

$$\tilde{d}_{n+1}^{(2)} = \int_{t_{n-1}}^{t_{n+1}} \Big(\tilde{A}\big(s,v(s)\big) - \widehat{\mathcal{M}}_n^\bullet\Big)v(t_n)\,\mathrm{d}s\,, \tag{8.71}$$

$$\tilde{d}_{n+1}^{(3)} = \int_{t_{n-1}}^{t_{n+1}} (s-t_n)\Big(\tilde{A}\big(s,v(s)\big) - \widehat{\mathcal{M}}_n^\bullet\Big)v'(t_n)\,\mathrm{d}s\,, \tag{8.72}$$

$$\tilde{d}_{n+1}^{(4)} = \int_{t_{n-1}}^{t_{n+1}} 2(\tau-s)\widehat{\mathcal{M}}_n\Big(\tilde{A}\big(s,v(s)\big) - \widehat{\mathcal{M}}_n^\bullet\Big)v(t_n)\,\mathrm{d}s\,, \tag{8.73}$$

$$\begin{aligned}\tilde{R}_{n+1} = &\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s}\int_{t_n}^{\sigma_1} \Big(\tilde{A}\big(s,v(s)\big) - \widehat{\mathcal{M}}_n^\bullet\Big)v''(\sigma_2)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,\mathrm{d}s\\ &+\int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} 2(\tau-s)\widehat{\mathcal{M}}_n\Big(\tilde{A}\big(s,v(s)\big) - \widehat{\mathcal{M}}_n^\bullet\Big)v'(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s\\ &+\int_{t_{n-1}}^{t_{n+1}} \big(2(\tau-s)\widehat{\mathcal{M}}_n\big)^2\varphi_2\big(2(\tau-s)\widehat{\mathcal{M}}_n\big)\Big(\tilde{A}\big(s,v(s)\big) - \widehat{\mathcal{M}}_n^\bullet\Big)v(s)\,\mathrm{d}s\,,\end{aligned}$$

By (8.3), (8.1) and (8.13), we have

$$\sum_{n=1}^{N}\left\|\tilde{d}_{n+1}^{(1)}\right\|_{\ell^1} \le \tau C(M_0)\sum_{n=1}^{N}\|\mathbf{e}_n\|_{\ell^1}\ , \tag{8.74}$$

with M_0 given in (3.14), cf. (8.24). Furthermore, we obtain

$$\sum_{n=1}^{N}\left\|\tilde{R}_{n+1}\right\|_{\ell^1} \le \tau^2\big(C(T,M_0) + \alpha C(T,M_2^v)\big)\,, \tag{8.75}$$

with (8.1), (8.63), (8.5) and Lemma 21 (Appendix A).

In the following, we deduce bounds for $\tilde{d}_{n+1}^{(2)}$, $\tilde{d}_{n+1}^{(3)}$ and $\tilde{d}_{n+1}^{(4)}$. Since all necessary ideas for these estimates have been demonstrated before, we omit a few details of the related computations.

Step 1. By (8.8), we have

$$\tilde{d}_{n+1}^{(2)} = \int_{t_{n-1}}^{t_{n+1}} \Big(\tilde{A}\big(s,v(s)\big) - \widehat{A}\big(s,v(t_n)\big)\Big)v(t_n)\,\mathrm{d}s\,,$$

and hence the m-th entry of $\tilde{d}_{n+1}^{(2)}$ can be split into

$$\{\tilde{d}_{n+1}^{(2)}\}_m = \{\tilde{S}_{n+1}^{(1)}\}_m - \{\tilde{S}_{n+1}^{(2)}\}_m\,,$$

with

$$\begin{aligned}\{\tilde{S}_{n+1}^{(1)}\}_m &= \mathrm{i}\sum_{I_m}\int_{t_{n-1}}^{t_{n+1}} \big(v_j(s)\overline{v}_k(s) - v_j(t_n)\overline{v}_k(t_n)\big)v_l(t_n) \\ &\qquad \exp(-\mathrm{i}\omega_{[jklm]}\alpha s)\,\mathrm{d}s\int_0^1 \exp(\mathrm{i}\omega_{[jklm]}\delta\xi)\,\mathrm{d}\xi\,, \qquad (8.76)\\ \{\tilde{S}_{n+1}^{(2)}\}_m &= \mathrm{i}\sum_{I_m} V_{jkl}(t_n)\int_{t_{n-1}}^{t_{n+1}} \exp(-\mathrm{i}\omega_{[jklm]}\alpha s) \\ &\qquad \left(\exp\left(-\mathrm{i}\omega_{[jklm]}\phi\left(\tfrac{s}{\varepsilon}\right)\right)\mathrm{d}\sigma - \int_0^1 \exp(\mathrm{i}\omega_{[jklm]}\delta\xi)\,\mathrm{d}\xi\right)\mathrm{d}s\,. \qquad (8.77)\end{aligned}$$

Because the term (8.77) is structured similarly to the term (5.87) in the proof of Theorem 11 part (iii) in Section 5.4.3, we obtain analogously the estimate

$$\sum_{n=1}^{N}\left\|\tilde{S}_{n+1}^{(2)}\right\|_{\ell^1} \le \alpha^2\frac{\varepsilon^2}{\delta}C(T, M_2^v)\,, \tag{8.78}$$

cf. (5.93). Moreover, we use the same principle as in (7.22) to decompose

$$\{\tilde{S}_{n+1}^{(1)}\}_m = \{\tilde{T}_{n+1}^{(1)}\}_m + \{\tilde{T}_{n+1}^{(2)}\}_m\,,$$

with

$$\begin{aligned}\{\tilde{T}_{n+1}^{(1)}\}_m &= \mathrm{i}\sum_{I_m}\int_0^1 \exp(\mathrm{i}\omega_{[jklm]}\delta\xi)\,\mathrm{d}\xi \\ &\qquad \int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} v_j(t_n)\overline{v}_k'(\sigma)v_l(t_n)\exp(-\mathrm{i}\omega_{[jklm]}\alpha s)\,\mathrm{d}\sigma\,\mathrm{d}s \qquad (8.79)\end{aligned}$$

and

$$\begin{aligned}\{\tilde{T}_{n+1}^{(2)}\}_m &= \mathrm{i}\sum_{I_m}\int_0^1 \exp(\mathrm{i}\omega_{[jklm]}\delta\xi)\,\mathrm{d}\xi \\ &\qquad \int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s} v_j'(\sigma)\overline{v}_k(s)v_l(t_n)\exp(-\mathrm{i}\omega_{[jklm]}\alpha s)\,\mathrm{d}\sigma\,\mathrm{d}s\,.\end{aligned}$$

There are two key observations for estimating the remaining error terms. First, expanding v_m' via the fundamental theorem of calculus is not critical because v_m' is independent of ε, cf. (3.9). Second, the double integral vanishes for constant integrands due to symmetry. Hence, fixing the integrands at t_n allows us to eliminate the constant leading order term. The remainder terms can then be estimated by Lemma 21 (Appendix A). We demonstrate the procedure for the term (8.79): fixing

$\overline{v}_k'(\sigma)$ at $\sigma = t_n$ followed by fixing $\exp(-\mathrm{i}\omega_{[jklm]}\alpha s)$ at $s = t_n$ yields the decomposition

$$\{\tilde{T}^{(1)}_{n+1}\}_m = \{\tilde{R}^{(1)}_{n+1}\}_m + \{\tilde{R}^{(2)}_{n+1}\}_m\,,$$

with

$$\begin{aligned}\{\tilde{R}^{(1)}_{n+1}\}_m &= \mathrm{i}\sum_{I_m}\int_0^1 \exp(\mathrm{i}\omega_{[jklm]}\delta\xi)\,\mathrm{d}\xi\\ &\qquad \int_{t_{n-1}}^{t_{n+1}}\int_{t_n}^{s}\int_{t_n}^{\sigma_1} v_j(t_n)\overline{v}_k''(\sigma_2)v_l(t_n)\exp(-\mathrm{i}\omega_{[jklm]}\alpha s)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,\mathrm{d}s\,,\\ \{\tilde{R}^{(2)}_{n+1}\}_m &= \alpha\sum_{I_m}\int_0^1 \exp(\mathrm{i}\omega_{[jklm]}\delta\xi)\,\mathrm{d}\xi\\ &\qquad \int_{t_{n-1}}^{t_{n+1}}(s-t_n)\int_{t_n}^{s}\omega_{[jklm]}v_j(t_n)\overline{v}_k'(t_n)v_l(t_n)\exp(-\mathrm{i}\omega_{[jklm]}\alpha\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s\,.\end{aligned}$$

Because estimates for

$$\big|v_j(t)\overline{v}_k''(t)v_l(t)\exp(-\mathrm{i}\omega_{[jklm]}\alpha t)\big| = \big|v_j(t)\overline{v}_k''(t)v_l(t)\big|$$

and

$$\big|\omega_{[jklm]}v_j(t)\overline{v}_k'(t)v_l(t)\exp(-\mathrm{i}\omega_{[jklm]}\alpha t)\big| = \big|\omega_{[jklm]}v_j(t)\overline{v}_k'(t)v_l(t)\big|$$

follow analogously to the estimates for $|V''_{jkl}(t)|$ and $|\omega_{[jklm]}V'_{jkl}(t)|$ in Lemma 21 (Appendix A), we infer

$$\Big\|\tilde{R}^{(1)}_{n+1}\Big\|_{\ell^1} \le \tau^3\big(C(M_0^v) + \alpha C(M_2^v)\big) \quad \text{and} \quad \Big\|\tilde{R}^{(2)}_{n+1}\Big\|_{\ell^1} \le \tau^3\alpha C(M_2^v)\,.$$

Hence, we obtain

$$\Big\|\tilde{T}^{(1)}_{n+1}\Big\|_{\ell^1} \le \tau^3\big(C(M_0^v) + \alpha C(M_2^v)\big)\,.$$

Analogously, we get the estimate

$$\Big\|\tilde{T}^{(2)}_{n+1}\Big\|_{\ell^1} \le \tau^3\big(C(M_0^v) + \alpha C(M_2^v)\big)\,,$$

and thus

$$\sum_{n=1}^{N}\Big\|\tilde{S}^{(1)}_{n+1}\Big\|_{\ell^1} \le \tau^2\big(C(T, M_0^v) + \alpha C(T, M_2^v)\big)\,. \tag{8.80}$$

Finally, combining (8.78) and (8.80) results in the bound

$$\sum_{n=1}^{N}\Big\|\tilde{d}^{(2)}_{n+1}\Big\|_{\ell^1} \le \big(\tfrac{\varepsilon^2}{\delta} + \tau^2\big)\big(C(T, M_0^v) + (\alpha+\alpha^2)C(T, M_2^v)\big)\,. \tag{8.81}$$

Step 2. The second summand in (8.72) vanishes due to the symmetry of the integral. Hence, it remains to estimate

$$\tilde{d}^{(3)}_{n+1} = \int_{t_{n-1}}^{t_{n+1}}(s-t_n)\tilde{A}\big(s, v(s)\big)v'(t_n)\,\mathrm{d}s\,.$$

As in step 1, one can estimate this term by fixing $\tilde{A}\big(s, v(s)\big)$ at $s = t_n$ and bounding the remainder terms by employing Lemma 21 (Appendix A). Ultimately, we obtain the estimate

$$\sum_{n=1}^{N} \left\| \tilde{d}_{n+1}^{(3)} \right\|_{\ell^1} \leq \tau^2 \big(C(T, M_0^v) + \alpha C(T, M_2^v) \big) . \tag{8.82}$$

Step 3. Thanks to (8.51) and (8.8), we have

$$\begin{aligned} \tilde{d}_{n+1}^{(4)} = &\int_{t_{n-1}}^{t_{n+1}} 2(\tau - s) \widehat{\mathcal{M}}_n \Big(\tilde{A}\big(s, v(s)\big) - \tilde{A}\big(s, v(t_n)\big) \Big) v(t_n) \, \mathrm{d}s \\ &- \int_{t_{n-1}}^{t_{n+1}} 2(s - t_n) \widehat{\mathcal{M}}_n \tilde{A}\big(s, v(t_n)\big) v(t_n) \, \mathrm{d}s \, . \end{aligned}$$

One can estimate the first term in (8.83) analogously to the term (8.53). Moreover, one can bound the second term by fixing $\tilde{A}\big(s, v(t_n)\big)$ at $s = t_n$. Then, the leading order term vanishes due to the symmetry of the integral and the remainder terms can be dealt with by Lemma 21 (Appendix A). Ultimately, we obtain the estimate

$$\sum_{n=1}^{N} \left\| \tilde{d}_{n+1}^{(4)} \right\|_{\ell^1} \leq \tau^2 \big(C(T, M_0^v) + \alpha C(T, M_2^v) \big) . \tag{8.83}$$

Finally, we combine (8.74), (8.81), (8.82), (8.83) and (8.75) and obtain

$$\|\mathbf{e}_N\|_{\ell^1} = \tau C(T, M_0) \sum_{n=0}^{N-1} \|\mathbf{e}_n\|_{\ell^1} + \big(\tfrac{\varepsilon^2}{\delta} + \tau^2 \big) \big(C(T, M_0) + (\alpha + \alpha^2) C(T, M_2) \big) .$$

Now, the assertion follows with the discrete Gronwall lemma. In particular, the constant improves as specified if $\alpha = 0$.

□

CHAPTER 9

Summary, final considerations and outlook

9.1. Summary

The goal of this thesis was to construct and analyze novel time-integration schemes for the DMNLS. To this end, we have introduced the tDMNLS in Chapter 2 as an equivalent problem and substantiated our view that it is beneficial to consider time-integration methods for the tDMNLS formulation instead of treating the DMNLS directly. In particular, we have pointed out the existence of a limit system for the tDMNLS in the limit $\varepsilon \to 0$ in Chapter 3 and analyzed the accuracy of solutions of the limit system considered as approximations for the tDMNLS. This accuracy is fixed *a priori* by the parameter ε, and hence the limit system does not allow for approximations of the tDMNLS in any desired accuracy.

Subsequently, we have started constructing numerical methods for the tDMNLS in Chapters 4 and 5. Here, we have introduced the adiabatic Euler method as a first step and then refined the time-integration scheme to obtain the adiabatic midpoint rule. For both methods we have provided a rigorous error analysis for the semi-discretization in time. We consider especially the error analysis of the adiabatic midpoint rule (Theorem 10 and Theorem 11) to be the first of two main results in this thesis: in terms of "classical" error analysis, the adiabatic midpoint rule is a first-order scheme with a constant independent of ε. However, in addition we have shown that approximating solutions of the tDMNLS by the adiabatic midpoint rule with step-sizes τ that are integer multiples of ε yields approximations in $\mathcal{O}(\tau^2)$. This is because approximating solutions of the tDMNLS in this case is equivalent to approximating solutions of the limit system by the explicit midpoint rule, and hence the precise knowledge about the accuracy of the limit system as approximation of the tDMNLS, gathered in Chapter 3, was required to analyze the error behavior of the adiabatic midpoint rule in this special case. Moreover, we have found out that the accuracy of the scheme also improves for step-sizes τ that are integer fractions of ε due to cancellation effects in the error terms. By thoroughly adding up these highly oscillatory local error terms, we have proven that these special step-sizes allow for approximations in $\mathcal{O}(\varepsilon\tau)$.

Because an exorbitant increase in computational cost due to nested multiple sums did not allow us to construct a viable second-order scheme with our approach (Chapter 6), we have redirected our attention to another class of methods in Chapters 7 and 8. Here, we have introduced exponential counterparts of the previous methods – the adiabatic exponential Euler method and the adiabatic exponential midpoint rule – and provided a rigorous error analysis for the semi-discretization in time. The result of the error analysis by itself indicates no clear advantage of the exponential methods over the non-exponential methods, but, our numerical experiments suggest that the exponential methods have a significantly smaller error constant in the global error bound. In addition, the exponential methods preserve the ℓ^2_0 norm of the initial value. We consider the error analysis of the adiabatic exponential midpoint rule (Theorem 19) to be the second main result of this thesis because new techniques and ideas have been required in order to exploit the cancellation effects of the local error terms appropriately. Again, we have shown that the accuracy of the approximations increases to $\mathcal{O}(\tau\varepsilon)$ for step-sizes τ that are integer fractions of ε and to $\mathcal{O}(\tau^2)$ for step-sizes τ that are integer multiples of ε.

So far, we have mainly focused on time-integration methods for the DMNLS that allow for reliable approximations and whose accuracy is not fixed by the value of ε. However, we have left out any discussion of our methods concerning their efficiency in terms of computational costs versus accuracy. We address this final matter to some extend in the next section.

9.2. Final considerations – efficiency

The most promising numerical methods introduced in this thesis are the adiabatic midpoint rule (Chapter 5) and the adiabatic exponential midpoint rule (Chapter 8). However, the underlying concept – approximating the tDMNLS instead of the original DMNLS – comes at a cost of more expensive evaluations of the right-hand side of the differential equation due to the nested sum. One appeal of using the Strang splitting with a very small step-size in order to approximate solutions of the DMNLS directly – despite a lack of a rigorous error analysis – is that in this case evaluations of the right-hand side are incredibly cheap.

Balancing both approaches, we consider two key opposing effects: on the one hand, the adiabatic methods benefit from decreasing values of ε, whereas small values of ε appear to disadvantage the Strang splitting method. On the other hand the adiabatic methods suffer disproportionately from increasing the number of grid points in the space discretization due to the nested summation in the integration schemes.

We investigate these effects in the following numerical example. Here, we consider the DMNLS with $\alpha = 0.1$, $\delta = 1$, $T = 1$ with initial value $u_0(x) = e^{-3x^2} e^{3ix}$ and 64, 128 and 256 equidistant grid points in the interval $[-\pi, \pi]$ for $\varepsilon = 0.005$ and $\varepsilon = 0.002$. To this setting, we apply all three variants of the adiabatic midpoint rule (Chapter 5) and all three variants of the adiabatic exponential midpoint rule (Chapter 8) as well as the Strang splitting method (Section 2.3). In this experiment, we solely consider step-sizes that are integer multiples or integer fractions of ε in accordance with the improved accuracy results from Theorem 10, Theorem 11 and Theorem 19 for the adiabatic methods[1]. The reference solution is computed by the Strang splitting with a large number of steps ($\approx 10^7$). We start all methods with 10 time-steps and conduct up to $\approx 5 \cdot 10^3$ time-steps of all adiabatic methods and up to 10^5 time-steps of the Strang splitting method.

Figure 9.1 shows the computational times in relation to the accuracy of the methods for $\varepsilon = 0.005$ and 64 grid points (top left), 128 grid points (top right) and 256 grid points (bottom left). We observe that increasing the number of grid points increases the computational cost of the adiabatic methods significantly as expected. At the same time, the computational cost of the Strang splitting increases only sightly. In particular, we observe that for larger step-sizes the adiabatic methods yield higher accuracy, and hence the adiabatic methods outperform the Strang splitting in terms of computational cost versus accuracy in the top left panel and to some extend also in the top right panel where the adiabatic exponential methods still perform better. However, the bottom left panel shows that if the number of grid points is too large the nested summation contained in the adiabatic schemes shifts the advantage to the Strang splitting scheme.

[1] We recognize that previous numerical experiments suggest that the Strang splitting provides particularly poor results for these step-sizes, and hence that a better performance of the Strang splitting might be obtained with a "lucky guess" for a better step-size.

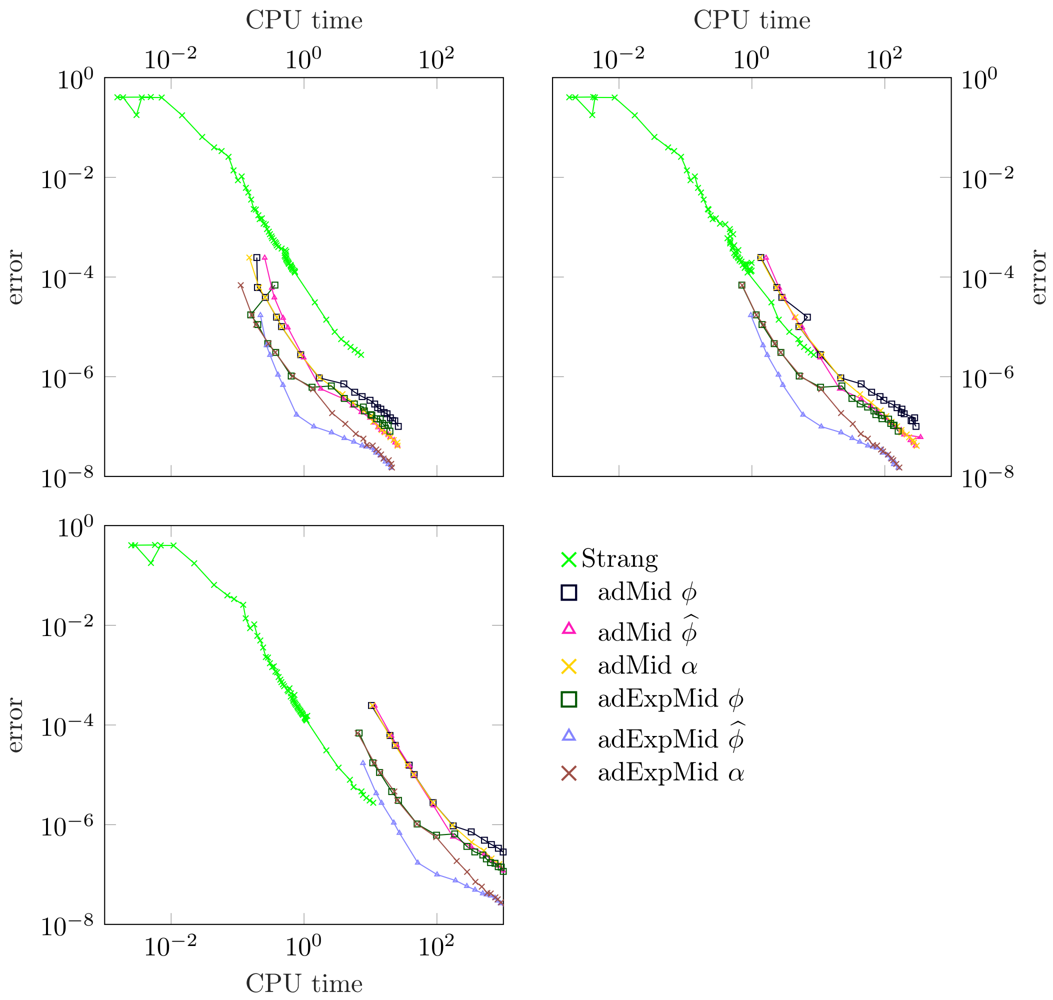

Figure 9.1: CPU-time versus maximal ℓ_0^2-error of the Strang splitting and all three variant of the adiabatic midpoint rule and of the adiabatic exponential midpoint rule for $\varepsilon = 0.005$ and 64 (top left), 128 (top right) and 256 (bottom left) equidistant grid points in space.

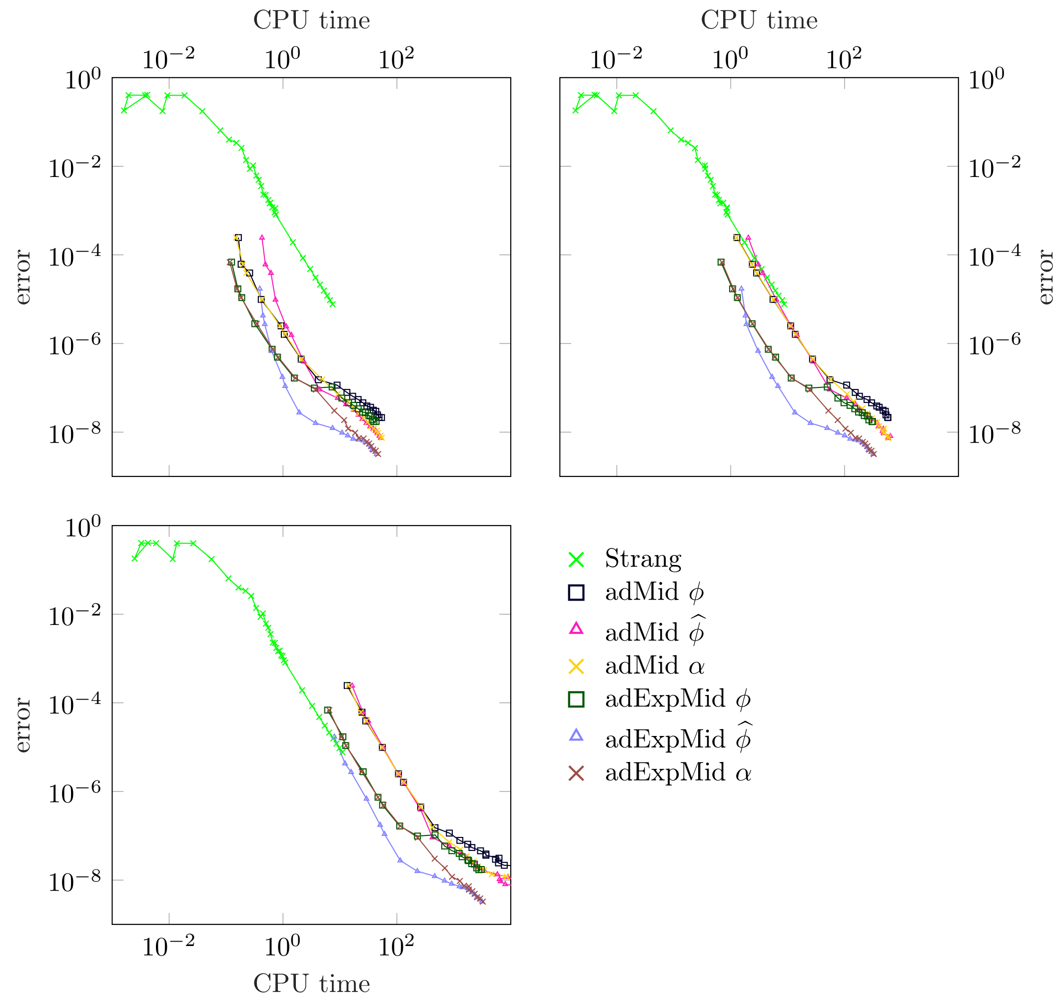

Figure 9.2: CPU-time versus maximal ℓ_0^2-error of the Strang splitting and all three variant of the adiabatic midpoint rule and of the adiabatic exponential midpoint rule for $\varepsilon = 0.002$ and 64 (top left), 128 (top right) and 256 (bottom left) equidistant grid points in space.

Figure 9.2 shows the same experiment but now the parameter ε is reduced to $\varepsilon = 0.002$. We observe that reducing the parameter ε benefits the adiabatic methods in terms of accuracy as stated in Theorem 10, Theorem 11 and Theorem 19, whereas we observe that the accuracy of the Strang splitting method is reduced. In this setting, we observe that the adiabatic methods significantly outperform the Strang splitting in terms of computational cost versus accuracy in the top left panel and top right panel. Moreover, the Strang splitting does not have an clear advantage over all adiabatic methods in the bottom left panel.

Remark. The bottom left panels in Figure 9.1 and Figure 9.2 suggest that one can use even more than 10^5 time-steps for the Strang splitting to increase the accuracy of the approximation to the same level of accuracy as for the adiabatic methods but at a lower computational cost. However, this is only true to a certain extend because at some point rounding errors prevent a higher accuracy of the method[2].

Conclusion. In general, investigating numerical methods in terms of work versus precession diagrams should be treated with caution because the results rely heavily on the underlying implementation of the methods and on the hardware. Hence, it is clear that the above experiment does not provide any conclusive information. It is also clear that increasing the number of grid points in space further increases the computational costs of the adiabatic methods severely. However, we take the liberty of concluding the following statement: the above experiment suggests that – depending on the value of ε and the number of grid points in space – the adiabatic methods introduced in this thesis are a worthwhile consideration for approximating solutions of the DMNLS. In particular, the adiabatic methods come with a rigorous error analysis ensuring reliable accuracy of the approximations.

9.3. Outlook

Concluding this chapter, we briefly address some open (and possibly interesting) questions that are not covered in this thesis.

The space discretization. In order to obtain a space discretization of the DMNLS and the tDMNLS for the numerical experiments, we have used the spectral collocation method (see Section 2.2.1) but we solely investigated the semi-discretization in time for all introduced numerical methods. A natural extension of this work is con-

[2] The accuracy of our implementation of the Strang splitting method starts to decrease for step-sizes $\tau < 10^{-7}$ in the setting of the above experiment.

sidering the full discretization of the tDMNLS, e.g., by investigating if and how the ideas and techniques from [20], where a full discretization of the NLS is considered, can be adapted.

Moreover, we have considered the DMNLS on the torus $\mathbb{T}$, whereas the classical DMNLS is considered on $\mathbb{R}$. It remains open whether and how our results can be extended to this setting.

Non-symmetric dispersion maps. Another possible starting point for future research is generalizing the dispersion map in the DMNLS, i.e. the function χ given in (1.3), in order to cover non-symmetric dispersion maps. For this purpose, one can consider a 2ε-periodic, piecewise constant function $\widetilde{\chi}$ with a positive section and a negative section of unequal length but still with zero mean over each 2ε-period. These more complicated dispersion maps are in fact considered in physics, [58].

Because exploiting the symmetric structure of the dispersion map is a crucial element for the improved error bound of the limit system (Theorem 3) and also for the improved error bounds of the adiabatic midpoint rule (Theorem 10 and 11) and the adiabatic exponential midpoint rule (Theorem 19), it remains open if and how our results can be adapted to this setting. Available results for the GTE with non-symmetric dispersion map (cf. [53]) suggest that it is unlikely to recover an improved error bound for the limit system in this setting. However, it might be possible to recover the cancellation effects in the local error terms by allowing more (possibly suitably weighted) evaluations of the right-hand side of the tDMNLS in each step of the (prospective) problem-adapted method.

Well-posedness of the limit system. Throughout this thesis we have assumed that the limit system (3.9) is globally well-posed in ℓ^2_s for $s \in \mathbb{N}$ with $0 \leq s \leq 5$, see Assumption 1. To prove this well-posedness of the limit system remains an open problem.

Competitiveness of the adiabatic methods. The multiple sum structure in the numeric scheme is the key limiting factor for the competitiveness of the adiabatic methods. Depending on the initial value, a considerable amount of summands in the multiple sum might only yield contributions close to zero. Hence, a natural idea is to introduce an adaptive selection mechanism into the scheme taking only summands with a substantial contribution to the entire sum into account. Preliminary tests indicate that this approach potentially leads to significantly lower computational costs for the adiabatic methods resulting in more competitive schemes.

APPENDIX A

Some technical estimates

In this section, we state and prove two lemmas containing rather technical estimates for various quantities arising frequently in the context of expanding the limit equation (3.9) and the tDMNLS (2.24) throughout this thesis.

The first lemma concerns various estimates for the triplet

$$V_{jkl}(t) = v_j(t)\overline{v}_k(t)v_l(t)$$

of entries of the solution v of the limit system, see (3.10). It has been published with Prof. Dr. Tobias Jahnke in the preprint [40].

Lemma 21. *Suppose that Assumption 1 holds. Let v be the solution of the limit system (3.9). Then, the product $V_{jkl}(t)$ fulfills the following estimates.*

If $v_0 \in \ell^2_1$, then

$$(i) \qquad \sum_{m\in\mathbb{Z}} \sum_{I_m} \left|V'_{jkl}(t)\right| \leq C(M_0^v)\,, \qquad \textit{for all} \quad t \in [0,T]\,.$$

If $v_0 \in \ell^2_3$, then

$$(ii) \qquad \sum_{m\in\mathbb{Z}} \sum_{I_m} \left|\omega_{[jklm]} V_{jkl}(t)\right| \leq C(M_2^v)\,, \qquad \textit{for all} \quad t \in [0,T]\,,$$

$$(iii) \qquad \sum_{m\in\mathbb{Z}} \sum_{I_m} \left|\omega_{[jklm]} V'_{jkl}(t)\right| \leq C(M_2^v)\,, \qquad \textit{for all} \quad t \in [0,T]\,,$$

$$(iv) \qquad \sum_{m\in\mathbb{Z}} \sum_{I_m} \left|V''_{jkl}(t)\right| \leq C(M_0^v) + \alpha C(M_2^v)\,, \qquad \textit{for all} \quad t \in [0,T]\,.$$

If $v_0 \in \ell^2_5$, then

$$(v) \qquad \sum_{m\in\mathbb{Z}} \sum_{I_m} \left|\omega^2_{[jklm]} V_{jkl}(t)\right| \leq C(M_4^v)\,, \qquad \textit{for all} \quad t \in [0,T]\,.$$

Proof. (i) Differentiating gives

$$V'_{jkl}(t) = v'_j(t)\overline{v}_k(t)v_l(t) + v_j(t)\overline{v}'_k(t)v_l(t) + v_j(t)\overline{v}_k(t)v'_l(t) \tag{A.1}$$

Moreover, we obtain by definition (3.9) the estimate

$$\left\|v'(t)\right\|_{\ell^1} = \sum_m \left|v'_m(t)\right| = \sum_{m\in\mathbb{Z}}\sum_{I_m} |v_j(t)|\,|\overline{v}_k(t)|\,|v_l(t)| \le C(M_0^v)\,, \tag{A.2}$$

and thus we acquire

$$\sum_{m\in\mathbb{Z}}\sum_{I_m} \left|V'_{jkl}(t)\right| \le C(M_0^v)\,. \tag{A.3}$$

(ii) Because we have for $(j,k,l)\in I_m$ the relation

$$\omega_{[jklm]} = (j^2 - k^2 + l^2 - m^2) = -2(k^2 + jk - jl + kl)\,, \tag{A.4}$$

we obtain

$$\begin{aligned}\sum_{m\in\mathbb{Z}}\sum_{I_m} \left|\omega_{[jklm]}V_{jkl}(t)\right| &= 2\sum_{m\in\mathbb{Z}}\sum_{I_m} \left|(k^2 + jk - jl + kl)V_{jkl}(t)\right| \\ &\le 2\big(\left\|v(t)\right\|^2_{\ell^1_0}\left\|v(t)\right\|_{\ell^1_2} + 3\left\|v(t)\right\|_{\ell^1_0}\left\|v(t)\right\|^2_{\ell^1_1}\big) \\ &\le C(M_2^v)\,. \end{aligned}\tag{A.5}$$

(iii) If we combine (A.4) with (A.1) and (A.2), then we get

$$\sum_{m\in\mathbb{Z}}\sum_{I_m} \left|\omega_{[jklm]}V'_{jkl}(t)\right| \le C(M_2^v)\,.$$

(iv) By differentiating (A.1), we obtain

$$\begin{aligned}V''_{jkl}(t) = {} & v''_j(t)\overline{v}_k(t)v_l(t) + v'_j(t)\overline{v}'_k(t)v_l(t) + v'_j(t)\overline{v}_k(t)v'_l(t) \\ & + v'_j(t)\overline{v}'_k(t)v_l(t) + v_j(t)\overline{v}''_k(t)v_l(t) + v_j(t)\overline{v}'_k(t)v'_l(t) \\ & + v'_j(t)\overline{v}_k(t)v'_l(t) + v_j(t)\overline{v}'_k(t)v'_l(t) + v_j(t)\overline{v}_k(t)v''_l(t)\,. \end{aligned}\tag{A.6}$$

Moreover, if we differentiate (3.9), we get

$$\left\|v''(t)\right\|_{\ell^1} \le \sum_{m\in\mathbb{Z}}\sum_{I_m} \left|V'_{jkl}(t) - \mathrm{i}\omega_{[jklm]}\alpha V_{jkl}(t)\right|\,, \tag{A.7}$$

and hence substituting (A.3) and (A.5) into (A.7) yields

$$\left\|v''(t)\right\|_{\ell^1} \le C(M_0^v) + \alpha C(M_2^v)\,. \tag{A.8}$$

Finally, combining (A.2) with (A.8) results in

$$\sum_{m\in\mathbb{Z}}\sum_{I_m}\left|V''_{jkl}(t)\right| \le C(M_0^v) + \alpha C(M_2^v)\,. \tag{A.9}$$

(v) A short computation starting from (A.4) leads to

$$\begin{aligned}\omega_{[jklm]}^2 &= 4(k^2+jk-jl+kl)^2\\ &= 4\big((k^2+jk)^2 - 2(k^2+jk)(jl+kl) + (jl+kl)^2\big)\\ &= 4\big(k^4+2k^3j+j^2k^2-2(k^3l+j^2kl+2k^2jl)+j^2l^2+2jkl^2+k^2l^2\big)\,.\end{aligned}$$

Hence, we obtain

$$\sum_{m\in\mathbb{Z}}\sum_{I_m}\left|\omega_{[jklm]}^2 V_{jkl}(t)\right| \le C(M_4^v)\,.$$

□

The second lemma concerns similar estimates for the products

$$Y_{jkl}(t) = y_j(t)\overline{y}_k(t)y_l(t) \quad \text{and} \quad Y_{pqrkl}(t) = y_p(t)\overline{y}_q(t)y_r(t)\overline{y}_k(t)y_l(t)$$

of entries of the solution y of the tDMNLS, see (2.23) and (5.41). It has been published with Prof. Dr. Tobias Jahnke in the preprint [40].

Lemma 22. *Let y be the solution of the tDMNLS* (2.24). *Then, $Y_{jkl}(t)$ and $Y_{pqrkl}(t)$ fulfill the following estimates.*

If $y_0 \in \ell_1^2$, then

$$\text{(i)}\quad \sum_{m\in\mathbb{Z}}\sum_{I_m}\left|Y'_{jkl}(t)\right| \le C(M_0^y)\,, \qquad \textit{for all} \quad t\in[0,T]\,,$$

$$\text{(ii)}\quad \sum_{m\in\mathbb{Z}}\sum_{I_m}\left|Y'_{pqrkl}(t)\right| \le C(M_0^y)\,, \qquad \textit{for all} \quad t\in[0,T]\,.$$

If $y_0 \in \ell_3^2$, then

$$\text{(iii)}\quad \sum_{m\in\mathbb{Z}}\sum_{I_m}\left|\omega_{[jklm]}Y_{jkl}(t)\right| \le C(M_2^y)\,, \qquad \textit{for all} \quad t\in[0,T]\,,$$

$$\text{(iv)}\quad \sum_{m\in\mathbb{Z}}\sum_{I_m}\left|\omega_{[jklm]}Y'_{jkl}(t)\right| \le C(M_2^y)\,, \qquad \textit{for all} \quad t\in[0,T]\,,$$

$$\text{(v)}\quad \sum_{m\in\mathbb{Z}}\sum_{I_m}\left|(\omega_{[jklm]}+\omega_{[pqrj]})Y_{pqrkl}(t)\right| \le C(M_2^y)\,, \qquad \textit{for all} \quad t\in[0,T]\,.$$

If $y_0 \in \ell_5^2$, then

$$\text{(vi)}\quad \sum_{m\in\mathbb{Z}}\sum_{I_m}\left|\omega_{[jklm]}^2 Y_{jkl}(t)\right| \le C(M_4^y)\,, \qquad \textit{for all} \quad t\in[0,T]\,.$$

The proof of Lemma 22 is largely analogous to the proof of Lemma 21 with straightforward minor modifications. For this reason, we omit the details.

APPENDIX B

An ℓ^1-bound for numerical solutions

A crucial ingredient for the error analysis of the numerical methods introduced in this thesis is the boundedness of the numerical scheme in ℓ^1. In this section, we state and prove a proposition ensuring this ℓ^1-boundedness under suitable conditions such that the proposition can be used to ensure the boundedness of all schemes in this thesis. In the proof, we rely on a well-known bootstrap-type argument (cf. [15,18,20,25,31]), which is accompanied by a step-size restriction for the respective numerical scheme.

Remark. Proposition 23 (below) has been published in a different context with Prof. Dr. Tobias Jahnke and Prof. Dr. Roland Schnaubelt in the preprint [41].

First, we denote by

$$\Psi_\theta^n(z) = \big(\psi_{\theta,m}(z)\big)_{m\in\mathbb{Z}} \tag{B.1}$$

$n \in \mathbb{N}$ steps of any numerical method with step-size τ starting at time θ with initial data $z = (z_m)_{m\in\mathbb{Z}}$. If $n = 1$, we simply write $\Psi_\theta(z)$ instead of $\Psi_\theta^1(z)$. Moreover, for $k, n \in \mathbb{N}$ the relations

$$\Psi_\theta^0(z) = z \quad \text{and} \quad \Psi_{t_k}^n(z) = \Psi_{t_{n+k-1}}\Big(\Psi_{t_k}^{n-1}(z)\Big)$$

follow directly form this definition, cf. Section 4.3 where we considered specifically the adiabatic Euler method.

The following proposition states boundedness of the numerical solution $\Psi\big(y(t_0)\big)$ in ℓ^1 for all $n \in \mathbb{N}$ for sufficiently small step-sizes τ.

Proposition 23. *Let $T > 0$ and y be a solution of the tDMNLS with initial value $y_0 \in \ell^1$. Furthermore, let* (B.1) *be a numerical scheme with the following properties.*

- *One step of the scheme applied to the tDMNLS is bounded by*

$$\big\|y(t_{n+1}) - \Psi_{t_n}\big(y(t_n)\big)\big\|_{\ell^1} \leq \tau^2 C_{loc} \tag{B.2}$$

with a constant $0 < C_{loc} < \infty$ *independent of* τ.

- *For* $\mu, \nu \in \ell^1$, *we have the bound*

$$\|\Psi_{t_0}(\mu) - \Psi_{t_0}(\nu))\|_{\ell^1} \leq e^{\tau C_{st}} \|\mu - \nu\|_{\ell^1} \tag{B.3}$$

with a constant $0 < C_{st} < \infty$ *depending only on* $\max\{\|\mu\|_{\ell^1}, \|\nu\|_{\ell^1}\}$.

Then, there exists $\tau_0 \in (0, T]$ *such that for step-sizes* $\tau \in (0, \tau_0]$ *the numerical solution* $\Psi_{t_0}^n(y_0)$ *stays bounded in* ℓ^1 *for* $n \in \mathbb{N}$ *with* $\tau n \leq T$.

Proof. The boundedness of the numerical solution is shown by an induction argument. First, we choose a constant $M_0^\star > M_0^y$. Clearly, the bound

$$\left\|\Psi_{t_0}^0(y_0)\right\|_{\ell^1} = \|y_0\|_{\ell^1} \leq M_0^\star$$

follows. Now, we assume that

$$\Psi_{t_p}^k(y(t_p)) \leq M_0^\star \quad \text{for all} \quad p \in \mathbb{N}, \quad k = 0, \dots, n-1, \quad t_{p+k} \leq T. \tag{B.4}$$

For the induction step, we prove that

$$\Psi_{t_p}^n(y(t_p)) \leq M_0^\star \quad \text{for all } p \in \mathbb{N}, \quad t_{p+k} \leq T$$

for sufficiently small step-sizes τ. Because our argument holds for arbitrary starting times t_p, we fix $p = 0$ with no loss of generality. Expressing $\Psi_{t_0}^n(y^{(0)})$ by the telescoping sum

$$\Psi_{t_0}^n(y^{(0)}) = y(t_n) - \sum_{k=0}^{n-1} \Psi_{t_{n-k}}^k(y(t_{n-k})) - \Psi_{t_{n-k-1}}^{k+1}(y(t_{n-k-1}))$$

allows us to estimate

$$\left\|\Psi_{t_0}^n(y^{(0)})\right\|_{\ell^1} \leq \|y(t_n)\|_{\ell^1} + \sum_{k=0}^{n-1} \left\|\Psi_{t_{n-k}}^k(y(t_{n-k})) - \Psi_{t_{n-k-1}}^{k+1}(y(t_{n-k-1}))\right\|_{\ell^1}. \tag{B.5}$$

On account of (B.4), we now apply the stability (B.3) of the numerical scheme for each summand in (B.5) and get

$$\begin{aligned}
&\left\|\Psi_{t_{n-k}}^k(y(t_{n-k})) - \Psi_{t_{n-k-1}}^{k+1}(y(t_{n-k-1}))\right\|_{\ell^1} \\
&\quad = \left\|\Psi_{t_{n-1}}\Big(\Psi_{t_{n-k}}^{k-1}(y(t_{n-k}))\Big) - \Psi_{t_{n-1}}\Big(\Psi_{t_{n-k-1}}^{k}(y(t_{n-k-1}))\Big)\right\|_{\ell^1} \\
&\quad \leq e^{\tau C(M_0^\star)} \left\|\Psi_{t_{n-k}}^{k-1}(y(t_{n-k})) - \Psi_{t_{n-k-1}}^{k}(y(t_{n-k-1}))\right\|_{\ell^1}.
\end{aligned}$$

We continue in this fashion obtaining recursively

$$\begin{aligned}&\left\|\Psi^{k}_{t_{n-k}}\big(y(t_{n-k})\big) - \Psi^{k+1}_{t_{n-k-1}}\big(y(t_{n-k-1})\big)\right\|_{\ell^1}\\&\qquad\le e^{TC(M_0^\star)}\left\|y(t_{n-k}) - \Psi_{t_{n-k-1}}\big(y(t_{n-k-1})\big)\right\|_{\ell^1}\,.\end{aligned}$$

Then, the bound of the local error (B.2) yields

$$\left\|\Psi^{k}_{t_{n-k}}\big(y(t_{n-k})\big) - \Psi^{k+1}_{t_{n-k-1}}\big(y(t_{n-k-1})\big)\right\|_{\ell^1} \le \tau^2 e^{TC(M_0^\star)} C_{loc}\,. \tag{B.6}$$

Finally, substituting (B.6) into (B.5) gives

$$\left\|\Psi^{n}_{t_0}\big(y^{(0)}\big)\right\|_{\ell^1} \le \|y(t_n)\|_{\ell^1} + n\tau^2 e^{TC(M_0^\star)} C_{loc} \le M_0^y + \tau T e^{TC(M_0^\star)} C_{loc}\,.$$

Hence, if τ is so small that

$$0 < \tau \le \tau_0 \coloneqq \frac{M_0^\star - M_0^y}{C_{loc} T} e^{-TC(M_0^\star)}\,, \tag{B.7}$$

we thus obtain $\Psi^{n}_{t_0}\big(y^{(0)}\big) \le M_0^\star$ as desired. □

Remark. Step-size restrictions in the manner of (B.7) are not a characteristic property of the tDMNLS nor specific for the introduced methods in this thesis. On the contrary, such restrictions typically arise in the context of numerical methods for nonlinear partial differential equations, cf. [15,18,20,25,31] and the references therein. Fortunately, the step-size restriction (B.7) is usually a worst-case estimate, and hence far too pessimistic in many applications.

APPENDIX C

Computation of a double integral

In this chapter, we compute the double integral

$$I(\tilde{\omega}, \omega) := \int_a^b \int_a^s \exp\left(-\mathrm{i}\tilde{\omega}\phi(\sigma)\right) \exp\left(-\mathrm{i}\omega\phi(s)\right) \mathrm{d}\sigma \, \mathrm{d}s \,. \tag{C.1}$$

This integral originates from (6.4) after substituting $\sigma = \sigma/\varepsilon$ and $s = s/\sigma$.

First, we single out the special case $\tilde{\omega} = 0$ because this is the relevant integral for the α-correction, see Section 6.2. Here, we have

$$I(\tilde{\omega}, \omega) = I_1(\omega) - a \int_a^b \exp\left(-\mathrm{i}\omega\phi(s)\right) \mathrm{d}s \,,$$

with

$$I_1(\omega) := \int_a^b s \exp\left(-\mathrm{i}\omega\phi(s)\right) \mathrm{d}s \,.$$

On account of Lemma 5, it thus remains to compute $I_1(\omega)$. Decomposing the integral into suitable sub-integrals combined with the following lemma allows us to compute this integral. We employ the abbreviation

$$E(z) := \exp(\mathrm{i}\omega\delta z) \,.$$

Lemma 24. *Let $\omega \neq 0$ and $a \in [\kappa, \kappa+1]$, $b \in [\kappa, \kappa+1]$ for $\kappa \in \mathbb{N}$.*

(i) If κ is even, then

$$I_1(\omega) = \frac{bE(b-\kappa) - aE(a-\kappa)}{\mathrm{i}\omega\delta} - \frac{E(b-\kappa) - E(a-\kappa)}{(\mathrm{i}\omega\delta)^2} \,.$$

(ii) If κ is odd, then

$$I_1(\omega) = \frac{bE(\kappa+1-b) - aE(\kappa+1-a)}{-\mathrm{i}\omega\delta} - \frac{E(\kappa+1-b) - E(\kappa+1-a)}{(\mathrm{i}\omega\delta)^2} \,.$$

Proof. We recall that

$$\phi(z) = \begin{cases} -\delta z & \text{if} \quad z \in [\kappa, \kappa+1) \quad \text{and} \quad \kappa \text{ even}\,, \\ -\delta(2-z) & \text{if} \quad z \in [\kappa, \kappa+1) \quad \text{and}\kappa \text{ odd}\,, \end{cases} \tag{C.2}$$

by (2.18). Because ϕ is periodic; cf. (2.18), we obtain for even κ

$$I_1(\omega) = \int_{a-\kappa}^{b-\kappa} (s+\kappa) \exp\left(-\mathrm{i}\omega\phi(s)\right) \mathrm{d}s = \int_{a-\kappa}^{b-\kappa} (s+\kappa) E(s)\, \mathrm{d}s\,.$$

Then, integration by parts and Lemma 5 give

$$\begin{aligned} I_1(\omega) = {} & \frac{(b-\kappa)E(b-\kappa) - (a-\kappa)E(a-\kappa)}{\mathrm{i}\omega\delta} - \frac{E(b-\kappa) - E(a-\kappa)}{(\mathrm{i}\omega\delta)^2} \\ & + \kappa \frac{E(b-\kappa) - E(a-\kappa)}{\mathrm{i}\omega\delta}\,, \end{aligned}$$

and thus adding up yields (i). Equation (ii) follows analogously. $\square$

The second and final lemma is devoted to the remaining cases of the integral (C.1). Here, we abbreviate

$$E_\theta(z) = \exp(\mathrm{i}\theta\delta z) \quad \text{for} \quad \theta \in \{\tilde{\omega}, \omega\}$$

for simplification.

Lemma 25. *Let $a \in [\kappa, \kappa+1]$ and $b \in [\kappa, \kappa+1]$ for $\kappa \in \mathbb{N}$.*

(a) Suppose that $\omega \neq 0$, $\tilde{\omega} \neq 0$ and $\omega + \tilde{\omega} \neq 0$.

(i) If κ is even, then

$$I(\tilde{\omega}, \omega) = \frac{1}{\mathrm{i}\tilde{\omega}\delta} \left(\frac{E_{\tilde{\omega}+\omega}(b-\kappa) - E_{\tilde{\omega}+\omega}(a-\kappa)}{\mathrm{i}(\tilde{\omega}+\omega)\delta} - \frac{E_{\tilde{\omega}}(a-\kappa)E_{\omega}(b-\kappa) - E_{\tilde{\omega}+\omega}(a-\kappa)}{\mathrm{i}\omega\delta} \right)\,.$$

(ii) If κ is odd, then

$$\begin{aligned} I(\tilde{\omega}, \omega) = \frac{1}{-\mathrm{i}\tilde{\omega}\delta} \Bigg(& \frac{E_{\tilde{\omega}+\omega}(\kappa+1-b) - E_{\tilde{\omega}+\omega}(\kappa+1-a)}{\mathrm{i}(\tilde{\omega}+\omega)\delta} \\ & - \frac{E_{\tilde{\omega}}(\kappa+1-a)E_{\omega}(\kappa+1-b) - E_{\tilde{\omega}+\omega}(\kappa+1-a)}{\mathrm{i}\omega\delta} \Bigg)\,. \end{aligned}$$

(b) Suppose that $\omega = 0$, $\tilde{\omega} \neq 0$.

(i) If κ is even, then

$$I(\tilde{\omega}, \omega) = \frac{1}{\mathrm{i}\tilde{\omega}\delta} \left(\frac{E_{\tilde{\omega}}(b-\kappa) - E_{\tilde{\omega}}(a-\kappa)}{\mathrm{i}\tilde{\omega}\delta} - (b-a)E_{\tilde{\omega}}(a-\kappa) \right)\,.$$

(ii) If κ is odd, then

$$I(\tilde{\omega},\omega) = \frac{1}{-\mathrm{i}\tilde{\omega}\delta}\left(\tfrac{E_{\tilde{\omega}}(\kappa+1-b)-E_{\tilde{\omega}}(\kappa+1-a)}{-\mathrm{i}\tilde{\omega}\delta} - (b-a)E_{\tilde{\omega}}(\kappa+1-a)\right) .$$

(c) Suppose that $\omega \neq 0$, $\tilde{\omega} \neq 0$ and $\omega + \tilde{\omega} = 0$.

(i) If κ is even, then

$$I(\tilde{\omega},\omega) = \frac{1}{\mathrm{i}\tilde{\omega}\delta}\left((b-a) - \frac{E_{\tilde{\omega}}(a-\kappa)E_{\omega}(b-\kappa)-1}{\mathrm{i}\omega\delta}\right) .$$

(ii) If κ is odd, then

$$I(\tilde{\omega},\omega) = \frac{1}{-\mathrm{i}\tilde{\omega}\delta}\left((b-a) - \frac{E_{\tilde{\omega}}(\kappa+1-a)E_{\omega}(\kappa+1-b)-1}{-\mathrm{i}\omega\delta}\right) .$$

Proof. We solely consider even κ because the case κ is odd follows with minor modifications. Straightforward calculation using (C.2) leads to:

(a)
$$\begin{aligned} I(\tilde{\omega},\omega) &= \int_{a-\kappa}^{b-\kappa}\int_{a-\kappa}^{s} E_{\tilde{\omega}}(\sigma)E_{\omega}(s)\,\mathrm{d}\sigma\,\mathrm{d}s \\ &= (\mathrm{i}\tilde{\omega}\delta)^{-1}\int_{a-\kappa}^{b-\kappa} E_{\tilde{\omega}+\omega}(s) - E_{\tilde{\omega}}(a-\kappa)E_{\omega}(s)\,\mathrm{d}s \\ &= (\mathrm{i}\tilde{\omega}\delta)^{-1}\left(\tfrac{E_{\tilde{\omega}+\omega}(b-\kappa)-E_{\tilde{\omega}+\omega}(a-\kappa)}{\mathrm{i}(\tilde{\omega}+\omega)\delta} - \tfrac{E_{\tilde{\omega}}(a-\kappa)E_{\omega}(b-\kappa)-E_{\tilde{\omega}+\omega}(a-\kappa)}{\mathrm{i}\omega\delta}\right) . \end{aligned}$$

(b)
$$\begin{aligned} I(\tilde{\omega},\omega) &= \int_{a-\kappa}^{b-\kappa}\int_{a-\kappa}^{s} E_{\tilde{\omega}}(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s \\ &= (\mathrm{i}\tilde{\omega}\delta)^{-1}\int_{a-\kappa}^{b-\kappa} E_{\tilde{\omega}}(s) - E_{\tilde{\omega}}(a-\kappa)\,\mathrm{d}s \\ &= (\mathrm{i}\tilde{\omega}\delta)^{-1}\left(\frac{E_{\tilde{\omega}}(b-\kappa)-E_{\tilde{\omega}}(a-\kappa)}{\mathrm{i}\tilde{\omega}\delta} - (b-a)E_{\tilde{\omega}}(a-\kappa)\right) . \end{aligned}$$

(c)
$$\begin{aligned} I(\tilde{\omega},\omega) &= \int_{a-\kappa}^{b-\kappa}\int_{a-\kappa}^{s} E_{\tilde{\omega}}(\sigma)E_{\omega}(s)\,\mathrm{d}\sigma\,\mathrm{d}s \\ &= (\mathrm{i}\tilde{\omega}\delta)^{-1}\int_{a-\kappa}^{b-\kappa} 1 - E_{\tilde{\omega}}(a-\kappa)E_{\omega}(s)\,\mathrm{d}s \\ &= (\mathrm{i}\tilde{\omega}\delta)^{-1}\left((b-a) - \frac{E_{\tilde{\omega}}(a-\kappa)E_{\omega}(b-\kappa)-1}{\mathrm{i}\omega\delta}\right) . \end{aligned}$$

$\square$

Danksagungen

An dieser Stelle bedanke ich mich bei allen, die mich während der Anfertigung meiner Dissertation unterstützt haben.

Mein besonderer Dank gilt dabei meinem Doktorvater Prof. Dr. Tobias Jahnke, der mir die Möglichkeit eröffnet und zudem das Vertrauen geschenkt hat, eine Promotion in Angriff zu nehmen. Die Betreuung meiner Promotion war stets vorbildlich. Selbst ein überfüllter Terminkalender und eine randvolle To-do-Liste konnten nicht verhindern, dass im Zweifelsfall immer ein Zeitfenster für fachliche sowie moralische Unterstützung geschaffen wurde. Neben allen fachlichen Kompetenzen, die ich während meiner Promotion erlernen durfte, empfand ich unsere gemeinsame Arbeit auch als persönliche Bereicherung.

Für die Übernahme des Korreferats danke ich Prof. Dr. Marlis Hochbruck. Ebenfalls vielen Dank für das stets offene Ohr für alle auftretenden Belange und Probleme der Promovierenden während meiner Arbeit im Konvent der Doktoranden/innen.

Für fachliche Unterstützung, speziell während meiner funktionalanalytischen Gehversuche, bedanke ich mich bei Luca Hornung, Johannes Ernesti und Christine Grathwohl. Ebenso Danke an Lydia Wagner, Christine Grathwohl, Johannes Ernesti, Dr. Daniel Weiß und Christian Rheinbay für konstruktive Kritik an verschiedenen Kapiteln dieser Arbeit.

Meine Zeit als wissenschaftlicher Mitarbeiter am IANM 3 wäre nicht, was sie ist, ohne alle Kollegen/innen, die ich hier kennen und schätzen lernen durfte. Als mittlerweile dienstältester Doktorand der Arbeitsgruppe blicke ich zurück auf eine Zeit, die vor gut vier Jahren in einem voll besetzten Viererbüro im Allianzgebäude begann und nun in einem neuen Einzelbüro im preisgekrönten Kollegiengebäude Mathematik ohne funktionsfähige Sonnensegel endet. Ich danke allen, die dafür gesorgt haben, dass mir diese Zeit in sehr guter Erinnerung bleiben wird.

Schließlich danke ich meiner Familie, die immer an mich geglaubt hat, und auch ohne mathematische Fachkenntnisse stets wusste, dass ich "das" schaffen werde. Abschließend ein großer Dank meiner Freundin Christine Stephan, die mir insbesondere in der heißen Phase den Rücken frei gehalten hat und zeitweise sogar meinen obligatorischen Staubsaugerdienst übernahm.

Marcel Mikl, Karlsruhe im Mai 2017

Bibliography

[1] A. Abdulle, E. Weinan, B. Engquist, and E. Vanden-Eijnden. The heterogeneous multiscale method. *Acta Numerica*, 21:1–87, 2012.

[2] M. J. Ablowitz and G. Biondini. Multiscale pulse dynamics in communication systems with strong dispersion management. *Optics Letters*, 23(21):1668–1670, 1998.

[3] G. P. Agrawal. *Fiber-optic communication systems.* John Wiley, New York, 2002.

[4] G. P. Agrawal. *Nonlinear fiber optics.* Elsevier, Academic Press, Amsterdam, 2013.

[5] P. Antonelli, J.-C. Saut, and C. Sparber. Well-Posedness and averaging of NLS with time-periodic dispersion management. Technical report, 2012. URL `https://arxiv.org/abs/1204.4468`.

[6] W. Auzinger, T. Kassebacher, O. Koch, and M. Thalhammer. Adaptive splitting methods for nonlinear Schrödinger equations in the semiclassical regime. *Numerical Algorithms*, 72(1):1–35, 2016.

[7] P. Bader, A. Iserles, K. Kropielnicka, and P. Singh. Efficient methods for linear Schrödinger equation in the semiclassical regime with time-dependent potential. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 472(2193), 2016.

[8] A. Biswas. Higher-order Gabitov–Turitsyn equation for solitons in optical fibers. *Optik - International Journal for Light and Electron Optics*, 118(3):120–133, 2007.

[9] A. Biswas, D. Milovic, and M. R. Edwards. *Mathematical theory of dispersion-managed optical solitons.* Nonlinear physical science. Higher Education Press Springer, Beijing Berlin New York, 2010.

[10] S. Blanes, F. Casas, J. Oteo, and J. Ros. The Magnus expansion and some of its applications. *Physics Reports*, 470(5):151–238, 2009.

[11] J. Bourgain. *Global solutions of nonlinear Schrödinger equations.* American Mathematical Society, Providence, R.I., 1999.

[12] S. Buchholz, L. Gauckler, V. Grimm, M. Hochbruck, and T. Jahnke. Closing the gap between trigonometric integrators and splitting methods for highly oscillatory differential equations. CRC 1173-Preprint 2016/22, Karlsruhe Institute of Technology, 2016. URL `http://www.waves.kit.edu/downloads/CRC1173_Preprint_2016-22.pdf`.

[13] M. Calvo, P. Chartier, A. Murua, and J. Sanz-Serna. Numerical stroboscopic averaging for ODEs and DAEs. *Applied Numerical Mathematics*, 61(10):1077–1095, 2011.

[14] F. Castella, P. Chartier, F. Méhats, and A. Murua. Stroboscopic Averaging for the Nonlinear Schrödinger Equation. *Foundations of Computational Mathematics*, 15(2):519–559, 2015.

[15] P. Chartier, F. Méhats, M. Thalhammer, and Y. Zhang. Improved error estimates for splitting methods applied to highly-oscillatory nonlinear Schrödinger equations. *Mathematics of Computation*, 85(302):2863–2885, 2016.

[16] D. Cohen, T. Jahnke, K. Lorenz, and C. Lubich. Numerical integrators for highly oscillatory Hamiltonian systems: a review. In *Analysis, Modeling and Simulation of Multiscale Problems*, pages 553–576. Springer, Berlin, 2006.

[17] J. N. Downing. *Fiber-optic communications.* Thomson/Delmar Learning, Clifton Park, NY, 2005.

[18] J. Eilinghoff, R. Schnaubelt, and K. Schratz. Fractional error estimates of splitting schemes for the nonlinear Schrödinger equation. *Journal of Mathematical Analysis and Applications*, 442(2):740–760, 2016.

[19] B. Engquist, A. Fokas, E. Hairer, and A. Iserles. *Highly Oscillatory Problems.* Cambridge University Press, New York, NY, USA, 1st edition, 2009.

[20] E. Faou. *Geometric numerical integration and Schrödinger equations.* Zurich Lectures in Advanced Mathematics. European Mathematical Society (EMS), Zürich, 2012.

[21] E. Faou, V. Gradinaru, and C. Lubich. Computing Semiclassical Quantum

Dynamics with Hagedorn Wavepackets. *SIAM Journal on Scientific Computing*, 31(4):3027–3041, 2009.

[22] G. Fibich. *The nonlinear Schrödinger equation.* Springer, Cham, 2015.

[23] I. Gabitov and S. K. Turitsyn. Averaged pulse dynamics in a cascaded transmission system with passive dispersion compensation. *Optics Letters*, 21(5): 327–329, 1996.

[24] I. Gabitov and S. K. Turitsyn. Breathing solitons in optical fiber links. *Journal of Experimental and Theoretical Physics Letters*, 63(10):861–866, 1996.

[25] L. Gauckler. Error Analysis of Trigonometric Integrators for Semilinear Wave Equations. *SIAM Journal on Numerical Analysis*, 53(2):1082–1106, 2015.

[26] W. R. Green and D. Hundertmark. Exponential Decay of Dispersion-Managed Solitons for General Dispersion Profiles. *Letters in Mathematical Physics*, 106 (2):221–249, 2016.

[27] V. S. Grigoryan, R. M. Mu, G. M. Carter, and C. R. Menyuk. Experimental demonstration of long-distance dispersion-managed soliton propagation at zero average dispersion. *IEEE Photonics Technology Letters*, 12(1):45–46, 2000.

[28] V. Grimm and M. Hochbruck. Error analysis of exponential integrators for oscillatory second-order differential equations. *Journal of Physics A: Mathematical and General*, 39(19):5495–5507, 2006.

[29] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration, Structure-Preserving Algorithms for Ordinary Differential Equations.* Springer, Berlin, Heidelberg, 2nd edition, 2006.

[30] E. Hairer, S. P. Nørsett, and G. Wanner. *Solving ordinary differential equations I: Nonstiff Problems.* Springer-Verlag, Berlin, second edition, corrected 3rd printing, 2008.

[31] E. Hansen and A. Ostermann. High-order splitting schemes for semilinear evolution equations. *BIT Numerical Mathematics*, 56(4):1303–1316, 2016.

[32] J. Hecht. *Understanding fiber optics.* Pearson Prentice Hall, Upper Saddle River, N.J, 2006.

[33] M. Hochbruck and C. Lubich. A Gautschi-type method for oscillatory second-order differential equations. *Numerische Mathematik*, 83(3):403–426, 1999.

[34] M. Hochbruck and A. Ostermann. Exponential integrators. *Acta Numerica*, 19: 209–286, 2010.

[35] D. Hundertmark and Y.-R. Lee. Decay Estimates and Smoothness for Solutions of the Dispersion Managed Non-linear Schrödinger Equation. *Communications in Mathematical Physics*, 286(3):851–873, 2009.

[36] A. Iserles, H. Z. Munthe-Kaas, S. P. Nørsett, and A. Zanna. Lie-group methods. *Acta Numerica 2000*, 9:215–365, 2000.

[37] T. Jahnke. *Numerische Verfahren für fast adiabatische Quantendynamik*. PhD thesis, Uni Tübingen, 2003.

[38] T. Jahnke. Long-Time-Step Integrators for Almost-Adiabatic Quantum Dynamics. *SIAM Journal on Scientific Computing*, 25(6):2145–2164, 2004.

[39] T. Jahnke and C. Lubich. Numerical integrators for quantum dynamics close to the adiabatic limit. *Numerische Mathematik*, 94(2):289–314, 2003.

[40] T. Jahnke and M. Mikl. Adiabatic midpoint rule for the dispersion-managed nonlinear Schrödinger equation. CRC 1173-Preprint 2016/28, Karlsruhe Institute of Technology, 2016. URL `http://www.waves.kit.edu/downloads/CRC1173_Preprint_2016-28.pdf`.

[41] T. Jahnke, M. Mikl, and R. Schnaubelt. Strang splitting for a semilinear Schrödinger equation with damping and forcing. CRC 1173-Preprint 2016/4, Karlsruhe Institute of Technology, 2016. URL `http://www.waves.kit.edu/downloads/CRC1173_Preprint_2016-4.pdf`.

[42] C. Lange, C. Behrens, E. Weis, J. Kraus, S. Krauss, M. Grigat, H. Droste, T. Rosowski, T. Monath, C. A. Bunge, E. Bogenfeld, M. Amend, N. Bayer, M. Dueser, F. J. Westphal, and A. Gladisch. Bridging the Last Mile. In *Broadband Coverage in Germany; 10. ITG-Symposium*, pages 1–8, 2016.

[43] C. Lin, H. Kogelnik, and L. G. Cohen. Optical-pulse equalization of low-dispersion transmission in single-mode fibers in the 1.3 - 1.7-microm spectral region. *Optics letters*, 5(11):476–8, 1980.

[44] C. Lubich. On splitting methods for Schrödinger-Poisson and cubic nonlinear Schrödinger equations. *Mathematics of computation*, 77(264):2141–2153, 2008.

[45] C. Lubich. *From quantum to classical molecular dynamics: reduced models and numerical analysis*. European Mathematical Society, Zürich, Switzerland, 2008.

[46] S. B. Medvedev and S. K. Turitsyn. Hamiltonian averaging and integrability in nonlinear systems with periodically varying dispersion. *Journal of Experimental and Theoretical Physics Letters*, 69(7):499–504, 1999.

[47] C. R. Menyuk. Application of multiple-length-scale methods to the study of optical fiber transmission. *Journal of Engineering Mathematics*, 36(1):113–136, 1999.

[48] L. F. Mollenauer, P. V. Mamyshev, J. Gripp, M. J. Neubelt, N. Mamysheva, L. Grüner-Nielsen, and T. Veng. Demonstration of massive wavelength-division multiplexing over transoceanic distances by use of dispersion-managed solitons. *Optics letters*, 25(10):704–706, 2000.

[49] L. F. Mollenauer, A. Grant, X. Liu, X. Wei, C. Xie, and I. Kang. Experimental test of dense wavelength-division multiplexing using novel, periodic-group-delay-complemented dispersion compensation and dispersion-managed solitons. *Optics letters*, 28(21):2043–2045, 2003.

[50] J. V. Moloney and A. C. Newell. *Nonlinear Optics*. Westview Press, Boulder, Colo, 2004.

[51] A. H. Nayfeh. *Perturbation methods*. Wiley, New York, 1973.

[52] A. Pazy. *Semigroups of linear operators and applications to partial differential equations*. Springer-Verlag, New York, 1983.

[53] D. Pelinovsky and V. Zharnitsky. Averaging of Dispersion-Managed Solitons: Existence and Stability. *SIAM Journal of Applied Mathematics*, 63(3):745–776, 2003.

[54] L. R. Petzold, L. O. Jay, and J. Yen. Numerical solution of highly oscillatory ordinary differential equations. *Acta Numerica*, 6:437–483, 1997.

[55] G. Strang. On the Construction and Comparison of Difference Schemes. *SIAM Journal on Numerical Analysis*, 5(3):506–517, 1968.

[56] L. N. Trefethen. *Spectral methods in MATLAB*. Society for Industrial and Applied Mathematics, Philadelphia, PA, 2000.

[57] S. K. Turitsyn, E. G. Shapiro, S. B. Medvedev, M. P. Fedoruk, and V. K. Mezentsev. Physics and mathematics of dispersion-managed optical solitons. *Comptes Rendus Physique*, 4(1):145–161, 2003.

[58] S. K. Turitsyn, B. G. Bale, and M. P. Fedoruk. Dispersion-managed solitons in fibre systems and lasers. *Physics Reports*, 521(4):135–203, 2012.

[59] D. Werner. *Funktionalanalysis*. Springer Berlin Heidelberg, 2007.

[60] V. Zharnitsky, E. Grenier, C. K. Jones, and S. K. Turitsyn. Stabilizing effects of dispersion management. *Physica D: Nonlinear Phenomena*, 152:794–817, 2001.