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Michael Kirn

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Referent: Prof. Dr. Tobias Jahnke
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Contents

Chapter 1

Introduction

In 1928, British physicist Paul Dirac proposed a new evolution equation [Dir28], with the aim of accurately describing the behavior of electrons and other spin-1/2 particles within the framework of special relativity. In particular, Dirac's equation, in contrast to the Schrödinger equation, also applies to particles travelling at velocities near the speed of light. It has not only become one of the fundamental equations in relativistic quantum mechanics, but also led to the prediction of antimatter as a new form of matter [And33].

The equation proposed by Dirac is nowadays known as the *free Dirac equation*. In dimensionless form, it can be written as

$$\partial_t \psi^\varepsilon(t,x) = -\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi^\varepsilon(t,x), \qquad \mathcal{T}_\varepsilon = -\mathrm{i}\varepsilon \sum_{j=1}^{3} \alpha_j \partial_j + \beta \tag{1.1}$$

for $t \geq 0, x \in \mathbb{R}^3$. Here, $\psi^\varepsilon = \psi^\varepsilon(t,x) \in \mathbb{C}^4$ is the vector-valued wave function. The operator $\mathcal{T}_\varepsilon$, sometimes called the *free Dirac operator*, is self-adjoint on the Sobolev space $\left(H^1(\mathbb{R}^3)\right)^4$ [Tha92, Theorem 1.1]. It contains the Dirac matrices α_j, $j = 1,2,3$, and β, which are given by

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \qquad j = 1,2,3, \qquad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}.$$

They in turn are determined by the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

A special role is played by the parameter $\varepsilon = v/c \in (0,1)$, which is the ratio of the velocity v of the moving particle and the speed of light c [BMP98; Bao+16b; Bao+17]. There are two important parameter regimes. The first one is the relativistic regime, where v is close to the speed of light, such that ε is close to 1. The other one is the *nonrelativistic limit regime*. This corresponds to quantum mechanical systems describing particles much slower than the speed of light. Thus, $\varepsilon \ll 1$ is small in this case, but it is not small enough to neglect relativistic effects. In this regime, solutions of the Dirac equation exhibit rapid oscillations in time with frequency proportional to $1/\varepsilon^2$. Understanding this oscillatory behavior will be crucial for this thesis, which is why we discuss it in detail at the end of the introduction.

In applications, it is interesting to observe how particles behave under an external electromagnetic field and when particle self-interaction is taken into account [HC09; Mer+10; Sol70;

Thi58]. Then, an electromagnetic potential W and a nonlinearity are included in the Dirac equation. The two most prominent examples for the latter are the Soler model [Sol70] and the Thirring model [Thi58]. In this work, we consider the *nonlinear Dirac equation (NLDE)* in the nonrelativistic limit regime $\varepsilon \ll 1$ in the form [Bao+16b; CW20]

$$\begin{aligned} \partial_t \psi^\varepsilon(t,x) &= -\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi^\varepsilon(t,x) - \mathrm{i}W(t,x)\psi^\varepsilon(t,x) - \mathrm{i}F(\psi^\varepsilon(t,x))\psi^\varepsilon(t,x), \\ \psi^\varepsilon(0,x) &= \psi^{\mathrm{init}}(x), \end{aligned} \tag{1.2}$$

with nonlinearity F given by

$$F(v) = \gamma_1 (v^* \beta v)\beta + \gamma_2 |v|^2 I_4.$$

The parameters $\gamma_1, \gamma_2 \in \mathbb{R}$ determine the kind of self interaction as well as the interaction strength. For $\gamma_1 = 0$, the Soler model is obtained, whereas the case $\gamma_2 = 0$ corresponds to the Thirring model. The electromagnetic potential $W = W(t,x) \in \mathbb{C}^{4\times 4}$ is composed of an electric scalar potential $V(t,x) \in \mathbb{R}$ and a magnetic vector potential $A(t,x) = (A_1(t,x), A_2(t,x), A_3(t,x))^T \in \mathbb{R}^3$. With the matrices from above, W is given by

$$W(t,x) = V(t,x) I_4 - \sum_{j=1}^{3} A_j(t,x)\alpha_j. \tag{1.3}$$

From an analytical point of view, it has been proven that there exist solutions of the NLDE on time intervals independent of ε [CW20; Naj92]. For smooth initial data, those solutions remain smooth in space, but as for the free Dirac equation, they oscillate rapidly in time with frequency proportional to $1/\varepsilon^2$ [Bao+16a; CW20]. The oscillations go hand in hand with time derivatives that are unbounded w.r.t. ε. In the left half of Figure 1.1, the temporal evolution of a typical solution of the NLDE is illustrated. Here, a version of the NLDE in one space dimension is considered, a point $x_0 \in \mathbb{R}$ in space is fixed, and the real part of the first component of a solution ψ^ε at x_0 is observed over time. Comparing the lines for the two different values of ε confirms that the frequency of the oscillations is proportional to $1/\varepsilon^2$.

Since solutions of the NLDE remain smooth in space, standard methods can be used for space discretization. However, the oscillatory nature of solutions poses major problems for time discretization. Standard time integration schemes typically face two issues when they are applied to oscillatory problems. On the one hand, some methods are only stable under a severe step size restriction. Even in the linear case where $\gamma_1 = \gamma_2 = 0$ in (1.2), stability of the leapfrog scheme, for example, is only obtained for small enough step sizes $\tau \leq C\varepsilon^2$ for some constant C dependent on the spatial mesh width [Bao+17]. Thus, for small values $\varepsilon \ll 1$, only tiny step sizes are possible. On the other hand, even if a method is stable, it might suffer from a poor accuracy. The reason is that error constants often depend on the size of time derivatives of the exact solution. Those derivatives grow very large in the case of the NLDE for small $\varepsilon \ll 1$ (corresponding to high frequencies of the oscillations). In [Bao+16b], several standard methods applied to the NLDE in the nonrelativistic limit regime were analyzed. For a Crank–Nicolson scheme, the authors did prove unconditional stability, but also that the error of the time discretization (in a suitable norm) is of order $\mathcal{O}(\tau^2/\varepsilon^6)$. Thus, even for tiny step sizes $\tau \approx \varepsilon^3$, good accuracies cannot be expected. For Strang splitting, they showed that the error is bounded by $C\tau^2/\varepsilon^4$ for some constant C. Even though this is an improvement, the same problems remain. All those methods thus require enormous computational costs for acceptable accuracies.

To obtain better results, tailor-made time integration schemes have to be constructed. This means that the schemes have to be adapted to the structure of the PDE under consideration.

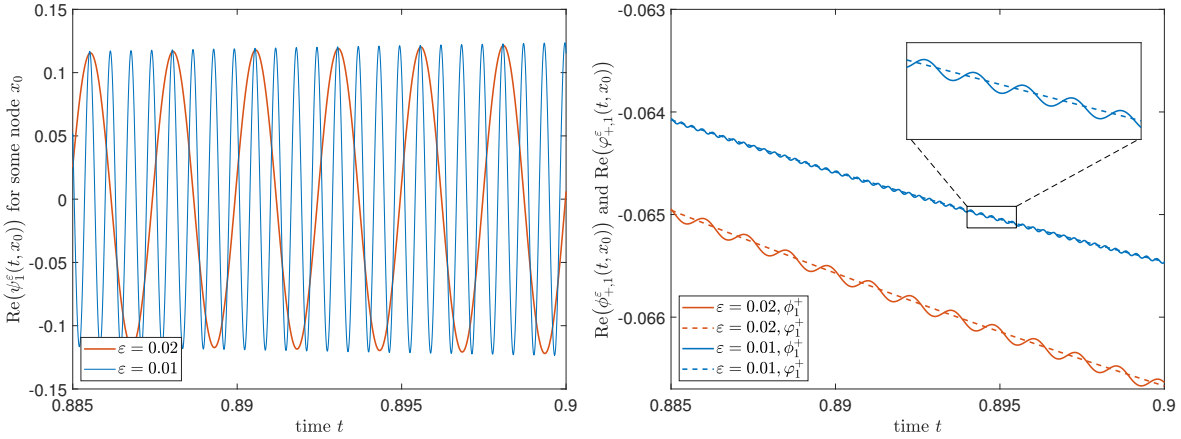

Figure 1.1: Temporal evolution of solutions of a 1D-analogue of the NLDE (left), the transformed Dirac equations (right, solid lines), and the semi-nonrelativistic limit system (right, dashed lines) for two different values of ε. All functions are considered for the same point x_0 in space, whereas time varies. Each line represents the real part of the first component of the respective function. Note that only a far smaller interval is shown on the y-axis in the right plot.

In the nonrelativistic limit regime, the ultimate goal must be to obtain error bounds that are independent of ε (*uniformly accurate schemes*) or even improve for smaller values of ε. There has been some progress in this direction. First of all, it was shown in [BCY21] that if no magnetic potential is present, i.e. $A_j = 0$ for $j = 1, 2, 3$ in (1.3), and if special, nonresonant step sizes are employed, then the error of Strang splitting improves to $\mathcal{O}\left(\tau^{3/2}\right)$ uniformly in ε. For the NLDE with magnetic potential, three other schemes have been proposed. In [CW18], the authors introduced the *multiscale time integrator* (MTI). They work with a multiscale formulation of the NLDE, which allows them to construct a time integration scheme with error in $\mathcal{O}(\min\{\tau^2 + \varepsilon^2, \tau^2/\varepsilon^2\})$. This implies that the error reduces quadratically with decreasing step size $\tau > \varepsilon$, until an accuracy of $\mathcal{O}(\varepsilon^2)$ is achieved for $\tau = \varepsilon$. For step sizes $\varepsilon^2 \leq \tau < \varepsilon$, no further improvement of the accuracy is expected. Only for step sizes $\tau < \varepsilon^2$, quadratic convergence in τ sets in again, but with an error constant proportional to $1/\varepsilon^2$. In view of this error behavior, the scheme is particularly interesting when an accuracy of order $\mathcal{O}(\varepsilon^2)$ is sufficient, which might be the case for small ε. However, the fine-scale corrections lead to a very complicated method, cf. [CW18, Eq. (2.29)-(2.31)]. A different strategy has been proposed in [LMZ17]. Here, the authors separate the fast and slow time scales in the NLDE, which leads to a non-oscillatory augmented problem, for which they are indeed able to construct a uniformly accurate method of second order in the time step size. However, this separation implies having an additional variable in the augmented problem. The extra dimension leads to far larger computational cost. In [CW22], the *second-order nested Picard iterative integrator* (NPI-2) has been presented. The NPI-2 also achieves second order convergence uniformly in ε. It is derived by first iterating Duhamel's formula, which yields representations of the solution involving several integrals. In those integrals, one carefully distinguishes slowly varying parts from highly oscillatory parts. The former ones can be approximated, whereas the latter parts are integrated exactly. If carried out correctly, the approximation errors in this strategy do not depend on the size of any time derivative of the solution. This is why it is very well suited for highly oscillatory problems from an accuracy point of view. However, the nonlinear nature of the PDE causes a large increase in the number of terms with each iteration of Duhamel's formula. The resulting method is very

complicated, in the sense that it takes the authors two pages to write down the final scheme in its full glory. This not only makes implementation and debugging extremely difficult, but also reduces the method's efficiency, since a large number of terms has to be computed in each time step. Furthermore, a rigorous error analysis would be very tedious, which is why the authors of [CW22] only presented it for a first-order scheme.

After having reviewed the few works that already exist on time integration of the NLDE in the nonrelativistic limit regime, it becomes clear why the subject is so difficult. The main challenge is to construct numerical schemes that can cope with both the oscillatory behavior of solutions and the nonlinear nature of the NLDE. Handling the oscillations requires special techniques, whilst the nonlinearity can make the application of said techniques very sophisticated. In this thesis, we propose and analyze three new time integration schemes for the NLDE. All of them take into account the special structure of the oscillations exhibited by solutions of the NLDE, and in some cases even exploit them to their advantage. None of the schemes is the best of the three. Instead, they all have their individual benefits. In particular, the method of choice depends on the level of accuracy that the user wants to achieve.

The first step in the construction of all three methods is a transformation of variables through which, roughly speaking, the dominating oscillations are filtered out. This transformation goes back to [BMP98] and [CW20]. The result is the *transformed Dirac equations*, which is a system of two coupled PDEs whose solutions ϕ_+^ε and ϕ_-^ε are "less oscillatory", in the sense that their first time derivatives are uniformly bounded w.r.t. ε. However, the second time derivative is still unbounded. This is illustrated by the solid lines in the right half of Figure 1.1. They show the temporal evolution of the function ϕ_+^ε from a solution of the transformed Dirac equations. It becomes apparent that ϕ_+^ε is still oscillatory. However, the amplitude of the oscillations decreases fast enough with decreasing ε such that the size of the first time derivative does not grow. The same holds for the function ϕ_-^ε. The solution of the original NLDE can exactly be reconstructed from a solution $(\phi_+^\varepsilon, \phi_-^\varepsilon)$ of the transformed system. More precisely, we have

$$\psi^\varepsilon(t,x) = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\phi_+^\varepsilon(t,x) + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\phi_-^\varepsilon(t,x). \tag{1.4}$$

The transformation is motivated by an eigenspace decomposition of the free Dirac operator in Fourier space and is fundamental for all methods in this thesis. This is why we will present it in detail at the end of this chapter.

Chapter 2 contains the paper [JK23]. Here, we consider time integration for the *semi-nonrelativistic limit system* from [CW20]. This is a simplified version of the transformed Dirac equations where a number of terms is omitted from the right-hand side of the PDEs. The simplification comes at the cost of an $\mathcal{O}(\varepsilon^2)$ approximation error. Considering (1.4), we thus have

$$\psi^\varepsilon(t,x) = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\varphi_+^\varepsilon(t,x) + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\varphi_-^\varepsilon(t,x) + \mathcal{O}\left(\varepsilon^2\right),$$

where $(\varphi_+^\varepsilon, \varphi_-^\varepsilon)$ is a solution of the new system. Here, $\mathcal{O}(\varepsilon^p)$, $p \in \mathbb{N}_0$, stands for a time- and space-dependent function for which a suitable Sobolev norm is bounded by $C\varepsilon^p$ at all times with some constant C independent of ε. As a consequence of the deliberations above, any method that approximates solutions of the semi-nonrelativistic limit system cannot achieve accuracies better than $\mathcal{O}(\varepsilon^2)$ for the original NLDE. For small values of ε, this will be sufficient in some applications. The benefit of this new system are the simpler PDEs, but also that the second time derivatives of its solutions are uniformly bounded w.r.t. ε. This is again confirmed by the right plot in Figure 1.1, where the dashed lines represent the function φ_+^ε

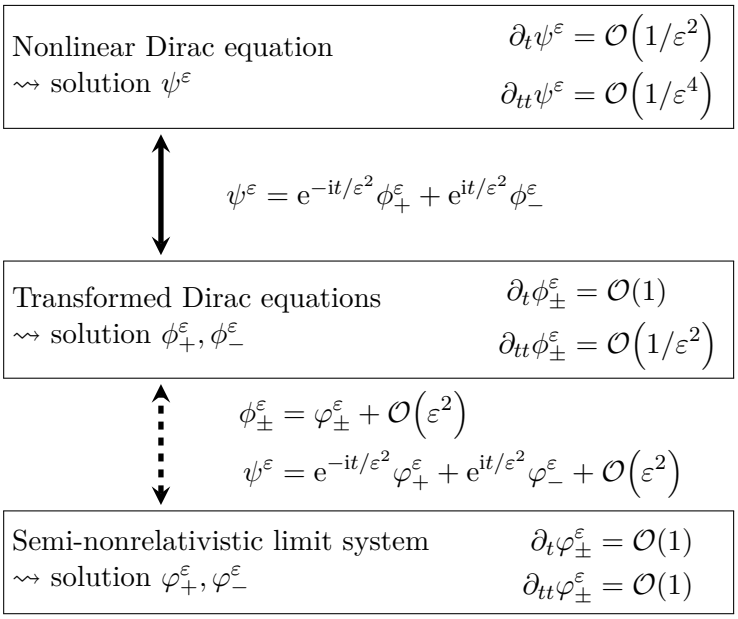

Figure 1.2: Systems under consideration, their relation to the original NLDE, and the size of their first two time derivatives w.r.t. ε.

from the semi-nonrelativistic limit system. No temporal oscillations are visible anymore, and the function ϕ_+^ε oscillates around φ_+^ε on a small scale. All three systems under consideration, their relation to the original NLDE, and the different temporal regularity of their solutions are summarized in Figure 1.2. We will present a uniformly accurate second order method for the semi-nonrelativistic limit system called the *explicit exponential midpoint rule* (EEMR). The method is an exponential integrator that perfectly exploits the additional temporal smoothness attained by considering the semi-nonrelativistic limit system. It is based on applying Duhamel's formula over a time interval of length 2τ, where τ is the time step size, and then approximating the resulting integrals via the midpoint rule. The approach requires one less iteration of Duhamel's formula than would normally be necessary to achieve the same error order. This brings large benefits considering that the PDEs are nonlinear. Overall, a two-step method with a very simple numerical flow is obtained. In particular, the EEMR is far simpler than the MTI or the NPI-2, and yet has the same accuracy as long as an error of $\mathcal{O}(\varepsilon^2)$ is sufficient.

The methods from Chapters 3 and 4 are developed for applications where an accuracy of $\mathcal{O}(\varepsilon^2)$ is not enough, such that the EEMR does not provide adequate results. The contents from Chapter 3 essentially correspond to the preprint [JK24], but it has been slightly modified during the review process of a scientific journal. Here, we first revisit the NPI-2 scheme from [CW22]. However, we formulate the method for the transformed Dirac equations instead of the original NLDE, and employ slightly different techniques to approximate the slowly varying parts. Working in the variables $\phi_\pm^\varepsilon$ allows us to identify terms in the NPI-2 scheme that are expected to have only a limited impact on the result if nonresonant step sizes are used. We then consider a simplified version of the NPI-2 scheme, where those terms are omitted. This results in the *nonresonant nested Picard iterative integrator* (NRNPI), which is the main accomplishment of this chapter. For $\tau \geq \pi\varepsilon^2/4$, the NRNPI has the same accuracy as the NPI-2 scheme if some a-priori known resonant step sizes are avoided. In particular, the error is proportional to τ^2 in this regime, and accuracies up to $\mathcal{O}(\varepsilon^4)$ can be achieved. For very small step sizes $\tau < \pi\varepsilon^2/4$, only linear convergence is observed, but with an error constant

that is proportional to ε^2. Altogether, the NRNPI performs especially well for very small values of ε. In the error analysis of the NRNPI, a detailed look into the error accumulation is necessary, since nonresonance effects that occur in the course of several time steps are exploited. The error analysis is only manageable since we introduce a sophisticated notation which allows writing both the full NPI-2 scheme and the NRNPI in a compact form. In fact, before discussing the NRNPI, the error of the NPI-2 scheme itself has to be analyzed first. This is worth mentioning since the authors of [CW22] refrained from doing so.

In Chapter 4, we introduce a new method based on splitting techniques. It is presented for the first time here in this thesis. Splitting methods are usually not suitable for oscillatory problems as their error constants grow very large with increasing frequency of the oscillations. For the classical splitting of the NLDE considered in [Bao+16b] and [BCY21], this was discussed previously. However, we suggest a special splitting of the transformed Dirac equation instead. The crucial benefit of this new ansatz is a reduced splitting error, which is not as heavily affected by rapid oscillations as the classical ansatz. We will analyze the resulting splitting error in detail. Furthermore, since the subproblems cannot be solved exactly, we will also introduce efficient schemes to approximate their solutions. This will lead to a method which we call the *oscillation-rewinding splitting method* (ORSM). The name is motivated by a different interpretation of the new splitting ansatz. After all, we are able to show that the error of the ORSM is in $\mathcal{O}(\tau^2/\varepsilon)$. Thus, second order convergence is achieved with an error constant that does increase with decreasing ε, but only linearly. This means that we expect the ORSM to outperform the NRNPI for very small step sizes, i.e. $\tau \leq \tau_0$ for some $\tau_0 < \varepsilon^2$. In numerical experiments, however, we will see that the error is in fact even in $\mathcal{O}(\tau^2)$ if certain resonant step sizes, which can easily be identified, are avoided. Note that in each time step of the ORSM, only the solutions of the subproblems have to be approximated. This brings considerable advantages compared to the approximation of solutions of the full (transformed) Dirac equation. In particular, it turns out that the ORSM also outperforms the NRNPI for step sizes $\tau > \tau_0$.

All three methods proposed in this thesis combined cover the entire spectrum of accuracies. If for a desired accuracy the most suitable of the three integrators is chosen, one can always outperform the methods that have previously been proposed in the literature for time integration of the NLDE in the nonrelativistic limit regime. To conclude this thesis, we provide a direct comparison of all three methods in Chapter 5, in particular in dependency of the computational costs invested. This once again clarifies the decision-making basis for choosing the right scheme.

Since Chapters 2 and 3 of this thesis consist of a peer-reviewed article and a preprint submitted for publication in a scientific journal, respectively, they are completely self-contained. Minor overlaps, especially in the introductions, are unavoidable. Chapter 4 was newly developed for this thesis and contains several references to previous chapters.

Decomposing the free Dirac operator

Before we begin discussing the time integration schemes, we want to understand the origin and the structure of the oscillations in solutions of the NLDE in the nonrelativistic limit regime. To this purpose, we will consider a decomposition of the free Dirac operator $\mathcal{T}_\varepsilon$. This decomposition also motivates the introduction of the transformed variables $\phi_\pm^\varepsilon$, which are fundamental throughout this thesis.

Let us omit the potential and the nonlinearity in the NLDE (1.2) for the moment. Thus, we

go back to the free Dirac equation (1.1). The effect of $\mathcal{T}_\varepsilon$ can be observed best in Fourier space. For a function $u = u(x) \in \left(H^1(\mathbb{R}^3)\right)^4$ with Fourier representation

$$u(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \mathrm{e}^{\mathrm{i}x\cdot\xi} \widehat{u}(\xi)\, \mathrm{d}\xi, \qquad \widehat{u}(\xi) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}x\cdot\xi} u(x)\, \mathrm{d}x, \quad \xi \in \mathbb{R}^3,$$

we have

$$\begin{aligned} \mathcal{T}_\varepsilon u(x) &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \Big(-\mathrm{i}\varepsilon \sum_{j=1}^{3} \alpha_j \partial_j + \beta \Big) \mathrm{e}^{\mathrm{i}x\cdot\xi} \widehat{u}(\xi) \mathrm{d}\xi \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \Big(\varepsilon \sum_{j=1}^{3} \alpha_j \xi_j + \beta \Big) \mathrm{e}^{\mathrm{i}x\cdot\xi} \widehat{u}(\xi)\, \mathrm{d}\xi. \end{aligned}$$

Thus, application of $\mathcal{T}_\varepsilon$ corresponds to multiplication of the Fourier transform at $\xi \in \mathbb{R}^3$ with the matrix

$$\mathcal{T}_\varepsilon(\xi) = \varepsilon \sum_{j=1}^{3} \alpha_j \xi_j + \beta \in \mathbb{C}^{4\times 4}.$$

Consequently, if we translate the PDE (1.1) into Fourier space, we obtain the ODE system

$$\partial_t \widehat{\psi}^\varepsilon(t,\xi) = -\frac{\mathrm{i}}{\varepsilon^2} \mathcal{T}_\varepsilon(\xi) \widehat{\psi}^\varepsilon(t,\xi) \tag{1.5}$$

for each $\xi \in \mathbb{R}^3$, with solution

$$\widehat{\psi}^\varepsilon(t,\xi) = \mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\mathcal{T}_\varepsilon(\xi)} \widehat{\psi}^\varepsilon(0,\xi). \tag{1.6}$$

It can easily be checked that α_j, $j = 1,2,3$ and β, and hence also $\mathcal{T}_\varepsilon(\xi)$, are Hermitian matrices. In particular, $\mathcal{T}_\varepsilon(\xi)$ is (unitarily) diagonalizable and only has real eigenvalues. The factor $1/\varepsilon^2$ in front of $\mathcal{T}_\varepsilon(\xi)$ enlarges the modulus of those eigenvalues considerably. However, considering the additional i in front of $\frac{1}{\varepsilon^2}\mathcal{T}_\varepsilon(\xi)$, it becomes apparent that the ODEs (1.5) are not exploding or stiff, but instead *highly oscillatory*. A more detailed insight into the oscillatory behavior can be gained by looking at the precise value of the eigenvalues. One can easily check that the matrices $\mathcal{T}_\varepsilon(\xi)$ have the two eigenvalues

$$\pm\Lambda_\varepsilon(\xi) \qquad \text{with} \qquad \Lambda_\varepsilon(\xi) = \sqrt{1 + \varepsilon^2 |\xi|^2}, \tag{1.7}$$

each of them with geometric multiplicity two [BMP98]. The orthogonal projections onto the two respective eigenspaces are given by

$$\Pi_\varepsilon^\pm(\xi) = \frac{1}{2}\left(I_4 \pm \frac{\mathcal{T}_\varepsilon(\xi)}{\Lambda_\varepsilon(\xi)} \right).$$

In particular, we have

$$\Pi_\varepsilon^\pm(\xi)^2 = \Pi_\varepsilon^\pm(\xi), \quad \Pi_\varepsilon^+(\xi) + \Pi_\varepsilon^-(\xi) = I_4, \quad \text{and} \quad \Pi_\varepsilon^+(\xi)\Pi_\varepsilon^-(\xi) = \Pi_\varepsilon^-(\xi)\Pi_\varepsilon^+(\xi) = 0. \tag{1.8}$$

Altogether, the matrix $\mathcal{T}_\varepsilon(\xi)$ can be decomposed as

$$\mathcal{T}_\varepsilon(\xi) = \Lambda_\varepsilon(\xi)\Pi_\varepsilon^+(\xi) - \Lambda_\varepsilon(\xi)\Pi_\varepsilon^-(\xi). \tag{1.9}$$

This can be used to rewrite the solution (1.6) of (1.5) as

$$\widehat{\psi}^\varepsilon(t,\xi) = \mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\Lambda_\varepsilon(\xi)}\Pi_\varepsilon^+(\xi)\widehat{\psi}^\varepsilon(0,\xi) + \mathrm{e}^{\frac{\mathrm{i}t}{\varepsilon^2}\Lambda_\varepsilon(\xi)}\Pi_\varepsilon^-(\xi)\widehat{\psi}^\varepsilon(0,\xi).$$

In particular, the solution is obtained by multiplying the two eigenspace components of $\widehat{\psi}^\varepsilon(0,\xi)$ with highly oscillatory phases with ξ-dependent frequencies of opposite sign. This suggests considering both eigenspace components separately, i.e. to write the solution as $\widehat{\psi}^\varepsilon(t,\xi) = \widehat{\psi}_+^\varepsilon(t,\xi) + \widehat{\psi}_-^\varepsilon(t,\xi)$ with $\widehat{\psi}_\pm^\varepsilon(t,\xi) = \Pi_\varepsilon^\pm(\xi)\widehat{\psi}^\varepsilon(t,\xi)$ given by

$$\widehat{\psi}_+^\varepsilon(t,\xi) = \mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\Lambda_\varepsilon(\xi)}\widehat{\psi}_+^\varepsilon(0,\xi), \qquad \widehat{\psi}_-^\varepsilon(t,\xi) = \mathrm{e}^{\frac{\mathrm{i}t}{\varepsilon^2}\Lambda_\varepsilon(\xi)}\widehat{\psi}_-^\varepsilon(0,\xi). \tag{1.10}$$

The different frequency components of $\widehat{\psi}^\varepsilon(\cdot,\xi)$ are now separated. The frequencies depend on the Fourier mode $\xi \in \mathbb{R}^3$. However, the estimate

$$|\Lambda_\varepsilon(\xi) - 1| = \left|\sqrt{1+\varepsilon^2\,|\xi|^2} - 1\right| = \left|\frac{\varepsilon^2\,|\xi|^2}{\sqrt{1+\varepsilon^2\,|\xi|^2}+1}\right| \leq \frac{\varepsilon^2\,|\xi|^2}{2} \tag{1.11}$$

shows that for all $\xi \in \mathbb{R}^3$, the main part of the frequencies $\mp\Lambda_\varepsilon(\xi)/\varepsilon^2$ is given by $\mp 1/\varepsilon^2$, and only a bounded (w.r.t. ε) part remains. In other words, if for each $\xi \in \mathbb{R}^3$ we multiply the functions $\widehat{\psi}_\pm^\varepsilon(\cdot,\xi)$ in (1.10) with $\exp\left(\pm \mathrm{i}t/\varepsilon^2\right)$, then the main temporal oscillations will be filtered out. This is why we define the new functions

$$\widehat{\phi}_+^\varepsilon(t,\xi) := \mathrm{e}^{+\frac{\mathrm{i}t}{\varepsilon^2}}\widehat{\psi}_+^\varepsilon(t,\xi), \qquad \widehat{\phi}_-^\varepsilon(t,\xi) := \mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}}\widehat{\psi}_-^\varepsilon(t,\xi), \qquad \xi \in \mathbb{R}^3,$$

for which we obtain the formulas

$$\widehat{\phi}_+^\varepsilon(t,\xi) = \exp\left(-\mathrm{i}t\,\frac{\Lambda_\varepsilon(\xi)-1}{\varepsilon^2}\right)\widehat{\psi}_+^\varepsilon(0,\xi), \qquad \widehat{\phi}_-^\varepsilon(t,\xi) = \exp\left(\mathrm{i}t\,\frac{\Lambda_\varepsilon(\xi)-1}{\varepsilon^2}\right)\widehat{\psi}_-^\varepsilon(0,\xi).$$

In view of (1.11), the frequencies of the temporal phases are now bounded w.r.t. ε.

All the considerations above can be translated to the original solution ψ^ε of the free Dirac equation (1.1) in physical space using pseudo-differential operators. Applying the operator $\Lambda_\varepsilon = \sqrt{\mathrm{Id} - \varepsilon^2\Delta}$ to a function $u \in (H^1(\mathbb{R}^3))^4$, for example, corresponds to multiplication of the Fourier transform of u at $\xi \in \mathbb{R}^3$ with the number $\Lambda_\varepsilon(\xi)$ from (1.7). Additionally defining the projection operators

$$\Pi_\varepsilon^\pm = \frac{1}{2}\left(\mathrm{Id} \pm \Lambda_\varepsilon^{-1}\mathcal{T}_\varepsilon\right) \tag{1.12}$$

in the same manner, we obtain the decomposition

$$\mathcal{T}_\varepsilon = \Lambda_\varepsilon\Pi_\varepsilon^+ - \Lambda_\varepsilon\Pi_\varepsilon^- \tag{1.13}$$

of the operator $\mathcal{T}_\varepsilon$, cf. Eq. (1.9). The properties of the projection matrices $\Pi_\varepsilon^\pm(\xi)$ from (1.8) transfer to the projection operators:

$$(\Pi_\varepsilon^\pm)^2 = \Pi_\varepsilon^\pm, \qquad \Pi_\varepsilon^+ + \Pi_\varepsilon^- = \mathrm{Id}, \qquad \text{and} \qquad \Pi_\varepsilon^+\Pi_\varepsilon^- = \Pi_\varepsilon^-\Pi_\varepsilon^+ = 0. \tag{1.14}$$

Further, analogously to before, we decompose the solution $\psi^\varepsilon = \psi_+^\varepsilon + \psi_-^\varepsilon$ into the two components $\psi_\pm^\varepsilon = \Pi_\varepsilon^\pm[\psi^\varepsilon]$ and define the two new functions $\phi_\pm^\varepsilon$ by

$$\phi_\pm^\varepsilon(t,x) = \mathrm{e}^{\pm\frac{\mathrm{i}t}{\varepsilon^2}}\psi_\pm^\varepsilon(t,x) = \mathrm{e}^{\pm\frac{\mathrm{i}t}{\varepsilon^2}}\Pi_\varepsilon^\pm\left[\psi^\varepsilon(t,x)\right]. \tag{1.15}$$

Since $\psi_{\pm}^{\varepsilon}(t,x) = \exp(\mp\frac{\mathrm{i}t}{\varepsilon^2}\Lambda_\varepsilon)\Pi_\varepsilon^{\pm}\left[\psi^\varepsilon(0,x)\right]$, they fulfill

$$\phi_{\pm}^{\varepsilon}(t,x) = \mathrm{e}^{\mp\mathrm{i}t\mathcal{D}_\varepsilon}\Pi_\varepsilon^{\pm}\left[\psi^\varepsilon(0,x)\right] \tag{1.16}$$

with the operator $\mathcal{D}_\varepsilon$ defined by

$$\mathcal{D}_\varepsilon = \frac{1}{\varepsilon^2}\left(\Lambda_\varepsilon - \mathrm{Id}\right). \tag{1.17}$$

To put it another way, the functions $\phi_{\pm}^{\varepsilon}$ solve the PDEs

$$\partial_t\phi_{\pm}^{\varepsilon} = \mp\mathrm{i}\mathcal{D}_\varepsilon\phi_{\pm}^{\varepsilon}, \qquad \phi_{\pm}^{\varepsilon}(0,x) = \Pi_\varepsilon^{\pm}\left[\psi^\varepsilon(0,x)\right].$$

Eq. (1.11) implies that $\mathcal{D}_\varepsilon$ is a uniformly (w.r.t. ε) bounded operator from H^{m+2} to H^m for any $m \geq 0$, in contrast to the unbounded operator $\frac{1}{\varepsilon^2}\mathcal{T}_\varepsilon$ in the free Dirac equation (1.1). The filtering of the main part of the oscillations therefore leads to a uniformly (w.r.t. ε) bounded first time derivative of the resulting functions $\phi_{\pm}^{\varepsilon}$.

In the full NLDE (1.2), the operator $\frac{1}{\varepsilon^2}\mathcal{T}_\varepsilon$ constitutes the dominant part of the right-hand side. This is why the transformation of variables from (1.15) will bring the same benefits for the temporal regularity. However, we are of course no longer able to write down the exact solution explicitly as in (1.16). Instead, from the original NLDE (1.2), we can derive two PDEs for the variables $\phi_{\pm}^{\varepsilon}$. Translating the potential term and the nonlinearity to the transformed variables will lead to a coupling between both PDEs, and to more complicated right-hand sides. Nevertheless, the resulting *transformed Dirac equations* are the cornerstone for all subsequent chapters. In Chapter 2, they form the basis for deriving an analytic approximation to solutions of the NLDE. Further, they make it possible to identify the different frequency components in solutions of the NLDE, which is fundamental for exploiting nonresonance effects to improve efficiency of a numerical scheme in Chapter 3. Finally, in Chapter 4, the transformed Dirac equations will give the motivation for a new kind of splitting ansatz which will result in a very efficient time integration scheme.

Chapter 2

On numerical methods for the semi-nonrelativistic limit system of the nonlinear Dirac equation

This chapter consists of the paper [JK23], which is joint work with Tobias Jahnke and was published in BIT Numerical Mathematics. In order to fit in with the rest of this thesis, the layout was adapted and minor changes have been made to the notation.

TOBIAS JAHNKE AND MICHAEL KIRN

Abstract: Solving the nonlinear Dirac equation in the nonrelativistic limit regime numerically is difficult, because the solution oscillates in time with frequency of $\mathcal{O}(\varepsilon^{-2})$, where $0 < \varepsilon \ll 1$ is inversely proportional to the speed of light. Yongyong Cai and Yan Wang have shown, however, that such solutions can be approximated up to an error of $\mathcal{O}(\varepsilon^2)$ by solving the semi-nonrelativistic limit system, which is a non-oscillatory problem. For this system, we construct a two-step method, called the *explicit exponential midpoint rule*, and prove second-order convergence of the semi-discretization in time. Furthermore, we construct a benchmark method based on standard techniques and compare the efficiency of both methods. Numerical experiments show that the new integrator reduces the computational costs per time step to 40% and within a given runtime improves the accuracy significantly.

2.1 Introduction

The Dirac equation describes the relativistic motion of spin-1/2 particles such as, e.g., electrons, positrons, protons, neutrons, and quarks, under the influence of external electromagnetic fields. Since its derivation by Dirac in [Dir28], it has become one of the cornerstones of relativistic quantum mechanics; cf. [Tha92]. Nonlinear versions of the Dirac equation have been proposed to model self-interaction of particles and other phenomena; see, e.g., [HC09; Mer+10; Sol70; Thi58]. In the nonrelativistic limit regime, the Dirac equation involves a small parameter $0 < \varepsilon \ll 1$ which is inversely proportional to the speed of light, and non-trivial solutions oscillate in time with frequency of $\mathcal{O}(\varepsilon^{-2})$. Using traditional numerical methods to approximate such solutions is inefficient, because then the oscillations have to be resolved with a tiny step size, which causes prohibitively large computational costs; cf. [Bao+16b]. Hence, constructing and analyzing numerical methods for the nonlinear Dirac equation in

the nonrelativistic limit regime is a considerable challenge.

In the special case that no magnetic potential is present, it was shown in [BCY21] that the classical Lie-Trotter and Strang splitting with step size τ have an error of $\mathcal{O}\left(\tau^{1/2}\right)$, but uniformly in ε. For nonresonant step sizes, the accuracy improves to $\mathcal{O}(\tau)$ for Lie-Trotter and $\mathcal{O}\left(\tau^{3/2}\right)$ for the Strang splitting. In the general case (with magnetic potential), uniformly accurate methods have been proposed and analyzed in [CW18; CW22; LMZ17]. Under certain assumptions, the error of the time discretization with the *multiscale time integrator pseudospectral method* from [CW18] is bounded by a constant times $\min\{\tau^2+\varepsilon^2, \frac{\tau^2}{\varepsilon^2}\}$, where τ is the step size. This yields second-order convergence if $\tau \geq \varepsilon$ or $\tau \ll \varepsilon$ and, what is more important, first-order convergence uniformly in ε. The *nested Picard iterative integrator* constructed in [CW22] converges even with order two in time and uniformly in ε. However, the correct implementation of both methods is not easy, because they are based on complicated expansions and involve a plethora of terms. A different approach was proposed in [LMZ17] in one space dimension. The idea is to consider an augmented problem where the slow and fast time scales are distinguished. A formal Chapman-Enskog expansion is used to construct initial data for the augmented problem such that the corresponding solution has three uniformly bounded time derivatives, which paves the way for the construction of a uniformly accurate second-order scheme. However, the price to pay is that the augmented problem involves one additional dimension representing the fast time scale, which increases the numerical work significantly.

The nonlinear Dirac equation in the nonrelativistic limit regime has also been intensively studied in analysis; cf. [CW20; MNO03; Mat95b; Mat95a; Naj92]. It was shown that the solution $\psi^\varepsilon(t,x) \in \mathbb{C}^4$ can be approximated by

$$\psi^\varepsilon(t,x) = e^{-\mathrm{i}t\beta/\varepsilon^2}\varphi(t,x) + \mathcal{O}(\varepsilon) \tag{2.1}$$

where $\beta = \operatorname{diag}(1,1,-1,-1) \in \mathbb{R}^{4\times 4}$ is a diagonal matrix, and where φ is the solution of a nonlinear Schrödinger equation which does not depend on ε and is thus easier to approximate numerically. A precise formulation of this result and its proof are given in [CW20, Theorem 2.3]. The main result of [CW20], however, is that a *better* approximation

$$\psi^\varepsilon(t,x) = e^{-\mathrm{i}t/\varepsilon^2}\varphi_+^\varepsilon(t,x) + e^{\mathrm{i}t/\varepsilon^2}\varphi_-^\varepsilon(t,x) + \mathcal{O}\left(\varepsilon^2\right) \tag{2.2}$$

can be obtained, where $\varphi_\pm^\varepsilon$ are the solutions of two coupled semilinear PDEs called the *semi-nonrelativistic limit system*; see [CW20, Theorem 2.2] or Theorem 2.3 below for details. In contrast to the above-mentioned nonlinear Schrödinger equation, the semi-nonrelativistic limit system does still involve the parameter ε, but in contrast to the original problem, the solution does not oscillate in time; cf. [CW20, Theorem 2.2]. Hence, (2.2) offers a way to approximate the highly oscillatory solution of the nonlinear Dirac equation without having to solve a highly oscillatory problem. Of course, one cannot expect the error of this approximation to be smaller than $\mathcal{O}(\varepsilon^2)$, but in this work we assume that this accuracy is sufficient. If a higher accuracy is required, one has to use the uniformly accurate integrators from [CW22; LMZ17] with a step size $\tau < \varepsilon$, which is computationally intense.

Solving the semi-nonrelativistic limit system numerically is much easier than solving the nonlinear Dirac equation in the nonrelativistic limit regime, but it is not straightforward. For example, explicit Runge-Kutta methods suffer from severe CFL conditions, whereas fully implicit methods come at the price of solving a large nonlinear system in every time step.

Constructing splitting methods[1] in a straightforward way is not an option, either, due to the particular structure of the semi-nonrelativistic limit system. These problems can be avoided with exponential integrators. Such integrators are typically constructed by applying variation of constants on the interval $[t_n, t_{n+1}]$ (where $t_n = n\tau$ are the times for which numerical approximations are supposed to be computed) and approximating the convolution integral, e.g. by expanding the nonlinearity in such a way that the integral can be solved analytically. The corresponding techniques are nowadays well-known in the context of dispersive equations and in particular highly oscillatory problems. Because of the special structure of the semi-nonrelativistic limit system, however, such a method requires many forward and backward Fourier transforms per time step, which is the dominating factor in the computational costs. In this paper, we propose a non-standard second-order exponential integrator. The idea is to apply variation of constants over the interval $[t_{n-1}, t_{n+1}]$, which simplifies the treatment of the nonlinearity a lot. This approach leads to a two-step method which we call the *explicit exponential midpoint rule*. The new method is time-symmetric, simpler to implement, and considerably more efficient than the standard second-order exponential integrator.

In Section 2.2 we introduce the nonlinear Dirac equation in the nonrelativistic limit regime and sketch the derivation of the semi-nonrelativistic limit system as presented in [CW20]. Moreover, we specify our assumptions and quote a number of important results from [CW20]. Time-integrators for the semi-nonrelativistic limit system are constructed in Section 2.3. The first method is an exponential integrator which is based on well-known techniques, and which is therefore considered as a benchmark method. The second method is the explicit exponential midpoint rule. For this integrator we carry out a detailed error analysis; cf. Theorem 2.10. In Section 2.4 we test the efficiency of both methods in a numerical experiment. It turns out that our new method reduces the computational costs per time step to about 40% and, within the same runtime as the benchmark method, improves the accuracy by a factor of about 4.6 in L^2 and 6 in H^1. We explain the reason for these improvements.

2.2 Problem setting

2.2.1 Nonlinear Dirac equation in the nonrelativistic limit regime

We consider the nonlinear Dirac equation (NLDE)

$$\begin{aligned} \partial_t \psi^\varepsilon(t,x) &= -\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi^\varepsilon(t,x) - \mathrm{i}W(t,x)\psi^\varepsilon(t,x) - \mathrm{i}F(\psi^\varepsilon(t,x))\psi^\varepsilon(t,x), \\ \psi^\varepsilon(0,x) &= \psi^{\mathrm{init}}(x) \end{aligned} \tag{2.3}$$

for $x \in \mathbb{R}^3$ and $t > 0$. In (2.3), $\psi^\varepsilon := \psi^\varepsilon(t,x) \in \mathbb{C}^4$ is the complex-valued vector wave function with initial data $\psi^{\mathrm{init}} = \psi^{\mathrm{init}}(x) \in \mathbb{C}^4$. The parameter $\varepsilon > 0$ is inversely proportional to the speed of light and thus is very small in the nonrelativistic limit regime. Furthermore, $\mathcal{T}_\varepsilon$ and W denote the free Dirac operator and the electromagnetic potential, respectively, given by

$$\mathcal{T}_\varepsilon = -\mathrm{i}\sum_{j=1}^{3} \varepsilon \alpha_j \partial_j + \beta, \qquad W(t,x) = V(t,x) I_4 - \sum_{j=1}^{3} A_j(t,x)\alpha_j, \tag{2.4}$$

[1] In [KSZ21] a splitting method for approximating the function φ in (2.1) was proposed. Our goal, however, is not to compute φ in (2.1), but $\varphi_\pm^\varepsilon$ in (2.2), because then an approximation of ψ^ε up to $\mathcal{O}(\varepsilon^2)$ is feasible.

where $V(t,x) \in \mathbb{R}$ is the electric scalar potential and $A(t,x) = (A_1(t,x), ..., A_3(t,x))^T$ is the magnetic vector potential. The Dirac matrices

$$\beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \qquad \alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}$$

are determined by the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Finally, F is the nonlinearity given by $F(v) = \gamma_1(v^*\beta v)\beta + \gamma_2 |v|^2 I_4$ for $\gamma_1, \gamma_2 \in \mathbb{R}$, where $v^* = \overline{v}^T$ denotes the conjugate transpose and $|v| = \sqrt{v^*v}$ the Euclidean norm of a vector v, respectively. This type of nonlinearity is motivated by numerous applications in physics and describes self-interaction of Dirac fermions; see, e.g., [HC09; Mer+10; Sol70; Thi58] and the references in [Bao+16b; BCY21; CW18; CW22; LMZ17]. For simplicity, we assume that $\gamma_1 = 0$ henceforth, but all results and proofs can be adapted to the case $\gamma_1 \neq 0$.

Throughout this paper, we will use the following notation: $\|v\|_{H^m}$ denotes the standard Sobolev norm of a scalar-valued function $v \in H^m(\mathbb{R}^3)$, whilst for a $\mathbb{C}^4$-valued function $v = (v_1, ..., v_4) \in (H^m(\mathbb{R}^3))^4$, we set

$$\|v\|_{H^m} = \sqrt{\|v_1\|_{H^m}^2 + ... + \|v_4\|_{H^m}^2}.$$

The following assumptions regarding the initial data and the potential W will be made. Recall that W is determined by V and A_j via (2.4).

Assumption 2.1. *Let $0 < T_0 < \infty$ be an arbitrary fixed time. For some $m \geq 2$, we assume that*

$$(A) \quad \psi^{\mathrm{init}} \in \left(H^m(\mathbb{R}^3)\right)^4,$$

$$(B) \quad V, A_j \in C\left([0,T_0], H^m(\mathbb{R}^3)\right), \qquad j = 1,2,3.$$

The following theorem quoted from [CW20, Theorem 2.1] provides well-posedness of the NLDE (2.3) and regularity of solutions.

Theorem 2.2. *[CW20, Theorem 2.1] Under the assumptions (A) and (B), there is a time $T_1 \in (0, T_0]$ such that for any $\varepsilon \in (0,1)$, the NLDE (2.3) admits a unique solution*

$$\psi^\varepsilon \in C\Big([0,T_1], (H^m(\mathbb{R}^3))^4\Big) \cap C^1\Big([0,T_1], (H^{m-1}(\mathbb{R}^3))^4\Big)$$

with uniform estimates

$$\sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T_1]} \|\psi^\varepsilon(t,\cdot)\|_{H^m} \leq C,$$

where C is independent of ε.

The original formulation of this result in [CW20] is slightly more general and applies also to the case where the initial data in (2.3) depend on ε to some extent.

Solving (2.3) numerically is a challenging task, because typical solutions oscillate in time with frequency of $\mathcal{O}(\varepsilon^{-2})$ due to the term $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon\psi^\varepsilon(t,x)$ on the right-hand side. Applying

traditional time-integrators such as, e.g., Runge-Kutta or standard multistep methods is inefficient, because such methods only achieve an acceptable accuracy if the ratio of the step size and the highest frequency is small; see, e.g., [Bao+16b]. One possibility to solve this problem is to construct special integrators which do not suffer from such a severe step size restriction. This has been done in [CW18; CW22; LMZ17], but the implementation of such methods is quite involved. In this paper we pursue a different goal. In [CW20] it was rigorously shown that in the limit $\varepsilon \to 0$ the solution of the NLDE (2.3) can be approximated up to $\mathcal{O}(\varepsilon^2)$ by solving a non-oscillatory system of PDEs known as the semi-nonrelativistic limit system; cf. (2.14) below. Since this accuracy is good enough in many applications, our main goal is to construct a particularly efficient method for the semi-nonrelativistic limit system. This is done in Section 2.3. Before that, we briefly outline the derivation of the semi-nonrelativistic limit system given in [CW20].

2.2.2 Transformed Dirac equation

In this and the next subsection we summarize the main results from [CW20].

By performing an eigenspace decomposition in Fourier space, the operator $\mathcal{T}_\varepsilon$ can be decomposed as [BMP98, Eq. (1.22)]

$$\mathcal{T}_\varepsilon = \Lambda_\varepsilon \Pi_\varepsilon^+ - \Lambda_\varepsilon \Pi_\varepsilon^- \tag{2.5}$$

with the scalar operator $\Lambda_\varepsilon = \sqrt{\mathrm{Id} - \varepsilon^2 \Delta}$ and the two projection operators $\Pi_\varepsilon^\pm$ given by

$$\Pi_\varepsilon^\pm = \frac{1}{2}\left(\mathrm{Id} \pm (\mathrm{Id} - \varepsilon^2\Delta)^{-\frac{1}{2}} \mathcal{T}_\varepsilon\right). \tag{2.6}$$

The identities $\Pi_\varepsilon^+ + \Pi_\varepsilon^- = Id$, $\Pi_\varepsilon^+ \Pi_\varepsilon^- = \Pi_\varepsilon^- \Pi_\varepsilon^+ = 0$ and $(\Pi_\varepsilon^\pm)^2 = \Pi_\varepsilon^\pm$ can easily be checked; cf. [CW20]. As a mapping from $(H^m(\mathbb{R}^3))^4$ to $(H^m(\mathbb{R}^3))^4$ the projectors $\Pi_\varepsilon^\pm$ are uniformly bounded w.r.t. ε; cf. [BMP98, Lemma 2.1]. The decomposition (2.5) allows us to filter out the main part of the temporal oscillations in a solution ψ^ε of the NLDE (2.3). This is achieved by considering the functions

$$\phi_\pm^\varepsilon(t,x) := e^{\pm \mathrm{i}t/\varepsilon^2} \Pi_\varepsilon^\pm [\psi^\varepsilon(t,x)] \tag{2.7}$$

instead of ψ^ε. Substituting (2.7) into the NLDE (2.3) shows that ϕ_+^ε and ϕ_-^ε are the solution of the two coupled PDEs

$$\begin{aligned} \partial_t \phi_\pm^\varepsilon &= \mp \mathrm{i} \mathcal{D}_\varepsilon \phi_\pm^\varepsilon - \mathrm{i}\Pi_\varepsilon^\pm \left[W\left(\phi_\pm^\varepsilon + e^{\pm 2\mathrm{i}t/\varepsilon^2}\phi_\mp^\varepsilon\right)\right] \\ &\quad - \mathrm{i}\gamma_2 \Pi_\varepsilon^\pm \left[g_\varepsilon(\phi_+^\varepsilon, \phi_-^\varepsilon, t)\left(\phi_\pm^\varepsilon + e^{\pm 2\mathrm{i}t/\varepsilon^2}\phi_\mp^\varepsilon\right)\right] \\ \phi_\pm^\varepsilon(0) &= \Pi_\varepsilon^\pm \left[\psi^{\mathrm{init}}\right] \end{aligned} \tag{2.8}$$

with the differential operator

$$\mathcal{D}_\varepsilon = \frac{1}{\varepsilon^2}(\Lambda_\varepsilon - \mathrm{Id}) = \frac{1}{\varepsilon^2}\left(\sqrt{\mathrm{Id} - \varepsilon^2\Delta} - \mathrm{Id}\right) \tag{2.9}$$

and nonlinearity

$$g_\varepsilon(\phi_+^\varepsilon, \phi_-^\varepsilon, t) = |\phi_+^\varepsilon|^2 + |\phi_-^\varepsilon|^2 + e^{2\mathrm{i}t/\varepsilon^2}(\phi_+^\varepsilon)^* \phi_-^\varepsilon + e^{-2\mathrm{i}t/\varepsilon^2}(\phi_-^\varepsilon)^* \phi_+^\varepsilon,$$

cf. [CW20, Sect. 2.1]. From the solution $\phi_\pm^\varepsilon$ of (2.8) we can reconstruct the solution ψ^ε of the NLDE (2.3) by

$$\psi^\varepsilon(t,x) = e^{-\mathrm{i}t/\varepsilon^2}\phi_+^\varepsilon(t,x) + e^{\mathrm{i}t/\varepsilon^2}\phi_-^\varepsilon(t,x). \tag{2.10}$$

In Fourier space, application of $\mathcal{D}_\varepsilon$ to a function v corresponds to multiplication of the Fourier transform of v at $\xi \in \mathbb{R}^3$ with

$$\delta_\varepsilon(\xi) := \frac{1}{\varepsilon^2}\left(\sqrt{1+\varepsilon^2|\xi|^2}-1\right) = \frac{|\xi|^2}{\sqrt{1+\varepsilon^2|\xi|^2}+1} \in \left[0, \frac{|\xi|^2}{2}\right]. \tag{2.11}$$

This yields the bound

$$\|\mathcal{D}_\varepsilon v\|_{H^n} \leq \frac{1}{2}\|v\|_{H^{n+2}} \qquad \forall\, v \in (H^{n+2}(\mathbb{R}^3))^4,\ n \in \mathbb{N}_0, \tag{2.12}$$

which means that the operator

$$\mathcal{D}_\varepsilon : (H^{n+2}(\mathbb{R}^3))^4 \to (H^n(\mathbb{R}^3))^4 \tag{2.13}$$

is uniformly bounded w.r.t. ε for all $n \in \mathbb{N}_0$. Hence, the first time derivative of a solution $\phi_\pm^\varepsilon$ is uniformly bounded w.r.t. ε, which is not true for a solution ψ^ε of the NLDE due to the factor $1/\varepsilon^2$ on the right-hand side. In this sense (2.8) is better suited for numerical purposes than the original form (2.3) of the NLDE. However, solving (2.8) with standard methods still suffers from severe step size restrictions, because the solution of (2.8) still oscillates with the same frequency as the original problem, albeit with smaller amplitude. In the next subsection, these oscillations are completely removed at the cost of an approximation error.

2.2.3 Semi-nonrelativistic limit system

Omitting the terms containing highly oscillatory exponential functions in (2.8) (including those in the nonlinearity g) yields the semi-nonrelativistic limit system [CW20, Eq. (2.14)]

$$\begin{aligned} \partial_t \varphi_\pm^\varepsilon &= \mp \mathrm{i}\mathcal{D}_\varepsilon \varphi_\pm^\varepsilon - \mathrm{i}\Pi_\varepsilon^\pm\left[W\varphi_\pm^\varepsilon\right] - \mathrm{i}\gamma_2\Pi_\varepsilon^\pm\left[\left(|\varphi_+^\varepsilon|^2 + |\varphi_-^\varepsilon|^2\right)\varphi_\pm^\varepsilon\right] \\ \varphi_\pm^\varepsilon(0) &= \Pi_\varepsilon^\pm\left[\psi^{\mathrm{init}}\right]. \end{aligned} \tag{2.14}$$

Well-posedness of (2.14) and regularity of solutions of (2.14) has been shown in [CW20]. Furthermore, the authors proved that solutions of (2.14) provide approximations to a solution of the original problem (2.3):

Theorem 2.3. *[CW20, Theorem 2.2] Under the assumptions (A) and (B), there is a time $T_2 \in (0, T_0]$ such that for any $\varepsilon \in (0,1)$, the semi-nonrelativistic limit system (2.14) admits a unique solution*

$$\varphi_\pm^\varepsilon \in C\left([0,T_2], \left(H^m(\mathbb{R}^3)\right)^4\right) \cap C^1\left([0,T_2], \left(H^{m-1}(\mathbb{R}^3)\right)^4\right)$$

with uniform estimates

$$\begin{aligned} \sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T_2]} \left\|\varphi_\pm^\varepsilon\right\|_{H^m} &\leq C, \\ \sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T_2]} \left\|\partial_t\varphi_\pm^\varepsilon\right\|_{H^{m-2}} &\leq C. \end{aligned}$$

Moreover, $\varphi_\pm^\varepsilon$ remain in the eigenspaces associated with $\Pi_\varepsilon^\pm$, respectively. If in addition the assumption $V, A_j \in C^1\left([0,T_0], H^{m-2}(\mathbb{R}^3)\right)$ holds for $j = 1,2,3$, then the approximation error is bounded by

$$\sup_{t\in[0,T]} \left\|\psi^\varepsilon - e^{-\mathrm{i}t/\varepsilon^2}\varphi_+^\varepsilon - e^{\mathrm{i}t/\varepsilon^2}\varphi_-^\varepsilon\right\|_{H^{m-2}} \leq C\varepsilon^2 \tag{2.15}$$

with $T = \min\{T_1, T_2\}$ *and for* $m \geq 4$ *we have*

$$\varphi_\pm^\varepsilon \in C^2\left([0,T_2], (H^{m-2}(\mathbb{R}^3))^4\right) \qquad \textit{with} \qquad \sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T_2]} \|\partial_{tt}\varphi_\pm^\varepsilon\|_{H^{m-4}} \leq C.$$

In [CW20] this theorem is formulated in a more general way which, however, exceeds our demands.

The inequality (2.15) implies that a solution of the NLDE (2.3) can be approximated up to $\mathcal{O}(\varepsilon^2)$ using a solution of the semi-nonrelativistic limit system. In this paper, we consider the case where ε is small enough such that this approximation is satisfactory. Thus, instead of developing time-integrators for the NLDE (2.3) or its transformed version (2.8), we can focus on the simpler semi-nonrelativistic limit system (2.14). Solutions of (2.14) are *not* affected by oscillations, because there is neither a factor ε^{-2} on the right-hand side (in contrast to (2.3)) nor oscillating exponentials (in contrast to (2.8)). The solution only depends on ε because the projectors $\Pi_\varepsilon^\pm$ and the differential operator $\mathcal{D}_\varepsilon$ do, but in a non-critical way. In spite of these advantages, solving (2.14) with standard methods is still not a good option. If explicit Runge-Kutta or multistep methods are used, then the spatial discretization of the differential operator $\mathcal{D}_\varepsilon$ causes severe CFL conditions, whereas a time step with an implicit method is somewhat costly due to the nonlinearity and the projectors $\Pi_\varepsilon^\pm$. Applying a splitting method to (2.14) in a straightforward way is not feasible, because the sub-problems involving the projectors $\Pi_\varepsilon^\pm$ cannot be propagated exactly or particularly efficiently. These disadvantages can be avoided by exponential integrators. Two such methods are presented and compared in the next section.

2.3 Time integration methods for the semi-nonrelativistic limit system

Our goal now is to compute approximations $\varphi_\pm^n \approx \varphi_\pm^\varepsilon(t_n)$ of the solution of the semi-nonrelativistic limit system at discrete times $t_n = n\tau$, where $\tau > 0$ is the step size. We propose two exponential integrators which converge with order two in τ. The first one is constructed by applying variation of constants over the interval $[t_n, t_{n+1}]$, approximating the integrand in a suitable way and computing the resulting integrals exactly. This strategy is, of course, not new, and the related techniques have been used for various types of PDEs, in particular in the context of highly oscillatory problems. We consider this first method only as a benchmark method, and for this reason we refrain from an extensive error analysis. The main contribution of this paper is the second time-integrator. The crucial idea is to use variation of constants over the time interval $[t_{n-1}, t_{n+1}]$ instead of $[t_n, t_{n+1}]$, which makes the approximation of the resulting integrals much easier. This leads to a novel exponential two-step method called the *explicit exponential midpoint rule* (EEMR). This time-integrator is time-symmetric, simple to implement, and considerably more efficient than the benchmark method. We present a detailed error analysis for the EEMR and explain the speed-up observed in numerical examples.

Assumptions and notation. In the end, we want to obtain error bounds in L^2. Our methods will rely on the uniform boundedness of the second time derivative of $\varphi_\pm$ in L^2. According to Theorem 2.3, this is given under the following assumptions that we will assume for the rest of the paper:

$$\text{(I)} \qquad \psi^{\text{init}} \in \left(H^4(\mathbb{R}^3)\right)^4,$$

$$\text{(II)} \quad V, A_j \in C\left([0,T_0], H^4(\mathbb{R}^3)\right), \qquad j=1,2,3.$$

$$\text{(III)} \quad V, A_j \in C^1\left([0,T_0], H^2(\mathbb{R}^3)\right), \qquad j=1,2,3.$$

In order to prove convergence of the methods, we will also require the assumption

$$\text{(IV)} \quad V, A_j \in C^2\left([0,T_0], L_2(\mathbb{R}^3)\right), \qquad j=1,2,3.$$

Assumptions (I) and (II) coincide with Assumption 2.1 for $m=4$.

To increase readability, we define the function space

$$\begin{aligned}\mathcal{S}_T := C([0,T],(H^4(\mathbb{R}^3))^4) \;&\cap\; C^1([0,T],(H^2(\mathbb{R}^3))^4)\\ &\cap\; C^2([0,T],(L^2(\mathbb{R}^3))^4)\end{aligned}$$

for $T=\min\{T_1,T_2\}$ from Theorem 2.3, which then states that if assumptions (I)–(III) hold, then $\varphi_\pm \in \mathcal{S}_T$ with uniform bounds in ε.

From now on we assume that ε is small but fixed. We can thus omit the index ε in our notation such that the semi-nonrelativistic limit system (2.14) reads

$$\begin{aligned}\partial_t\varphi_\pm &= \mp \mathrm{i}\mathcal{D}\varphi_\pm - \mathrm{i}\Pi^\pm\left[W\varphi_\pm\right] - \mathrm{i}\gamma_2\Pi^\pm\left[\left(|\varphi_+|^2+|\varphi_-|^2\right)\varphi_\pm\right]\\ \varphi_\pm(0) &= \Pi^\pm\left[\psi^{\mathrm{init}}\right].\end{aligned} \tag{2.16}$$

All bounds presented below are uniformly in ε in the sense that the constants do not depend on ε.

Let $\tau \in (0,T)$ be the time step size and let $t_n = n\tau$, $n=0,1,...,\lfloor T/\tau \rfloor$. To improve readability, we omit the spatial variable x on the solution and the potential in the following. For a function $f_\varepsilon = f_\varepsilon(s)$, we write $f_\varepsilon = \mathcal{O}(s^p)$ for some $p \in \mathbb{N}_0$ to express that

$$\|f_\varepsilon(s)\|_{L^2} \leq Cs^p$$

for $s \to 0$ with some constant C which does not dependent on s and ε.

We will repeatedly use that there is a constant C such that

$$\|vw\|_{L^2} \leq C\|v\|_{L^2}\|w\|_{H^2} \tag{2.17}$$

for all $v \in L^2(\mathbb{R}^3)$, $w \in H^2(\mathbb{R}^3)$ (where one of the functions may also be $\mathbb{C}^4$-valued), and

$$\|v^*w\|_{L^2} \leq C\|v\|_{L^2}\|w\|_{H^2} \tag{2.18}$$

for all $v \in (L^2(\mathbb{R}^3))^4$, $w \in (H^2(\mathbb{R}^3))^4$. These inequalities follow from the Sobolev embedding $H^2(\mathbb{R}^3) \subset L_\infty(\mathbb{R}^3)$.

2.3.1 The benchmark method

Using variation of constants, we can express the solution $\varphi_\pm$ of the semi-nonrelativistic limit system (2.16) at time $t_n+\tau$ as

$$\varphi_\pm(t_n+\tau) = e^{\mp \mathrm{i}\tau\mathcal{D}}\varphi_\pm(t_n) - \mathrm{i}I_1^\pm(\varphi_+,\varphi_-,t_n) - \mathrm{i}\gamma_2 I_2^\pm(\varphi_+,\varphi_-,t_n) \tag{2.19}$$

with $I_j^\pm = I_j^\pm(\varphi_+, \varphi_-, t_n)$ given by

$$I_1^\pm = \int_0^\tau e^{\mp \mathrm{i}(\tau-s)\mathcal{D}} \Pi^\pm \left[W(t_n+s)\, \varphi_\pm(t_n+s) \right] ds,$$
$$I_2^\pm = \int_0^\tau e^{\mp \mathrm{i}(\tau-s)\mathcal{D}} \Pi^\pm \left[\left(|\varphi_+(t_n+s)|^2 + |\varphi_-(t_n+s)|^2 \right) \varphi_\pm(t_n+s) \right] ds.$$

The operators $e^{\mp \mathrm{i}(\tau-s)\mathcal{D}}$ and $\Pi^\pm$ are both bounded in $(L^2(\mathbb{R}^3))^4$. Thus, in order to obtain a third-order approximation (in τ) to the integrals, we need a second-order approximation (in s) to the integrands. Under assumption (IV), $W(t_n+s)$ can be replaced by the Taylor expansion

$$W(t_n+s) = W(t_n) + s\partial_t W(t_n) + \mathcal{O}\left(s^2\right). \tag{2.20}$$

Since the second time derivative of $\varphi_\pm$ is bounded in $(L^2(\mathbb{R}^3))^4$ under assumptions (I)–(III), we can also expand

$$\varphi_\pm(t_n+s) = \varphi_\pm(t_n) + s\Theta_\pm(\varphi_+(t_n), \varphi_-(t_n), t_n) + \mathcal{O}\left(s^2\right), \tag{2.21}$$

with

$$\Theta_\pm = \Theta_\pm(\varphi_+(t_n), \varphi_-(t_n), t_n) := \partial_t \varphi_\pm(t_n)$$

being the first time derivative of $\varphi_\pm$ at time t_n. It is obtained by evaluating the right-hand side of the PDE (2.16) at time t_n:

$$\begin{aligned}\Theta_\pm(\varphi_+(t_n), \varphi_-(t_n), t_n) = {} & \mp \mathrm{i}\mathcal{D}\varphi_\pm(t_n) - \mathrm{i}\Pi^\pm \left[W(t_n)\varphi_\pm(t_n) \right] \\ & - \mathrm{i}\gamma_2 \Pi^\pm \left[\left(|\varphi_+(t_n)|^2 + |\varphi_-(t_n)|^2 \right) \varphi_\pm(t_n) \right].\end{aligned} \tag{2.22}$$

Before we continue by inserting (2.20) and (2.21) into (2.19), let us quickly comment on an alternative approach to construct a second-order approximation to $\varphi_\pm(t_n+s)$. Using variation of constants once again, but now over a time interval of length s, and fixing $\varphi_\pm$ as well as W at time t_n inside the integrals yields

$$\begin{aligned}\varphi_\pm(t_n+s) = {} & e^{\mp \mathrm{i}s\mathcal{D}}\varphi_\pm(t_n) - \mathrm{i}\int_0^s e^{\mp \mathrm{i}(s-r)\mathcal{D}} \Pi^\pm \left[W(t_n)\varphi_\pm(t_n) \right] dr \\ & - \mathrm{i}\int_0^s e^{\mp \mathrm{i}(s-r)\mathcal{D}} \Pi^\pm \left[\gamma_2 \left(|\varphi_+(t_n)|^2 + |\varphi_-(t_n)|^2 \right) \varphi_\pm(t_n) \right] dr + \mathcal{O}\left(s^2\right).\end{aligned} \tag{2.23}$$

This approach does only rely on boundedness of the first time derivative of $\varphi_\pm$ and thus is, at first glance, feasible under lower regularity assumptions on the potential W and the initial data. Unfortunately, inserting (2.23) into (2.19) leads to integrals which cannot be computed analytically. In order to avoid this problem, we could use the formal approximations

$$e^{\mp \mathrm{i}s\mathcal{D}}\varphi_\pm(t_n) = \varphi_\pm(t_n) \mp \mathrm{i}s\mathcal{D}\varphi_\pm(t_n) + \mathcal{O}\left(s^2\right),$$
$$\int_0^s e^{\mp \mathrm{i}(s-r)\mathcal{D}} \Pi^\pm [v]\, dr = s\Pi^\pm [v] + \mathcal{O}\left(s^2\right)$$

which can be rigorously justified for $\varphi_\pm \in \left(H^4(\mathbb{R}^3)\right)^4$ and $v \in \left(H^2(\mathbb{R}^3)\right)^4$. Using these approximations in (2.23), however, yields exactly the same second-order approximation to $\varphi_\pm(t_n+s)$ as (2.21) together with (2.22).

Now we continue the construction of the benchmark method. Inserting (2.20) and (2.21) into $I_1^\pm$ yields

$$I_1^\pm(\varphi_+, \varphi_-, t_n) = \widehat{I}_1^\pm(\varphi_+(t_n), \varphi_-(t_n), t_n) + \mathcal{O}\Big(\tau^3\Big)$$

where $\widehat{I}_1^\pm = \widehat{I}_1^\pm(\varphi_+(t_n), \varphi_-(t_n), t_n)$ is given by

$$\begin{aligned}\widehat{I}_1^\pm &= \int_0^\tau e^{\mp \mathrm{i}(\tau-s)\mathcal{D}} \Pi^\pm \left[W(t_n)\varphi_\pm(t_n)\right] \, ds \\ &\quad + \int_0^\tau s e^{\mp \mathrm{i}(\tau-s)\mathcal{D}} \Pi^\pm \left[W(t_n)\Theta_\pm + \partial_t W(t_n)\varphi_\pm(t_n)\right] \, ds \\ &= \tau p_1(\mp \mathrm{i}\tau\mathcal{D})\, \Pi^\pm \left[W(t_n)\varphi_\pm(t_n)\right] \\ &\quad + \tau^2 p_2(\mp \mathrm{i}\tau\mathcal{D})\, \Pi^\pm \left[W(t_n)\Theta_\pm + \partial_t W(t_n)\varphi_\pm(t_n)\right].\end{aligned}$$

The functions p_1 and p_2 are defined by

$$p_1(z) = \int_0^1 e^{(1-\theta)z} d\theta, \qquad p_2(z) = \int_0^1 \theta e^{(1-\theta)z} d\theta, \qquad z \in \mathbb{C}, \tag{2.24}$$

cf. [HO10, Eq. (2.10) and (2.11)]. They can be computed as

$$p_1(z) = \begin{cases} \frac{e^z-1}{z} & \text{for } z \neq 0, \\ 1 & \text{for } z = 0 \end{cases} \qquad \text{and} \qquad p_2(z) = \begin{cases} \frac{e^z-z-1}{z^2} & \text{for } z \neq 0, \\ \frac{1}{2} & \text{for } z = 0. \end{cases}$$

When inserting (2.21) into $I_2^\pm$, we can additionally drop all $\mathcal{O}(s^2)$-terms in the integrand that arise due to the nonlinearity. Overall, we obtain

$$I_2^\pm(\varphi_+, \varphi_-, t_n) = \widehat{I}_2^\pm(\varphi_+(t_n), \varphi_-(t_n), t_n) + \mathcal{O}\Big(\tau^3\Big)$$

where $\widehat{I}_2^\pm = \widehat{I}_2^\pm(\varphi_+(t_n), \varphi_-(t_n), t_n)$ is given by

$$\begin{aligned}\widehat{I}_2^\pm &= \int_0^\tau e^{\mp \mathrm{i}(\tau-s)\mathcal{D}} \Pi^\pm \left[\zeta_\pm + s\zeta'_\pm\right] \, ds \\ &= \tau p_1\left(\mp \mathrm{i}\tau\mathcal{D}\right) \Pi^\pm \left[\zeta_\pm\right] + \tau^2 p_2\left(\mp \mathrm{i}\tau\mathcal{D}\right) \Pi^\pm \left[\zeta'_\pm\right]\end{aligned}$$

with $\zeta_\pm = \zeta_\pm\left(\varphi_+(t_n), \varphi_-(t_n), t_n\right)$ and $\zeta'_\pm = \zeta'_\pm\left(\varphi_+(t_n), \varphi_-(t_n), t_n\right)$ defined by

$$\begin{aligned}\zeta_\pm &= \left(|\varphi_+(t_n)|^2 + |\varphi_-(t_n)|^2\right) \varphi_\pm(t_n) \\ \zeta'_\pm &= \left(|\varphi_+(t_n)|^2 + |\varphi_-(t_n)|^2\right) \Theta_\pm + 2\,\mathrm{Re}\left((\Theta_+)^*\varphi_+(t_n) + (\Theta_-)^*\varphi_-(t_n)\right)\varphi_\pm(t_n)\end{aligned}$$

and $\Theta_\pm$ from (2.22). A third-order approximation to $\varphi_\pm(t_n + \tau)$ is obtained by simply replacing the integrals $I_1^\pm$ and $I_2^\pm$ in (2.19) by their approximations $\widehat{I}_1^\pm$ and $\widehat{I}_2^\pm$:

$$\begin{aligned}\varphi_\pm(t_n + \tau) = e^{\mp \mathrm{i}\tau\mathcal{D}}\varphi_\pm(t_n) &- \mathrm{i}\widehat{I}_1^\pm(\varphi_+(t_n), \varphi_-(t_n), t_n) \\ &- \mathrm{i}\gamma_2 \widehat{I}_2^\pm(\varphi_+(t_n), \varphi_-(t_n), t_n) + \mathcal{O}\Big(\tau^3\Big).\end{aligned} \tag{2.25}$$

This approximation suggests a numerical method with local error of order $\mathcal{O}(\tau^3)$ which, however, would not be stable. The reason for this instability is the term $\mp \mathrm{i}\mathcal{D}\varphi_\pm(t_n)$, which appears in $\Theta_\pm$, cf. (2.22), and thus also in $\zeta'_\pm$. A bound for the norm of $\mathcal{D}$ that is independent of ε can only be established when interpreting $\mathcal{D}$ as mapping from H^2 to L^2, cf. (2.13). Hence, the L^2-norm of $\Theta_\pm$ and thus $\zeta'_\pm$, $\widehat{I}_1^\pm$ and $\widehat{I}_2^\pm$ can only be bounded using the H^2-norm

of $\varphi_\pm(t_n)$, which would not be sufficient for stability. This is why we replace $\mathcal{D}$ in $\Theta_\pm$ by a filtered version

$$\widetilde{\mathcal{D}}(\tau) = \frac{\sin(\tau\mathcal{D})}{\tau} \tag{2.26}$$

as, e.g., in [CW19; CW22]. It is not difficult to show that for every $\tau > 0$, $\widetilde{\mathcal{D}}(\tau)$ is a bounded operator from L^2 to L^2 with $\|\widetilde{\mathcal{D}}(\tau)\| \leq \frac{1}{\tau}$, and that

$$\left\|(\mathcal{D} - \widetilde{\mathcal{D}}(\tau))v\right\|_{L^2} \leq \frac{\tau}{2}\|v\|_{H^4}$$

for all $v \in (H^4(\mathbb{R}^3))^4$. Since Theorem 2.3 yields that $\varphi_\pm \in C([0,T_2],(H^4(\mathbb{R}^3))^4)$ under assumptions (I) and (II), it follows that replacing $\mathcal{D}$ by $\widetilde{\mathcal{D}}(\tau)$ in $\Theta_\pm$ and hence also in $\zeta'_\pm$ causes an error of $\mathcal{O}(\tau)$. But in $\widehat{I}_1^\pm$ and $\widehat{I}_2^\pm$, the terms including $\Theta_\pm$ or $\zeta'_\pm$ are multiplied by a factor τ^2. Thus, substituting $\widetilde{\mathcal{D}}(\tau)$ for $\mathcal{D}$ in the right-hand side of (2.25) causes only an additional error of $\mathcal{O}(\tau^3)$ and hence does not affect the overall approximation error. All in all, this yields the numerical method

$$\varphi_\pm^{n+1} = \Phi_\tau^\pm(\varphi_+^n, \varphi_-^n, t_n), \qquad n \in \mathbb{N}_0, \tag{2.27}$$

with the numerical flow

$$\Phi_\tau^\pm(\varphi_+^n, \varphi_-^n, t_n) = e^{\mp \mathrm{i}\tau\mathcal{D}}\varphi_\pm^n - \mathrm{i}\widetilde{I}_1^\pm(\varphi_+^n, \varphi_-^n, t_n) - \mathrm{i}\gamma_2\widetilde{I}_2^\pm(\varphi_+^n, \varphi_-^n, t_n). \tag{2.28}$$

$\widetilde{I}_1^\pm$ and $\widetilde{I}_2^\pm$ correspond to $\widehat{I}_1^\pm$ and $\widehat{I}_2^\pm$, respectively, but with $\mathcal{D}$ replaced by $\widetilde{\mathcal{D}}(\tau)$ in $\Theta_\pm$ and $\zeta'_\pm$, i.e.

$$\begin{aligned}
\widetilde{I}_1^\pm(\varphi_+^n, \varphi_-^n, t_n) &= \tau p_1(\mp\mathrm{i}\tau\mathcal{D})\,\Pi^\pm\left[W(t_n)\varphi_\pm^n\right] \\
&\quad + \tau^2 p_2(\mp\mathrm{i}\tau\mathcal{D})\,\Pi^\pm\left[W(t_n)\widetilde{\Theta}_\pm + \partial_t W(t_n)\varphi_\pm^n\right], \\
\widetilde{I}_2^\pm(\varphi_+^n, \varphi_-^n, t_n) &= \tau p_1\left(\mp\mathrm{i}\tau\mathcal{D}\right)\Pi^\pm\left[\zeta_\pm\right] + \tau^2 p_2\left(\mp\mathrm{i}\tau\mathcal{D}\right)\Pi^\pm\left[\widetilde{\zeta'_\pm}\right],
\end{aligned}$$

with

$$\begin{aligned}
\zeta_\pm = \zeta_\pm\left(\varphi_+^n, \varphi_-^n, t_n\right) &= \left(|\varphi_+^n|^2 + |\varphi_-^n|^2\right)\varphi_\pm^n, \\
\widetilde{\Theta}_\pm = \widetilde{\Theta}_\pm(\varphi_+^n, \varphi_-^n, t_n) &= \mp\mathrm{i}\widetilde{\mathcal{D}}(\tau)\varphi_\pm^n - \mathrm{i}\Pi^\pm\left[W(t_n)\varphi_\pm^n + \gamma_2\zeta_\pm\right], \\
\widetilde{\zeta'_\pm} = \widetilde{\zeta'_\pm}(\varphi_+^n, \varphi_-^n, t_n) &= \left(|\varphi_+^n|^2 + |\varphi_-^n|^2\right)\widetilde{\Theta}_\pm + 2\,\mathrm{Re}\left((\widetilde{\Theta}_+)^*\varphi_+^n + (\widetilde{\Theta}_-)^*\varphi_-^n\right)\varphi_\pm^n.
\end{aligned}$$

For an efficient implementation, the two integrals $\widetilde{I}_1^\pm$ and $\gamma_2\widetilde{I}_2^\pm$ can be combined to

$$\begin{aligned}
\widetilde{I}^\pm(\varphi_+^n, \varphi_-^n, t_n) &= \widetilde{I}_1^\pm(\varphi_+^n, \varphi_-^n, t_n) + \gamma_2\widetilde{I}_2^\pm(\varphi_+^n, \varphi_-^n, t_n) \\
&= \tau p_1\left(\mp\mathrm{i}\tau\mathcal{D}\right)\Pi^\pm\left[W(t_n)\varphi_\pm^n + \gamma_2\zeta_\pm\right] \\
&\quad + \tau^2 p_2\left(\mp\mathrm{i}\tau\mathcal{D}\right)\Pi^\pm\left[W(t_n)\widetilde{\Theta}_\pm + \partial_t W(t_n)\varphi_\pm^n + \gamma_2\widetilde{\zeta'_\pm}\right].
\end{aligned}$$

Under assumptions (I)–(IV) the local error in L^2 is bounded by $C\tau^3$ by construction. With well-known techniques, it can be shown that under assumptions (I)–(IV) there are constants $\tau_0 > 0$ and C such that for all step sizes $\tau \in (0, \tau_0]$ the bound

$$\left\|\varphi_\pm^n - \varphi_\pm(t_n)\right\|_{L^2} \leq C\tau^2, \qquad n = 1, 2, ..., \lfloor T/\tau \rfloor$$

for the global error holds. We omit the proof, because our focus is not on the benchmark method. The step size restriction $\tau \leq \tau_0$ is required to obtain uniform boundedness of the numerical approximations in $H^2(\mathbb{R}^3)$, which is required for stability; for the EEMR this issue is discussed in the proof of Theorem 2.10.

Remark 2.4. *The method (2.27)–(2.28) is certainly not new. We have described the construction only for the convenience of the reader and in order to keep the paper self-contained. In fact, (2.27)–(2.28) coincides with a "part" of the multiscale method for the NLDE (2.3) which has been proposed in [CW18]. The idea is, roughly speaking, to make the ansatz*

$$\psi^\varepsilon(t,x) = e^{-\mathrm{i}t/\varepsilon^2}\varphi_+(t,x) + e^{\mathrm{i}t/\varepsilon^2}\varphi_-(t,x) + r(t,x),$$

i.e. to decompose the solution of (2.3) into the part provided by the semi-nonrelativistic limit system plus a rest $r(t,x)$ which, according to (2.15), is only $\mathcal{O}(\varepsilon^2)$. Substituting this ansatz into the NLDE and replacing $\partial_t\varphi_\pm$ by (2.16) yields a PDE for $r(t,x)$ with a rather complicated right-hand side. Then, a numerical method for $\varphi_\pm$ and r is constructed in [CW18]. Within this method the part which approximates $\varphi_\pm$ is almost identical to what we call the benchmark method. The only differences are that instead of (2.26) a different filter is used in [CW18], and that the authors consider the full discretization in time and space.

Remark 2.5. *In this work we only consider time discretizations. For a full discretization in time and space on the torus, the benchmark method (2.27)–(2.28) can be combined with a Fourier pseudospectral method, such that $\varphi_\pm^n$ is approximated by a trigonometric polynomial. All operators involving spatial derivatives (which includes the projectors $\Pi^\pm$) are applied in Fourier space, whereas pointwise multiplications of functions such as, e.g., $W(t_n)\varphi_\pm^n$ or $W(t_n)\widetilde{\Theta}_\pm$ correspond to entry-wise multiplications of vectors. In order to compute all terms required for one time step, the fast Fourier transform (FFT) or its inverse has to be applied quite a number of times, and in spite of the efficiency of the FFT, this causes the dominating part of the numerical work.*

2.3.2 Explicit exponential midpoint rule

We will now propose and analyze a new exponential integrator which converges with order two under the same regularity assumptions as the benchmark method, but which is conceptually simpler, easier to implement and significantly faster. The new integrator is time-symmetric, in contrast to the benchmark method. For time-dependent potentials, the new method does not require evaluations of $\partial_t W$, which is convenient in situations where no explicit formula for $W(t,x)$ is available.

Construction

We again use variation of constants to express the solution $\varphi_\pm$ of the semi-nonrelativistic limit system at time $t_n+\tau$, but now over a time interval of length 2τ. This yields

$$\varphi_\pm(t_n+\tau) = e^{\mp 2\mathrm{i}\tau\mathcal{D}}\varphi_\pm(t_n-\tau) - \mathrm{i}I_1^\pm(\varphi_+,\varphi_-,t_n) - \mathrm{i}\gamma_2 I_2^\pm(\varphi_+,\varphi_-,t_n) \tag{2.29}$$

with $I_1^\pm = I_1^\pm(\varphi_+,\varphi_-,t_n)$, $I_2^\pm = I_2^\pm(\varphi_+,\varphi_-,t_n)$ given by[2]

$$I_1^\pm = \int_{-\tau}^{\tau} e^{\mp\mathrm{i}(\tau-s)\mathcal{D}}\Pi^\pm\left[W(t_n+s)\varphi_\pm(t_n+s)\right]\,ds,$$
$$I_2^\pm = \int_{-\tau}^{\tau} e^{\mp\mathrm{i}(\tau-s)\mathcal{D}}\Pi^\pm\left[\left(|\varphi_+(t_n+s)|^2 + |\varphi_-(t_n+s)|^2\right)\varphi_\pm(t_n+s)\right]\,ds.$$

[2]Note that $I_1^\pm$ and $I_2^\pm$ are different from the integral terms which were denoted with $I_1^\pm$ and $I_2^\pm$ in the previous section. Many other objects which appeared in the previous section such as, e.g., $\widehat{I}_1^\pm$, $\widehat{I}_2^\pm$, $\Phi_\tau^\pm$, Φ_τ etc., will be re-defined in a different way in this section.

Under the assumptions (I)–(III), we know that $\varphi_\pm \in \mathcal{S}_T$ with uniformly bounded (w.r.t. ε) derivatives according to Theorem 2.3. If additionally assumption (IV) is fulfilled, then according to the estimates (2.17) and (2.18) the same holds for the functions

$$\Pi^\pm [W\varphi_\pm] \qquad \text{and} \qquad \gamma_2 \Pi^\pm \left[\left(|\varphi_+|^2 + |\varphi_-|^2 \right) \varphi_\pm \right]$$

which appear in the integrands of $I_1^\pm$ and $I_2^\pm$. For a function $v \in \mathcal{S}_T$, a third-order approximation to integrals of the form $\int_{-\tau}^{\tau} e^{\mp \mathrm{i}(\tau - s)\mathcal{D}} v(t_n + s)\, ds$ is obtained by fixing v at the midpoint t_n, as the following lemma confirms.

Lemma 2.6. *Let $v \in \mathcal{S}_T$ and $\tau \in (0, T)$. Then,*

$$\left\| \int_{-\tau}^{\tau} e^{\mp \mathrm{i}(\tau - s)\mathcal{D}} v(t_n + s)\, ds - \int_{-\tau}^{\tau} e^{\mp \mathrm{i}(\tau - s)\mathcal{D}} v(t_n)\, ds \right\|_{L^2} \leq C\tau^3$$

for some constant C that only depends on $\|\partial_t v\|_{H^2}$ and $\|\partial_{tt} v\|_{L^2}$.

Proof. Since v is twice continuously differentiable, Taylor's theorem yields

$$v(t_n + s) = v(t_n) + s\partial_t v(t_n) + \int_0^s (s - r)\partial_{tt} v(t_n + r)\, dr, \qquad s \in \mathbb{R}.$$

Thus,

$$\int_{-\tau}^{\tau} e^{\mp \mathrm{i}(\tau - s)\mathcal{D}} v(t_n + s)\, ds = \int_{-\tau}^{\tau} e^{\mp \mathrm{i}(\tau - s)\mathcal{D}} v(t_n)\, ds + \mathcal{R}_1(v, t_n, \tau) + \mathcal{R}_2(v, t_n, \tau)$$

with the remainders

$$\begin{aligned} \mathcal{R}_1(v, t_n, \tau) &= \int_{-\tau}^{\tau} s e^{\mp \mathrm{i}(\tau - s)\mathcal{D}} \partial_t v(t_n)\, ds, \\ \mathcal{R}_2(v, t_n, \tau) &= \int_{-\tau}^{\tau} e^{\mp \mathrm{i}(\tau - s)\mathcal{D}} \int_0^s (s - r)\partial_{tt} v(t_n + r)\, dr\, ds. \end{aligned}$$

For $\mathcal{R}_2$, we can derive the bound

$$\begin{aligned} \|\mathcal{R}_2(v, t_n, \tau)\|_{L^2} &\leq \int_{-\tau}^{\tau} \left| \int_0^s s - r\, dr \right| ds \max_{r \in [-\tau, \tau]} \|\partial_{tt} v(t_n + r)\|_{L^2} \\ &= \frac{\tau^3}{3} \max_{r \in [-\tau, \tau]} \|\partial_{tt} v(t_n + r)\|_{L^2} \leq C\tau^3. \end{aligned} \tag{2.30}$$

We analyze the norm of $\mathcal{R}_1$ in Fourier space. Recall that application of $\mathcal{D}$ corresponds to multiplication with $\delta_\varepsilon(\xi)$ in Fourier space, cf. (2.11). This yields

$$\begin{aligned} \|\mathcal{R}_1(v, t_n, \tau)\|_{L^2}^2 &= \int_{\mathbb{R}^3} \left| \int_{-\tau}^{\tau} s e^{\mp \mathrm{i}(\tau - s)\delta_\varepsilon(\xi)}\, ds \right|^2 \left| \widehat{\partial_t v(t_n)}(\xi) \right|^2 d\xi \\ &= \int_{\mathbb{R}^3} \left| \int_{-\tau}^{\tau} s e^{\pm \mathrm{i} s \delta_\varepsilon(\xi)}\, ds \right|^2 \left| \widehat{\partial_t v(t_n)}(\xi) \right|^2 d\xi, \end{aligned}$$

where $\widehat{\partial_t v(t_n)}$ is the Fourier transform of $\partial_t v(t_n)$. Using $e^{\pm \mathrm{i} s \delta_\varepsilon(\xi)} = 1 \pm \mathrm{i} s \delta_\varepsilon(\xi)\, p_1(\pm \mathrm{i} s \delta_\varepsilon(\xi))$ and $|p_1(\mathrm{i}x)| \leq 1 \, \forall\, x \in \mathbb{R}$, we have

$$\begin{aligned} \left| \int_{-\tau}^{\tau} s e^{\pm \mathrm{i} s \delta_\varepsilon(\xi)}\, ds \right| &\leq \left| \int_{-\tau}^{\tau} s\, ds \right| + \left| \int_{-\tau}^{\tau} s^2 \delta_\varepsilon(\xi) p_1(\pm \mathrm{i} s \delta_\varepsilon(\xi))\, ds \right| \\ &\leq 0 + \frac{2\tau^3}{3} |\delta_\varepsilon(\xi)| \leq \frac{\tau^3}{3} |\xi|^2, \end{aligned}$$

where we used the bound (2.11) on $\delta_\varepsilon(\xi)$ in the last step. Overall, we have

$$\begin{aligned}\|\mathcal{R}_1(v,t_n,\tau)\|_{H^m}^2 &\le \int_{\mathbb{R}^3}\left(\frac{\tau^3}{3}|\xi|^2\right)^2 \left|\widehat{\partial_t v(t_n)}(\xi)\right|^2 d\xi \\ &\le \left(\frac{\tau^3}{3}\right)^2 \|\partial_t v(t_n)\|_{H^2}^2 . \end{aligned} \tag{2.31}$$

Since $v \in \mathcal{S}_T$, the assertion follows from (2.30) and (2.31). □

After fixing v at the midpoint as in the previous lemma, the remaining integral can be computed as

$$\int_{-\tau}^{\tau} e^{\mp \mathrm{i}(\tau-s)\mathcal{D}} v(t_n)\, ds = 2\tau\, p_1(\mp 2\mathrm{i}\tau\mathcal{D}) v(t_n)$$

with p_1 from (2.24). Applying the lemma to the integrals $I_1^\pm$ and $I_2^\pm$ in (2.29) thus yields

$$\varphi_\pm(t_n+\tau) = e^{\mp 2\mathrm{i}\tau\mathcal{D}}\varphi_\pm(t_n-\tau) - \mathrm{i}\widehat{I}_1^\pm - \mathrm{i}\gamma_2\widehat{I}_2^\pm + \mathcal{O}\left(\tau^3\right)$$

with $\widehat{I}_1^\pm = \widehat{I}_1^\pm(\varphi_+(t_n),\varphi_-(t_n),t_n)$ and $\widehat{I}_2^\pm = \widehat{I}_2^\pm(\varphi_+(t_n),\varphi_-(t_n))$ given by

$$\widehat{I}_1^\pm = 2\tau p_1(\mp 2\mathrm{i}\tau\mathcal{D})\Pi^\pm\left[W(t_n)\varphi_\pm(t_n)\right], \tag{2.32}$$

$$\widehat{I}_2^\pm = 2\tau p_1(\mp 2\mathrm{i}\tau\mathcal{D})\Pi^\pm\left[\left(|\varphi_+(t_n)|^2 + |\varphi_-(t_n)|^2\right)\varphi_\pm(t_n)\right]. \tag{2.33}$$

Omitting the $\mathcal{O}(\tau^3)$-terms and replacing exact solutions with approximations $\varphi_\pm^n \approx \varphi_\pm(t_n)$ leads to the integrator

$$\varphi_\pm^{n+1} = \Phi_\tau^\pm\left(\varphi_+^n,\varphi_-^n,\varphi_+^{n-1},\varphi_-^{n-1},t_n\right), \qquad n\in\mathbb{N} \tag{2.34}$$

with the numerical flow

$$\begin{aligned}\Phi_\tau^\pm\left(\varphi_+^n,\varphi_-^n,\varphi_+^{n-1},\varphi_-^{n-1},t_n\right) = e^{\mp 2\mathrm{i}\tau\mathcal{D}}\varphi_\pm^{n-1} &- \mathrm{i}\widehat{I}_1^\pm(\varphi_+^n,\varphi_-^n,t_n) \\ &- \mathrm{i}\gamma_2\widehat{I}_2^\pm(\varphi_+^n,\varphi_-^n).\end{aligned} \tag{2.35}$$

For an efficient implementation, we can again combine the two integrals $\widehat{I}_1^\pm$ and $\gamma_2\widehat{I}_2^\pm$ to

$$\begin{aligned}\widehat{I}^\pm(\varphi_+^n,\varphi_-^n,t_n) &= \widehat{I}_1^\pm(\varphi_+^n,\varphi_-^n,t_n) + \gamma_2\widehat{I}_2^\pm(\varphi_+^n,\varphi_-^n) \\ &= 2\tau p_1\left(\mp 2\mathrm{i}\tau\mathcal{D}\right)\Pi^\pm\left[W(t_n)\varphi_\pm^n + \gamma_2\left(|\varphi_+^n|^2 + |\varphi_-^n|^2\right)\varphi_\pm^n\right].\end{aligned}$$

When using a Fourier pseudospectral method for space discretization on the torus, only one FFT per time step is required in the computation of $\widehat{I}^\pm$ before being able to apply the operators $p_1\left(\mp 2\mathrm{i}\tau\mathcal{D}\right)\Pi^\pm$. If the approximations obtained in the two previous steps are saved in physical as well as in Fourier space, only one inverse FFT is necessary for retransforming the result of (2.34)–(2.35) into physical space.

We call this method the *explicit exponential midpoint rule* (EEMR), because it can be regarded as the exponential counterpart of the classical explicit midpoint rule. Since (2.34)–(2.35) is a two-step method, the first approximation $\varphi_\pm^1 \approx \varphi_\pm(t_1)$ has to be computed with a starting step. Only an accuracy of $\mathcal{O}(\tau^2)$ is required for $\varphi_\pm^1$, and this can be achieved easily by using variation of constants over a time span of length τ as in the benchmark method and

then approximating the integrals via the rectangle rule. After omitting the $\mathcal{O}(\tau^2)$-terms and replacing $\varphi_\pm(t_1)$ with $\varphi_\pm^1$ we obtain

$$\varphi_\pm^1 = e^{\mp \mathrm{i}\tau\mathcal{D}}\varphi_\pm^0 - \mathrm{i}\tau e^{\mp \mathrm{i}\tau\mathcal{D}}\Pi^\pm\left[\left(W + \gamma_2\left(\left|\varphi_\pm^0\right|^2 + \left|\varphi_\pm^0\right|^2\right)\right)\varphi_\pm^0\right]. \tag{2.36}$$

To improve the accuracy of $\varphi_\pm^1$, one can replace (2.36) by $\eta \in \mathbb{N}$ such steps with step size τ/η.

Remark 2.7. *The idea to construct exponential multistep methods by applying variation of constants over the time-interval $[(n-\ell)\tau, (n+1)\tau]$ for some $\ell \geq 1$ has already been used in [CP06; Jah04; JM19], but the PDEs and the methods considered in these references are completely different. The exponential multistep methods reviewed in [HO10, Section 2.5] are of Adams type, which is different from what we propose here.*

Error analysis

Our goal is to prove that the EEMR (2.34)–(2.36) is indeed second-order convergent under the regularity assumptions (I)–(IV), which are also required for the benchmark method. For this purpose we reformulate the EEMR as a one-step method by introducing the vectors

$$u(t) = \begin{pmatrix} \varphi_+(t) \\ \varphi_-(t) \\ \varphi_+(t-\tau) \\ \varphi_-(t-\tau) \end{pmatrix}, \qquad u_n = \begin{pmatrix} \varphi_+^n \\ \varphi_-^n \\ \varphi_+^{n-1} \\ \varphi_-^{n-1} \end{pmatrix}, \qquad n \in \mathbb{N}.$$

We then have $u_{n+1} = \Phi_\tau(u_n, t_n)$ for $n \in \mathbb{N}$ with the numerical flow

$$\Phi_\tau(u_n, t_n) = \begin{pmatrix} \Phi_\tau^+(\varphi_+^n, \varphi_-^n, \varphi_+^{n-1}, \varphi_-^{n-1}, t_n) \\ \Phi_\tau^-(\varphi_+^n, \varphi_-^n, \varphi_+^{n-1}, \varphi_-^{n-1}, t_n) \\ \varphi_+^n \\ \varphi_-^n \end{pmatrix} \tag{2.37}$$

with $\Phi_\tau^\pm$ defined by (2.35). For vectors of the form $v = (v_1, ..., v_4)^T$ with four functions $v_1, ..., v_4 \in (L^2(\mathbb{R}^3))^4$, we define the norm

$$|||v|||_{L^2} = \sum_{j=1}^4 \|v_j\|_{L^2}$$

and analogously for the H^m-norm for some $m > 0$. The following bounds for the local error and the starting step are an immediate consequence of the construction of the EEMR.

Lemma 2.8. *(a) Local error: Under assumptions (I)–(IV) there is a constant C_{E_1} such that the inequality*

$$|||u(t_n + \tau) - \Phi_\tau(u(t_n), t_n)|||_{L^2} \leq C_{E_1}\tau^3 \tag{2.38}$$

holds for all $\tau > 0$ and all $n = 1, 2 \ldots, \lfloor T/\tau \rfloor$.

(b) Starting step: Let $\varphi_\pm^0 = \varphi_\pm(0)$ and let $\varphi_\pm^1$ be computed with the starting step (2.36). Under assumptions (I)–(IV) there is a constant C_{E_2} such that the inequality

$$|||u(t_1) - u_1|||_{L^2} \leq C_{E_2}\tau^2 \tag{2.39}$$

holds for some constant C_{E_2}.

Proof. By definition of u, Φ_τ and $|||\cdot|||_{L^2}$ we have

$$\begin{aligned}
&|||u(t_n+\tau) - \Phi_\tau(u(t_n),t_n)|||_{L^2} \\
&\quad = \left\|\varphi_+(t_n+\tau) - \Phi_\tau^+\left(\varphi_+(t_n),\varphi_-(t_n),\varphi_+(t_n-\tau),\varphi_-(t_n-\tau),t_n\right)\right\|_{L^2} \\
&\qquad + \left\|\varphi_-(t_n+\tau) - \Phi_\tau^-\left(\varphi_+(t_n),\varphi_-(t_n),\varphi_+(t_n-\tau),\varphi_-(t_n-\tau),t_n\right)\right\|_{L^2}.
\end{aligned}$$

Since all approximations made during the construction of the method are $\mathcal{O}(\tau^3)$, the bound (2.38) follows. In a similar way, the bound for

$$|||u(t_1) - u_1|||_{L^2} = \left\|\varphi_+(t_1) - \varphi_+^1\right\|_{L^2} + \left\|\varphi_-(t_1) - \varphi_-^1\right\|_{L^2} \tag{2.40}$$

can be shown with standard arguments. □

Next, we discuss stability. In order to simplify presentation, we will henceforth assume that the electromagnetic potential W does not depend on time. In this case, the semi-nonrelativistic limit system (2.14) is *autonomous*, and as a consequence the numerical flows $\Phi_\tau^\pm$ defined in (2.35) and Φ_τ defined in (2.37) do not depend on t, either. This allows us to omit the last variable in $\Phi_\tau^\pm$ and Φ_τ, which makes the following equations easier to read. We stress, however, that under Assumption (I)–(IV) the following proofs could be extended to a time-dependent W at the cost of a more involved notation.

Lemma 2.9. *Let $W(t) = W$ be constant in time. Let $v_\ell^\pm, w_\ell^\pm \in (H^2(\mathbb{R}^3))^4$ for $\ell \in \{0,1\}$ and set $v = (v_1^+, v_1^-, v_0^+, v_0^-)^T$ and $w = (w_1^+, w_1^-, w_0^+, w_0^-)^T$. Under assumptions (I)–(II) there is a constant C_S such that the stability estimate*

$$|||\Phi_\tau(v) - \Phi_\tau(w)|||_{L^2} \le (1 + C_S\tau)\,|||v - w|||_{L^2} \tag{2.41}$$

holds for all $\tau > 0$. The constant C_S depends on $\|V\|_{H^2}$, $\|A_j\|_{H^2}$, $j = 1,2,3$, $\left\|v_1^\pm\right\|_{H^2}$ and $\left\|w_1^\pm\right\|_{H^2}$, but not on τ.

Proof. It follows from (2.37) and (2.35) that

$$\begin{aligned}
&|||\Phi_\tau(v) - \Phi_\tau(w)|||_{L^2} \\
&\quad \le \left|\left|\left| \begin{pmatrix} e^{-2i\tau\mathcal{D}}\begin{pmatrix} v_0^+ - w_0^+ \\ v_0^- - w_0^- \end{pmatrix} \\ e^{+2i\tau\mathcal{D}}\begin{pmatrix} v_0^+ - w_0^+ \\ v_0^- - w_0^- \end{pmatrix} \\ v_1^+ - w_1^+ \\ v_1^- - w_1^- \end{pmatrix} \right|\right|\right|_{L^2} + \left|\left|\left| \begin{pmatrix} \widehat{I}_1^+(v_1^+,v_1^-) - \widehat{I}_1^+(w_1^+,w_1^-) \\ \widehat{I}_1^-(v_1^+,v_1^-) - \widehat{I}_1^-(w_1^+,w_1^-) \\ 0 \\ 0 \end{pmatrix} \right|\right|\right|_{L^2} \\
&\qquad + \left|\left|\left| \begin{pmatrix} \widehat{I}_2^+(v_1^+,v_1^-) - \widehat{I}_2^+(w_1^+,w_1^-) \\ \widehat{I}_2^-(v_1^+,v_1^-) - \widehat{I}_2^-(w_1^+,w_1^-) \\ 0 \\ 0 \end{pmatrix} \right|\right|\right|_{L^2}.
\end{aligned} \tag{2.42}$$

Since $e^{\mp 2i\tau\mathcal{D}}$ is an isometry in L^2, the first term on the right-hand side equals $|||v - w|||_{L^2}$. Now we insert the definition (2.32) of $\widehat{I}_1^\pm$ and use that $p_1(\mp 2i\tau\mathcal{D})$ and the projectors $\Pi^\pm$ are bounded operators in L^2. Applying the estimate (2.17) for the product with the potential W yields the inequality

$$\left\|\widehat{I}_1^\pm(v_1^+,v_1^-) - \widehat{I}_1^\pm(w_1^+,w_1^-)\right\|_{L^2} \le C\tau\left\|v_1^\pm - w_1^\pm\right\|_{L^2} \tag{2.43}$$

for some constant C which depends on $\|V\|_{H^2}$ and $\|A_j\|_{H^2}$, $j = 1, 2, 3$, but not on τ.

Now we will prove such a bound for the term $\widehat{I}_2^{\pm}$ containing the nonlinearity. The estimates (2.17) and (2.18) imply the inequality

$$\begin{aligned} &\left\| \left(\left|v_1^+\right|^2 + \left|v_1^-\right|^2 \right) v_1^{\pm} - \left(\left|w_1^+\right|^2 + \left|w_1^-\right|^2 \right) w_1^{\pm} \right\|_{L^2} \\ &\leq C \left(\left\|v_1^+ - w_1^+\right\|_{L^2} + \left\|v_1^- - w_1^-\right\|_{L^2} \right) \end{aligned} \tag{2.44}$$

with a constant C which depends on $\left\|v_1^{\pm}\right\|_{H^2}$ and $\left\|w_1^{\pm}\right\|_{H^2}$. Together with the arguments mentioned above, we obtain

$$\left\| \widehat{I}_2^{\pm}(v_1^+, v_1^-) - \widehat{I}_2^{\pm}(w_1^+, w_1^-) \right\|_{L^2} \leq C\tau \left(\left\|v_1^+ - w_1^+\right\|_{L^2} + \left\|v_1^- - w_1^-\right\|_{L^2} \right) \tag{2.45}$$

for some constant C which depends on $\left\|v_1^{\pm}\right\|_{H^2}$ and $\left\|w_1^{\pm}\right\|_{H^2}$. Combining (2.42), (2.43) and (2.45) proves the assertion. □

We are now in a position to prove second-order convergence for the EEMR.

Theorem 2.10 (Global error of the EEMR)**.** *Assume that assumptions (I) and (II) hold and that W does not depend on t. Let $\tau > 0$ be the step size and let $\varphi_{\pm}^n$ be the approximations obtained by (2.34) and (2.36) with step size τ and initial data $\varphi_{\pm}^0 = \varphi_{\pm}(0) = \Pi^{\pm}\left[\psi^{\text{init}}\right]$. Then, there are constants C and $\tau_0 > 0$ such that the global error bound*

$$\left\|\varphi_{\pm}^n - \varphi_{\pm}(t_n)\right\|_{L^2} \leq C\tau^2, \qquad n = 1, 2, ..., \lfloor T/\tau \rfloor$$

holds for all $\tau \in (0, \tau_0]$.

Remark 2.11. *Under the assumptions (I)–(IV) the theorem remains true for a time-dependent potential $W = W(t)$.*

Remark 2.12. *Under stronger regularity assumptions on the initial data and the potentials, one could of course obtain error bounds in higher-order Sobolev spaces. More precisely, to obtain an identical error bound in H^m, $m \geq 0$, one would require the initial data ψ^{init} and the potentials V, A_j to be in H^{m+4} with*

$$V, A_j \in C^1([0, T_0], H^{m+2}(\mathbb{R}^3)) \ \cap \ C^2([0, T_0], H^m(\mathbb{R}^3)), \quad j = 1, 2, 3.$$

Proof. Set $\Phi_\tau^0(v) = v$ and define $\Phi_\tau^n(v) = \Phi_\tau(\Phi_\tau^{n-1}(v))$ recursively for $n \in \mathbb{N}$, such that $\Phi_\tau^n(v)$ denotes the result of n steps of the EEMR in the one-step formulation with initial data v.

In order to prove the global error bound, we combine the local error bounds (2.38) and (2.39) with the stability estimate (2.41) in the classical construction known as Lady Windermere's fan. Using a telescopic sum, we have for $n = 1, 2, ..., \lfloor T/\tau \rfloor$

$$\begin{aligned} \left|\!\left|\!\left| u(t_n) - u_n \right|\!\right|\!\right|_{L^2} &= \left|\!\left|\!\left| \Phi_\tau^0(u(t_n)) - \Phi_\tau^{n-1}(u_1) \right|\!\right|\!\right|_{L^2} \\ &\leq \sum_{k=0}^{n-2} \left|\!\left|\!\left| \Phi_\tau^k(u(t_{n-k})) - \Phi_\tau^{k+1}(u(t_{n-k-1})) \right|\!\right|\!\right|_{L^2} \\ &\quad + \left|\!\left|\!\left| \Phi_\tau^{n-1}(u(t_1)) - \Phi_\tau^{n-1}(u_1) \right|\!\right|\!\right|_{L^2}. \end{aligned} \tag{2.46}$$

At this point, we would like to control the term

$$\left|\!\left|\!\left|\Phi_\tau^k(u(t_{n-k})) - \Phi_\tau^{k+1}(u(t_{n-k-1}))\right|\!\right|\!\right|_{L^2} = \left|\!\left|\!\left|\Phi_\tau^k(u(t_{n-k})) - \Phi_\tau^k(\Phi_\tau(u(t_{n-k-1})))\right|\!\right|\!\right|_{L^2} \tag{2.47}$$

by applying the stability estimate (2.41) k times. A minor technical difficulty is the fact that the constant C_S in (2.41) depends on the H^2-norms of the two functions involved, which in our situation are $\Phi_\tau^j(u(t_{n-k}))$ and $\Phi_\tau^{j+1}(u(t_{n-k-1}))$, respectively, with $j = 0, \dots, k-1$. In order to obtain a corresponding bound for (2.47) with a constant which does not depend on n, k or τ, we need that there are constants τ_0 and C such that

$$\max_{\substack{j,\ell=0,\dots,\lfloor T/\tau\rfloor \\ j+\ell\le\lfloor T/\tau\rfloor}} \left|\!\left|\!\left|\Phi_\tau^j(u(t_\ell))\right|\!\right|\!\right|_{H^2} \le C \qquad \text{for all } \tau \in (0,\tau_0]. \tag{2.48}$$

This estimate states, roughly speaking, that for a sufficiently small step size the numerical approximations, starting from the exact solution at time t_ℓ, remain uniformly bounded in H^2 on the time interval $[0,T]$.

In order to prove (2.48), two auxiliary results are needed. Firstly, under the assumptions of Lemma 2.9, the inequality

$$\left|\!\left|\!\left|\Phi_\tau(v) - \Phi_\tau(w)\right|\!\right|\!\right|_{H^2} \le (1 + c_s\tau)\left|\!\left|\!\left|v - w\right|\!\right|\!\right|_{H^2} \tag{2.49}$$

holds for some constant c_s which depends on $|||v|||_{H^2}$ and $|||w|||_{H^2}$. Note that in contrast to (2.41), the H^2-norm is used on both sides of (2.49). The estimate can be shown by adjusting the proof of Lemma 2.9. Secondly, one has to prove that under the assumptions of Lemma 2.8, the local error bound

$$\left|\!\left|\!\left|u(t_n+\tau) - \Phi_\tau(u(t_n))\right|\!\right|\!\right|_{H^2} \le C_{E_3}\tau^2 \tag{2.50}$$

holds for some constant C_{E_3} and for all $\tau > 0$ and $n = 1, 2, ..., \lfloor T/\tau\rfloor$. In contrast to (2.38), the local error is measured in the H^2-norm instead of L^2, but the power of τ is only 2 instead of 3. The proof of (2.50) is straightforward. Having established (2.49) and (2.50), one can prove (2.48) by induction. Since the procedure is essentially the same as, e.g., in [Lub08] or [JMS17, Section 8], we omit this part.

Now we return to (2.46). Combining (2.48) with the stability estimate (2.41) yields under the condition $\tau \le \tau_0$ that

$$\begin{aligned}\left|\!\left|\!\left|u(t_n) - u_n\right|\!\right|\!\right|_{L^2} \le& \sum_{k=0}^{n-2}(1+C_\star\tau)^k \left|\!\left|\!\left|u(t_{n-k}) - \Phi_\tau(u(t_{n-k-1}))\right|\!\right|\!\right|_{L^2} \\ &+ (1+C_\star\tau)^{n-1}\left|\!\left|\!\left|u(t_1) - u_1\right|\!\right|\!\right|_{L^2}\end{aligned}$$

with a constant $C_\star$ which only depends on $\|V\|_{H^2}$, $\|A_j\|_{H^2}$, $j = 1, 2, 3$, and on C from (2.48). Applying the local error bound (2.38) as well as the bound (2.39) for the starting step and using that $(n-1)\tau = t_{n-1} \le T$ shows that

$$\begin{aligned}\left|\!\left|\!\left|u(t_n) - u_n\right|\!\right|\!\right|_{L^2} \le& \sum_{k=0}^{n-2}\left(1+\frac{C_\star t_n}{n}\right)^k C_{E_1}\tau^3 + \left(1+\frac{C_\star t_n}{n}\right)^{n-1} C_{E_2}\tau^2 \\ \le& \sum_{k=0}^{n-2} e^{C_\star t_n} C_{E_1}\tau^3 + e^{C_\star t_n} C_{E_2}\tau^2 \le e^{C_\star t_n}\left(t_n C_{E_1}\tau^2 + C_{E_2}\tau^2\right) \\ \le& (T+1)e^{C_\star T} C_E \tau^2\end{aligned}$$

with $C_E = \max\{C_{E_1}, C_{E_2}\}$. This implies that $|||u(t_n) - u_n|||_{L^2} = \mathcal{O}(\tau^2)$ for all $n \ge 1$ and thus $\|\varphi_\pm(t_n) - \varphi_\pm^n\|_{L^2} = \mathcal{O}(\tau^2)$. □

The EEMR for the semi-nonrelativistic limit system is thus indeed second-order accurate. Both the solution and the numerical approximation still depend on ε (see the remark at the beginning of this section), but all bounds are uniform in ε.

2.4 Numerical experiments

In this section, we present numerical results to illustrate our error analysis, and to compare the efficiency of the EEMR and the benchmark method. For simplicity, we conduct our experiments in one space dimension, where the NLDE can be reduced to the system

$$\partial_t \psi^\varepsilon(t,x) = -\frac{\mathrm{i}}{\varepsilon^2}\widetilde{\mathcal{T}}\psi^\varepsilon(t,x) - \mathrm{i}\widetilde{W}(t,x)\psi^\varepsilon(t,x) - \mathrm{i}\widetilde{F}(\psi^\varepsilon)\psi^\varepsilon(t,x),$$

$t > 0$, $x \in \mathbb{R}$, for a two-component solution $\psi^\varepsilon(t,x) \in \mathbb{C}^2$ with initial data $\psi^\varepsilon(0,x) = \widetilde{\psi}^0(x) \in \mathbb{C}^2$ (see e.g. [Bao+16b]). Here, the differential operator $\widetilde{\mathcal{T}}$, the potential $\widetilde{W}$ and the nonlinearity $\widetilde{F}$ are given by

$$\widetilde{\mathcal{T}} = -\mathrm{i}\varepsilon\sigma_1\partial_x + \sigma_3, \qquad \widetilde{W}(t,x) = V(t,x)I_2 - A_1(t,x)\sigma_1, \qquad \widetilde{F}(v) = \gamma_2 |v|^2 I_2.$$

For simplicity, we omit the $\widetilde{\ }$ in the following, and we chose $\gamma_2 = 1$. The properties of the semi-nonrelativistic limit system, the construction of the numerical methods presented above as well as the obtained error results can be formulated for this reduced system in exactly the same manner.

As is common practice [Alv92; Bao+16b; BCY21; HL06], we truncate the whole space problem to a bounded interval $\Omega = [a,b]$ which is large enough such that the truncation error is negligible. We impose periodic boundary conditions and discretize Ω through the grid points $x_j = (a+b)/2 + jh$, $j = -M, ..., M-1$ with mesh size $h = (b-a)/2M$ for some $M \in \mathbb{N}$. All spatial derivatives are then computed by Fourier pseudospectral techniques. For our experiments, we utilize $2M = 256$ grid points in space. We use the data from [Bao+16b; CW22], i.e. we choose the interval $\Omega = [-16, 16]$, the initial data

$$\psi_1^{\mathrm{init}}(x) = e^{-x^2/2}, \qquad \psi_2^{\mathrm{init}}(x) = e^{-(x-1)^2/2}, \qquad x \in \Omega$$

and the (time-independent) potential functions

$$V(t,x) = \frac{1-x}{1+x^2}, \qquad A_1(t,x) = \frac{(x+1)^2}{1+x^2}, \qquad x \in \Omega, \quad t \geq 0.$$

For all following error plots, we compute approximations to solutions at time $T = 1$ using the presented methods, and compare them to reference solutions computed via MATLAB's `ode45` routine using the same spatial grid and very small tolerances. The error is always computed in the L^2-norm, approximated by $\|v\|_{L^2}^2 \approx \sum_{k=-M}^{M-1} |\widehat{v}_k|^2$ for a scalar periodic function $v \in L_2(\Omega)$ and $\|v\|_{L^2} = \sqrt{\|v^+\|_{L^2}^2 + \|v^-\|_{L^2}^2}$ for a vector $v = (v^+, v^-)$ of two scalar periodic functions $v^\pm \in L_2(\Omega)$.

Performing various numerical experiments, we have observed that an even number of time steps gives slightly better results for the two-step method. Therefore, in all following plots, the step sizes are chosen such that the number of time steps T/τ is even. The quality of approximations after many time steps can be further improved by a very good approximation to the solution at time t_1. In the experiments below, we always use $\eta = 3$ substeps in the starting step (2.36) to obtain an approximation at time t_1. Increasing η further did not improve the results significantly.

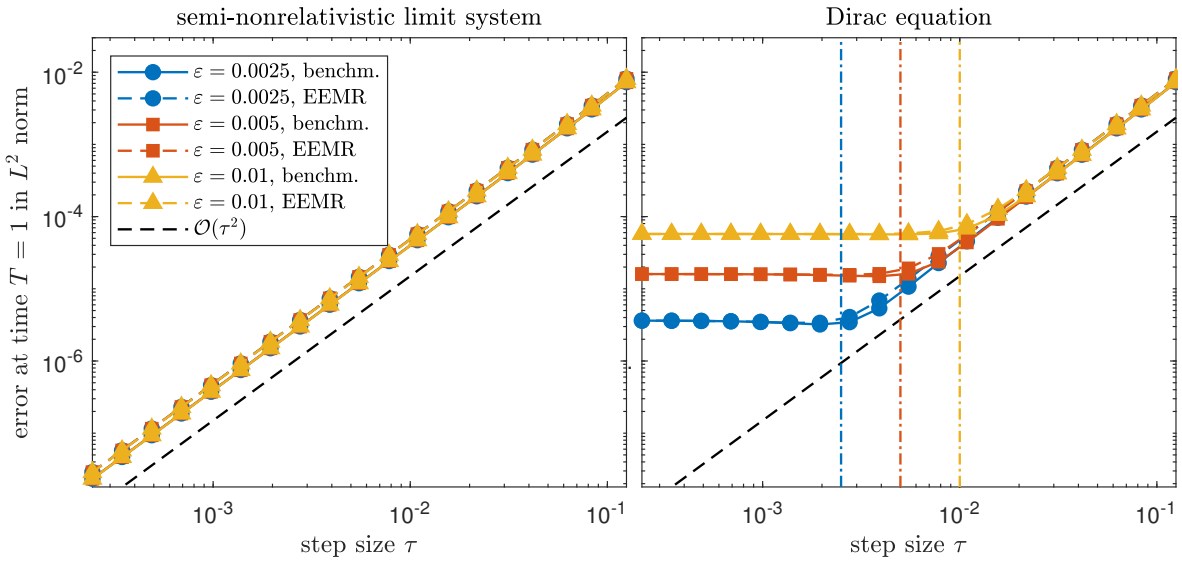

Figure 2.1: Global error of the numerical methods presented in Section 2.3 at time $T = 1$. *Left:* In comparison to a reference solution $\varphi_\pm$ of the semi-nonrelativistic limit system (2.16). *Right:* In comparison to a reference solution ψ^ε of the NLDE (2.3).

Accuracy. Figure 2.1 shows the global error of both methods in dependency of the step size τ in logarithmic axes. On the left-hand side, the approximations obtained by both methods are compared to a reference solution $\varphi_\pm$ of the semi-nonrelativistic limit system (2.16). The solid lines represent the benchmark method, the colored dashed lines the EEMR. Different values of ε are depicted through different colors, but the six lines coincide almost. The results confirm that both methods are second-order accurate in the step size τ, and that the error constants do not depend on ε. For a fixed step size τ, both methods yield approximations of nearly the same accuracy in this example. On the right-hand side of Figure 2.1, the approximations are compared to a reference solution of the NLDE (2.3). Here the numerical approximations $\varphi_\pm^n$ are interpreted as approximations to a solution $\phi_\pm$ of the transformed Dirac equation (2.8). Then, according to (2.10) the function

$$\psi^n := e^{-\mathrm{i}t_n/\varepsilon^2}\varphi_+^n + e^{\mathrm{i}t_n/\varepsilon^2}\varphi_-^n, \qquad n \geq 1,$$

approximates a solution of the original problem (2.3). Since

$$\begin{aligned}\|\psi^n - \psi(t_n)\|_{L^2} &= \left\| e^{-\mathrm{i}t_n/\varepsilon^2}\left(\varphi_+^n - \phi_+(t_n)\right) + e^{\mathrm{i}t_n/\varepsilon^2}\left(\varphi_-^n - \phi_-(t_n)\right)\right\|_{L^2} \\ &\leq \|\varphi_+^n - \phi_+(t_n)\|_{L^2} + \|\varphi_-^n - \phi_-(t_n)\|_{L^2},\end{aligned}$$

the overall error is composed of two parts:

- the approximation error of the numerical methods in comparison to the exact solution of the semi-nonrelativistic limit system, which is of order $\mathcal{O}(\tau^2)$,
- the difference between solutions of the semi-nonrelativistic limit system and the transformed NLDE, which, for a fixed time T, is of order $\mathcal{O}(\varepsilon^2)$.

The overall approximation error is thus of order $\mathcal{O}(\tau^2) + \mathcal{O}(\varepsilon^2)$. Consequently, the $\mathcal{O}(\tau^2)$-terms are dominating for large step sizes $\tau > \varepsilon$, and we observe second-order convergence w.r.t. τ until $\tau = \varepsilon$ (this value is indicated by the vertical dashed-dotted lines). For $\tau < \varepsilon$ however, the $\mathcal{O}(\varepsilon^2)$-terms are dominating, and no further convergence is achieved when the

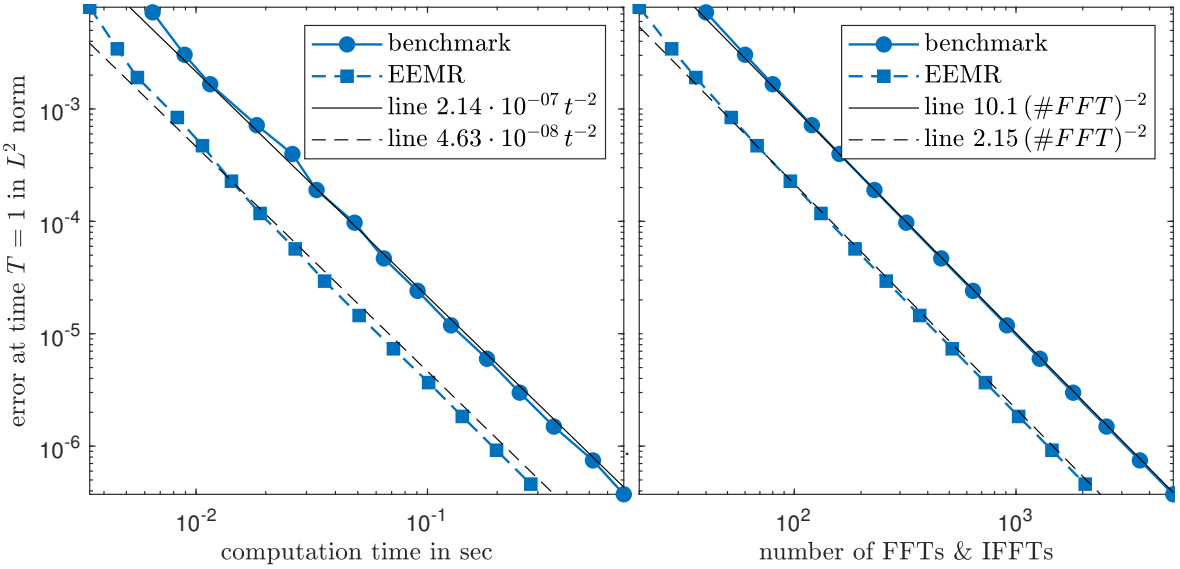

Figure 2.2: Global error of the numerical methods presented in Section 2.3 at time $T = 1$ for $\varepsilon = 0.01$. *Left:* Error over computation time. *Right:* Error over number of required Fourier and inverse Fourier transforms.

step size τ is reduced. Thus, applying the two methods to the semi-nonrelativistic limit system allows us to compute very accurate approximations to the highly oscillatory solution of the original NLDE in the nonrelativistic regime, where ε is very small.

Efficiency. Whilst the experiments above suggest that both methods perform equally well, they do not take into account the computational effort required for one time step in each method. In the EEMR, we have symmetry of the integration interval of the integrals $I_1^{\pm}$ and $I_2^{\pm}$ in the variation of constants formula. This is why the required accuracy was achieved by essentially only keeping the constant term of the Taylor expansions of the integrands. In contrast to that, in the benchmark method, the linear terms of such Taylor expansions had to be taken into account as well. Those terms include several pointwise multiplications of space-dependent functions (with the potential W or with the functions $\varphi_{\pm}$ itself) as well as applications of the projectors $\Pi^{\pm}$. Whilst the former has to be done in physical space, the latter can only be done in Fourier space. Consequently, computing those linear terms requires additional (inverse) Fourier transforms, which are the dominating operations in computational costs; cf. Remark 2.5. One time step of the benchmark method is thus significantly more expensive than of the EEMR. In an efficient implementation, one time step of the EEMR can be done using one Fourier and one inverse Fourier transform (where we count one transformation of a function $v = (v^+, v^-)^T$, $v^{\pm} \in (L^2(\Omega))^2$, into or out of Fourier space as one transform). One time step of the benchmark method, however, requires three Fourier and two inverse Fourier transforms. Hence, the computational cost of a time step of the benchmark method is about $\frac{5}{2}$ times larger than one of the EEMR.

Figure 2.2 shows the results of numerical experiments comparing the efficiency of both methods. For the plot on the left-hand side, both methods have been applied using different step sizes and their computation time has been measured. To lower the impact of background processes, the average of multiple runs is taken, and the different step sizes are used in random order. For each method, a reference line has been added that fits best to the measurement points. Comparing the constants of those lines, one can see that for a given computation time,

the error of the benchmark method is about 4.6 times larger than the error of the EEMR, despite the fact that for this specific data, the EEMR performs a little worse for a fixed time step size than the benchmark method. On the right-hand side, the number of Fourier and inverse Fourier transforms is counted. Again, for a fixed number of Fourier transforms, the error of the benchmark method is about 4.7 times larger than the error of the EEMR.

If the error is measured in the discrete H^1-norm instead (cf. Remark 2.12), then the accuracy of both methods for a fixed time step is almost indistinguishable for this model problem (data not shown). For a fixed computation time, the error of the benchmark method in the discrete H^1-norm is six times larger than the error of EEMR (data not shown).

The reason for the observed factors is the following. Let $w_j(N_j)$ be the numerical work (measured in runtime or in number of FFTs) required for N_j steps with the benchmark method ($j = 1$) or the EEMR ($j = 2$), respectively. For a given N we have $w_1(N) \approx \frac{5}{2}cN$ and $w_2(N) \approx cN$ with some constant $c > 0$. If we fix the numerical work $w > 0$ we can thus perform $N_1 \approx \frac{2w}{5c}$ steps with the benchmark method and $N_2 \approx \frac{w}{c}$ with the EEMR. According to Figure 2.1 the error $err_j(N_j)$ of both methods is $err_j(N_j) \approx C_j N_j^{-2}$ with some error constant C_j. Hence, the errors for a fixed numerical work w are

$$err_1(N_1) \approx C_1 \left(\frac{5c}{2w}\right)^2 \qquad \text{and} \qquad err_2(N_2) \approx C_2 \left(\frac{c}{w}\right)^2.$$

This implies that $err_1(N_1) \approx \frac{C_1}{C_2}\frac{25}{4} err_2(N_2)$. For the error in the L^2-norm, the ratio $\frac{C_1}{C_2} \approx 0.8$ can be calculated from Figure 2.1, which yields $err_1(N_1) \approx 5 err_2(N_2)$. For the error in H^1, we have that $\frac{C_1}{C_2} \approx 1$, which yields $err_1(N_1) \approx 6.25 err_2(N_2)$. Although the values 5 and 6.25 are a bit larger than the observed factors 4.7 and 6, they predict approximately the improvement obtained with EEMR.

Chapter 3

Employing nonresonant step sizes for time integration of highly oscillatory nonlinear Dirac equations

This chapter is based on the preprint [JK24], which was written in collaboration with Tobias Jahnke and has since been accepted for publication in the IMA Journal of Numerical Analysis (IMAJNA). The present version contains minor revisions to the preprint that were made during the review process.

In contrast to the rest of this work and to other literature on the Dirac equation, in this chapter the projectors onto the eigenspaces are defined by $\Pi^\varepsilon_{\mp 1} = \frac{1}{2}\left(\mathrm{Id} \pm \Lambda_\varepsilon^{-1}\mathcal{T}_\varepsilon\right)$ instead of (1.12). In particular, the role of "+" and "−" is interchanged in the notation, and to avoid confusion with exponents, the indices ∓ 1 are attached below. Similarly, the transformed eigenspace components $\phi^\varepsilon_\pm$ of a solution of the NLDE are now referred to as $\phi^\varepsilon_{\mp 1}$. This change in notation will allow a compact representation of otherwise complicated expressions in Section 3.2.3 and thereafter. Furthermore, the functions p_1 and p_2 from (2.24) are from now on called by their common names φ_1 and φ_2. This was not done previously to avoid confusion with the solution $\varphi^\varepsilon_\pm$ of the semi-nonrelativistic limit system, which will no longer play a role in the following chapters.

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Abstract: In the nonrelativistic limit regime, nonlinear Dirac equations involve a small parameter $\varepsilon > 0$ which induces rapid temporal oscillations with frequency proportional to ε^{-2}. Efficient time integrators are challenging to construct, since their accuracy has to be independent of ε or improve with smaller values of ε. Yongyong Cai and Yan Wang have presented a nested Picard iterative integrator (NPI-2), which is a uniformly accurate second-order scheme. We propose a novel method called the *nonresonant nested Picard iterative integrator (NRNPI)*, which takes advantage of cancellation effects in the global error to significantly simplify the NPI-2. We prove that for nonresonant step sizes $\tau \geq \frac{\pi}{4}\varepsilon^2$, the NRNPI has the same accuracy as the NPI-2 and is thus more efficient. Moreover, we show that for arbitrary $\tau < \frac{\pi}{4}\varepsilon^2$ the error decreases proportionally to $\varepsilon^2\tau$. We provide numerical experiments to illustrate the error behavior as well as the efficiency gain.

3.1 Introduction

One of the most important partial differential equations (PDE) in particle physics are the Dirac equations, which represents a well-established model for relativistic dynamics of electrons, protons, neutrons, and other spin-1/2 particles in an external electromagnetic field [Dir28; Tha92]. In order to include effects related to self-interaction of particles and other phenomena, nonlinear versions have been introduced in [HC09; Mer+10; Sol70; Thi58]. After a proper nondimensionalization, nonlinear Dirac equations involve a parameter $\varepsilon > 0$ inversely proportional to the speed of light; cf. [Bao+16b]. In the nonrelativistic limit regime, this parameter is very small, and solutions exhibit rapid oscillations in time with frequency proportional to ε^{-2}. In this situation, traditional time integrators require a tiny step size $\tau \sim \varepsilon^{-2}$ and thus a huge number of time steps to produce an acceptable accuracy; see [Bao+16b] for details.

The construction of numerical methods with a better convergence behavior is a major challenge. Several attempts have been made in this direction. If an accuracy of $\mathcal{O}(\varepsilon^2)$ is sufficient, then one can solve the semi-nonrelativistic limit system, which is a non-oscillatory problem and enables the approximation of solutions of nonlinear Dirac equations with said accuracy [CW20]. For this purpose, the *explicit exponential midpoint rule* was proposed in [JK23], which is a second-order integrator and consequently yields a total accuracy of $\mathcal{O}(\varepsilon^2 + \tau^2)$. For very small step sizes $\tau < \varepsilon^2$, better accuracies can be achieved with the *multiscale time integrator pseudospectral method* from [CW18], which has an error of $\mathcal{O}(\min\{\tau^2 + \varepsilon^2, \tau^2/\varepsilon^2\})$. This implies that the method is uniformly accurate with order one, i.e. that the error can be bounded by $C\tau$ with a constant C that does not depend on ε. Splitting methods for nonlinear Dirac equations in the nonrelativistic limit regime were analyzed in [BCY21]. Although such methods usually suffer from a severe order reduction when applied to highly oscillatory problems, it was shown that using special nonresonant step sizes yields convergence of the Lie-Trotter splitting with the full order 1 and of the Strang splitting with order 3/2 independently of ε. However, the analysis in [BCY21] is based on the assumption that there is no magnetic field.

Two second-order uniformly accurate methods were proposed in [LMZ17] and [CW22]. The authors of [LMZ17] devised an approach which allows them to replace the highly oscillatory Dirac equations by a non-oscillatory augmented problem. The price to pay is that the augmented problem has one additional dimension, which originates from the separation of the fast and slow timescales. In [CW22], uniformly accurate *nested Picard iterative integrators (NPI)* of first and second order were constructed. This is done by iterating Duhamel's formula, approximating the slowly varying parts of the integrands, but integrating all highly oscillatory phases exactly. However, the fact that the solution has to be expanded in a suitable way and appears three times in the nonlinearity has the consequence that the number of terms in the numerical flow of the first-order scheme (NPI-1) is already rather large (cf. Section 2.2 in [CW22]). For the second-order method (NPI-2), where Duhamel's formula has to be used twice, the ansatz leads to a plethora of complicated terms (cf. Section 2.3 in [CW22]). This makes the implementation and debugging of the integrator quite difficult and causes considerable numerical costs per time step.

In this work we construct and analyze a new method called the *nonresonant nested Picard iterative integrator (NRNPI)*. This method is a modification of the NPI-2, but contains only a small portion of the terms in its numerical flow. In spite of this simplification, our integrator has essentially the same accuracy as the NPI-2 if the step size is not extremely small and is chosen in such a way that resonances in the error accumulation are avoided. The construc-

tion is carried out for the transformed form of the nonlinear Dirac equations introduced in [CW20]. We consider two different representations of this PDE and show how to use them to reformulate the NPI-2 scheme for the transformed problem in a very compact and structured way. This reformulation is crucial, because it allows us to identify all terms in the numerical flow which are of $\mathcal{O}(\tau^2)$ and contain a factor of the type $\mathrm{e}^{\mathrm{i}qt_n/\varepsilon^2}$ for some $q \neq 0$, where $n \in \mathbb{N}$ and $t_n = n\tau$ are the time points where the solution is approximated. Then, we obtain the new NRNPI by simply omitting all these terms. In contrast to the NPI-2, the local error of the NRNPI is clearly not of $\mathcal{O}(\tau^3)$ anymore, such that second-order convergence in the classical sense cannot be expected. Nevertheless, we prove that the NRNPI behaves like a second-order method for step sizes which are moderately small ($\tau \geq \pi\varepsilon^2/4$) and not close to certain resonant values. The reason is that for such choices of τ the omitted terms do not sum up critically in the error accumulation due to the exponential factor $\mathrm{e}^{\mathrm{i}qt_n/\varepsilon^2}$. A similar yet different technique has been used in [BCY21; Buc+18; GH06; HL99; JM19; JL03]. The fact that the NRNPI achieves the same accuracy as the NPI-2 with a significantly smaller number of terms improves the efficiency and facilitates implementation and debugging. We remark that choosing a nonresonant step size is easy, because both the resonant and the optimal step sizes are known *a priori*. For very small step sizes $\tau < \frac{\pi}{4}\varepsilon^2$, we prove that the NRNPI has an error of $\mathcal{O}(\varepsilon^2\tau)$. In this range, the error of the second-order NPI-2 is smaller, but this is only relevant if an extremely small error of $\mathcal{O}(\varepsilon^4)$ or less is required.

The paper is structured as follows. In Section 2 we introduce the nonlinear Dirac equations in the nonrelativistic limit regime. We recall the transformation of variables from [CW20] and present the two different representations of the resulting PDEs. With these representations, we formulate the NPI-2 in the transformed variables and derive the NRNPI in Section 3.3. In Section 3.4, we present a rigorous error analysis for the NRNPI. Our main results are the global error bounds in Theorem 3.12 and Corollary 3.14. In particular, we show why there is no significant error accumulation for nonresonant step sizes due to cancellation effects. To keep the focus on the essentials, the proofs of a number of auxiliary results are postponed to Section 3.6. In Section 3.5, we present several numerical experiments which corroborate our error analysis and reveal certain interesting effects, which we discuss briefly. Finally, we test the efficiency gain achieved with NRNPI.

3.2 Problem setting

3.2.1 Nonlinear Dirac equations in the nonrelativistic limit regime

The nonlinear Dirac equations (NLDE)

$$\partial_t \psi^\varepsilon = -\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi^\varepsilon - \mathrm{i}W\psi^\varepsilon - \mathrm{i}F(\psi^\varepsilon)\psi^\varepsilon, \qquad x \in \mathbb{R}^3, \quad t > 0, \tag{3.1}$$

with initial data $\psi^\varepsilon(0,x) = \psi^{\mathrm{init}}(x)$ describe the evolution of a complex-valued vector wave function $\psi^\varepsilon = \psi^\varepsilon(t,x) \in \mathbb{C}^4$. The solution ψ^ε depends on the value of a parameter $\varepsilon \in (0,1)$. In the nonrelativistic limit regime, this parameter is very small as it is inversely proportional to the speed of light. The operator $\mathcal{T}_\varepsilon$ and the function $W = W(t,x)$ are the free Dirac operator and the electromagnetic potential, respectively. They are given by

$$\mathcal{T}_\varepsilon = -\mathrm{i}\sum_{j=1}^{3} \varepsilon\alpha_j\partial_j + \beta, \qquad W(t,x) = V(t,x)I_4 - \sum_{j=1}^{3} A_j(t,x)\alpha_j. \tag{3.2}$$

where $V(t,x) \in \mathbb{R}$ is the electric scalar potential and $A(t,x) = (A_1(t,x), ..., A_3(t,x))^T$ is the magnetic vector potential. The matrices

$$\beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \qquad \alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \qquad j = 1,2,3,$$

are the Dirac matrices, which are determined by the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Further, F is a nonlinearity of the form $F(u) = \gamma_1(u^*\beta u)\beta + \gamma_2 |u|^2 I_4$ for $\gamma_1, \gamma_2 \in \mathbb{R}$. Here, $u^* = \overline{u}^T$ denotes the conjugate transpose and $|u| = \sqrt{u^*u}$ the Euclidean norm of a vector u, respectively. This type of nonlinearity is motivated by numerous applications in physics and models self-interaction of Dirac fermions; see, e.g., [HC09; Mer+10; Sol70; Thi58] and the references in [Bao+16b; BCY21; CW18; CW22; LMZ17]. In the rest of this paper, we limit ourselves to the second type of nonlinearity, i.e. $\gamma_1 = 0$. However, analogous results could be obtained for the case $\gamma_1 \neq 0$. With no loss of generality, we set $\gamma_2 = 1$.

The kinetic part $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon\psi^\varepsilon$ of (3.1) causes oscillations in time with frequency of $\mathcal{O}(\varepsilon^{-2})$. As a consequence, classical numerical schemes can only be expected to converge if the step size is significantly smaller than ε^2, which results in prohibitive numerical costs.

3.2.2 Function spaces and assumptions

Throughout, the Fourier transform of $u \in L^2(\mathbb{R}^3)$ or $u \in \left(L^2(\mathbb{R}^3)\right)^4$ and the inverse transform are defined by

$$\widehat{u}(\xi) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}x\cdot\xi} u(x)\,\mathrm{d}x \qquad \text{and} \qquad u(x) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \mathrm{e}^{\mathrm{i}x\cdot\xi} \widehat{u}(\xi)\,\mathrm{d}\xi,$$

respectively. For $m \geq 0$ we equip the Sobolev spaces $H^m(\mathbb{R}^3)$ and $\left(H^m(\mathbb{R}^3)\right)^4$ with the norm

$$\|u\|_{H^m} = \left(\int_{\mathbb{R}^3} \left(1 + |\xi|_2^2\right)^m |\widehat{u}(\xi)|_2^2 \,\mathrm{d}\xi \right)^{1/2}.$$

Since we will later decompose a solution of (3.1) into two components, we further define the space

$$\mathbf{H^m} = \left(H^m(\mathbb{R}^3)\right)^4 \times \left(H^m(\mathbb{R}^3)\right)^4$$

for tuples $u = (u_{-1}, u_{+1})$ of two functions $u_{-1}, u_{+1} \in \left(H^m(\mathbb{R}^3)\right)^4$, and equip it with the norm

$$|||u|||_{\mathbf{H^m}} = \|u_{-1}\|_{H^m} + \|u_{+1}\|_{H^m}.$$

In the special case $m = 0$ we have $\mathbf{H^0} = \left(L^2(\mathbb{R}^3)\right)^4 \times \left(L^2(\mathbb{R}^3)\right)^4$, and we write $\mathbf{L^2}$ instead of $\mathbf{H^0}$ for clarity. Finally, we define $\mathbf{B^m}(R) = \{u \in \mathbf{H^m} : |||u|||_{\mathbf{H^m}} \leq R\}$ to be the closed ball of radius R in $\mathbf{H^m}$.

Having established the necessary notation, we collect some important Sobolev inequalities that we will use frequently. There is a constant $C_S > 0$ such that

$$\|uv\|_{H^2} \leq C_S \|u\|_{H^2} \|v\|_{H^2}, \qquad u \in H^2(\mathbb{R}^3),\ v \in H^2(\mathbb{R}^3), \tag{3.3}$$

$$\|uv\|_{L^2} \leq C_S \|u\|_{L^2} \|v\|_{H^2}, \qquad u \in L^2(\mathbb{R}^3),\ v \in H^2(\mathbb{R}^3). \tag{3.4}$$

In both cases, one of the functions may also be $\mathbb{C}^4$-valued. The first inequality (3.3) is the classical bilinear estimate in a Banach algebra; cf. Theorem 4.39 in [AF03]. The second inequality (3.4) follows from the Sobolev embedding $H^2(\mathbb{R}^3) \subset L^\infty(\mathbb{R}^3)$ via $\|uv\|_{L^2} \leq \|u\|_{L^2} \|v\|_{L^\infty} \leq C_S \|u\|_{L^2} \|v\|_{H^2}$; cf. Theorem 4.12 in [AF03]. The counterparts of (3.3) and (3.4) for two vector-valued functions read

$$\|u^* v\|_{H^2} \leq C_S \|u\|_{H^2} \|v\|_{H^2}, \qquad u \in \left(H^2(\mathbb{R}^3)\right)^4,\ v \in \left(H^2(\mathbb{R}^3)\right)^4, \tag{3.5}$$

$$\|u^* v\|_{L^2} \leq C_S \|u\|_{L^2} \|v\|_{H^2}, \qquad u \in \left(L^2(\mathbb{R}^3)\right)^4,\ v \in \left(H^2(\mathbb{R}^3)\right)^4. \tag{3.6}$$

The following assumptions regarding regularity of the initial data and the potential W (determined by V and A_j via (3.2)) are crucial in the construction of our methods and will thus be made henceforth.

Assumption 3.1. *Let $0 < T < \infty$ be an arbitrary fixed time. We assume that*

$$\text{(A)} \qquad V, A_j \in L^\infty([0,T], H^2(\mathbb{R}^3))$$

and that there is a constant $M_{\mathrm{ex}} > 0$ independent of ε such that for the exact solution ψ^ε of (3.1), we have

$$\text{(B)} \qquad \sup_{\varepsilon \in (0,1)} \sup_{t \in [0,T]} \|\psi^\varepsilon(t,\cdot)\|_{H^4} \leq M_{\mathrm{ex}}.$$

We remark that assumption (B) is always fulfilled for some $T > 0$ if the potential and the initial data are sufficiently regular, in particular if $V, A_j \in L^\infty([0,\widetilde{T}], H^4(\mathbb{R}^3))$ for some $\widetilde{T} > T$ and if $\psi^{\mathrm{init}} \in H^4(\mathbb{R}^3)$, see [CW20, Theorem 2.1].

Assumption (A) together with the inequalities (3.3)–(3.6) yields the existence of some constant $C_W > 0$ such that for all $t \in [0,T]$, we have

$$\begin{aligned} \|W(t,\cdot)u\|_{L^2} &\leq C_W \|u\|_{L^2}, \quad u \in \left(L^2(\mathbb{R}^3)\right)^4, \\ \|W(t,\cdot)u\|_{H^2} &\leq C_W \|u\|_{H^2}, \quad u \in \left(H^2(\mathbb{R}^3)\right)^4. \end{aligned} \tag{3.7}$$

3.2.3 Transformed Dirac equations

Whilst the uniform boundedness of solutions in (B) is a reasonable assumption, the time derivative of a solution is in general unbounded w.r.t. ε due to the term $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi^\varepsilon$ on the right-hand side of (3.1). In this subsection, we introduce a transformation of variables proposed in [CW20] and state the PDEs for the new variables. These PDEs have the advantage that for sufficiently smooth solutions, the right-hand side is uniformly bounded in ε, which is favorable for numerical approximation. A key step in the systematic formulation of the methods in Section 3.3 will be to write those PDEs in an appropriate representation. In fact, it will later turn out that two different representations of the PDEs are useful as each of them has its individual advantages.

The transformation of variables used in [CW20] is based on the decomposition

$$\mathcal{T}_\varepsilon = \Lambda_\varepsilon \Pi^\varepsilon_{-1} - \Lambda_\varepsilon \Pi^\varepsilon_{+1} \tag{3.8}$$

with the scalar operator Λ_ε and the two projection operators $\Pi^\varepsilon_{\mp 1}$ given by

$$\Lambda_\varepsilon = \sqrt{\mathrm{Id} - \varepsilon^2 \Delta}, \qquad \Pi^\varepsilon_{\mp 1} = \frac{1}{2}\left(\mathrm{Id} \pm (\mathrm{Id} - \varepsilon^2\Delta)^{-\frac{1}{2}} \mathcal{T}_\varepsilon\right).$$

Here and below, Id denotes the identity operator. These pseudo-differential operators are defined in Fourier space, for example

$$\Lambda_\varepsilon u(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}x\cdot\xi} \sqrt{1 + \varepsilon^2 |\xi|_2^2}\, \widehat{u}(\xi) \mathrm{d}\xi,$$

and similar for $\Pi^\varepsilon_{\mp 1}$. The decomposition (3.8) is obtained by performing an eigenspace decomposition in Fourier space, see [BMP98, Eq. (1.22)] and [CW20, Section 2]. It was shown in [BMP98] that for any $m \geq 0$ the operators

$$\Pi^\varepsilon_{\mp 1} : \left(H^m(\mathbb{R}^3)\right)^4 \to \left(H^m(\mathbb{R}^3)\right)^4$$

are indeed projectors, i.e. $(\Pi^\varepsilon_{\mp 1})^2 = \Pi^\varepsilon_{\mp 1}$, and that $\|\Pi^\varepsilon_{\mp 1}\| = 1$.

The decomposition (3.8) allows us to filter out the main part of the temporal oscillations in a solution ψ^ε of the NLDE (3.1). This is achieved by introducing two new functions ϕ^ε_{-1} and ϕ^ε_{+1} defined by

$$\phi^\varepsilon_{-1}(t,x) = \mathrm{e}^{\mathrm{i}t/\varepsilon^2} \Pi^\varepsilon_{-1}\left[\psi^\varepsilon(t,x)\right], \qquad \phi^\varepsilon_{+1}(t,x) = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2} \Pi^\varepsilon_{+1}\left[\psi^\varepsilon(t,x)\right] \tag{3.9}$$

for $t \geq 0$ and $x \in \mathbb{R}^3$. To increase readability, we will omit the variable x from now on. Assumption (B) together with the boundedness of the projectors immediately implies

$$\sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T]} \left\|\phi^\varepsilon_{-1}(t)\right\|_{H^4} \leq M_{\mathrm{ex}}, \qquad \sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T]} \left\|\phi^\varepsilon_{+1}(t)\right\|_{H^4} \leq M_{\mathrm{ex}}. \tag{3.10}$$

The original variable ψ^ε is determined from the pair $\phi^\varepsilon = (\phi^\varepsilon_{-1}, \phi^\varepsilon_{+1})$ via

$$\psi^\varepsilon(t) = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\phi^\varepsilon_{-1}(t) + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\phi^\varepsilon_{+1}(t) = \sum_{j\in\{-1,+1\}} \mathrm{e}^{\mathrm{j}\mathrm{i}t/\varepsilon^2}\phi^\varepsilon_j(t). \tag{3.11}$$

Taking the derivative w.r.t. time in (3.9) and inserting the Dirac equations (3.1) yields the PDEs

$$\begin{aligned}
\partial_t \phi^\varepsilon_{-1} &= -\mathrm{i}\mathcal{D}_\varepsilon \phi^\varepsilon_{-1} - \mathrm{i}\mathrm{e}^{+\mathrm{i}t/\varepsilon^2}\Pi^\varepsilon_{-1}\left[W\psi^\varepsilon\right] - \mathrm{i}\mathrm{e}^{+\mathrm{i}t/\varepsilon^2}\Pi^\varepsilon_{-1}\left[|\psi^\varepsilon|^2\psi^\varepsilon\right], \quad \phi^\varepsilon_{-1}(0) = \Pi^\varepsilon_{-1}\left[\psi^{\mathrm{init}}\right], \\
\partial_t \phi^\varepsilon_{+1} &= +\mathrm{i}\mathcal{D}_\varepsilon \phi^\varepsilon_{+1} - \mathrm{i}\mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi^\varepsilon_{+1}\left[W\psi^\varepsilon\right] - \mathrm{i}\mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi^\varepsilon_{+1}\left[|\psi^\varepsilon|^2\psi^\varepsilon\right], \quad \phi^\varepsilon_{+1}(0) = \Pi^\varepsilon_{+1}\left[\psi^{\mathrm{init}}\right]
\end{aligned}$$

with operator

$$\mathcal{D}_\varepsilon = \frac{1}{\varepsilon^2}\left(\sqrt{1 - \varepsilon^2\Delta} - \mathrm{Id}\right).$$

In fact, considering the very similar structure of both PDEs allows us to write them in a general way as

$$\partial_t \phi^\varepsilon_\sigma = \sigma\mathrm{i}\mathcal{D}_\varepsilon \phi^\varepsilon_\sigma - \mathrm{i}\mathrm{e}^{-\sigma\mathrm{i}t/\varepsilon^2}\Pi^\varepsilon_\sigma\left[W\psi^\varepsilon\right] - \mathrm{i}\mathrm{e}^{-\sigma\mathrm{i}t/\varepsilon^2}\Pi^\varepsilon_\sigma\left[|\psi^\varepsilon|^2\psi^\varepsilon\right], \qquad \sigma \in \{-1,+1\}. \tag{3.12}$$

By expanding the product, we can represent the nonlinearity in terms of ϕ^ε as

$$\begin{aligned}
|\psi^\varepsilon|^2\psi^\varepsilon &= \left(\mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\phi^\varepsilon_{-1} + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\phi^\varepsilon_{+1}\right)^* \left(\mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\phi^\varepsilon_{-1} + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\phi^\varepsilon_{+1}\right)\left(\mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\phi^\varepsilon_{-1} + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\phi^\varepsilon_{+1}\right) \\
&= \sum_{\substack{j=-3 \\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J} \\ \#J=j}} \mathrm{e}^{\mathrm{i}jt/\varepsilon^2} (\phi^\varepsilon_{-j_1})^* \phi^\varepsilon_{j_2}\phi^\varepsilon_{j_3},
\end{aligned}$$

where $\mathcal{J} = \{-1,+1\}^3$ is the set of all multi-indices and $\#J = j_1 + j_2 + j_3$ denotes the sum of the entries of $J = (j_1, j_2, j_3) \in \mathcal{J}$. Additionally replacing ψ^ε in the potential-term of (3.12), we obtain the *transformed Dirac equations*

$$\begin{aligned}\partial_t \phi_\sigma^\varepsilon = \sigma \mathrm{i} \mathcal{D}_\varepsilon \phi_\sigma^\varepsilon &- \mathrm{i} \sum_{j \in \{-1,1\}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2} \Pi_\sigma^\varepsilon \left[W \phi_j^\varepsilon \right] \\ &- \mathrm{i} \sum_{\substack{j=-3 \\ j \text{ odd}}}^{3} \sum_{\substack{J \in \mathcal{J} \\ \#J = j}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2} \Pi_\sigma^\varepsilon \left[(\phi_{-j_1}^\varepsilon)^* \phi_{j_2}^\varepsilon \phi_{j_3}^\varepsilon \right] \end{aligned} \tag{3.13}$$

for $\sigma \in \{-1,+1\}$. In contrast to the operator $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon$ in (3.1), the leading differential operator $\mathcal{D}_\varepsilon$ in (3.13) is uniformly bounded w.r.t. ε when considered as an operator from $H^{m+2}(\mathbb{R}^3)$ to $H^m(\mathbb{R}^3)$ for $m \geq 0$; cf. [CW20]. More precisely, it fulfills the estimate

$$\left\| \mathcal{D}_\varepsilon u \right\|_{H^m} \leq \frac{1}{2} \left\| u \right\|_{H^{m+2}}, \qquad u \in (H^{m+2}(\mathbb{R}^3)), \tag{3.14}$$

see [JK23, Eq. (2.8)]. Thus, Assumption 3.1 implies that the first time derivative of ϕ_{-1}^ε and ϕ_{+1}^ε is uniformly bounded in H^2 w.r.t. ε, i.e. for $\sigma \in \{-1,+1\}$ we have

$$\sup_{\varepsilon \in (0,1)} \sup_{t \in [0,T]} \left\| \partial_t \phi_\sigma^\varepsilon(t) \right\|_{H^2} \leq C_D \tag{3.15}$$

for some constant C_D. The same then obviously holds in the L^2-norm. This fact will be crucial in the construction and error analysis of our methods.

In the PDEs (3.13), one can clearly recognize the origin of each term, but the double sum makes the right-hand sides somewhat complicated. An alternative representation of the PDEs for ϕ_{-1}^ε and ϕ_{+1}^ε can be obtained by sorting the terms in (3.13) according to the arguments in the exponential functions. For example, in the equation for ϕ_{-1}^ε, i.e. $\sigma = -1$ in (3.13), the argument $2\mathrm{i}t/\varepsilon^2$ is obtained by the value $j = +1$. Next, one can check which terms appear with the associated prefactor $\mathrm{e}^{2\mathrm{i}t/\varepsilon^2}$. In the first sum in (3.13), this is

$$\Pi_{-1}^\varepsilon \left[W \phi_{+1}^\varepsilon \right],$$

because for $\sigma = -1$ and $j = +1$ the summand is $\mathrm{e}^{2\mathrm{i}t/\varepsilon^2} \Pi_{-1}^\varepsilon \left[W \phi_{+1}^\varepsilon \right]$. In the second sum, we have to take into account all multi-indices $J = (j_1, j_2, j_3) \in \mathcal{J} = \{-1,+1\}^3$ with $\#J = 1$. Those are $(+1,+1,-1)$, $(+1,-1,+1)$ and $(-1,+1,+1)$, leading to the terms

$$\Pi_{-1}^\varepsilon \left[(\phi_{-1}^\varepsilon)^* \phi_{+1}^\varepsilon \phi_{-1}^\varepsilon \right], \qquad \Pi_{-1}^\varepsilon \left[(\phi_{-1}^\varepsilon)^* \phi_{-1}^\varepsilon \phi_{+1}^\varepsilon \right], \qquad \text{and} \qquad \Pi_{-1}^\varepsilon \left[(\phi_{+1}^\varepsilon)^* \phi_{+1}^\varepsilon \phi_{+1}^\varepsilon \right].$$

Carefully proceeding similarly for all other exponents and for both values of σ, one can obtain the alternative representation

$$\begin{aligned}\partial_t \phi_\sigma^\varepsilon = \sigma \mathrm{i} \mathcal{D}_\varepsilon \phi_\sigma^\varepsilon &- \mathrm{i} \mathrm{e}^{-4\sigma \mathrm{i} t/\varepsilon^2} \Pi_\sigma^\varepsilon \left[(\phi_\sigma^\varepsilon)^* \phi_{-\sigma}^\varepsilon \phi_{-\sigma}^\varepsilon \right] \\ &- \mathrm{i} \mathrm{e}^{-2\sigma \mathrm{i} t/\varepsilon^2} \left(\Pi_\sigma^\varepsilon \left[W \phi_{-\sigma}^\varepsilon \right] + \Pi_\sigma^\varepsilon \left[\left(\left| \phi_{-1}^\varepsilon \right|^2 + \left| \phi_{+1}^\varepsilon \right|^2 \right) \phi_{-\sigma}^\varepsilon + (\phi_\sigma^\varepsilon)^* \phi_{-\sigma}^\varepsilon \phi_\sigma^\varepsilon \right] \right) \\ &- \mathrm{i} \left(\Pi_\sigma^\varepsilon \left[W \phi_\sigma^\varepsilon \right] + \Pi_\sigma^\varepsilon \left[\left(\left| \phi_{-1}^\varepsilon \right|^2 + \left| \phi_{+1}^\varepsilon \right|^2 \right) \phi_\sigma^\varepsilon + (\phi_{-\sigma}^\varepsilon)^* \phi_\sigma^\varepsilon \phi_{-\sigma}^\varepsilon \right] \right) \\ &- \mathrm{i} \mathrm{e}^{+2\sigma \mathrm{i} t/\varepsilon^2} \Pi_\sigma^\varepsilon \left[(\phi_{-\sigma}^\varepsilon)^* \phi_\sigma^\varepsilon \phi_\sigma^\varepsilon \right]. \end{aligned} \tag{3.16}$$

This can be written in the more compact form

$$\partial_t \phi_\sigma^\varepsilon = \sigma \mathrm{i} \mathcal{D}_\varepsilon \phi_\sigma^\varepsilon + \sum_{\substack{p=-4 \\ p \text{ even}}}^{2} \mathrm{e}^{p\sigma \mathrm{i} t/\varepsilon^2} G_\sigma^{(p)}(\phi^\varepsilon)[\phi^\varepsilon], \qquad \sigma \in \{-1,+1\}, \tag{3.17}$$

where for each $u = (u_{-1}, u_{+1}) \in \mathbf{H^2}$, $\sigma \in \{-1, +1\}$ and $p \in \{-4, -2, 0, 2\}$, the operators $G_\sigma^{(p)}(u)$ are defined by

$$\begin{aligned}
G_\sigma^{(-4)}(u)[v] &:= -\mathrm{i}\Pi_\sigma^\varepsilon \left[(u_\sigma)^* u_{-\sigma} v_{-\sigma}\right], \\
G_\sigma^{(-2)}(u)[v] &:= -\mathrm{i}\Pi_\sigma^\varepsilon \left[W v_{-\sigma}\right] - \mathrm{i}\Pi_\sigma^\varepsilon \left[\left(|u_{-1}|^2 + |u_{+1}|^2\right) v_{-\sigma} + (u_\sigma)^* u_{-\sigma} v_\sigma\right], \\
G_\sigma^{(0)}(u)[v] &:= -\mathrm{i}\Pi_\sigma^\varepsilon \left[W v_\sigma\right] - \mathrm{i}\Pi_\sigma^\varepsilon \left[\left(|u_{-1}|^2 + |u_{+1}|^2\right) v_\sigma + (u_{-\sigma})^* u_\sigma v_{-\sigma}\right], \\
G_\sigma^{(2)}(u)[v] &:= -\mathrm{i}\Pi_\sigma^\varepsilon \left[(u_{-\sigma})^* u_\sigma v_\sigma\right]
\end{aligned}$$

for $v = (v_{-1}, v_{+1}) \in \mathbf{L^2}$. The linearity of the projectors $\Pi_{\mp 1}^\varepsilon$ and the estimates (3.3)-(3.7) imply that for every $u \in \mathbf{H^2}$, $G_\sigma^{(p)}(u)$ are linear operators that map a tuple from $\mathbf{L^2}$ to a function in $\left(L^2(\mathbb{R}^3)\right)^4$ and a tuple from $\mathbf{H^2}$ to a function in $\left(H^2(\mathbb{R}^3)\right)^4$.

In the derivation of our methods, we always consider the operators $G_\sigma^{(p)}$ with argument $\phi^\varepsilon(t)$, which are applied to the same function $\phi^\varepsilon(t)$. In short, we consider $G_\sigma^{(p)}(\phi^\varepsilon(t))[\phi^\varepsilon(t)]$ where $\phi^\varepsilon(t) = (\phi_{-1}^\varepsilon(t), \phi_{+1}^\varepsilon(t))$ is a solution of (3.13) (or, equivalently, (3.17)) at some time $t \geq 0$. We just write $G_\sigma^{(p)}(t)$ in this case to increase readability. However, in our error analysis, the distinction between the argument of $G_\sigma^{(p)}$ and the function to which it is applied to will be crucial.

The representation (3.17) is the most compact form to write the PDEs for ϕ_σ^ε, involving only four addends in the sum. However, there is no common structure of the individual addends $G_\sigma^{(p)}$ for different values of p. In contrast to that, each addend in the sums of (3.13) has exactly the same structure, and only the indices j or j_1, j_2, j_3, determining which solution component to be employed, differ. On the other hand, the representation in (3.13) is more involved due to the distinction between the potential and the nonlinearity parts and the more complicated composition of the exponents. In the next section, we will use both representations to make the best possible use of their individual advantages.

3.3 Construction of time integration methods

In this section, we present the construction of two different time integration methods for the NLDE. Both methods are based on the transformed Dirac equations (3.13) or (3.17) and will therefore yield approximations

$$\phi^n = (\phi_{-1}^n, \phi_{+1}^n) \approx (\phi_{-1}^\varepsilon(t_n), \phi_{+1}^\varepsilon(t_n)) = \phi^\varepsilon(t_n)$$

with $t_n = n\tau$ for $n = 0, 1, 2, \ldots$ and a step size $\tau > 0$. The relation (3.11) between ϕ^ε and ψ^ε can then be used to construct approximations $\psi^n \approx \psi^\varepsilon(t_n)$ by

$$\psi^n := \mathrm{e}^{-\mathrm{i}t_n/\varepsilon^2} \phi_{-1}^n + \mathrm{e}^{\mathrm{i}t_n/\varepsilon^2} \phi_{+1}^n, \qquad n = 0, 1, \ldots. \tag{3.18}$$

Since

$$\begin{aligned}
\|\psi^n - \psi^\varepsilon(t_n)\|_{L^2} &= \left\| \mathrm{e}^{-\mathrm{i}t_n/\varepsilon^2} \left(\phi_{-1}^n - \phi_{-1}^\varepsilon(t_n)\right) + \mathrm{e}^{\mathrm{i}t_n/\varepsilon^2} \left(\phi_{+1}^n - \phi_{+1}^\varepsilon(t_n)\right) \right\|_{L^2} \\
&\leq \left\|\phi_{-1}^n - \phi_{-1}^\varepsilon(t_n)\right\|_{L^2} + \left\|\phi_{+1}^n - \phi_{+1}^\varepsilon(t_n)\right\|_{L^2} = \left|\!\left|\!\left|\phi^n - \phi^\varepsilon(t_n)\right|\!\right|\!\right|_{\mathbf{L^2}},
\end{aligned} \tag{3.19}$$

any error bound concerning the accuracy of ϕ^n transfers directly to ψ^n.

The first method constructed in this section is a uniformly accurate second-order time integrator. It is similar and not superior to the NPI-2 from [CW22]. However, we formulate

the method in the transformed variables $(\phi^\varepsilon_{-1}, \phi^\varepsilon_{+1})$ instead of the original variable ψ^ε. This allows us to write the recursion formula in a special structure, which is fundamental for the construction of the *nonresonant nested Picard iterative integrator* (NRNPI) in the second part of this section. The NRNPI is a simplification of the first method, but in many cases has the same accuracy and thus improved efficiency.

To make the formulas a little simpler, we assume that the potential W is time-independent throughout the rest of the paper. We will explain later how and under which assumptions the methods can be extended to time-dependent potentials. In case of a time-independent potential, assumption (A) simplifies to $V, A_j \in H^2(\mathbb{R}^3)$.

We write $f_\varepsilon = \mathcal{O}(t^p)$ for a function $f_\varepsilon = f_\varepsilon(t,x)$ and some $p \in \mathbb{N}_0$ to express that

$$\|f_\varepsilon(t,\cdot)\|_{L^2} \le Ct^p$$

for $t \to 0$ with some constant C which does not depend on t and ε.

3.3.1 Iterating Duhamel's formula for the transformed Dirac equations

The method we present here is based on the idea of iterating Duhamel's formula for the *transformed Dirac equations* (3.13) twice, and then only approximating the slowly varying parts in the integrals, whereas the highly oscillatory parts are integrated exactly. The same strategy has been used in [CW22] and for oscillatory Klein-Gordon equations also in, e.g., [BFS18; CS22; Wan22; CZ22].

Duhamel's formula for (3.13) yields the representation

$$\begin{aligned}\phi^\varepsilon_\sigma(t_n+\tau) = \mathrm{e}^{\sigma \mathrm{i}\tau \mathcal{D}_\varepsilon}\phi^\varepsilon_\sigma(t_n) - \mathrm{i}\sum_{j\in\{-1,1\}}\int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon}\mathrm{e}^{\mathrm{i}(j-\sigma)(t_n+s)/\varepsilon^2}\Pi^\varepsilon_\sigma\left[W\phi^\varepsilon_j(t_n+s)\right]\mathrm{d}s \\ - \mathrm{i}\sum_{\substack{j=-3\\ j\text{ odd}}}^{3}\sum_{\substack{J\in\mathcal{J}\\ \#J=j}}\int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon}\mathrm{e}^{\mathrm{i}(j-\sigma)(t_n+s)/\varepsilon^2}\Pi^\varepsilon_\sigma\Big[\\ \phi^\varepsilon_{-j_1}(t_n+s)^*\phi^\varepsilon_{j_2}(t_n+s)\phi^\varepsilon_{j_3}(t_n+s)\Big]\mathrm{d}s \qquad (3.20)\end{aligned}$$

for the solution ϕ^ε_σ, $\sigma \in \{-1,+1\}$, at time $t_{n+1} = t_n + \tau$. In order to obtain a uniformly accurate second-order method, the main challenge is to approximate the highly oscillatory integrals up to $\mathcal{O}(\tau^3)$ by an expression where the unknown solution $\phi^\varepsilon_{\mp1}$ is only evaluated at the current time t_n. The first step to achieve this is to construct a sufficiently accurate approximation to $\phi^\varepsilon_{-1}(t_n+s)$ and $\phi^\varepsilon_{+1}(t_n+s)$ by using Duhamel's formula once again and approximating non-oscillatory parts. To ensure stability, the differential operator $\mathcal{D}_\varepsilon : H^{m+2}(\mathbb{R}^3) \to H^m(\mathbb{R}^3)$ is replaced by a filtered version in the second step. In the third step, we insert this representation into (3.20) and compute all remaining oscillatory integrals analytically.

Step 1: approximation of $\phi^\varepsilon_{\mp1}(t_n+s)$

In order to approximate $\phi^\varepsilon_{\mp1}(t_n+s)$, we apply Duhamel's formula again, but this time to the representation (3.17) of the PDEs for ϕ^ε_σ. This yields

$$\phi^\varepsilon_\sigma(t_n+s) = \mathrm{e}^{\sigma\mathrm{i}s\mathcal{D}_\varepsilon}\phi^\varepsilon_\sigma(t_n) + \sum_{\substack{p=-4\\ p\text{ even}}}^{2}\int_0^s \mathrm{e}^{\sigma\mathrm{i}(s-r)\mathcal{D}_\varepsilon}\mathrm{e}^{p\sigma\mathrm{i}(t_n+r)/\varepsilon^2}G^{(p)}_\sigma(t_n+r)\,\mathrm{d}r. \qquad (3.21)$$

Thanks to (3.15), we have

$$\phi_\sigma^\varepsilon(t_n + r) = \phi_\sigma^\varepsilon(t_n) + \mathcal{O}(r)\,, \qquad r > 0 \tag{3.22}$$

for $\sigma \in \{-1, +1\}$. Using (3.22) and the fact that the exact solution is uniformly bounded in H^2 at all times (even in H^4 by assumption (B)), we obtain

$$\phi_{j_1}^\varepsilon(t_n + r)^* \phi_{j_2}^\varepsilon(t_n + r)\phi_{j_3}^\varepsilon(t_n + r) = \phi_{j_1}^\varepsilon(t_n)^* \phi_{j_2}^\varepsilon(t_n)\phi_{j_3}^\varepsilon(t_n) + \mathcal{O}(r)$$

for any $j_1, j_2, j_3 \in \{-1, +1\}$ and thus $G_\sigma^{(p)}(t_n + r) = G_\sigma^{(p)}(t_n) + \mathcal{O}(r)$. Considering the surrounding integral, fixing the solutions at time t_n in the functions $G_\sigma^{(p)}$ in (3.21) produces an error of $\mathcal{O}(s^2)$. Further, we can use the following

Lemma 3.2. *For any $s \in \mathbb{R}$, we have*

$$\left\| \mathrm{e}^{\mathrm{i}s\mathcal{D}_\varepsilon} u - u \right\|_{L^2} \leq \frac{1}{2} s \left\| u \right\|_{H^2}\,, \qquad u \in \left(H^2(\mathbb{R}^3)\right)^4,$$
$$\left\| \mathrm{e}^{\mathrm{i}s\mathcal{D}_\varepsilon} u - (\mathrm{Id} + \mathrm{i}s\mathcal{D}_\varepsilon) u \right\|_{L^2} \leq \frac{1}{8} s^2 \left\| u \right\|_{H^4}\,, \qquad u \in \left(H^4(\mathbb{R}^3)\right)^4.$$

Proof. Apply Taylor's theorem in Fourier space. □

Using the first estimate inside and the second estimate outside the integrals in (3.21), we overall obtain

$$\phi_\sigma^\varepsilon(t_n + s) = \phi_\sigma^\varepsilon(t_n) + \sigma \mathrm{i}s\mathcal{D}_\varepsilon \phi_\sigma^\varepsilon(t_n) + \sum_{\substack{p=-4 \\ p \text{ even}}}^{2} \int_0^s \mathrm{e}^{p\sigma \mathrm{i}(t_n + r)/\varepsilon^2}\, \mathrm{d}r\, G_\sigma^{(p)}(t_n) + \mathcal{O}\Big(s^2\Big)\,. \tag{3.23}$$

Step 2: filtered operator

Whilst the order of accuracy in (3.23) is sufficient, using this representation would lead to instabilities of the methods we are about to construct. The reason is that the operator $\mathcal{D}_\varepsilon$ maps from $H^{m+2}(\mathbb{R}^3)$ to $H^m(\mathbb{R}^3)$ for $m \geq 0$, and hence causes a loss of regularity; cf. (3.14). This is why we replace $\mathcal{D}_\varepsilon$ by the filtered version

$$\widehat{\mathcal{D}_\varepsilon}(\tau) : H^m(\mathbb{R}^3) \to H^m(\mathbb{R}^3), \qquad \widehat{\mathcal{D}_\varepsilon}(\tau) = \frac{\sin(\tau \mathcal{D}_\varepsilon)}{\tau}, \qquad \tau > 0$$

as, e.g., in [CW19; CW22]. The filtered operator $\widehat{\mathcal{D}_\varepsilon}(\tau)$ has the properties that

$$\left\| \widehat{\mathcal{D}_\varepsilon}(\tau) u \right\|_{H^m} \leq \frac{1}{\tau} \left\| u \right\|_{H^m}\,, \qquad u \in \left(H^m(\mathbb{R}^3)\right)^4, \tag{3.24}$$
$$\left\| \widehat{\mathcal{D}_\varepsilon}(\tau) u \right\|_{H^m} \leq \frac{1}{2} \left\| u \right\|_{H^{m+2}}\,, \qquad u \in \left(H^{m+2}(\mathbb{R}^3)\right)^4 \tag{3.25}$$

for any $m \geq 0$. The first inequality is obvious, whereas the second one can easily be shown by using Taylor's theorem in Fourier space. Moreover, using the same techniques, it is not difficult so show that

$$\left\| \left(\mathcal{D}_\varepsilon - \widehat{\mathcal{D}_\varepsilon}(\tau) \right) u \right\|_{L^2} \leq \frac{\tau}{2} \left\| u \right\|_{H^4} \tag{3.26}$$

for all $u \in \left(H^4(\mathbb{R}^3)\right)^4$ (see [CW19, Proof of Lemma 3.2]). Since the exact solution is assumed to be in H^4, property (3.26) implies that replacing $\mathcal{D}_\varepsilon$ by $\widehat{\mathcal{D}_\varepsilon}$ in (3.23) introduces an $\mathcal{O}(s\tau)$

error, which is unproblematic in view of the error order we want to achieve. Further, combining the term $\sigma \mathrm{i} s \widehat{\mathcal{D}_\varepsilon}(\tau)\phi_\sigma^\varepsilon(t_n)$ with $G_\sigma^{(0)}(t_n) = G_\sigma^{(0)}(\phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]$ motivates the definition of the operators $\widehat{G}_\sigma^{(p)}(u)$ for each $u = (u_{-1}, u_{+1}) \in \mathbf{H^2}$ by

$$\begin{aligned} \widehat{G}_\sigma^{(0)}(u)[v] &:= G_\sigma^{(0)}(u)[v] + \sigma \mathrm{i} \widehat{\mathcal{D}_\varepsilon}(\tau) v_\sigma, \\ \widehat{G}_\sigma^{(p)}(u)[v] &:= G_\sigma^{(p)}(u)[v], \qquad p \in \{-4, -2, 2\} \end{aligned} \tag{3.27}$$

for $v = (v_{-1}, v_{+1}) \in \mathbf{L^2}$. This leads to the representation

$$\phi_\sigma^\varepsilon(t_n + s) = \phi_\sigma^\varepsilon(t_n) + \sum_{\substack{p=-4 \\ p \text{ even}}}^{2} \int_0^s \mathrm{e}^{p\sigma \mathrm{i}(t_n + r)/\varepsilon^2} \, \mathrm{d}r \, \widehat{G}_\sigma^{(p)}(t_n) + \mathcal{O}\Big(s^2 + s\tau\Big), \tag{3.28}$$

where we wrote $\widehat{G}_\sigma^{(p)}(t_n)$ instead of $\widehat{G}_\sigma^{(p)}(\phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]$ similar to before. Property (3.24) ensures that for each $u \in \mathbf{H^2}$, $\widehat{G}_\sigma^{(0)}(u)$ are indeed well-defined operators mapping from and to $\mathbf{L^2}$ (details on this and other properties of the operators $\widehat{G}_\sigma^{(p)}$ are discussed in Lemma 3.17 in Section 3.6). With the function φ_1 given by

$$\varphi_1(z) = \int_0^1 e^{\theta z} \, d\theta = \begin{cases} \frac{e^z - 1}{z} & \text{for } z \in \mathbb{C}, z \neq 0, \\ 1 & \text{for } z = 0, \end{cases}$$

Eq. (3.28) can equivalently be expressed as

$$\phi_\sigma^\varepsilon(t_n + s) = \phi_\sigma^\varepsilon(t_n) + \sum_{\substack{p=-4 \\ p \text{ even}}}^{2} \mathrm{e}^{p\sigma \mathrm{i} t_n/\varepsilon^2} s \varphi_1\Big(\frac{p\sigma \mathrm{i} s}{\varepsilon^2}\Big) \widehat{G}_\sigma^{(p)}(t_n) + \mathcal{O}\Big(s^2 + s\tau\Big). \tag{3.29}$$

Step 3: Approximating the integrals in (3.20)

Eq. (3.29) can now be inserted into (3.20). At this point, it becomes clear why we established two different representations of the PDEs for ϕ_σ^ε: We would like our $\mathcal{O}(s^2)$-approximation of $\phi_\sigma^\varepsilon(t_n + s)$ to be as simple as possible, which was achieved by using the representation (3.17). When inserting (3.29) into (3.20), however, the similar structure of all terms provided by representation (3.13) is essential such that we can take care of all of them at once instead of considering every term individually, which would be very cumbersome as the nonlinearity increases the number of terms even further.

When inserting (3.29) into the nonlinearity in (3.20), this gives rise to a number of $\mathcal{O}(s^2)$ terms which lead to a total error of $\mathcal{O}(\tau^3)$. After all, we can express each component of the exact solution $\phi^\varepsilon = (\phi_{-1}^\varepsilon, \phi_{+1}^\varepsilon)$ at time $t_n + \tau$ as

$$\phi_\sigma^\varepsilon(t_n + \tau) = \mathrm{e}^{\sigma \mathrm{i} \tau \mathcal{D}_\varepsilon} \phi_\sigma^\varepsilon(t_n) - \mathrm{i} I_\sigma^1(t_n, \phi^\varepsilon(t_n)) - \mathrm{i} I_\sigma^2(t_n, \phi^\varepsilon(t_n)) + \mathcal{O}\Big(\tau^3\Big), \tag{3.30}$$

$\sigma \in \{-1, +1\}$. Here, we define

$$\begin{aligned} I_\sigma^1(t, u) = &\sum_{j \in \{-1,1\}} \mathrm{e}^{\mathrm{i}(j-\sigma)\frac{t}{\varepsilon^2}} \int_0^\tau \mathrm{e}^{\sigma \mathrm{i}(\tau - s)\mathcal{D}_\varepsilon} \mathrm{e}^{\mathrm{i}(j-\sigma)\frac{s}{\varepsilon^2}} \, \mathrm{d}s \, \Pi_\sigma^\varepsilon \left[W u_j\right] \\ &+ \sum_{j \in \{-1,1\}} \sum_{\substack{p=-4 \\ p \text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj)\frac{t}{\varepsilon^2}} \int_0^\tau \mathrm{e}^{\sigma \mathrm{i}(\tau - s)\mathcal{D}_\varepsilon} \mathrm{e}^{\mathrm{i}(j-\sigma)\frac{s}{\varepsilon^2}} s \varphi_1\Big(\frac{pj\mathrm{i}s}{\varepsilon^2}\Big) \, \mathrm{d}s \, \Pi_\sigma^\varepsilon \Big[W \widehat{G}_j^{(p)}(u)[u]\Big] \end{aligned}$$

for $t \geq 0$ and $u = (u_{-1}, u_{+1}) \in \mathbf{H^2}$, such that $I^1_\sigma(t_n, \phi^\varepsilon(t_n))$ is the $\mathcal{O}(\tau^3)$-approximation to the integrals in (3.20) containing products with the potential W. Further, I^2_σ is given by

$$
\begin{aligned}
I^2_\sigma(t,u) = &\sum_{\substack{j=-3\\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathrm{e}^{\mathrm{i}(j-\sigma)\frac{t}{\varepsilon^2}} \int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon} \mathrm{e}^{\mathrm{i}(j-\sigma)\frac{s}{\varepsilon^2}} \,\mathrm{d}s\, \Pi^\varepsilon_\sigma \left[u^*_{-j_1} u_{j_2} u_{j_3}\right] \\
&+ \sum_{\substack{j=-3\\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \sum_{\substack{p=-4\\ p \text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj_1)\frac{t}{\varepsilon^2}} \int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon} \mathrm{e}^{\mathrm{i}(j-\sigma)\frac{s}{\varepsilon^2}} s\varphi_1\Big(\frac{pj_1\mathrm{i}s}{\varepsilon^2}\Big) \,\mathrm{d}s\, \Pi^\varepsilon_\sigma \left[\big(\widehat{G}^{(p)}_{-j_1}(u)[u]\big)^* u_{j_2} u_{j_3}\right] \\
&+ \sum_{\substack{j=-3\\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \sum_{\substack{p=-4\\ p \text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj_2)\frac{t}{\varepsilon^2}} \int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon} \mathrm{e}^{\mathrm{i}(j-\sigma)\frac{s}{\varepsilon^2}} s\varphi_1\Big(\frac{pj_2\mathrm{i}s}{\varepsilon^2}\Big) \,\mathrm{d}s\, \Pi^\varepsilon_\sigma \left[u^*_{-j_1} \widehat{G}^{(p)}_{j_2}(u)[u] u_{j_3}\right] \\
&+ \sum_{\substack{j=-3\\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \sum_{\substack{p=-4\\ p \text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj_3)\frac{t}{\varepsilon^2}} \int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon} \mathrm{e}^{\mathrm{i}(j-\sigma)\frac{s}{\varepsilon^2}} s\varphi_1\Big(\frac{pj_3\mathrm{i}s}{\varepsilon^2}\Big) \,\mathrm{d}s\, \Pi^\varepsilon_\sigma \left[u^*_{-j_1} u_{j_2} \widehat{G}^{(p)}_{j_3}(u)[u]\right],
\end{aligned}
$$

which means that $I^2_\sigma(t_n, \phi^\varepsilon(t_n))$ is the $\mathcal{O}(\tau^3)$-approximation to the integrals in (3.20) accounting for the nonlinearity. The integrals in I^1_σ and I^2_σ do no longer involve the exact solution ϕ^ε. Instead, they are operators that can be computed and applied analytically. For $\delta, \zeta \in \mathbb{Z}$, we have

$$
\begin{aligned}
\mathcal{A}_\sigma(\delta) &:= \int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon} \mathrm{e}^{\mathrm{i}\delta s/\varepsilon^2} \,\mathrm{d}s = \tau \mathrm{e}^{\mathrm{i}\delta\tau/\varepsilon^2} \varphi_1\Big(\mathrm{i}\tau\Big(\sigma\mathcal{D}_\varepsilon - \frac{\delta}{\varepsilon^2}\mathrm{Id}\Big)\Big), \\
\mathcal{B}_\sigma(\delta,\zeta) &:= \int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon} s \mathrm{e}^{\mathrm{i}\delta s/\varepsilon^2} \varphi_1\Big(\frac{\zeta\mathrm{i}s}{\varepsilon^2}\Big) \,\mathrm{d}s \qquad (3.31) \\
&= \begin{cases} \mathrm{i}\tau\dfrac{\varepsilon^2}{\zeta} \mathrm{e}^{\mathrm{i}\tau\delta/\varepsilon^2} \left(\varphi_1\Big(\mathrm{i}\tau\Big(\sigma\mathcal{D}_\varepsilon - \dfrac{\delta}{\varepsilon^2}\mathrm{Id}\Big)\Big) - \mathrm{e}^{\mathrm{i}\tau\zeta/\varepsilon^2} \varphi_1\Big(\mathrm{i}\tau\Big(\sigma\mathcal{D}_\varepsilon - \dfrac{\delta+\zeta}{\varepsilon^2}\mathrm{Id}\Big)\Big)\right), & \zeta \neq 0, \\ \tau^2 \mathrm{e}^{\mathrm{i}\tau\delta/\varepsilon^2} \varphi_2\Big(\mathrm{i}\tau\Big(\sigma\mathcal{D}_\varepsilon - \dfrac{\delta}{\varepsilon^2}\mathrm{Id}\Big)\Big), & \zeta = 0, \end{cases}
\end{aligned}
$$

where the function φ_2 is given by

$$
\varphi_2(z) = \int_0^1 \theta e^{(1-\theta)z} \, d\theta = \begin{cases} \frac{\varphi_1(z)-1}{z} & \text{for } z \in \mathbb{C}, z \neq 0, \\ \frac{1}{2} & \text{for } z = 0. \end{cases}
$$

Thus, we obtain

$$
\begin{aligned}
I^1_\sigma(t,u) = &\sum_{j\in\{-1,1\}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2} \mathcal{A}_\sigma(j-\sigma) \Pi^\varepsilon_\sigma \left[W u_j\right] \\
&+ \sum_{j\in\{-1,1\}} \sum_{\substack{p=-4\\ p \text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj)t/\varepsilon^2} \mathcal{B}_\sigma(j-\sigma, pj) \Pi^\varepsilon_\sigma \left[W \widehat{G}^{(p)}_j(u)[u]\right] \qquad (3.32)
\end{aligned}
$$

and

$$
\begin{aligned}
I^2_\sigma(t,u) = &\sum_{\substack{j=-3\\ j\text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2} \mathcal{A}_\sigma(j-\sigma)\Pi^\varepsilon_\sigma\left[(u_{-j_1})^* u_{j_2} u_{j_3}\right] \\
&+ \sum_{\substack{j=-3\\ j\text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \sum_{\substack{p=-4\\ p\text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj_1)t/\varepsilon^2} \mathcal{B}_\sigma(j-\sigma,pj_1)\Pi^\varepsilon_\sigma\left[\left(\widehat{G}^{(p)}_{-j_1}(u)[u]\right)^* u_{j_2} u_{j_3}\right] \\
&+ \sum_{\substack{j=-3\\ j\text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \sum_{\substack{p=-4\\ p\text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj_2)t/\varepsilon^2} \mathcal{B}_\sigma(j-\sigma,pj_2)\Pi^\varepsilon_\sigma\left[(u_{-j_1})^* \widehat{G}^{(p)}_{j_2}(u)[u] u_{j_3}\right] \\
&+ \sum_{\substack{j=-3\\ j\text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \sum_{\substack{p=-4\\ p\text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj_3)t/\varepsilon^2} \mathcal{B}_\sigma(j-\sigma,pj_3)\Pi^\varepsilon_\sigma\left[(u_{-j_1})^* u_{j_2} \widehat{G}^{(p)}_{j_3}(u)[u]\right]. \qquad (3.33)
\end{aligned}
$$

Specification of the time integrator and local error bound

Eq. (3.30) immediately suggests a time integrator: Replacing $\phi^\varepsilon(t_n)$ by numerical approximations $\phi^n = (\phi^n_{-1}, \phi^n_{+1})$ (thus also replacing $\widehat{G}^{(p)}_\sigma(t_n) = \widehat{G}^{(p)}_\sigma(\phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]$ by $\widehat{G}^{(p)}_\sigma(\phi^n)[\phi^n]$) and omitting the $\mathcal{O}(\tau^3)$ terms yields the recursion

$$
\phi^{n+1} = \Phi_{\mathrm{NPI}}(t_n, \phi^n), \qquad n = 0, 1, 2, \dots \qquad (3.34)
$$

with the numerical flow[1]

$$
\Phi_{\mathrm{NPI}}(t,u) = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\tau\mathcal{D}_\varepsilon} u_{-1} - \mathrm{i} I^1_{-1}(t,u) - \mathrm{i} I^2_{-1}(t,u) \\ \mathrm{e}^{+\mathrm{i}\tau\mathcal{D}_\varepsilon} u_{+1} - \mathrm{i} I^1_{+1}(t,u) - \mathrm{i} I^2_{+1}(t,u) \end{pmatrix}. \qquad (3.35)
$$

The operator Φ_{NPI} does of course depend on the step size τ and on ε (as $I^1_{\pm1}$ and $I^2_{\pm1}$ do). However, we refrain from marking this dependency explicitly in order to keep the notation simple. The method (3.34) is fully explicit. If the exact solution $\phi^\varepsilon = (\phi^\varepsilon_{-1}, \phi^\varepsilon_{+1})$ of (3.13) is in $\mathbf{H^4}$ for all times, then by construction its local error

$$
\ell^{n+1}_{\mathrm{NPI}} := \phi^\varepsilon(t_{n+1}) - \Phi_{\mathrm{NPI}}(t_n, \phi^\varepsilon(t_n)), \qquad n \in \mathbb{N}_0,
$$

is bounded by

$$
\left\| \ell^{n+1}_{\mathrm{NPI}} \right\|_{\mathbf{L^2}} \le C\tau^3 \qquad (3.36)
$$

for some constant C that is independent of τ and ε. This is one of the ingredients which would be necessary to prove that the scheme is second-order accurate independently of ε, which, however, is not our objective. Instead, this estimate will turn out to be useful for the error analysis of the NRNPI in the next subsection.

Remark 3.3. *If the potential $W = W(t,x)$ is time-dependent, a similar method can easily be derived. In the inner application of Duhamel's formula, that is Eq. (3.21) in step 1, the potential W appearing in $G^{(-2)}_\sigma$ and $G^{(0)}_\sigma$ is then evaluated at time $t_n + r$, but approximating $W(t_n + r) \approx W(t_n)$ is sufficiently accurate here. In the outer application of Duhamel's formula from (3.20), W is evaluated at time $t_n + s$. For a sufficient accuracy, the linearization $W(t_n + s) \approx W(t_n) + s\partial_t W(t_n)$ has to be employed here. In step 3, the strategies remain*

[1] In general, we combine two functions $u_{-1}, u_{+1} \in H^m(\mathbb{R}^3)$ to a tuple $(u_{-1}, u_{+1}) \in \mathbf{H^m}$. Only occasionally, we stack two such functions into a vector for the sake of presentation.

unaltered, but the additional term $s\partial_t W(t_n)$ has to be taken into account. One can check that the additional assumptions

$$V, A_j \in C^1([0,T], H^2(\mathbb{R}^3)), \qquad V, A_j \in C^2([0,T], L^2(\mathbb{R}^3))$$

are necessary for a rigorous local error and stability analysis in $\mathbf{L^2}$.

Remark 3.4. *The NPI-2 proposed in [CW22] is based on the same ideas. There are however some differences. Firstly, they work in the context of the* original Dirac equations (3.1). *This means that they cannot apply an approximation of the type $\psi^\varepsilon(t_n + r) \approx \psi^\varepsilon(t_n)$ (as we did for the transformed variables, cf. (3.22)), since this would induce large errors when ε is small due to the oscillatory dynamics of ψ^ε. This is why in [CW22], the approximation*

$$\psi^\varepsilon(t_n + r) = \left(\mathrm{e}^{-\mathrm{i}r/\varepsilon^2}\Pi^\varepsilon_{-1} + \mathrm{e}^{\mathrm{i}r/\varepsilon^2}\Pi^\varepsilon_{+1}\right)\psi^\varepsilon(t_n) + \mathcal{O}(r)\,, \qquad r > 0$$

was used instead, which is again motivated by Duhamel's formula together with the decomposition (3.8). Secondly, they employed slightly different strategies for approximating the remaining, slowly varying parts. In the end, their NPI-2 scheme is still very similar to the method we presented in (3.34), which is why we will also refer to our version as NPI-2. However, having formulated the method in the transformed variables $\phi = (\phi^\varepsilon_{-1}, \phi^\varepsilon_{+1})$ allows us to have a detailed look at the frequencies of the highly oscillatory phases involved. This will be crucial for the derivation and analysis of our simplified method in the following section.

3.3.2 Nonresonant nested Picard iterative integrator (NRNPI)

For the NPI-2 (3.34), one can derive a second-order global error bound with a constant that does not depend on ε, as mentioned in [CW22, Sec. 4]. To do so, one has to combine the local error bound (3.36) with suitable stability estimates and a standard Lady Windermere's fan argument. Even though second-order convergence uniformly in ε is a very favorable property, the efficiency of the NPI-2 is to some extent limited by the huge amount of terms that have to be computed in each time step: the numerical flow (3.35) contains evaluations of $I^1_\pm$ and $I^2_\pm$, which in turn involve multiple sums. Each addend then requires the computation of a product of several functions in physical space and the application of operators in Fourier space. The total numerical work to compute one time step of this method is thus very large.

Our goal now is to omit a significant number of terms in the numerical flow without affecting the accuracy, or only to a small extent. For this purpose, we return to the representation (3.30) of an exact solution $\phi^\varepsilon = (\phi^\varepsilon_{-1}, \phi^\varepsilon_{+1})$ of (3.13) at time $t_n + \tau$, which provided the basis for the method from the previous section. Here, it is worthwhile to consider the structure of the actual addends that appear in the sums of $I^1_\pm$ and $I^2_\pm$ more closely. Let us take a look, for instance, at the last three lines of I^2_σ, cf. Eq. (3.33). If I^2_σ is evaluated with arguments t_n and $\phi^\varepsilon(t_n)$ as in (3.30), then each of the addends is of the type

$$\mathrm{e}^{\mathrm{i}qt_n/\varepsilon^2}\mathcal{B}_\sigma(\delta,\zeta)\Pi^\varepsilon_\sigma\left[z(t_n)\right] \tag{3.37}$$

for some $q \in \{-6,-4,-2,0,2,4,6\}$, $\delta, \zeta \in \mathbb{Z}$ and some function z of the form

$$z(t) = u(t)^* v(t) w(t) \tag{3.38}$$

where u, v and w each are either ϕ^ε_σ for some $\sigma \in \{-1,+1\}$ or $\widehat{G}^{(p)}_\sigma(\phi^\varepsilon(\cdot))[\phi^\varepsilon(\cdot)]$ for some $\sigma \in \{-1,+1\}$, $p \in \{-4,-2,0,2\}$. We suggest a method where all terms of the type (3.37) with $q \neq 0$ are omitted, and are thus included in the local error instead. This may come as a

surprise since those terms are only in $\mathcal{O}(\tau^2)$ due to the norm bound of $\mathcal{B}_\sigma(\delta,\zeta)$. Hence, in a standard error analysis based on the classical Lady Windermere's fan argument, neglecting such terms would reduce the global error order from two to one. However, we expect that actually such terms will not critically sum up in the error accumulation. The reasons for this conjecture are the following: Firstly, the terms in (3.37) contain the prefactor $\mathrm{e}^{\mathrm{i}q t_n/\varepsilon^2}$. This is a complex number oscillating on the unit circle throughout the time steps. For $q \neq 0$, two consecutive numbers $\mathrm{e}^{\mathrm{i}q t_n/\varepsilon^2}$ and $\mathrm{e}^{\mathrm{i}q t_{n+1}/\varepsilon^2} = \mathrm{e}^{\mathrm{i}q\tau/\varepsilon^2}\mathrm{e}^{\mathrm{i}q t_n/\varepsilon^2}$ do not point in the same direction in the complex plane as long as a *nonresonant* step size is chosen, meaning that

$$\mathrm{e}^{\mathrm{i}q\tau/\varepsilon^2} \not\approx 1, \qquad \text{i.e.,} \qquad \tau \not\approx k\frac{2\pi\varepsilon^2}{q} \qquad \text{for all } k \in \mathbb{Z}.$$

Secondly, the boundedness of the first time derivative of a solution $\phi^\varepsilon = (\phi^\varepsilon_{-1}, \phi^\varepsilon_{+1})$ of (3.13) implies that z only varies slowly (in a sense that is made precise later on) in the course of several time steps. The same holds for $\mathcal{B}_\sigma(\delta,\zeta)\Pi^\varepsilon_\sigma[z(t_n)]$ since the operator $\mathcal{B}_\sigma(\delta,\zeta)\Pi^\varepsilon_\sigma$ does not depend on n. Those two facts are later used in a summation-by-parts argument (cf. proof of Thm. 3.12) to show that neglecting terms of the form (3.37) with nonzero exponent in the prefactor, i.e. $q \neq 0$, has indeed only little impact on the accuracy. Terms of a similar structure that we will also omit are additionally found in $I^1_\sigma(t_n, \phi^\varepsilon(t_n))$.

Let us now establish our new method in detail. In each of the last three lines of I^2_σ, defined in (3.33), we only *keep* the terms for the value of p for which the exponent in the prefactor *is* zero. In the second line of I^2_σ, for example, we only keep the term for the value of p for which $j - \sigma + pj_1 = 0$. Since $1/j_1 = j_1$ for $j_1 \in \{-1,+1\}$, this is the case for $p = j_1(\sigma - j)$. Thus, for each multi-index $J \in \mathcal{J}$, there is exactly one value of p for which the exponent is zero, whereas the terms for the other three values of p are omitted in our simplified method.

Analogously, in the third and fourth line of I^2_σ, we only keep the term for $p = j_2(\sigma - j)$ or $p = j_3(\sigma - j)$, respectively. In the second line of I^1_σ, we keep the term for the value of p for which $j - \sigma + pj = 0$, i.e. $p = \sigma j - 1$. Thus, as before, we always keep exactly one out of four terms here. Overall, we replace $I^1_\sigma(t,u)$ and $I^2_\sigma(t,u)$ in the numerical flow (3.35) of the full method by $J^1_\sigma(t,u)[u]$ and $J^2_\sigma(t,u)[u]$ where for $u = (u_{-1}, u_{+1}) \in \mathbf{H^2}$ the operators $J^1_\sigma(t,u)$ and $J^2_\sigma(t,u)$ are given by

$$\begin{aligned} J^1_\sigma(t,u)[v] = &\sum_{j\in\{-1,1\}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2}\mathcal{A}_\sigma(j-\sigma)\Pi^\varepsilon_\sigma[Wv_j] \\ &+ \sum_{j\in\{-1,1\}} \mathcal{B}_\sigma(j-\sigma,\sigma-j)\Pi^\varepsilon_\sigma\left[W\widehat{G}^{(\sigma j-1)}_j(u)[v]\right], \end{aligned} \tag{3.39}$$

$$\begin{aligned} J^2_\sigma(t,u)[v] = &\sum_{\substack{j=-3\\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2}\mathcal{A}_\sigma(j-\sigma)\Pi^\varepsilon_\sigma\left[u^*_{-j_1}u_{j_2}v_{j_3}\right] \\ &+ \sum_{\substack{j=-3\\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathcal{B}_\sigma(j-\sigma,\sigma-j)\Pi^\varepsilon_\sigma\left[\left(\widehat{G}^{(j_1(\sigma-j))}_{-j_1}(u)[u]\right)^* u_{j_2}v_{j_3}\right] \\ &+ \sum_{\substack{j=-3\\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathcal{B}_\sigma(j-\sigma,\sigma-j)\Pi^\varepsilon_\sigma\left[u^*_{-j_1}\widehat{G}^{(j_2(\sigma-j))}_{j_2}(u)[u]v_{j_3}\right] \\ &+ \sum_{\substack{j=-3\\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathcal{B}_\sigma(j-\sigma,\sigma-j)\Pi^\varepsilon_\sigma\left[u^*_{-j_1}u_{j_2}\widehat{G}^{(j_3(\sigma-j))}_{j_3}(u)[v]\right], \end{aligned} \tag{3.40}$$

$v = (v_{-1}, v_{+1}) \in \mathbf{L^2}$. The reason why we distinguished between the arguments u and v is that now, for every $u \in \mathbf{H^2}$, $J^1_\sigma(t,u)$ and $J^2_\sigma(t,u)$ are linear operators. This will be crucial in the error analysis.

After all, the *nonresonant nested Picard iterative integrator (NRNPI)* is given by the recursion

$$\phi^{n+1} = \Phi_{\mathrm{NRNPI}}(t_n, \phi^n)[\phi^n], \qquad n = 0, 1, 2, \dots$$

with the numerical flow

$$\Phi_{\mathrm{NRNPI}}(t,u)[v] = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\tau\mathcal{D}_\varepsilon} v_{-1} - \mathrm{i}J^1_{-1}(t,u)[v] - \mathrm{i}J^2_{-1}(t,u)[v] \\ \mathrm{e}^{+\mathrm{i}\tau\mathcal{D}_\varepsilon} v_{+1} - \mathrm{i}J^1_{+1}(t,u)[v] - \mathrm{i}J^2_{+1}(t,u)[v] \end{pmatrix} \tag{3.41}$$

for $u \in \mathbf{H^2}$ and $v \in \mathbf{L^2}$. Again, we do not express the dependency of Φ_{NRNPI} on τ and ε explicitly. The linearity of $J^1_\sigma(t,u)$ and $J^2_\sigma(t,u)$ directly implies the linearity of $\Phi_{\mathrm{NRNPI}}(t,u)$ for fixed $u \in \mathbf{H^2}$.

Remark 3.5. *The terms J^1_σ and J^2_σ have to be computed in every time step. They include products of the numerical approximations ϕ^n_σ with the potential and with themselves in the nonlinearity. Those products have to be computed in physical space. The result has to be transformed to Fourier space, since afterward the projectors and the operators $\mathcal{A}_\sigma$ or $\mathcal{B}_\sigma$ have to be applied. Considering the computational effort, (inverse) Fourier transforms are the dominating operations in each time step. It is thus crucial to reduce their number as much as possible. In the second line of J^1_σ and the last three lines of J^2_σ, for each $j \in \{-3,-1,1,3\}$, the respective operator is always identical. Consequently, by a reordering of the sums, only two Fourier transforms per index j are required (one for the case $\sigma = -1$ and $\sigma = +1$ respectively). The same holds for the first lines of J^1_σ and J^2_σ.*

Remark 3.6. *Again, the method can easily be extended to time-dependent potentials $W = W(t,x)$. To do so, one can take the corresponding extension of the full NPI-2 from Remark 3.3 and omit terms according to the strategies from above. Consequently, the same additional assumptions on the potential W as in Remark 3.3 are required.*

Remark 3.7. *The techniques from this section can be used to construct similar time integrators for other equations, such as the Klein-Gordon-Dirac system.*

3.4 Convergence of the NRNPI

In this section, we analyze the convergence of the NRNPI. First, we discuss the local error. In contrast to the NPI-2, the NRNPI involves local error terms which are only in $\mathcal{O}(\tau^2)$, but have a special structure in return. This will be the topic of the first lemma in this section. Then, we state two technical lemmas concerning stability of the numerical flow. The proofs of those lemmas are postponed to Section 3.6. Instead, we will continue by presenting and proving our main theorem, which is a convergence result for the NRNPI. In particular, we show that although the local error of the NRNPI is increased, its special structure ensures that the global error is not affected in many cases (in a sense to be made precise below). In all proofs, C always denotes a constant that may change from line to line, but is independent of τ and ε.

The local error

$$\ell^{n+1} := \phi^\varepsilon(t_{n+1}) - \Phi_{\mathrm{NRNPI}}(t_n, \phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]$$

of the NRNPI in the $(n+1)$-st step can be decomposed into two parts: The local errors $\ell_{\mathrm{NPI}}^{n+1}$ of the full NPI-2 and those originating from omitting terms of the full method (3.34), which we collect in $\ell_{\mathrm{diff}}^{n+1}$, i.e.

$$\ell^{n+1} = \underbrace{\phi^\varepsilon(t_{n+1}) - \Phi_{\mathrm{NPI}}(t_n, \phi^\varepsilon(t_n))}_{=\ell_{\mathrm{NPI}}^{n+1}} + \underbrace{\Phi_{\mathrm{NPI}}(t_n, \phi^\varepsilon(t_n)) - \Phi_{\mathrm{NRNPI}}(t_n, \phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]}_{=:\ell_{\mathrm{diff}}^{n+1}}. \tag{3.42}$$

From (3.36), we have $\left|\!\left|\!\left| \ell_{\mathrm{NPI}}^{n+1} \right|\!\right|\!\right|_{\mathbf{L^2}} \le C\tau^3$. Comparing (3.35) and (3.41), we further find

$$\begin{aligned}\ell_{\mathrm{diff}}^{n+1} = \mathrm{i} &\begin{pmatrix} J_{-1}^1(t_n, \phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)] - I_{-1}^1(t_n, \phi^\varepsilon(t_n)) \\ J_{+1}^1(t_n, \phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)] - I_{+1}^1(t_n, \phi^\varepsilon(t_n)) \end{pmatrix} \\ + \mathrm{i} &\begin{pmatrix} J_{-1}^2(t_n, \phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)] - I_{-1}^2(t_n, \phi^\varepsilon(t_n)) \\ J_{+1}^2(t_n, \phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)] - I_{+1}^2(t_n, \phi^\varepsilon(t_n)) \end{pmatrix}.\end{aligned}$$

This representation allows us to derive the following lemma concerning the structure and properties of $\ell_{\mathrm{diff}}^{n+1}$.

Lemma 3.8. *Let Assumption 3.1 hold and let ϕ^ε be the exact solution of (3.13). Set $\mathcal{Q} = \{-6, -4, -2, 2, 4, 6\}$. Then, we can write*

$$\ell_{\mathrm{diff}}^{n+1} = \sum_{q \in \mathcal{Q}} \tau^2 \mathrm{e}^{\mathrm{i}qt_n/\varepsilon^2} E_q^n \tag{3.43}$$

for some $E_q^n \in \mathbf{H^2}$ that fulfill

$$\left|\!\left|\!\left| E_q^n \right|\!\right|\!\right|_{\mathbf{H^2}} \le C \qquad \text{and} \qquad \left|\!\left|\!\left| E_q^{n+1} - E_q^n \right|\!\right|\!\right|_{\mathbf{L^2}} \le C\tau$$

for $n = 0, 1, ..., \lfloor T/\tau \rfloor$ with some constant C independent of τ, n and ε.

The proof can be found in Section 3.6. The next lemma addresses the stability of the numerical flow Φ_{NRNPI}.

Lemma 3.9. *Let Assumption 3.1 (A) hold. Then, for $R > 0$, we have*

$$\begin{aligned}
&(i) && \left|\!\left|\!\left| \Phi_{\mathrm{NRNPI}}(t,u)[v] \right|\!\right|\!\right|_{\mathbf{L^2}} \le (1 + C\tau) \left|\!\left|\!\left| v \right|\!\right|\!\right|_{\mathbf{L^2}}, && u \in \mathbf{B^2}(R), v \in \mathbf{L^2}, \\
&(ii) && \left|\!\left|\!\left| (\Phi_{\mathrm{NRNPI}}(t,u) - \mathrm{Id})[v] \right|\!\right|\!\right|_{\mathbf{L^2}} \le C\tau \left|\!\left|\!\left| v \right|\!\right|\!\right|_{\mathbf{H^2}}, && u \in \mathbf{B^2}(R), v \in \mathbf{H^2}, \\
&(iii) && \left|\!\left|\!\left| \Phi_{\mathrm{NRNPI}}(t,u)[v] - \Phi_{\mathrm{NRNPI}}(t,\widetilde{u})[v] \right|\!\right|\!\right|_{\mathbf{L^2}} \le C\tau \left|\!\left|\!\left| u - \widetilde{u} \right|\!\right|\!\right|_{\mathbf{L^2}}, && u, \widetilde{u}, v \in \mathbf{B^2}(R),
\end{aligned}$$

for all $t \ge 0$. In all cases, the constant C depends on R, but not on τ and ε.

Lemma 3.8 implies that the local error of the NRNPI is at least in $\mathcal{O}(\tau^2)$ for *all* step sizes τ. A Lady Windermere's fan argument and Lemma 3.9 yield a first-order global error bound which is uniform in ε. We will see later, however, that the accuracy of NRNPI is actually much better; cf. Corollary 3.14.

In preparation for the following lemma, we define the (linear) operators $\Phi_{\mathrm{NRNPI}}^{n,k}$ for $n, k \in \mathbb{N}_0$ by

$$\begin{aligned}
&\Phi_{\mathrm{NRNPI}}^{n,k}[u] = \Phi_{\mathrm{NRNPI}}(t_{n-1}, \phi^{n-1})\Big[\Phi_{\mathrm{NRNPI}}(t_{n-2}, \phi^{n-2})\Big[\ \dots \ \Phi_{\mathrm{NRNPI}}(t_k, \phi^k)[u]\Big]\Big], && k < n \\
&\Phi_{\mathrm{NRNPI}}^{n,k}[u] = u, && k \ge n
\end{aligned}$$

for $u \in \mathbf{L^2}$. If $u = \phi^k$ is the numerical approximation after k steps, then application of $\Phi^{n,k}_{\mathrm{NRNPI}}$ with $n > k$ corresponds to performing another $n-k$ steps, such that $\Phi^{n,k}_{\mathrm{NRNPI}}(\phi^k) = \phi^n$ is the numerical approximation after n steps. However, note that even if $u \neq \phi^k$ is an arbitrary function, the numerical approximations $\phi^k, \dots, \phi^n$ are used in the numerical flow operators Φ_{NRNPI}. In order to be able to state a stability estimate for $\Phi^{n,k}_{\mathrm{NRNPI}}$ and in the further error analysis, we require the following

Assumption 3.10. *There is a constant τ_0 independent of ε such that for all $\tau \leq \tau_0$ and $\varepsilon \in (0,1)$, the numerical approximations ϕ^n remain uniformly bounded in $\mathbf{H^2}$:*

$$\phi^n \in \mathbf{B^2}(M_{\mathrm{num}}) \qquad \text{for all } n = 0, 1, ..., \lfloor T/\tau \rfloor$$

for some constant M_{num} independent of τ and ε.

In fact, one can prove with a bootstrapping argument that this assumption is indeed fulfilled if the step size is sufficiently small, cf. [JK23; Lub08]. This step size restriction is not critical, since it is independent of ε.

Lemma 3.11. *Under Assumptions 3.1 (A) and 3.10, we have for all $k, n \in \mathbb{N}$ with $k, n \leq \lfloor T/\tau \rfloor$ that*

$$\left|\!\left|\!\left| \Phi^{n,k}_{\mathrm{NRNPI}}[u] \right|\!\right|\!\right|_{\mathbf{L^2}} \leq \mathrm{e}^{Ct_n} \left|\!\left|\!\left| u \right|\!\right|\!\right|_{\mathbf{L^2}} \qquad \text{for all } u \in \mathbf{L^2}$$

for some constant C independent of n, k, τ and ε.

In the proof of this lemma (see Section 3.6.4), Lemma 3.9 (i) will be applied recursively. Assumption 3.10 guarantees that the constant C therein can always be chosen identically, and in particular independently of τ and ε.

We are now in a position to state and prove an error estimate for the NRNPI, which is the main result of this paper.

Theorem 3.12. *Let Assumptions 3.1 and 3.10 hold and let τ_0 be the constant from the latter. Further, for $\varepsilon \in (0,1)$ arbitrary, let ϕ^ε be the exact solution of (3.13) and let ϕ^n be the numerical approximations of the NRNPI for any step size $\tau \leq \tau_0$ with $\tau \notin \{\frac{k}{2}\pi\varepsilon^2, \frac{k}{3}\pi\varepsilon^2, k \in \mathbb{N}\}$. Then, the error bound*

$$\left|\!\left|\!\left| \phi^\varepsilon(t_n) - \phi^n \right|\!\right|\!\right|_{\mathbf{L^2}} \leq C_\star \left(1 + \frac{1}{K(\tau,\varepsilon)}\right) \tau^2, \qquad n = 0, 1, ..., \lfloor T/\tau \rfloor,$$

holds for some constant $C_\star$ independent of τ and ε and with

$$K(\tau,\varepsilon) := \min_{q \in \{2,4,6\}} \left| \mathrm{e}^{\mathrm{i}q\tau/\varepsilon^2} - 1 \right|. \tag{3.44}$$

According to (3.19), the theorem directly yields an error bound for the approximations $\psi^n \approx \psi^\varepsilon(t_n)$ defined in (3.18):

Corollary 3.13. *Under the assumptions of and with the constant $C_\star$ from Theorem 3.12, we have*

$$\left\| \psi^n - \psi^\varepsilon(t_n) \right\|_{L^2} \leq C_\star \left(1 + \frac{1}{K(\tau,\varepsilon)}\right) \tau^2, \qquad n = 0, 1, ..., \lfloor T/\tau \rfloor.$$

Before we continue with the proof of Theorem 3.12, it is crucial to note that the right-hand side of the estimate contains the τ-dependent number $1/K(\tau,\varepsilon)$, which might be very large if an unsuitable step size is chosen. We now discuss to what extent ensuring $K(\tau,\varepsilon) \not\approx 0$ is possible. For a fixed value of ε, we distinguish two cases. If $\tau \geq \frac{\pi}{4}\varepsilon^2$, then one can choose the step sizes

$$\tau = \frac{(2k-1)}{4}\pi\varepsilon^2, \qquad k \in \mathbb{N}. \tag{3.45}$$

It follows from (3.44) that $K(\tau,\varepsilon) = \sqrt{2}$ for this choice of τ. One can check that this is the maximal possible value, which is why we call the step sizes (3.45) *optimal*. On the other hand, one should avoid the *resonant step sizes*

$$\tau = \frac{k}{2}\pi\varepsilon^2 \qquad \text{or} \qquad \tau = \frac{k}{3}\pi\varepsilon^2, \qquad k \in \mathbb{N}, \tag{3.46}$$

for which $K(\tau,\varepsilon) = 0$. This is the reason why these step sizes were excluded in Theorem 3.12. For a step size in between the optimal and the resonant ones, the size of $1/K(\tau,\varepsilon)$ and thus of the error bound depends on how close it is to a resonant step size. This is illustrated in Figure 3.1 (a) in Section 3.5, where the function $\tau \mapsto \frac{\tau^2}{K(\tau,\varepsilon)}$ is plotted for $\varepsilon = 0.01$ together with markers of the optimal and the resonant step sizes. In practice, however, we recommend replacing a given step size by the closest optimal step size, which is at most $\frac{\pi}{4}\varepsilon^2$ away.

If $\tau < \frac{\pi}{4}\varepsilon^2$, on the other hand, it is no longer possible to ensure that $K(\tau,\varepsilon) \not\approx 0$ since $K(\tau,\varepsilon) \to 0$ for $\tau \to 0$. Instead, we can only show the lower bound

$$K(\tau,\varepsilon) = \min_{q\in\{2,4,6\}} \left|\mathrm{e}^{\mathrm{i}q\tau/\varepsilon^2} - 1\right| = \left|\mathrm{e}^{\mathrm{i}2\tau/\varepsilon^2} - 1\right| = 2\sin(\tau/\varepsilon^2) > \frac{4\sqrt{2}}{\pi}\frac{\tau}{\varepsilon^2},$$

where we used that

$$|\mathrm{e}^{\mathrm{i}x} - 1| = \sqrt{(\cos(x)-1)^2 + \sin^2(x)} = \sqrt{2 - 2\cos(x)} = 2\sin\left(\tfrac{x}{2}\right) \qquad \text{for } x \in [0, 2\pi]$$

and that $\sin(x) > \frac{2\sqrt{2}}{\pi}x$ for $x \in (0, \frac{\pi}{4})$. This implies

$$\left(1 + \frac{1}{K(\tau,\varepsilon)}\right)\tau^2 < \tau^2 + \frac{\pi}{4\sqrt{2}}\varepsilon^2\tau < \left(1 + \frac{1}{\sqrt{2}}\right)\frac{\pi}{4}\varepsilon^2\tau,$$

which means that the error of the NRNPI decreases only linearly, but in return, the error constant is proportional to ε^2. Altogether, we obtain the following

Corollary 3.14. *In the setting of Corollary 3.13, we have*

$$\|\psi^n - \psi^\varepsilon(t_n)\|_{L^2} \leq C_\star\left(1 + \frac{1}{\sqrt{2}}\right)\tau^2 \qquad \text{for optimal } \tau \geq \frac{\pi}{4}\varepsilon^2,$$
$$\|\psi^n - \psi^\varepsilon(t_n)\|_{L^2} \leq C_\star\left(1 + \frac{1}{\sqrt{2}}\right)\frac{\pi}{4}\varepsilon^2\tau \qquad \text{for } \tau < \frac{\pi}{4}\varepsilon^2.$$

In the first case, the error of the NRNPI is not larger than the one of the full NPI-2, even though many terms have been omitted from the numerical flow. Only if extremely small errors of less than $\mathcal{O}(\varepsilon^4)$ are required, the second case, where the NRNPI is inferior, becomes relevant.

Proof of Theorem 3.12. Let $e^n = \phi^\varepsilon(t_n) - \phi^n$ be the global error at time t_n. The linearity of $\Phi_{\mathrm{NRNPI}}(t,u)$ for fixed u allows decomposing e^n as

$$e^n = \phi^\varepsilon(t_n) - \Phi_{\mathrm{NRNPI}}(t_{n-1},\phi^{n-1})[\phi^{n-1}] = \ell^n + d^n + \Phi_{\mathrm{NRNPI}}(t_{n-1},\phi^{n-1})[e^{n-1}]$$

with $\ell^n = \phi^\varepsilon(t_n) - \Phi_{\mathrm{NRNPI}}(t_{n-1},\phi^\varepsilon(t_{n-1}))[\phi^\varepsilon(t_{n-1})]$ being the local error and

$$d^n := \Phi_{\mathrm{NRNPI}}(t_{n-1},\phi^\varepsilon(t_{n-1}))[\phi^\varepsilon(t_{n-1})] - \Phi_{\mathrm{NRNPI}}(t_{n-1},\phi^{n-1})[\phi^\varepsilon(t_{n-1})] \tag{3.47}$$

accounting for perturbations in the linear flow operator Φ_{NRNPI}. Dissolving the recursion formula yields

$$\begin{aligned} e^n &= \ell^n + d^n + \Phi_{\mathrm{NRNPI}}(t_{n-1},\phi^{n-1})\left[\ell^{n-1} + d^{n-1} + \Phi_{\mathrm{NRNPI}}(t_{n-2},\phi^{n-2})[e^{n-2}]\right] \\ &= \ldots = \sum_{k=1}^n \Phi_{\mathrm{NRNPI}}^{n,k}[\ell^k] + \sum_{k=1}^n \Phi_{\mathrm{NRNPI}}^{n,k}[d^k]. \end{aligned} \tag{3.48}$$

Here, we used the definition and linearity of $\Phi_{\mathrm{NRNPI}}^{n,k}$ and that $e^0 = \phi^\varepsilon(t_0) - \phi^0 = 0$. Again using the linearity of $\Phi_{\mathrm{NRNPI}}^{n,k}$ and the decomposition of the local error ℓ^k from (3.42), the first sum can be decomposed to

$$\sum_{k=1}^n \Phi_{\mathrm{NRNPI}}^{n,k}[\ell^k] = \sum_{k=1}^n \Phi_{\mathrm{NRNPI}}^{n,k}[\ell_{\mathrm{NPI}}^k] + \sum_{k=1}^n \Phi_{\mathrm{NRNPI}}^{n,k}[\ell_{\mathrm{diff}}^k]. \tag{3.49}$$

Now, the lemmas established before allow deriving suitable bounds for the norm of each of the sums appearing in (3.48) or (3.49). In the first sum of (3.49), we can "afford" to lose one τ since ℓ_{NPI}^k is in $\mathcal{O}(\tau^3)$. Thus, we can use triangle inequality together with Lemma 3.11 to obtain

$$\begin{aligned} \left\|\!\left|\sum_{k=1}^n \Phi_{\mathrm{NRNPI}}^{n,k}\left[\ell_{\mathrm{NPI}}^k\right]\right|\!\right\|_{\mathbf{L^2}} &\le \sum_{k=1}^n \left\|\!\left|\Phi_{\mathrm{NRNPI}}^{n,k}\left[\ell_{\mathrm{NPI}}^k\right]\right|\!\right\|_{\mathbf{L^2}} \le \sum_{k=1}^n \mathrm{e}^{Ct_n}\left\|\!\left|\ell_{\mathrm{NPI}}^k\right|\!\right\|_{\mathbf{L^2}} \\ &\le \sum_{k=1}^n C\mathrm{e}^{Ct_n}\tau^3 \le CT\mathrm{e}^{CT}\tau^2. \end{aligned} \tag{3.50}$$

To control the second sum in (3.49), however, we rely on cancellation of errors from different time steps, such that a more sophisticated analysis is required here. Recalling the structure of ℓ_{diff}^k from Lemma 3.8 and using summation by parts, we have

$$\begin{aligned} \sum_{k=1}^n \Phi_{\mathrm{NRNPI}}^{n,k}\left[\ell_{\mathrm{diff}}^k\right] &= \tau^2 \sum_{q\in\mathcal{Q}}\sum_{k=1}^n \mathrm{e}^{\mathrm{i}qt_{k-1}/\varepsilon^2}\Phi_{\mathrm{NRNPI}}^{n,k}\left[E_q^{k-1}\right] \\ &= \tau^2 \sum_{q\in\mathcal{Q}} \Phi_{\mathrm{NRNPI}}^{n,n}\left[E_q^{n-1}\right]\sum_{k=1}^n \mathrm{e}^{\mathrm{i}qt_{k-1}/\varepsilon^2} \\ &\quad + \tau^2 \sum_{q\in\mathcal{Q}}\sum_{k=1}^{n-1}\left(\Phi_{\mathrm{NRNPI}}^{n,k}\left[E_q^{k-1}\right] - \Phi_{\mathrm{NRNPI}}^{n,k+1}\left[E_q^{k}\right]\right)\sum_{j=1}^k \mathrm{e}^{\mathrm{i}qt_{j-1}/\varepsilon^2}. \end{aligned}$$

Since $\Phi_{\mathrm{NRNPI}}^{n,n}[\cdot] = \mathrm{Id}$, we obtain

$$\begin{aligned} \left\|\!\left|\sum_{k=1}^n \Phi_{\mathrm{NRNPI}}^{n,k}\left[\ell_{\mathrm{diff}}^k\right]\right|\!\right\|_{\mathbf{L^2}} &\le \tau^2 \sum_{q\in\mathcal{Q}}\left\|\!\left|E_q^{n-1}\right|\!\right\|_{\mathbf{L^2}}\left|\sum_{k=1}^n \mathrm{e}^{\mathrm{i}qt_{k-1}/\varepsilon^2}\right| \\ &\quad + \tau^2 \sum_{q\in\mathcal{Q}}\sum_{k=1}^{n-1}\left\|\!\left|\Phi_{\mathrm{NRNPI}}^{n,k}\left[E_q^{k-1}\right] - \Phi_{\mathrm{NRNPI}}^{n,k+1}\left[E_q^{k}\right]\right|\!\right\|_{\mathbf{L^2}}\left|\sum_{j=1}^k \mathrm{e}^{\mathrm{i}qt_{j-1}/\varepsilon^2}\right|. \end{aligned}$$

In the first term, only the complex numbers oscillating on the unit circle are summed up. For nonresonant step sizes, the modulus of this sum does not grow with n since by the geometric sum formula, we have

$$\left|\sum_{k=1}^{n} \mathrm{e}^{\mathrm{i}q t_{k-1}/\varepsilon^2}\right| = \left|\sum_{k=0}^{n-1} \mathrm{e}^{\mathrm{i}q t_k/\varepsilon^2}\right| = \left|\sum_{k=0}^{n-1} \left(\mathrm{e}^{\mathrm{i}q\tau/\varepsilon^2}\right)^k\right| = \left|\frac{\mathrm{e}^{\mathrm{i}q t_n/\varepsilon^2}-1}{\mathrm{e}^{\mathrm{i}q\tau/\varepsilon^2}-1}\right| \leq \frac{2}{\left|\mathrm{e}^{\mathrm{i}q\tau/\varepsilon^2}-1\right|} \leq \frac{2}{K(\tau,\varepsilon)}$$

for all $q \in \mathcal{Q}$. Together with the uniform bound for the norm of E_q^{n-1} from Lemma 3.8, we infer that the first term is in $\mathcal{O}\left(\frac{\tau^2}{K(\tau,\varepsilon)}\right)$. Further, using the properties of Φ_{NRNPI} and $\Phi_{\mathrm{NRNPI}}^{n,k}$ from Lemmas 3.9 and 3.11, respectively, and the properties for the error components E_q from Lemma 3.8, we obtain for $k \leq n-1$ that

$$\begin{aligned}
&\left\|\!\left|\Phi_{\mathrm{NRNPI}}^{n,k}\left[E_q^{k-1}\right] - \Phi_{\mathrm{NRNPI}}^{n,k+1}\left[E_q^{k}\right]\right|\!\right\|_{\mathbf{L^2}} \\
&\quad \leq \left\|\!\left|\Phi_{\mathrm{NRNPI}}^{n,k}\left[E_q^{k-1}\right] - \Phi_{\mathrm{NRNPI}}^{n,k}\left[E_q^{k}\right]\right|\!\right\|_{\mathbf{L^2}} + \left\|\!\left|\Phi_{\mathrm{NRNPI}}^{n,k}\left[E_q^{k}\right] - \Phi_{\mathrm{NRNPI}}^{n,k+1}\left[E_q^{k}\right]\right|\!\right\|_{\mathbf{L^2}} \\
&\quad = \left\|\!\left|\Phi_{\mathrm{NRNPI}}^{n,k}\left[E_q^{k-1} - E_q^{k}\right]\right|\!\right\|_{\mathbf{L^2}} + \left\|\!\left|\Phi_{\mathrm{NRNPI}}^{n,k+1}\left[\Phi_{\mathrm{NRNPI}}(t_k,\phi^k)\left[E_q^{k}\right] - E_q^{k}\right]\right|\!\right\|_{\mathbf{L^2}} \\
&\quad \leq \mathrm{e}^{Ct_n}\left\|\!\left|E_q^{k-1} - E_q^{k}\right|\!\right\|_{\mathbf{L^2}} + \mathrm{e}^{Ct_n}\left\|\!\left|\left(\Phi_{\mathrm{NRNPI}}(t_k,\phi^k) - \mathrm{Id}\right)\left[E_q^{k}\right]\right|\!\right\|_{\mathbf{L^2}} \\
&\quad \leq \mathrm{e}^{Ct_n} C\tau + \mathrm{e}^{Ct_n} C\tau \left\|\!\left|\left[E_q^{k}\right]\right|\!\right\|_{\mathbf{H^2}} \leq C\tau \mathrm{e}^{CT}.
\end{aligned}$$

Overall, we have

$$\left\|\!\left|\sum_{k=1}^{n} \Phi_{\mathrm{NRNPI}}^{n,k}\left[\ell_{\mathrm{diff}}^k\right]\right|\!\right\|_{\mathbf{L^2}} \leq \tau^2 \sum_{q\in\mathcal{Q}} C\frac{2}{K(\tau,\varepsilon)} + \tau^2 \sum_{q\in\mathcal{Q}} \sum_{k=1}^{n-1} C\tau \mathrm{e}^{CT}\frac{2}{K(\tau,\varepsilon)} \leq \tau^2 \frac{CT\mathrm{e}^{CT}}{K(\tau,\varepsilon)}. \quad (3.51)$$

Now, it remains to control the second sum in (3.48). Recall the definition of d^k from (3.47). Since $\phi^\varepsilon(t_{k-1}) \in \mathbf{B^2}(M_{\mathrm{ex}})$ and $\phi^{k-1} \in \mathbf{B^2}(M_{\mathrm{num}})$ by Assumptions 3.1 and 3.10, respectively, we can use Lemma 3.9 (iii) with $R = \max\{M_{\mathrm{ex}}, M_{\mathrm{num}}\}$ to obtain

$$\left\|\!\left|d_k\right|\!\right\|_{\mathbf{L^2}} \leq C\tau \left\|\!\left|\phi^\varepsilon(t_{k-1}) - \phi^{k-1}\right|\!\right\|_{\mathbf{L^2}} = C\tau \left\|\!\left|e^{k-1}\right|\!\right\|_{\mathbf{L^2}}.$$

The triangle inequality together with Lemma 3.11 then yields

$$\left\|\!\left|\sum_{k=1}^{n} \Phi_{\mathrm{NRNPI}}^{n,k}[d^k]\right|\!\right\|_{\mathbf{L^2}} \leq \mathrm{e}^{Ct_n} \sum_{k=1}^{n} \left\|\!\left|d^k\right|\!\right\|_{\mathbf{L^2}} \leq C\mathrm{e}^{CT}\tau \sum_{k=1}^{n} \left\|\!\left|e^{k-1}\right|\!\right\|_{\mathbf{L^2}}. \quad (3.52)$$

Finally, combining (3.48) - (3.52), we have

$$\left\|\!\left|e^n\right|\!\right\|_{\mathbf{L^2}} \leq C\tau^2\left(1 + \frac{1}{K(\tau,\varepsilon)}\right) + C\tau \sum_{k=1}^{n} \left\|\!\left|e^{k-1}\right|\!\right\|_{\mathbf{L^2}}.$$

The discrete Gronwall Lemma inequality implies

$$\left\|\!\left|e^n\right|\!\right\|_{\mathbf{L^2}} \leq C\tau^2\left(1 + \frac{1}{K(\tau,\varepsilon)}\right)\mathrm{e}^{nC\tau} \leq C\tau^2\left(1 + \frac{1}{K(\tau,\varepsilon)}\right)\mathrm{e}^{CT},$$

which completes the proof. □

Remark 3.15. *Since the local errors of the NRNPI contain those of the NPI-2 (ℓ_{NPI}^k) and additionally the terms that have been omitted from it (ℓ_{diff}^k), the error analysis of the NRNPI is more involved than of the full NPI-2. Nevertheless, we were able to present it in detail*

in the proof above. This is worth mentioning since in the work [CW22], where the authors presented the original version of the NPI-2, they refrained from an error analysis due to the plethora of terms in the numerical flow. It was the structured formulation of the NPI-2 and the NRNPI in (3.32)-(3.35) and (3.39)-(3.41), respectively, that made the error analysis in this section manageable. In fact, Lemmas 3.9, 3.11 and 3.17 could easily be extended to the NPI-2. A uniform second-order global error bound could then be proven with standard techniques and without requiring summation by parts.

Remark 3.16. *The entire error analysis can also be carried out in H^r instead of L^2 if more regularity is available. For error bounds in H^r, we only have to replace H^2 by H^{2+r} in Assumptions 3.1 (A) and 3.10 as well as H^4 by H^{4+r} in Assumption 3.1 (B). If $r > 3/2$, then H^r is an algebra, which simplifies things because (3.3) and (3.4) can then be replaced by the single inequality*

$$\|uv\|_{H^r} \leq C_S \|u\|_{H^r} \|v\|_{H^r}, \qquad u \in H^r(\mathbb{R}^3),\ v \in H^r(\mathbb{R}^3),$$

and (3.5) and (3.6) by

$$\|u^* v\|_{H^r} \leq C_S \|u\|_{H^r} \|v\|_{H^r}, \qquad u \in \left(H^r(\mathbb{R}^3)\right)^4,\ v \in \left(H^r\mathbb{R}^3)\right)^4.$$

3.5 Numerical illustrations

In this section, we illustrate the results of our error analysis for the NRNPI by numerical experiments. Furthermore, we compare the efficiency of the NRNPI and the NPI-2.

3.5.1 Problem setting and details about the numerical computations

For simplicity, we consider the NLDE in one space dimension, where it can be reduced to

$$\partial_t \psi^\varepsilon(t,x) = -\frac{\mathrm{i}}{\varepsilon^2}\widetilde{\mathcal{T}}_\varepsilon \psi^\varepsilon(t,x) - \mathrm{i}\widetilde{W}(t,x)\psi^\varepsilon(t,x) - \mathrm{i}\widetilde{F}(\psi^\varepsilon)\psi^\varepsilon(t,x), \qquad t > 0,\ x \in \mathbb{R}$$

with a two-component solution $\psi^\varepsilon(t,x) \in \mathbb{C}^2$ and

$$\widetilde{\mathcal{T}}_\varepsilon = -\mathrm{i}\varepsilon\sigma_1\partial_x + \sigma_3, \qquad \widetilde{W}(t,x) = V(t,x)I_2 - A_1(t,x)\sigma_1, \qquad \widetilde{F}(u) = |u|^2 I_2,$$

see e.g. [Bao+16b]. To keep notation simple, we omit the tilde in the following. For this reduced system, the construction of the NRNPI as well as the error analysis can be carried out in exactly the same manner.

In the numerical computations, we have to replace the unbounded domain by a sufficiently large, but bounded interval $\Omega = [a,b]$ and impose periodic boundary conditions as, e.g., in [Bao+16b; BCY21; CW22]. For the space discretization, we define grid points $x_j = (a+b)/2 + jh$, $j = -M, ..., M-1$, with mesh size $h = (b-a)/2M$ for $M = 128$ and compute all spatial derivatives by Fourier pseudospectral techniques.

The initial data, the potential functions and the interval Ω are chosen as in [Bao+16b; CW22], i.e.

$$\psi_1^{\text{init}}(x) = e^{-x^2/2}, \quad \psi_2^{\text{init}}(x) = e^{-(x-1)^2/2}, \quad V(x) = \frac{1-x}{1+x^2}, \quad A_1(x) = \frac{(x+1)^2}{1+x^2}$$

for $x \in \Omega = [-16, 16]$. We consider time intervals $[0,T]$ with two slightly different values of T which are specified below. All numerical computations on $[0,T]$ are carried out with

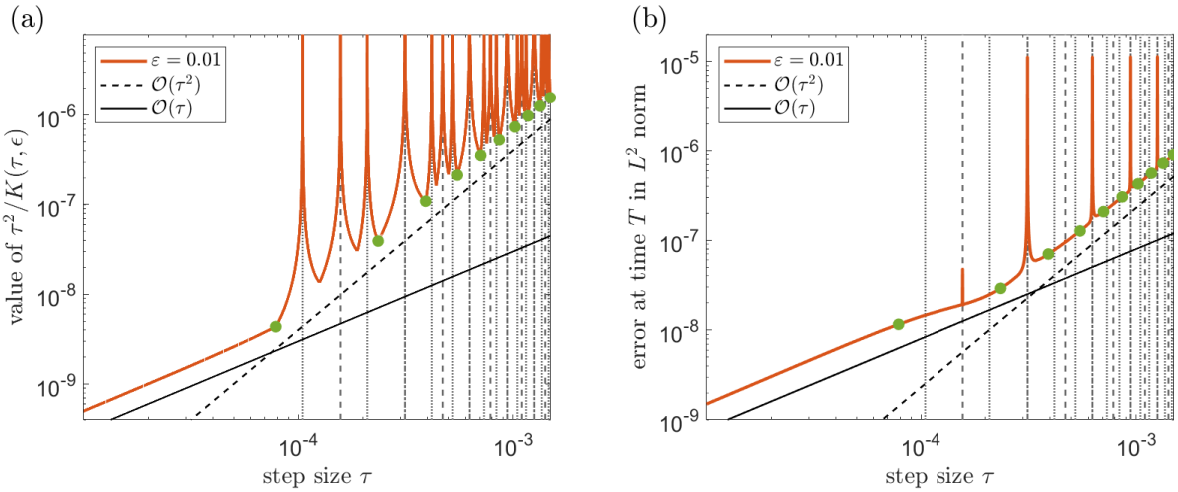

Figure 3.1: The behavior of the function $\tau \mapsto \frac{\tau^2}{K(\tau,\varepsilon)}$ (left) compared to the error at time $T = 0.3360\pi$ of the NRNPI (right) for $\varepsilon = 0.01$. In both plots, the axis limits for the step size τ are the same. The green dots depict the function values for the optimal step sizes (3.45). Further, the vertical gray lines mark the resonant step sizes (3.46), where we distinguish between the multiples of $\pi\varepsilon^2$ (dash-dotted) and the additional multiples of $\frac{\pi\varepsilon^2}{2}$ (dashed) or $\frac{\pi\varepsilon^2}{3}$ (dotted). The black lines are first (solid) and second (dashed) order reference lines.

step sizes $\tau = T/N$, where $N \in \mathbb{N}$ is the number of time steps. This means, in particular, that not all positive real numbers are possible step sizes, which will be important later on. We apply both the NPI-2 and the NRNPI to compute approximations $\psi^1, \dots, \psi^N$ via (3.18). For all error plots, we then compare the approximations ψ^N at the final time $t_N = T$ with a reference solution $\psi(T)$ of the NLDE. To compute the latter, we use the same spatial grid and applied MATLAB's `ode45` routine with very small absolute and relative tolerances. All errors are measured in the L^2-norm, which is approximated by $\|u\|_{L^2}^2 \approx \sum_{k=-M}^{M-1} |\widehat{u}_k|^2$ for a periodic function $u \in \left(L^2(\Omega)\right)^2$ with Fourier coefficients $\widehat{u}_k \in \mathbb{C}^2, k \in \mathbb{Z}$.

3.5.2 Accuracy

First, we want to observe how the accuracy of the NRNPI depends on the step size τ. While doing so, we pay special attention to the performance of the NRNPI for optimal step sizes (3.45) and for resonant step sizes (3.46). This is why we choose T in such a way that for $\varepsilon \in \{0.005, 0.01, 0.02\}$, many of the optimal and resonant step sizes are hit by $\tau = T/N$ for some $N \in \mathbb{N}$. A suitable choice is $T = 0.336\pi \approx 1$. Then, for $\varepsilon = 0.02$, the resonant step sizes $\tau = \frac{k}{2}\pi\varepsilon^2$ with $k \in \mathbb{N}$ have the form $\tau = T/N$ for some $N \in \mathbb{N}$ if

$$N = \frac{2T}{k\pi}\varepsilon^{-2} = \frac{T}{2k\pi}10^4 = \frac{3360}{2k} \tag{3.53}$$

is an integer, which is true if $k \in \{1, \dots, 8, 10, 12, 14, 15, 16 \dots\}$. The same holds for $\varepsilon = 0.01$ or $\varepsilon = 0.005$, because dividing ε by 2 in (3.53) simply corresponds to multiplying N by 4. Similar considerations can be made for resonant step sizes of the form $\tau = \frac{k}{3}\pi\varepsilon^2$ and for the optimal step sizes (3.45).

Figure 3.1 (b) shows the L^2-error of the NRNPI for $\varepsilon = 0.01$ at the final time $T = 0.336\pi$ in dependency of the time step size τ. By comparing the red line with the black dashed reference line, one can see that for $\tau \geq \frac{\pi}{4}\varepsilon^2$, the error of the NRNPI is indeed proportional

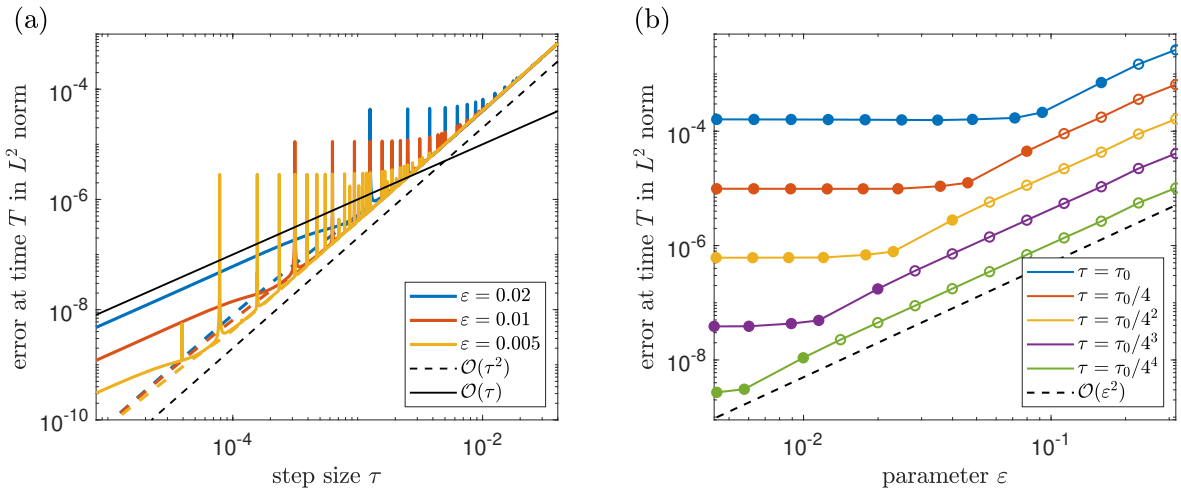

Figure 3.2: Left: L^2-error of the NRNPI (solid) and the NPI-2 (dashed) at time $T = 0.3360\pi$ in dependency of the step size τ for three different values of ε. Right: L^2-error of the NRNPI at time $T = 1$ in dependency of ε for five different step sizes τ, namely $\tau_0 = 0.02$ and fractions thereof. The filled markers correspond to ε-values for which the respective step size is optimal.

to τ^2 if optimal step sizes (represented by the green markers) are chosen. The error can, however, be much larger for step sizes close to the resonant step sizes (depicted by the gray vertical lines). For $\tau < \frac{\pi}{4}\varepsilon^2$ (i.e. left of the leftmost green marker), only linear convergence is observed. This error behavior agrees perfectly with the Corollaries 3.13 and 3.14. What comes as a surprise is that *not all* resonant step sizes seem to be harmful, because in contrast to the function $\tau \mapsto \frac{\tau^2}{K(\tau,\varepsilon)}$ depicted in (a), the error plot in (b) does only have a spike at *some* of the resonant step sizes. This interesting effect will be discussed below.

The way how this error behavior changes for other values of ε is illustrated in Figure 3.2 (a). The red line is the same as in Figure 3.1 (b), but the corresponding results for $\varepsilon = 0.02$ (blue) and $\varepsilon = 0.005$ (yellow) are added. It can be seen that the error constant of the linear convergence for $\tau < \frac{\pi}{4}\varepsilon^2$ decreases significantly with ε, which again corroborates our error analysis; cf. Corollaries 3.13 and 3.14. The dashed lines in blue, red, and yellow show the error of the full NPI-2. As expected, all of them almost coincide, because the NPI-2 is uniformly accurate. Comparing the solid colored lines with the dashed ones shows that for nonresonant step sizes the NRNPI has almost exactly the same accuracy as the NPI-2, although a huge number of terms of the latter have been omitted in the former. Only for very small step sizes, the accuracy of the NPI-2 is better, because then the $\mathcal{O}(\tau\varepsilon^2)$-errors of the NRNPI are larger than the $\mathcal{O}(\tau^2)$-errors of the NPI-2. More precisely, this is the case if $\tau < C\varepsilon^2$ for some constant C. In this experiment, the value $C \approx \frac{3\pi}{4}$ can be observed. However, we emphasize that at the threshold $\tau = C\varepsilon^2$ the error has already been reduced to $\mathcal{O}(\varepsilon^4)$, which should be sufficient for most applications.

Figure 3.2 (b) illustrates how the error of the NRNPI scales for several fixed step sizes, but varying values of ε. Here, the special choice of T made before is no longer necessary, such that we use $T = 1$ instead. In the regime $\varepsilon \leq \left(\frac{4\tau}{\pi}\right)^{1/2}$, i.e. for $\tau \geq \frac{\pi}{4}\varepsilon^2$, only values of ε have been chosen for which the respective step size is one of the optimal step sizes $\tau = \frac{2k-1}{4}\pi\varepsilon^2$ from Eq. (3.45), i.e. $\varepsilon = \left(\frac{4\tau}{(2k-1)\pi}\right)^{1/2}$ for some $k \in \mathbb{N}$. Those values of ε are depicted by the filled markers. The numbers $k = 1, 2, 3$ (furthermost right filled markers)

and $k = 6, 11, 21, 41, ...$ (other filled markers) were chosen for a suitable distribution on the logarithmic axis. Apart from the one for $k = 1$, all markers for the same step size are nearly at the same height, which again confirms that the error is independent of ε for optimal step sizes $\tau \geq \frac{\pi}{4}\varepsilon^2$, in accordance with Corollary 3.14. In contrast, in the regime $\tau < \frac{\pi}{4}\varepsilon^2$ (empty markers), a comparison with the reference line yields that the error scales quadratically with ε, as predicted by Corollary 3.14.

All in all, the numerical experiments agree nicely with the main results of our error analysis. However, these experiments also suggest that in practice, the performance of the NRNPI is even better than predicted by theory. The following three aspects are interesting in this context.

Resonant but harmless step sizes. In view of Figure 3.1, it seems that not all resonant step sizes (3.46) do indeed cause a large error. In fact, apart from the furthermost left, all spikes appear at multiples of $\pi\varepsilon^2$, and there are no spikes at those multiples of $\frac{\pi\varepsilon^2}{2}$ or $\frac{\pi\varepsilon^2}{3}$ that are not a multiple of $\pi\varepsilon^2$ as well. Those step sizes had to be excluded such that the terms of the form (3.37) for $q = \pm 4$ or $q = \pm 6$, respectively, do indeed have prefactors pointing in different directions on the complex plane. As an example, we analyze the term in the second line of (3.33). Here, one combination of indices leading to the value $q = 6$ in the exponent is $J = (1, 1, 1)$, $\sigma = -1$ and $p = 2$. The corresponding term that has been omitted for the flow of the NRNPI, evaluated for a solution $u = \phi^\varepsilon(t_n) = (\phi^\varepsilon_{-1}(t_n), \phi^\varepsilon_{+1}(t_n))$ of the transformed Dirac equations, is

$$\mathrm{e}^{6\mathrm{i}t/\varepsilon^2}\mathcal{B}_{-1}(4,2)\Pi^\varepsilon_{-1}\left[\left(\widehat{G}^{(2)}_{-1}(\phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]\right)^* \phi^\varepsilon_{+1}(t_n)\phi^\varepsilon_{+1}(t_n)\right] \tag{3.54}$$

with

$$\widehat{G}^{(2)}_{-1}(\phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)] = -\mathrm{i}\Pi^\varepsilon_{-1}\left[(\phi^\varepsilon_{+1}(t_n))^*\phi^\varepsilon_{-1}(t_n)\phi^\varepsilon_{-1}(t_n)\right].$$

Noting that ϕ^ε_{-1} and ϕ^ε_{+1} are in the range of the opposing projectors Π^ε_{-1} and Π^ε_{+1}, respectively, and considering an expansion of $\Pi^\varepsilon_{\mp 1}$ w.r.t. ε, it was shown in [CW19, Eq. (3.25) and (3.26)], however, that

$$\left\|(\phi^\varepsilon_{+1}(s))^*\phi^\varepsilon_{-1}(s)\right\|_{L^2} \leq C\varepsilon, \quad \left\|\Pi^\varepsilon_{-1}\left[u\phi^\varepsilon_{+1}(s)\right]\right\|_{L^2} \leq C\varepsilon, \quad \left\|\Pi^\varepsilon_{+1}\left[u\phi^\varepsilon_{-1}(s)\right]\right\|_{L^2} \leq C\varepsilon$$

for any $s \in [0, T]$, any sufficiently regular, scalar-valued function u, and a constant C independent of ε. This yields

$$\left\|\widehat{G}^{(2)}_{-1}(\phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]\right\|_{L^2} \leq C\varepsilon, \quad \left\|\Pi^\varepsilon_{-1}\left[\left(\widehat{G}^{(2)}_{-1}(\phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]\right)^* \phi^\varepsilon_{+1}(t_n)\phi^\varepsilon_{+1}(t_n)\right]\right\|_{L^2} \leq C\varepsilon^2.$$

Thus, the terms in (3.54) are actually not only in $\mathcal{O}(\tau^2)$, but even in $\mathcal{O}(\tau^2\varepsilon^2)$ and hence also in $\mathcal{O}(\tau^3)$ for $\tau \geq \frac{\pi}{4}\varepsilon^2$. Consequently, in our error analysis, we do not rely on non-accumulation of the error terms obtained by omitting terms of the form (3.54). All other terms with $q = 6$ or $q = -6$ in the exponent can be analyzed in a similar way, which explains the absence of spikes at

$$\tau = \frac{k}{3}\pi\varepsilon^2, \qquad k \in \mathbb{N} \setminus \{3, 6, 9, \ldots\}$$

in Figures 3.1 (b) and 3.2 (a), and which implies that the corresponding step size restriction *is actually not necessary*. A corresponding analysis for $q = \pm 4$, however, does not cover all terms, such that we do not have a full explanation for the other missing spikes.

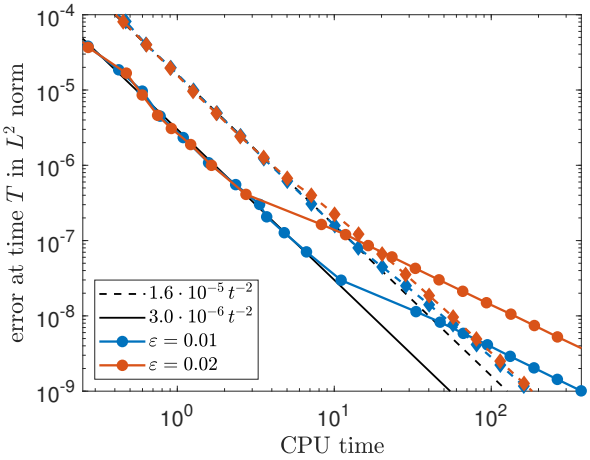

Figure 3.3: L^2-error of the NRNPI (solid, circles) and the NPI-2 (dashed, diamonds) at time $T = 1$ in dependency of the computing time for two different values of ε. Each marker corresponds to an approximation with a different step size.

Bounded error for resonant step sizes. By definition of $K(\tau, \varepsilon)$, the function $\tau \mapsto \tau^2/K(\tau, \varepsilon)$ has a singularity at the resonant step sizes (3.46), which is illustrated in Figure 3.1 (a). Hence, Corollary 3.13 suggests that the error of the NRNPI would be unbounded if a resonant step size was used. In contrast, Figure 3.1 (b) reveals that even at those resonant step sizes where spikes indeed appear, the error grows only to a finite level. There are two explanations for this. First, NRNPI is a first-order uniformly accurate method for *all* step sizes τ, as we have seen in the discussion after Lemma 3.9. Indeed, the furthermost left large spikes for the different values of ε in Figure 3.2 (a) could be capped by a first-order reference line. Secondly, an alternative error bound can be derived by once more analyzing the norm of the operators $\mathcal{B}_\sigma(\delta, \zeta)$ contained in the terms (3.37) that have been omitted from the numerical flow of the full NPI-2. By the definition of $\mathcal{B}_\sigma(\delta, \zeta)$, cf. (3.31), and of the φ_1-function, we have

$$\mathcal{B}_\sigma(\delta, \zeta) = \frac{\varepsilon^2}{\mathrm{i}\zeta} \int_0^\tau \mathrm{e}^{\sigma \mathrm{i}(\tau - s)\mathcal{D}_\varepsilon} \mathrm{e}^{\mathrm{i}\delta s/\varepsilon^2} \left(\mathrm{e}^{\mathrm{i}\zeta s/\varepsilon^2} - 1 \right) \mathrm{d}s$$

for $\zeta \neq 0$, such that an $\mathcal{O}(\tau\varepsilon^2)$ bound in operator norm follows. In the case $\zeta = 0$, the same bound easily follows by integration by parts. Together with the local error terms from the full NPI-2, the local error of the NRNPI can be shown to be in $\mathcal{O}(\tau\varepsilon^2 + \tau^3)$, which in turn can be used to derive the bound $C(\varepsilon^2 + \tau^2)$ for the global error. In particular, for $\tau \leq \varepsilon$ (including resonant τ), the error is limited by $C\varepsilon^2$. This explains the constant height of all spikes for a given value of ε.

Accuracy for non-optimal but nonresonant step sizes. Whilst the optimal step sizes (3.45) provide a suitable choice for τ, many other nonresonant step sizes yield equally good results.

3.5.3 Efficiency

In the convergence analysis and the illustrations before, we have seen that for optimal step sizes in the regime $\tau \geq \frac{\pi}{4}\varepsilon^2$, the NRNPI yields equally accurate results as the NPI-2 applied with the same step size. However, since the numerical flow of the NRNPI was obtained by omitting many terms of the flow of the NPI-2, each time step of the former is significantly

cheaper than of the latter. In other words, if a certain computing time is available, more steps of the NRNPI can be conducted, yielding an improved accuracy. To show this effect, we apply both methods for different step sizes and then evaluate the error in dependency of the computing times required. In the regime $\tau \geq \frac{\pi}{4}\varepsilon^2$, only nonresonant step sizes are used. The results are depicted in Figure 3.3. A comparison of the constants of the two second-order reference lines therein shows that for large step sizes, the error of the NRNPI is approximately $3/16 = 18.75\%$ of the one of the NPI-2 for a fixed computing time. Conversely, to achieve a given accuracy which is not extremely high (i.e. errors not smaller than ε^4, up to a constant), the necessary computing time of the NRNPI is around $\sqrt{3/16} \approx 43.3\%$ of that of the NPI-2. In fact, it can be checked that the numerical flow of the NRNPI contains only around 32% of the terms of the flow of the NPI-2. The reason why this does not quite correspond to the improvement in terms of computing time is some computational overhead which is equally expensive for both methods, such as, e.g., the evaluation of all $\widehat{G}_\sigma^{(p)}$-operators or the evolution of the kinetic part.

For $\tau < \frac{\pi}{4}\varepsilon^2$ the error of the NRNPI is bounded by $C_1\varepsilon^2\tau$ with a constant C_1 according to Corollary 3.14, whereas the error of the NPI-2 is bounded by $C_2\tau^2$ for some C_2. Hence, the NPI-2 is more accurate for $\tau \leq (C_1/C_2)\varepsilon^2$. This means that if τ is sufficiently small, the full second order of NPI-2 starts to pay off and compensates the higher costs per time step, such that the NPI-2 outperforms the NRNPI. This is reflected by Figure 3.3: The point where the solid line crosses the dashed line of the same color has an ordinate (= error at time T) of approximately ε^4, i.e. 10^{-8} for the blue lines ($\varepsilon = 0.01$) and $1.6 \cdot 10^{-7}$ for the red lines ($\varepsilon = 0.02$). Since ε is assumed to be small, however, we believe that such a high accuracy is not required in many applications.

All in all, the NRNPI offers a significant efficiency gain as long as the desired accuracy is not extremely high. Moreover, the substantial reduction of the number of terms facilitates the implementation and in particular the debugging.

3.6 Proof of auxiliary lemmas

In this chapter, we present the proofs of the Lemmas 3.8, 3.9 and 3.11. In preparation thereto, we prove an additional lemma concerning properties of the operators $\widehat{G}_\sigma^{(p)}$ in Section 3.6.1. In several parts of the proofs, we will have to use that differences of two identically-structured products of two or three functions can be related to differences of the individual functions by inserting intermediate terms. In particular, we have

$$u^* v - \widetilde{u}^* \widetilde{v} = u^* (v - \widetilde{v}) + (u - \widetilde{u})^* \widetilde{v}, \tag{3.55}$$

$$u^* v w - \widetilde{u}^* \widetilde{v} \widetilde{w} = u^* v (w - \widetilde{w}) + u^* (v - \widetilde{v}) \widetilde{w} + (u - \widetilde{u})^* \widetilde{v} \widetilde{w} \tag{3.56}$$

for $u, v, w, \widetilde{u}, \widetilde{v}, \widetilde{w} \in \left(L^2(\mathbb{R}^3)\right)^4$.

3.6.1 Properties of the operators $\widehat{G}_\sigma^{(p)}$

Lemma 3.17. *Let Assumption 3.1 hold and let $R > 0$. For each $u \in \mathbf{B^2}(R)$, $p \in \{-4, -2, 0, 2\}$ and $\sigma \in \{-1, 1\}$, the operators $\widehat{G}_\sigma^{(p)}(u)$ are linear operators with the properties*

$$(i) \qquad \left\| \widehat{G}_\sigma^{(p)}(u)[v] \right\|_{L^2} \leq \frac{C}{\tau} |||v|||_{\mathbf{L^2}} \quad \text{for all } v \in \mathbf{L^2},$$

$$(ii) \qquad \left\| \widehat{G}_\sigma^{(p)}(u)[v] \right\|_{H^2} \leq \frac{C}{\tau} |||v|||_{\mathbf{H^2}} \quad \text{for all } v \in \mathbf{H^2},$$

$$(iii) \qquad \left\| \widehat{G}_\sigma^{(p)}(u)[v] \right\|_{H^2} \leq C \, |||v|||_{\mathbf{H^4}} \quad \textit{for all } v \in \mathbf{H^4}.$$

Moreover, the inequalities

$$(iv) \qquad \left\| \widehat{G}_\sigma^{(p)}(u)[u] - \widehat{G}_\sigma^{(p)}(\widetilde{u})[\widetilde{u}] \right\|_{L^2} \leq \frac{C}{\tau} \, |||u - \widetilde{u}|||_{\mathbf{L^2}} \,,$$

$$(v) \qquad \left\| \widehat{G}_\sigma^{(p)}(u)[u] - \widehat{G}_\sigma^{(p)}(\widetilde{u})[\widetilde{u}] \right\|_{L^2} \leq C \, |||u - \widetilde{u}|||_{\mathbf{H^2}} \,,$$

$$(vi) \qquad \left\| \widehat{G}_\sigma^{(p)}(u)[v] - \widehat{G}_\sigma^{(p)}(\widetilde{u})[v] \right\|_{L^2} \leq C \, |||u - \widetilde{u}|||_{\mathbf{L^2}}$$

hold for all $u, \widetilde{u}, v \in \mathbf{B^2}(R)$*. In all cases, the constant* C *does depend on* R*, but not on* τ *and* ε*.*

Proof. *(i)* Let $u = (u_{-1}, u_{+1}) \in \mathbf{B^2}(R)$ and $v = (v_{-1}, v_{+1}) \in \mathbf{L^2}$. Then, for three indices $j_1, j_2, j_3 \in \{-1, +1\}$, the inequalities (3.4) and (3.6) yield

$$\left\| u_{j_1}^* u_{j_2} v_{j_3} \right\|_{L^2} \leq C_S^2 \, \|u_{j_1}\|_{H^2} \, \|u_{j_2}\|_{H^2} \, \|v_{j_3}\|_{L^2} \leq C_S^2 R^2 \, \|v_{j_3}\|_{L^2} \,.$$

Together with the bound (3.7) for products with the potential W, the fact that $\|\Pi_{\mp 1}^\varepsilon\| = 1$, and the estimate (3.24) for the norm of $\widehat{\mathcal{D}_\varepsilon}(\tau)$, the assertion follows from the definition of $\widehat{G}_\sigma^{(p)}$.

(ii) As in (i), but using that H^2 is an algebra instead of inequalities (3.4) and (3.6).

(iii) As in (ii), but using the estimate (3.25) instead of (3.24) for $\widehat{\mathcal{D}_\varepsilon}(\tau)$.

(iv) Let $u, \widetilde{u} \in \mathbf{B^2}(R)$. First, note that with (3.24), we have

$$\left\| \sigma \mathrm{i} \widehat{\mathcal{D}_\varepsilon}(\tau) u_\sigma - \sigma \mathrm{i} \widehat{\mathcal{D}_\varepsilon}(\tau) \widetilde{u}_\sigma \right\|_{L^2} \leq \left\| \widehat{\mathcal{D}_\varepsilon}(\tau) \, [u_\sigma - \widetilde{u}_\sigma] \right\|_{L^2} \leq \frac{1}{\tau} \, |||u - \widetilde{u}|||_{\mathbf{L^2}} \,.$$

For three indices $j_1, j_2, j_3 \in \{-1, +1\}$, a decomposition of the form 3.56 together with the inequalities (3.4) and (3.6) imply that

$$\left\| u_{j_1}^* u_{j_2} u_{j_3} - \widetilde{u}_{j_1}^* \widetilde{u}_{j_2} \widetilde{u}_{j_3} \right\|_{L^2} \leq 3 C_S^2 R^2 \, |||u - \widetilde{u}|||_{\mathbf{L^2}} \,.$$

On top of that, (3.7) yields

$$\|W u_j - W \widetilde{u}_j\|_{L^2} = \|W \, (u_j - \widetilde{u}_j)\|_{L^2} \leq C_W \, |||u - \widetilde{u}|||_{\mathbf{L^2}}$$

for $j \in \{-1, +1\}$. Now the assertion follows from $\|\Pi_{\mp 1}^\varepsilon\| = 1$ and the definition of $\widehat{G}_\sigma^{(p)}$.

(v) Instead of (3.24), we use the estimate (3.25) to obtain

$$\left\| \sigma \mathrm{i} \widehat{\mathcal{D}_\varepsilon}(\tau) u_\sigma - \sigma \mathrm{i} \widehat{\mathcal{D}_\varepsilon}(\tau) \widetilde{u}_\sigma \right\|_{L^2} \leq \left\| \widehat{\mathcal{D}_\varepsilon}(\tau) \, [u_\sigma - \widetilde{u}_\sigma] \right\|_{L^2} \leq \frac{1}{2} \, |||u - \widetilde{u}|||_{\mathbf{H^2}} \,.$$

Considering that the L^2-norm is bounded by H^2-norm, the rest then follows exactly as in (iii).

(vi) Let $u, \widetilde{u}, v \in \mathbf{B^2}(R)$. Since here $\widehat{G}_\sigma^{(p)}(u)$ and $\widehat{G}_\sigma^{(p)}(\widetilde{u})$ are applied to the same function v, the terms including the operator $\widehat{\mathcal{D}_\varepsilon}$ or the potential W vanish. For the remaining terms, one can proceed similarly as in (iii). □

3.6.2 Lemma 3.8: structure of the local error of the NRNPI

Proof of Lemma 3.8. Let $\sigma \in \{-1,+1\}$. The terms that have been omitted in $J_\sigma^2(t_n,\phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]$ compared to $I_\sigma^2(t_n,\phi^\varepsilon(t_n))$ are exactly those of the form (3.37) with $q \neq 0$, i.e. $q \in \mathcal{Q}$, and with z given by (3.38). Those terms omitted in $J_\sigma^1(t_n,\phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]$ compared to $I_\sigma^1(t_n,\phi^\varepsilon(t_n))$ are also of the form (3.37) with $q \in \mathcal{Q}$, but with

$$z(t) = W\widehat{G}_j^{(p)}(\phi^\varepsilon(t))[\phi^\varepsilon(t)] \tag{3.57}$$

for some $j \in \{-1,+1\}$, $p \in \{-4,-2,0,2\}$. For each $q \in \mathcal{Q}$, collecting all corresponding terms of the form $\mathcal{B}_\sigma(\delta,\zeta)\Pi_\sigma^\varepsilon[z(t_n)]$, combining those for $\sigma=-1$ and for $\sigma=+1$ in a tuple and extracting the factor τ^2 defines the functions E_q^n.

Considering that the time derivative of $\phi_{\pm1}^\varepsilon$ is uniformly bounded w.r.t. ε in H^2, Taylor's theorem yields $\left\|\phi_j^\varepsilon(t_{n+1})-\phi_j^\varepsilon(t_n)\right\|_{H^2} \leq C\tau$ and thus also

$$\left\|\phi_j^\varepsilon(t_{n+1})-\phi_j^\varepsilon(t_n)\right\|_{L^2} \leq C\tau \tag{3.58}$$

with the constant $C = C_D$ from (3.15). Further, since for all $t \in [0,T]$, $\left\|\phi_j^\varepsilon(t)\right\|_{H^4} \leq M_{\mathrm{ex}}$ by (3.10), we have $\phi^\varepsilon(t) = (\phi_{-1}^\varepsilon(t),\phi_{+1}^\varepsilon(t)) \in \mathbf{B^4}(2M_{\mathrm{ex}}) \subset \mathbf{B^2}(2M_{\mathrm{ex}})$. Now it follows from Lemma 3.17 (v) that

$$\left\|\widehat{G}_j^{(p)}(\phi^\varepsilon(t_{n+1}))[\phi^\varepsilon(t_{n+1})]-\widehat{G}_j^{(p)}(\phi^\varepsilon(t_n))[\phi^\varepsilon(t_n)]\right\|_{L^2} \leq C\,|||\phi^\varepsilon(t_{n+1})-\phi^\varepsilon(t_n)|||_{\mathbf{H^2}} \leq C\tau \tag{3.59}$$

for $j \in \{-1,+1\}$ and some constant C which depends on M_{ex}, but not on τ and ε.

Now, we first analyze the case where z is of the type (3.38). Regardless of whether $u=\phi_\sigma^\varepsilon$ or $u=\widehat{G}_\sigma^{(p)}(\phi^\varepsilon(\cdot))[\phi^\varepsilon(\cdot)]$, from (3.10) and Lemma 3.17 (iii), we know that $u(t_n) \in \left(H^2(\mathbb{R}^3)\right)^4$ with uniform bound in ε and n. The same holds for $v(t_n)$ and $w(t_n)$ and thus for $z(t_n)$. On top of that, the estimates (3.58) and (3.59) yield

$$\|u(t_{n+1})-u(t_n)\|_{L^2} \leq C\tau$$

and the same estimate for the functions v and w. Consequently, for the difference

$$z(t_{n+1})-z(t_n) = (u(t_{n+1}))^* v(t_{n+1})w(t_{n+1}) - (u(t_n))^* v(t_n)w(t_n),$$

a decomposition of the form (3.56) together with the Sobolev inequalities (3.4) and (3.6) yields

$$\|z(t_{n+1})-z(t_n)\|_{L^2} \leq C\tau.$$

When z is of the form (3.57), the same estimate follows from (3.59) together with the bounds for products with the potential (3.7). Since $\|\Pi_{\pm1}^\varepsilon\| = 1$ and since $\mathcal{B}_\sigma$ are linear operators with norm proportional to τ^2, we obtain

$$\|\mathcal{B}_\sigma(\delta,\zeta)\Pi_\sigma^\varepsilon[z(t_n)]\|_{H^2} \leq C\tau^2, \qquad \|\mathcal{B}_\sigma(\delta,\zeta)\Pi_\sigma^\varepsilon[z(t_{n+1})]-\mathcal{B}_\sigma(\delta,\zeta)\Pi_\sigma^\varepsilon[z(t_n)]\|_{L^2} \leq C\tau^3,$$

such that the assertion follows. □

3.6.3 Lemma 3.9: stability of the numerical flow of the NRNPI

Proof of Lemma 3.9. *(i)* Let $u \in \mathbf{B^2}(R)$ and $v = (v_{-1}, v_{+1}) \in \mathbf{L^2}$. Since $\mathrm{e}^{i\sigma\tau\mathcal{D}_\varepsilon}$ is an isometry in L^2, we obtain

$$\begin{aligned}|||\Phi_{\mathrm{NRNPI}}(t,u)[v]|||_{\mathbf{L^2}} &\leq \sum_{\sigma\in\{-1,+1\}} \Big(\left\| \mathrm{e}^{\sigma \mathrm{i}\tau\mathcal{D}_\varepsilon} v_\sigma \right\|_{L^2} + \left\| J^1_\sigma(t,u)[v] \right\|_{L^2} + \left\| J^2_\sigma(t,u)[v] \right\|_{L^2} \Big) \\ &= |||v|||_{\mathbf{L^2}} + \sum_{\sigma\in\{-1,+1\}} \Big(\left\| J^1_\sigma(t,u)[v] \right\|_{L^2} + \left\| J^2_\sigma(t,u)[v] \right\|_{L^2} \Big).\end{aligned}$$

Each addend of $J^1_\sigma(t,u)[v]$ and $J^2_\sigma(t,u)[v]$ contains an operator $\mathcal{A}_\sigma$ or $\mathcal{B}_\sigma$. We know that $\|\mathcal{A}_\sigma(\delta)\| \leq C\tau$ and $\|\mathcal{B}_\sigma(\delta,\zeta)\| \leq C\tau^2$ for all $\sigma \in \{-1,+1\}$, $\zeta, \delta \in \mathbb{Z}$. According to Lemma 3.17 (i), we have $\left\| \widehat{G}^{(p)}_\sigma(u)[v] \right\|_{L^2} \leq C\,|||v|||_{\mathbf{L^2}}$ for some constant C that depends on R, but not on τ. Using that $u \in \mathbf{B^2}(R)$ together with the estimates (3.4), (3.6) and (3.7) yields

$$\left\| J^1_\sigma(t,u)[v] \right\|_{L^2} \leq C\tau\,|||v|||_{\mathbf{L^2}}\,, \qquad \left\| J^2_\sigma(t,u)[v] \right\|_{L^2} \leq C\tau\,|||v|||_{\mathbf{L^2}}$$

for some constant C that depends on R, but not on τ. The assertion then follows.

(ii) Let $u \in \mathbf{B^2}(R)$ and $v = (v_{-1}, v_{+1}) \in \mathbf{H^2}$. Then, we have

$$\begin{aligned}&|||(\Phi_{\mathrm{NRNPI}}(t,u) - \mathrm{Id})\,[v]|||_{\mathbf{L^2}} \\ &\quad\leq \sum_{\sigma\in\{-1,+1\}} \Big(\left\| \mathrm{e}^{\sigma \mathrm{i}\tau\mathcal{D}_\varepsilon} v_\sigma - v_\sigma \right\|_{L^2} + \left\| J^1_\sigma(t,u)[v] \right\|_{L^2} + \left\| J^2_\sigma(t,u)[v] \right\|_{L^2} \Big).\end{aligned}$$

Since $v_\sigma \in \left(H^2(\mathbb{R}^3)\right)^4$ for $\sigma \in \{-1,+1\}$, Lemma 3.2 yields

$$\left\| \mathrm{e}^{\sigma \mathrm{i}\tau\mathcal{D}_\varepsilon} v_\sigma - v_\sigma \right\|_{L^2} \leq C\tau\,\|v_\sigma\|_{H^2}\,.$$

Moreover, we know from the proof of part (i) that

$$\left\| J^1_\sigma(t,u)[v] \right\|_{L^2} \leq C\tau\,|||v|||_{\mathbf{H^2}}\,, \qquad \left\| J^2_\sigma(t,u)[v] \right\|_{L^2} \leq C\tau\,|||v|||_{\mathbf{H^2}}$$

because $|||v|||_{\mathbf{L^2}} \leq |||v|||_{\mathbf{H^2}}$. Altogether, the assertion follows.

(iii) Let $u = (u_{-1}, u_{+1})$, $\widetilde{u} = (\widetilde{u}_{+1}, \widetilde{u}_{-1})$, $v = (v_{-1}, v_{+1}) \in \mathbf{B^2}(R)$. Since in *both* $\Phi_{\mathrm{NRNPI}}(t,u)[v]$ and $\Phi_{\mathrm{NRNPI}}(t,\widetilde{u})[v]$, the evolution operators $\mathrm{e}^{\pm \mathrm{i}\tau\mathcal{D}_\varepsilon}$ act on the components v_{-1} and v_{+1} of the *same* function v, we have

$$\begin{aligned}|||\Phi_{\mathrm{NRNPI}}(t,u)[v] - \Phi_{\mathrm{NRNPI}}(t,\widetilde{u})[v]|||_{\mathbf{L^2}} \leq \sum_{\sigma\in\{-1,+1\}} \Big(&\left\| J^1_\sigma(t,u)[v] - J^1_\sigma(t,\widetilde{u})[v] \right\|_{L^2} \\ &+ \left\| J^2_\sigma(t,u)[v] - J^2_\sigma(t,\widetilde{u})[v] \right\|_{L^2} \Big).\end{aligned}$$

We proceed by discussing the second term first. Both $J^2_\sigma(t,u)[v]$ and $J^2_\sigma(t,\widetilde{u})[v]$ are given by (3.40), only with u replaced by $\widetilde{u}$ in the latter case (whereas the function v in the second argument is the same). Combing the corresponding double sums, the difference of $J^2_\sigma(t,u)[v]$ and $J^2_\sigma(t,\widetilde{u})[v]$ consists of four double sums which we analyze individually. The first one is given by

$$\sum_{\substack{j=-3 \\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J} \\ \#J=j}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2} \mathcal{A}_\sigma(j-\sigma)\Pi^\varepsilon_\sigma \left(u^*_{-j_1} u_{j_2} - \widetilde{u}^*_{-j_1} \widetilde{u}_{j_2} \right) v_{j_3}. \tag{3.60}$$

With (3.4) and the fact that $\|v_{j_3}\|_{H^2} \leq |||v|||_{\mathbf{H^2}} \leq R$, we obtain

$$\left\| \left(u_{-j_1}^* u_{j_2} - \widetilde{u}_{-j_1}^* \widetilde{u}_{j_2} \right) v_{j_3} \right\|_{L^2} \leq C_S R \left\| u_{-j_1}^* u_{j_2} - \widetilde{u}_{-j_1}^* \widetilde{u}_{j_2} \right\|_{L^2} .$$

A decomposition of the form (3.55) together with (3.6) and $\|u_j\|_{H^2} \leq |||u|||_{\mathbf{H^2}} \leq R$ for $j \in \{-1, +1\}$ leads to

$$\left\| u_{-j_1}^* u_{j_2} - \widetilde{u}_{-j_1}^* \widetilde{u}_{j_2} \right\|_{L^2} \leq 2 C_S R \, |||u - \widetilde{u}|||_{\mathbf{L^2}} .$$

Combining both estimates and considering that the operators $\mathcal{A}_\sigma$ and $\Pi^\varepsilon_{\mp 1}$ have norm bounded by $C\tau$ and 1, respectively, yields a bound of the form $C\tau \, |||u - \widetilde{u}|||_{\mathbf{L^2}}$ for the L^2-norm of the first double sum (3.60).

The second double sum in the difference $J^2_\sigma(t,u)[v] - J^2_\sigma(t,\widetilde{u})[v]$ is

$$\sum_{\substack{j=-3 \\ j \text{ odd}}}^{3} \sum_{\substack{J \in \mathcal{J} \\ \#J = j}} \mathcal{B}_\sigma(j-\sigma, \sigma-j) \Pi^\varepsilon_\sigma \left[\left(\left(\widehat{G}^{(j_1(\sigma-j))}_{-j_1}(u)[u] \right)^* u_{j_2} - \left(\widehat{G}^{(j_1(\sigma-j))}_{-j_1}(\widetilde{u})[\widetilde{u}] \right)^* \widetilde{u}_{j_2} \right) v_{j_3} \right] .$$

First using a decomposition of the form (3.55) together with estimate (3.6) and then applying Lemma 3.17 (ii) and (iv), we find

$$\begin{aligned}
&\left\| \left(\widehat{G}^{(j_1(\sigma-j))}_{-j_1}(u)[u] \right)^* u_{j_2} - \left(\widehat{G}^{(j_1(\sigma-j))}_{-j_1}(\widetilde{u})[\widetilde{u}] \right)^* \widetilde{u}_{j_2} \right\|_{L^2} \\
&\quad \leq C_S \Big(\left\| \widehat{G}^{(j_1(\sigma-j))}_{-j_1}(u)[u] - \widehat{G}^{(j_1(\sigma-j))}_{-j_1}(\widetilde{u})[\widetilde{u}] \right\|_{L^2} \|u_{j_3}\|_{H^2} \\
&\qquad\quad + \left\| \widehat{G}^{(j_1(\sigma-j))}_{-j_1}(\widetilde{u})[\widetilde{u}] \right\|_{H^2} \|u_{j_2} - \widetilde{u}_{j_2}\|_{L^2} \Big) \\
&\quad \leq \frac{C}{\tau} \, |||u - \widetilde{u}|||_{\mathbf{L^2}}
\end{aligned}$$

for some constant C dependent on R. Having established this bound, estimating the L^2-norm of the second double sum works in the same way as for the first one. The τ in the denominator is not a problem, since it is compensated by the extra τ we get from the bound of the norm of $\mathcal{B}_\sigma$. Analogously, one can proceed for the third double sum in the difference of $J^2_\sigma(t,u)[v]$ and $J^2_\sigma(t,\widetilde{u})[v]$.

In the fourth double sum

$$\sum_{\substack{j=-3 \\ j \text{ odd}}}^{3} \sum_{\substack{J \in \mathcal{J} \\ \#J = j}} \mathcal{B}_\sigma(j-\sigma, \sigma-j) \Pi^\varepsilon_\sigma \left[u_{-j_1}^* u_{j_2} \widehat{G}^{(j_3(\sigma-j))}_{j_3}(u)[v] - \widetilde{u}_{-j_1}^* \widetilde{u}_{j_2} \widehat{G}^{(j_3(\sigma-j))}_{j_3}(\widetilde{u})[v] \right] ,$$

the functions u or $\widetilde{u}$ appear in all three factors of the products. Thus, a decomposition of the form (3.56) instead of (3.55) is required here. Apart from that, the same arguments as for the previous sums lead to a bound of the form $C\tau \, |||u - \widetilde{u}|||_{\mathbf{L^2}}$ for some constant C independent of τ and ε.

It remains to analyze the difference of $J^1_\sigma(t,u)[v]$ and $J^1_\sigma(t,\widetilde{u})[v]$. Each of them consist of two sums, cf. Eq. (3.39). Since both $J^1_\sigma(t,u)$ and $J^1_\sigma(t,\widetilde{u})$ are applied to the same function v, the first sums vanish in the difference. The difference of the remaining sums can be treated similarly as those above. □

3.6.4 Lemma 3.11: Stability of $\Phi^{n,k}_{\mathrm{NRNPI}}$

Proof of Lemma 3.11. Let $u \in \mathbf{L^2}$. For $k \geq n$ the assertion is trivial because $\Phi^{n,k}_{\mathrm{NRNPI}} = \mathrm{Id}$. For $k < n$, $\Phi^{n,k}_{\mathrm{NRNPI}}$ is given by

$$\Phi^{n,k}_{\mathrm{NRNPI}}(u) = \Phi_{\mathrm{NRNPI}}(t_{n-1}, \phi^{n-1})\Big[\Phi_{\mathrm{NRNPI}}(t_{n-2}, \phi^{n-2})\Big[\ \ldots\ \Phi_{\mathrm{NRNPI}}(t_k, \phi^k)[u]\Big]\Big].$$

Now, we can apply Lemma 3.9 (i) for $\Phi_{\mathrm{NRNPI}}(t_k, \phi^k)$, then for $\Phi_{\mathrm{NRNPI}}(t_{k+1}, \phi^{k+1})$ and so forth. The constant of the lemma can be chosen identically each time by Assumption 3.10. Thus, we obtain

$$\left|\!\left|\!\left|\Phi^{n,k}_{\mathrm{NRNPI}}(u)\right|\!\right|\!\right|_{\mathbf{L^2}} \leq (1 + C\tau)^{n-k} \left|\!\left|\!\left|u\right|\!\right|\!\right|_{\mathbf{L^2}} \leq \left(1 + \frac{Ct_n}{n}\right)^n \left|\!\left|\!\left|u\right|\!\right|\!\right|_{\mathbf{L^2}} \leq \mathrm{e}^{Ct_n} \left|\!\left|\!\left|u\right|\!\right|\!\right|_{\mathbf{L^2}},$$

which proves the assertion. □

Chapter 4

Splitting methods for (transformed) Dirac equations

4.1 Introduction

The technique of *iterating Duhamel's formula*, which built the basis in constructing the NPI-2 scheme in the previous chapter, is a very powerful tool as it allows finding explicit approximations of the solution after a time step of given size τ. More precisely, it is possible to construct approximations of arbitrary order in τ that are independent of the highest occurring frequency of the temporal oscillations, see [CW19] and [CW22] for the linear and nonlinear Dirac equation.

However, this technique has the major disadvantage that the approximations (and thus the numerical time integrators) become more and more complicated with increasing order in τ. In the case of the transformed Dirac equation, the $\mathcal{O}(s^2)$ approximation (3.29) of $\phi_\sigma^\varepsilon(t_n+s)$, $\sigma \in \{-1,+1\}$ is still rather clear. However, inserting this representation in the integrals of Duhamel's formula once again (especially in the integral containing the nonlinearity) led to the very involved third order approximation (3.30) of $\phi_\sigma^\varepsilon(t_n+\tau)$. The enormous amount of resulting terms was only manageable by a sophisticated notation. Implementation and debugging of the resulting method and the limited efficiency caused by the large computational effort required for each time step remain drawbacks of this ansatz. The NRNPI scheme brought significant improvements on those issues, but the remaining number of terms is still not particularly small.

Splitting methods are in strong contrast to this. They divide the considered PDE into two (or more) subproblems and propagate each of them after the other in a specific order. Solutions of the individual subproblems are typically far easier to approximate than of the full PDE. Ideally, one can exploit special properties of the subproblems that even allow solving each of them exactly. The NLDE (1.2), for example, can be split into the two subproblems

$$\partial_t \psi^\varepsilon = -\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi^\varepsilon, \qquad \partial_t \psi^\varepsilon = -\mathrm{i}W\psi^\varepsilon - \mathrm{i}F(\psi^\varepsilon)\psi^\varepsilon. \tag{4.1}$$

Both of them can indeed be solved exactly in the case $\gamma_1 = 0$ [Bao+16b]. For the first subproblem, the decomposition (1.13) yields that

$$\psi^\varepsilon(t_0+t) = \mathrm{e}^{-t\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon}\psi^\varepsilon(t_0) = \left(\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon^2}t}\mathrm{e}^{-\mathrm{i}t\mathcal{D}_\varepsilon}\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}}{\varepsilon^2}t}\mathrm{e}^{\mathrm{i}t\mathcal{D}_\varepsilon}\Pi_\varepsilon^-\right)\psi^\varepsilon(t_0) \tag{4.2}$$

for all $t_0 \geq 0$ and $t > 0$. The operators $\mathrm{e}^{\pm \mathrm{i}t\mathcal{D}_\varepsilon}$ and $\Pi_\varepsilon^\pm$ can easily be applied in Fourier space. Further, if $\gamma_1 = 0$, one can check that $F(\psi^\varepsilon)$ remains constant in time within the second subproblem, which allows solving it exactly. If the potential W is time-independent, then the solution is given by

$$\psi^\varepsilon(t_0 + t) = \mathrm{e}^{-\mathrm{i}tW - \mathrm{i}tF(\psi^\varepsilon(t_0))}\psi^\varepsilon(t_0). \tag{4.3}$$

Here, the argument of the exponential function is a 4×4-matrix for each $x \in \mathbb{R}^3$, and its exponential can easily be computed using a diagonalization [Bao+16b]. Numerical schemes can be constructed by combining the exact flows (4.2) and (4.3), e.g., using Strang splitting. For a given step size τ, approximations $\psi^n \approx \psi^\varepsilon(t_n)$ to the exact solution at the discrete time points $t_n = n\tau$, $n = 0, 1, ...$, are then computed via the procedure

$$\psi^{①} = \mathrm{e}^{-\frac{\tau}{2}\cdot\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon}\psi^n, \qquad \psi^{②} = \mathrm{e}^{-\mathrm{i}\tau W - \mathrm{i}\tau F(\psi^{①})}\psi^{①}, \qquad \psi^{n+1} = \mathrm{e}^{-\frac{\tau}{2}\cdot\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon}\psi^{②}. \tag{4.4}$$

Together with space discretization by Fourier spectral methods, the resulting scheme was named time-splitting Fourier pseudospectral method (TSFP) by the authors of [Bao+16b]. The iteration (4.4) is very simple, and each time step is very cheap to compute. If only the last approximation ψ^N at some final time T_N is of interest, then both half steps can be combined, such that only one Fourier transform/inverse Fourier transform is required before/after each application of the operator $\mathrm{e}^{-\tau\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon}$.

However, also spitting methods come with a major drawback, namely that they are usually not suitable for oscillatory problems as the error constant is strongly affected by fast oscillations. In the case of the NLDE, it was shown in [Bao+16b] that the error of the TSFP scheme is in $\mathcal{O}(\tau^2/\varepsilon^4)$. Useful results can therefore only be expected for small step sizes $\tau \leq \varepsilon^2$. Further, the authors proved that there exists a number $K_0 \in \mathbb{N}$ such that the error is in $\mathcal{O}(\tau^2/\varepsilon^2)$ if the *special* step size $\tau = 2\pi\varepsilon^2/K$ is employed for some $K \in \mathbb{N}$ with $K \geq K_0$. Despite this being a significant improvement, the occurrence of ε^2 in the denominator is a serious disadvantage. A more detailed understanding of the error behavior of the TSFP scheme can be obtained by looking at a numerical experiment. To this purpose, we again consider the NLDE in one space dimension as in Sections 2.4 and 3.5.1 with the same initial data and potentials, and approximate its solution using Strang splitting with different step sizes τ. The resulting L^2-error at the final time $T = 1$ in dependency of τ is illustrated in Figure 4.1. For step sizes $\tau > \varepsilon^2$, a very irregular error behavior is observed. The error oscillates within a corridor with upper bound of $\mathcal{O}(1)$ and lower bound of $\mathcal{O}(\tau)$, cf. the black dotted reference line. Only for $\tau \leq \varepsilon^2$, second order convergence is observed. However, the error constant indeed is proportional to ε^{-2} as a comparison with the dashed reference lines reveals. This seems to hold for *all* step sizes $\tau \leq \varepsilon^2$, not only for the *special* step sizes $\tau = 2\pi\varepsilon^2/K$, $K_0 \leq K \in \mathbb{N}$.

For the sake of completeness, we note that the error bounds improve if no magnetic potential is present [BCY21]. However, since this is not the case we are interested in, we refrain from further details.

In this chapter, we will employ a different strategy of splitting the NLDE than the one briefly discussed above. The crucial advantage of this new strategy is that the splitting error behaves far more favorable than before, in the sense that it is less critically affected by the oscillatory nature of solutions of the NLDE. More precisely, we will prove that the error is in

$$\mathcal{O}\left(\min\left\{\frac{\tau^2}{\varepsilon}, \max\left\{\tau\varepsilon, \tau^2\right\}\right\}\right)$$

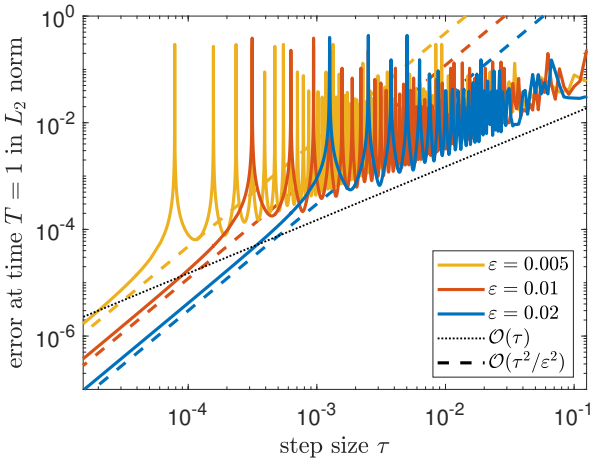

Figure 4.1: L^2-error of the TSFP scheme at time $T = 1$ in dependency of the time step size τ for three different values of ε. The dashed reference lines are of the form $C\frac{\tau^2}{\varepsilon^2}$ for a joint constant C.

and thus in particular in $\mathcal{O}(\frac{\tau^2}{\varepsilon})$. This means that the error constant only increases linearly if ε decreases (no matter if $\tau \leq \varepsilon^2$ or $\tau > \varepsilon^2$). In numerical experiments, we will even see that the error is in $\mathcal{O}(\tau^2)$ uniformly in ε if some specific resonant step sizes are avoided. This improvement comes at the cost of more challenging subproblems than those in (4.1). In fact, approximating the solution of each of them will again require the technique of iterating Duhamel's formula. It will turn out, however, that applying said technique only to the subproblems instead of the full NLDE will bring notable improvements.

Overall, the method we construct and analyze in this chapter is an *interplay between iterating Duhamel's formula and splitting methods*. It makes use of the advantages of both techniques, whereas their disadvantages only occur to a small extent.

As in the previous chapters, we only consider the case $\gamma_1 = 0$ for the nonlinearity of the NLDE (1.2) and set $\gamma_2 = 1$ without loss of generality. Further, we present details only for time-independent potentials, but later give a remark on how to incorporate time-dependent potentials as well.

The new splitting strategy is described very simply: We divide the transformed Dirac equation (2.8) into the two subproblems

$$\partial_t \phi_\pm^{\mathrm{LDE}} = \mp \mathrm{i}\mathcal{D}_\varepsilon \phi_\pm^{\mathrm{LDE}} - \mathrm{i}\Pi_\varepsilon^\pm \left[W \left(\phi_\pm^{\mathrm{LDE}} + \mathrm{e}^{\pm 2\mathrm{i}t/\varepsilon^2} \phi_\mp^{\mathrm{LDE}} \right) \right], \tag{4.5}$$

$$\partial_t \phi_\pm^{\mathrm{NL}} = -\mathrm{i}\Pi_\varepsilon^\pm \left[g_\varepsilon(\phi_+^{\mathrm{NL}}(t), \phi_-^{\mathrm{NL}}(t), t) \left(\phi_\pm^{\mathrm{NL}} + \mathrm{e}^{\pm 2\mathrm{i}t/\varepsilon^2} \phi_\mp^{\mathrm{NL}} \right) \right], \tag{4.6}$$

i.e. the linear transformed Dirac equations and the PDEs containing only the nonlinear terms. Then, in order to obtain an approximation $\phi_\pm^{n+1} \approx \phi_\pm^\varepsilon(t_{n+1})$ to the solution $\phi_\pm^\varepsilon$ of the full transformed Dirac equation at the next time step $t_{n+1} = t_n + \tau$ out of the previous iterate $\phi_\pm^n \approx \phi_\pm^\varepsilon(t_n)$, both subproblems are combined via Strang splitting in the following

way:

$$\left.\begin{aligned}
&1.\ \text{Solve (4.6) (nonlinearity) for } t \in [t_n, t_n + \tfrac{\tau}{2}] \text{ with initial data } \phi_\pm^n.\\
&\quad\ \text{Denote the result by } \phi_\pm^{①}.\\
&2.\ \text{Solve (4.5) (transformed LDE) for } t \in [t_n, t_{n+1}] \text{ with initial data } \phi_\pm^{①}.\\
&\quad\ \text{Denote the result by } \phi_\pm^{②}.\\
&3.\ \text{Solve (4.6) (nonlinearity) for } t \in [t_n + \tfrac{\tau}{2}, t_{n+1}] \text{ with initial data } \phi_\pm^{②}.\\
&\quad\ \text{Denote the result by } \phi_\pm^{③} =: \phi_\pm^{n+1}.
\end{aligned}\right\} \tag{4.7}$$

Note that the specification of the precise time interval is necessary as the PDEs (4.5) and (4.6) are not autonomous. The role of both subproblems in Strang splitting could, of course, also be interchanged, see Remark 4.15 for a motivation of our choice. The improved smoothness of the transformed Dirac equation (which was discussed in Sections 2.2.2 and 3.2.3) gives hope for a lower splitting error. However, the presence of the operator $\mathcal{D}_\varepsilon$ and the projectors $\Pi_\varepsilon^\pm$ makes solving the subproblems non-trivial.

We will proceed as follows in this chapter. First, we will translate the splitting ansatz (4.5) - (4.6) into the original variables ψ^ε in Section 4.2. On the one hand, this will give an interesting new perspective on the splitting ansatz. On the other hand, we will also conduct the analysis of the splitting error in the original variables in Section 4.3. For this analysis, we will still assume that the subproblems can be solved exactly, but this is not the case in practice. Instead, we will discuss numerical methods to approximate their solutions in sections 4.4.1 and 4.4.2. This will allow us to present our proposed time integrator for the NLDE in Section 4.4.3. We then conduct a full error analysis in Section 4.5 and finally illustrate our estimates in numerical experiments in Section 4.6.

4.2 Splitting ansatz in original variables

Recall that the transformed Dirac equation was derived by introducing the new variables $\phi_\pm^\varepsilon(t) = \mathrm{e}^{\pm \mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^\pm[\psi^\varepsilon(t)]$. Thus, by definition, $\phi_\pm^\varepsilon(t)$ is in the range of $\Pi_\varepsilon^\pm$ for all $t \geq 0$. The original variable ψ^ε can always be reconstructed by $\psi^\varepsilon(t) = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\phi_+^\varepsilon(t) + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\phi_-^\varepsilon(t)$.

Now, let $\phi_\pm^{\mathrm{LDE}}$ and $\phi_\pm^{\mathrm{NL}}$ be the solution of the subproblems (4.5) or (4.6), respectively. By the structure of both PDEs, it is obvious that if the initial data is in the range of $\Pi_\varepsilon^\pm$, then the same holds for the solutions $\phi_\pm^{\mathrm{LDE}}$ and $\phi_\pm^{\mathrm{NL}}$ of the subproblems at any later time. Thus, if we *define* the new variables ψ^{LDE} and ψ^{NL} by

$$\psi^{\mathrm{LDE}}(t) = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\phi_+^{\mathrm{LDE}}(t) + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\phi_-^{\mathrm{LDE}}(t), \qquad \psi^{\mathrm{NL}}(t) = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\phi_+^{\mathrm{NL}}(t) + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\phi_-^{\mathrm{NL}}(t),$$

then it is always possible to reconstruct $\phi_\pm^{\mathrm{LDE}}$ and $\phi_\pm^{\mathrm{NL}}$ by

$$\phi_\pm^{\mathrm{LDE}}(t) = \mathrm{e}^{\pm \mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^\pm\left[\psi^{\mathrm{LDE}}(t)\right], \qquad \phi_\pm^{\mathrm{NL}}(t) = \mathrm{e}^{\pm \mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^\pm\left[\psi^{\mathrm{NL}}(t)\right].$$

With ψ^{LDE} and ψ^{NL}, it is possible to write the subproblems (4.5) and (4.6) more conveniently as

$$\begin{aligned}
\partial_t \phi_\pm^{\mathrm{LDE}} &= \mp \mathrm{i}\mathrm{e}^{\pm \mathrm{i}t/\varepsilon^2}\mathcal{D}_\varepsilon\Pi_\varepsilon^\pm\left[\psi^{\mathrm{LDE}}\right] - \mathrm{i}\mathrm{e}^{\pm \mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^\pm\left[W\psi^{\mathrm{LDE}}\right],\\
\partial_t \phi_\pm^{\mathrm{NL}} &= -\mathrm{i}\mathrm{e}^{\pm \mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^\pm\left[F(\psi^{\mathrm{NL}})\psi^{\mathrm{NL}}\right],
\end{aligned}$$

which in turn can be used to derive the PDEs

$$\begin{aligned}\partial_t \psi^{\mathrm{LDE}} &= -\frac{\mathrm{i}}{\varepsilon^2}\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right)[\psi^{\mathrm{LDE}}] - \mathrm{i}\mathcal{D}_\varepsilon\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right)[\psi^{\mathrm{LDE}}] - \mathrm{i}W\psi^{\mathrm{LDE}},\\ \partial_t \psi^{\mathrm{NL}} &= -\frac{\mathrm{i}}{\varepsilon^2}\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right)[\psi^{\mathrm{NL}}] - \mathrm{i}F(\psi^{\mathrm{NL}})\psi^{\mathrm{NL}}.\end{aligned} \tag{4.8}$$

Since the differential operator $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon$ from the NLDE (1.2) can be decomposed as

$$-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon = -\mathrm{i}\left(\mathcal{D}_\varepsilon + \frac{1}{\varepsilon^2}\mathrm{Id}\right)\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right) = -\frac{\mathrm{i}}{\varepsilon^2}\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right) - \mathrm{i}\mathcal{D}_\varepsilon\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right),$$

cf. (1.13) and (1.17), the first PDE is, unsurprisingly, the linear Dirac equation in the original variables. However, for the further analysis, it will be more convenient to distinguish the unbounded part (w.r.t. ε)

$$\mathcal{P}_\varepsilon := -\frac{\mathrm{i}}{\varepsilon^2}\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right)$$

of the operator $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon$ from the bounded part $-\mathrm{i}\mathcal{D}_\varepsilon\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right)$. Instead, we combine the latter part with the potential W by introducing the linear operator

$$\mathcal{L}_\varepsilon := -\mathrm{i}\mathcal{D}_\varepsilon\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right) - \mathrm{i}W. \tag{4.9}$$

The PDEs from (4.8) can then be written as

$$\begin{aligned}\partial_t \psi^{\mathrm{LDE}} &= \mathcal{P}_\varepsilon\psi^{\mathrm{LDE}} + \mathcal{L}_\varepsilon\psi^{\mathrm{LDE}},\\ \partial_t \psi^{\mathrm{NL}} &= \mathcal{P}_\varepsilon\psi^{\mathrm{NL}} - \mathrm{i}F(\psi^{\mathrm{NL}})\psi^{\mathrm{NL}}.\end{aligned}$$

Thus, in the second PDE, the nonlinearity appears together with the dominating part of the operator $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon$. Using the notation introduced above, the full NLDE (1.2) can be written as

$$\partial_t \psi^\varepsilon = \mathcal{P}_\varepsilon\psi^\varepsilon + \mathcal{L}_\varepsilon\psi^\varepsilon - \mathrm{i}F(\psi^\varepsilon)\psi^\varepsilon. \tag{4.10}$$

We can now tell how the PDEs (4.5) and (4.6) of both subproblems look like in the original variables ψ^{LDE} and ψ^{NL}. However, since the definition of those variables explicitly depends on time, one has to take special care to appropriately choose the initial data in each substep. Consider, e.g., the transition from the first to the second step in (4.7). Since $\phi_\pm^{①}$ is the solution of the first substep at time $t_n + \frac{\tau}{2}$, the corresponding value in the variable ψ^{NL} is

$$\psi^{①} := \mathrm{e}^{-\mathrm{i}(t_n+\frac{\tau}{2})/\varepsilon^2}\phi_+^{①} + \mathrm{e}^{\mathrm{i}(t_n+\frac{\tau}{2})/\varepsilon^2}\phi_-^{①}.$$

In the second substep in (4.7), however, $\phi_\pm^{①}$ is taken as initial data at time t_n. The corresponding value in the variable ψ^{LDE} thus is

$$\mathrm{e}^{-\mathrm{i}t_n/\varepsilon^2}\phi_+^{①} + \mathrm{e}^{\mathrm{i}t_n/\varepsilon^2}\phi_-^{①} = \mathrm{e}^{-\mathrm{i}\frac{\tau}{2}/\varepsilon^2}\Pi_\varepsilon^+[\psi^{①}] + \mathrm{e}^{\mathrm{i}\frac{\tau}{2}/\varepsilon^2}\Pi_\varepsilon^-[\psi^{①}] = \mathrm{e}^{-\frac{\tau}{2}\mathcal{P}_\varepsilon}\psi^{①}, \tag{4.11}$$

where we used that

$$\mathrm{e}^{t\mathcal{P}_\varepsilon} = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right)} = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^+ + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^-$$

for all $t \in \mathbb{R}$ due to the special properties of the projectors (1.14). Since the function in (4.11) is the solution of the initial value problem

$$\partial_t \psi^{\mathrm{RO}} = -\mathcal{P}_\varepsilon\psi^{\mathrm{RO}}, \qquad \psi^{\mathrm{RO}}(0) = \psi^{①}$$

after a time interval of length $\frac{\tau}{2}$, this means that the transition of the data between the substeps in the variables ψ^{LDE} and ψ^{NL} can be interpreted as "rewinding" the dominating part of the operator $\mathcal{T}_\varepsilon$, or, in other words, "**R**ewinding the dominating **O**scillations (**RO**)". The same considerations hold for the transition between the second and third substep in (4.7).

All in all, the splitting given by (4.5) - (4.7) can equivalently be interpreted as splitting the full NLDE (4.10) into the three subproblems

$$\begin{aligned} \partial_t \psi^{\mathrm{LDE}} &= \mathcal{P}_\varepsilon \psi^{\mathrm{LDE}} + \mathcal{L}_\varepsilon \psi^{\mathrm{LDE}}, \\ \partial_t \psi^{\mathrm{RO}} &= -\mathcal{P}_\varepsilon \psi^{\mathrm{RO}}, \\ \partial_t \psi^{\mathrm{NL}} &= \mathcal{P}_\varepsilon \psi^{\mathrm{NL}} - \mathrm{i}F(\psi^{\mathrm{NL}})\psi^{\mathrm{NL}} \end{aligned} \tag{4.12}$$

and combining their solutions according to the scheme

$$\psi^n \xrightarrow{\Psi^{\mathrm{NL}}_{\frac{\tau}{2}}} \psi^{①} \xrightarrow{\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}} \psi^{②} \xrightarrow{\Psi^{\mathrm{LDE}}_{\tau}} \psi^{④} \xrightarrow{\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}} \psi^{⑤} \xrightarrow{\Psi^{\mathrm{NL}}_{\frac{\tau}{2}}} \psi^{⑥} =: \psi^{n+1}, \qquad n = 0, 1, \dots, \tag{4.13}$$

where Ψ^{LDE}_t, Ψ^{RO}_t and Ψ^{NL}_t are the *exact* flows of the three (autonomous) subproblems in (4.12), respectively, over a time interval of length t. The value $\psi^{③}$ has not been introduced so far on purpose, since we will divide the full LDE-step into two substeps for the analysis of the splitting error later. Combining all right-hand sides in (4.12) yields the right-hand side of the full NLDE (4.10) again. Thus, (4.12) can be considered as a special splitting of the NLDE into three terms, and (4.13) is the corresponding Strang splitting scheme.

Although the motivation for this kind of splitting originates from the transformed Dirac equation, we will work in the original variables for the rest of this chapter. The reasons for this are, on the one hand, the more compact form of the PDEs from the LDE- and the NL-subproblem and, on the other hand, the autonomy of all subproblems. Both make notation considerably easier. The fact that we have to consider a three-term instead of a two-term splitting does not cause any significant problems, since the solution of the RO-subproblem is trivial.

4.3 Local splitting error

Before we discuss how the solutions of all three subproblems in (4.12) can be approximated, we analyze the local splitting error of the approach (4.13) under the assumption that each subproblem could be solved exactly. To this purpose, let $u_0 = \psi^\varepsilon(t_n)$ be the exact solution of the full NLDE at some time t_n. We analyze the difference between $\Psi_\tau(u_0)$ and $u^{⑥}$ in dependency of τ and ε, where Ψ_t is the exact flow of the NLDE over a time interval of length t and $u^{⑥}$ is defined according to the scheme

$$u_0 \xrightarrow{\Psi^{\mathrm{NL}}_{\frac{\tau}{2}}} u^{①} \xrightarrow{\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}} u^{②} \xrightarrow{\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}} u^{③} \xrightarrow{\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}} u^{④} \xrightarrow{\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}} u^{⑤} \xrightarrow{\Psi^{\mathrm{NL}}_{\frac{\tau}{2}}} u^{⑥}. \tag{4.14}$$

In contrast to (4.13), we used that the exact flow of the LDE-subproblem fulfills $\Psi^{\mathrm{LDE}}_\tau = \Psi^{\mathrm{LDE}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}$ and introduced the intermediate value $u^{③}$.

Of course, establishing an error bound requires some assumptions. First of all, for the initial data u_0 and for all $\varepsilon \in (0, 1)$, the exact solution of the NLDE must exist on the whole time interval $[0, \tau]$. Furthermore, the solution has to be sufficiently regular in space, with uniform norm bounds in ε. Both properties are non-trivial considering the nonlinear nature of the

PDE, but for sufficiently small time intervals, these properties are guaranteed by Theorem 2.2 under suitable assumptions on the potential W and on u_0. But also the NL-subproblem in (4.12) is, of course, nonlinear, and the same properties as for the full NLDE are required for its solutions on time intervals of length $\frac{\tau}{2}$. Here, we additionally have to keep in mind that the NL-subproblem appears twice in (4.14), with initial data $v_0 = u_0$ or with $v_0 = u^{⑤}$. Furthermore, we will divide the full time step into two half steps for the analysis at some point. This is why the initial data $v_0 = \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{LDE}}_{\frac{\tau}{2}} \left(u\left(\frac{\tau}{2}\right)\right)$, where $u(t) = \Psi_t(u_0)$, will be relevant as well. For all those choices of v_0 and all $\varepsilon \in (0,1)$, we have to assume that the solution of the NL-subproblem exists on the time interval $[0, \frac{\tau}{2}]$, is sufficiently smooth in space, and remains uniformly bounded w.r.t. ε and t. Again, this is not a far-fetched assumption. Instead, one could show with a standard fixed point argument that this is true at least for all $\tau \leq \tau_0$ for some number $\tau_0 > 0$ independent of ε. All precise requirements are listed in the following.

Assumption 4.1. *For some $\widehat{m} \geq 2$, let*

(A) $V, A_j \in H^{\widehat{m}+6}(\mathbb{R}^3)$, $j = 1,2,3$,

(B) $u_0 \in \left(H^{\widehat{m}+6}(\mathbb{R}^3)\right)^4$.

Further, let $T_1 > 0$ such that the NLDE with initial data u_0 admits a solution u on $[0,T_1]$ for all $\varepsilon \in (0,1)$ that remains uniformly bounded in $\left(H^{\widehat{m}+6}(\mathbb{R}^3)\right)^4$ w.r.t. ε and t. For this value of T_1, assume that

(C) $\tau \leq T_1$,

(D) for each $\varepsilon \in (0,1)$ and for all the initial data

$$v_0 \in \left\{u_0,\, u^{⑤},\, \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{LDE}}_{\frac{\tau}{2}} \left(u\left(\frac{\tau}{2}\right)\right)\right\}, \tag{4.15}$$

the NL-subproblem admits a solution on the time interval $[0, \frac{\tau}{2}]$ that is uniformly bounded in $H^{\widehat{m}+6}$ w.r.t. ε and t.

Those assumptions will allow us to show the following bound for the local splitting error in $H^{\widehat{m}}$, whose proof is the main objective of this section.

Lemma 4.2. *Let Assumption 4.1 hold. Further, let $u^{⑥}$ be the result after one splitting step according to the scheme (4.14). Then, the local error estimate*

$$\left\|\Psi_\tau(u_0) - u^{⑥}\right\|_{H^{\widehat{m}}} \leq C \min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\}$$

holds for some constant C independent of τ and ε.

A short discussion of the right-hand side of this error bound will follow in Subsection 4.3.5. Here, we focus on its proof, which we divide into several steps by establishing multiple preliminary lemmas. First, we will derive expansions of the flow of each subproblem and of the exact solution up to terms of order $\mathcal{O}(\tau^3)$ uniformly in ε, cf. Subsection 4.3.1. Those of the subproblems are then combined to expansions of the flows of Lie splitting steps in Subsection 4.3.2. This is fundamental since the Strang splitting step (4.14) can be divided into two consecutive Lie splitting steps with reversed order of the subproblems. In Subsection 4.3.3, we will then analyze the error in the Lie splitting steps by comparing the expansions of their flows to those of the exact solution. Further, we will combine the results to find that the error in the Strang splitting step only involves few remainder terms (apart from $\mathcal{O}(\tau^3)$

terms). Finally, in Subsection 4.3.4, we will use the special structure of the projectors to show that all those remainders combined fulfill the desired bound from Lemma 4.2. After having established the error bound, we then also observe the local splitting error in a numerical experiment in Subsection 4.3.5 and compare it with the analytical estimate.

A major challenge in the analysis of the splitting error will be to keep track of the spatial regularity of all terms involved (especially of the remainder terms). To facilitate this, we introduce the following notation: For a $\mathbb{C}^4$-valued time- and space-dependent function $f_\varepsilon = f_\varepsilon(t,x)$, we write

$$f_\varepsilon(t,\cdot) = \mathcal{O}^m(t^p\varepsilon^q)$$

for some $m \in N_0$ and $p,q \in \mathbb{Z}$ if $f_\varepsilon(t,\cdot) \in \left(H^m(\mathbb{R}^3)\right)^4$ with $\|f_\varepsilon(t,\cdot)\|_{H^m} \leq Ct^p\varepsilon^q$ for some constant C independent of t and ε.

4.3.1 Step 1: Expansions of the flows of the NLDE and all subproblems

We first discuss the flows of the subproblems from (4.12) and then the flow of the full NLDE. Whenever the operator $\mathcal{T}_\varepsilon$ is involved in a problem (that is, in the LDE-subproblem and in the full NLDE), Assumption 4.1 (B) will be particularly important since the additional regularity of the solution ($H^{\widehat{m}+6}$ for an error bound in $H^{\widehat{m}}$) is required here in order to obtain uniform bounds in ε. In contrast to that, in the NL- and the RO-subproblem, less strict assumptions than Assumption 4.1 (B) would be sufficient. In fact, when discussing those two subproblems, we will always work with initial data in H^m for a generic value $m \geq 2$, while having in mind that $m = \widehat{m}+6$ would be one admissible value.

RO-subproblem

The PDE of the RO-subproblem in (4.12) was chosen in such a way that it corresponds to the flow $\Psi_t^{\mathrm{RO}} = \mathrm{e}^{-t\mathcal{P}_\varepsilon}$. In particular, the flow is known and we do not require an expansion. Instead, we only discuss an important property.

Lemma 4.3. *For any $m \geq 0$ and any $t \in \mathbb{R}$, the flow $\Psi_t^{\mathrm{RO}} = \mathrm{e}^{-t\mathcal{P}_\varepsilon}$ of the RO-subproblem in (4.12) is an isometry from and to $\left(H^m(\mathbb{R}^3)\right)^4$.*

Proof. Application of the operator $\mathrm{e}^{-t\mathcal{P}_\varepsilon}$ corresponds to multiplication of the Fourier transform at $\xi \in \mathbb{R}^3$ with the matrix $\exp\left(\frac{\mathrm{i}t}{\varepsilon^2}\left(\Pi_\varepsilon^+(\xi) - \Pi_\varepsilon^-(\xi)\right)\right)$, where

$$\Pi_\varepsilon^\pm(\xi) = \frac{1}{2}\left[I_4 \pm \frac{\mathcal{T}_\varepsilon(\xi)}{\sqrt{1+\varepsilon^2\left|\xi\right|^2}}\right], \qquad \mathcal{T}_\varepsilon(\xi) = \varepsilon\sum_{j=1}^3 \alpha_j\xi_j + \beta.$$

Since α_j, $j = 1,2,3$, and β are Hermitian, the same holds for the matrices $\mathcal{T}_\varepsilon(\xi)$, $\Pi_\varepsilon^\pm(\xi)$ and $\Pi_\varepsilon^+(\xi) - \Pi_\varepsilon^-(\xi)$. The assertion then follows with a unitary diagonalization of $\Pi_\varepsilon^+(\xi) - \Pi_\varepsilon^-(\xi)$. □

LDE-subproblem

Next, we tackle the LDE-subproblem in (4.12). To express its expansions in a compact form, we define the auxiliary operator

$$\Upsilon_t^{\mathrm{LDE}} : C\left([0,t], \left(H^2(\mathbb{R}^3)\right)^4\right) \longrightarrow \left(L^2(\mathbb{R}^3)\right)^4, \qquad \Upsilon_t^{\mathrm{LDE}}(v) = \int_0^t \mathrm{e}^{-s\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{s\mathcal{P}_\varepsilon}v(s)\,\mathrm{d}s \quad (4.16)$$

for any $t \geq 0$. We will usually just write $\Upsilon_t^{\mathrm{LDE}}(v(s))$ instead of $\Upsilon_t^{\mathrm{LDE}}\big(s \mapsto v(s)\big)$ to increase readability. Further, for a time-independent function $v_0 \in \big(H^2(\mathbb{R}^3)\big)^4$, we write $\Upsilon_t^{\mathrm{LDE}}(v_0)$ meaning that $\Upsilon_t^{\mathrm{LDE}}$ is applied to the constant function $v(s) \equiv v_0$, $s \in [0,t]$.

Having introduced the auxiliary operator above, we can now discuss different expansions of Ψ_t^{LDE}. This will be part (ii) of the following lemma. As a preparation, however, we first have to consider some technical properties of $\Upsilon_t^{\mathrm{LDE}}$ in part (i).

Lemma 4.4. *Let Ass. 4.1 (A) hold.*

(i) For any $t \geq 0$, $\Upsilon_t^{\mathrm{LDE}}$ is a well-defined, linear operator. Further, for any $0 \leq m \leq \widehat{m}+4$, we have

$$\left\|\Upsilon_t^{\mathrm{LDE}}(v)\right\|_{H^m} \leq Ct \sup_{s\in[0,t]} \|v(s)\|_{H^{m+2}}, \qquad v \in C\left([0,t], \big(H^{m+2}(\mathbb{R}^3)\big)^4\right) \tag{4.17}$$

and for any $0 \leq m \leq \widehat{m}+2$

$$\left\|\Upsilon_t^{\mathrm{LDE}}\left(\Upsilon_s^{\mathrm{LDE}}(v)\right)\right\|_{H^m} \leq Ct^2 \|v\|_{H^{m+4}}, \qquad v \in \big(H^{m+4}(\mathbb{R}^3)\big)^4 \tag{4.18}$$

for a constant C independent of t, ε and v.

(ii) Let $v_0 \in \big(H^{\widehat{m}+6}(\mathbb{R}^3)\big)^4$. Then, for the flow Ψ_t^{LDE} of the LDE-subproblem in (4.12), we have

$$\Psi_t^{\mathrm{LDE}}(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + t\mathcal{R}_1^{\mathrm{LDE}}, \tag{4.19}$$

$$\Psi_t^{\mathrm{LDE}}(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon}\Upsilon_t^{\mathrm{LDE}}(v_0) + t^2\mathcal{R}_2^{\mathrm{LDE}}, \tag{4.20}$$

$$\Psi_t^{\mathrm{LDE}}(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon}\Upsilon_t^{\mathrm{LDE}}(v_0) + \mathrm{e}^{t\mathcal{P}_\varepsilon}\Upsilon_t^{\mathrm{LDE}}\left(\Upsilon_s^{\mathrm{LDE}}(v_0)\right) + t^3\mathcal{R}_3^{\mathrm{LDE}} \tag{4.21}$$

for $t \geq 0$, where $\mathcal{R}_j^{\mathrm{LDE}} \in \big(H^{\widehat{m}+6-2j}(\mathbb{R}^3)\big)^4$ are remainders with $\left\|\mathcal{R}_j^{\mathrm{LDE}}\right\|_{H^{\widehat{m}+6-2j}} \leq C$, $j = 1,2,3$, for some constant C that depends on v_0, but is independent of t and ε.

Proof. (i) It is clear that the operator $\mathcal{L}_\varepsilon$ defined in (4.9) is linear and is uniformly bounded w.r.t. ε from H^{m+2} to H^m for any $0 \leq m \leq \widehat{m}+4$ since the same holds for D and since W is in $H^{\widehat{m}+6}$ by assumption. Together with the properties of $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ from Lemma 4.3, it then follows from the definition that $\Upsilon_t^{\mathrm{LDE}}$ is well-defined on $C\left([0,t], \big(H^2(\mathbb{R}^3)\big)^4\right)$, that it is linear and that the first estimate from the assertion holds. The second estimate follows by applying the first estimate twice.

(ii) Let $v(s) = \Psi_s^{\mathrm{LDE}}(v_0)$, $s \in [0,t]$, be the solution of the LDE-subproblem with initial data $v_0 \in \big(H^{\widehat{m}+6}(\mathbb{R}^3)\big)^4$. The regularity of the potentials guarantees that the solution v remains uniformly bounded w.r.t. ε in $\big(H^{\widehat{m}+6}(\mathbb{R}^3)\big)^4$ for all $s \in [0,t]$ [BMP98, Lemma 2.2]. Further, Duhamel's formula yields

$$\Psi_t^{\mathrm{LDE}}(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon} \int_0^t \mathrm{e}^{-s\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon v(s)\,\mathrm{d}s. \tag{4.22}$$

The first equation (4.19) thus follows directly from the properties of $\mathcal{L}_\varepsilon$ and $\mathrm{e}^{t\mathcal{P}_\varepsilon}$. Iterating Duhamel's formula once again in (4.22) and using the linearity of all operators involved yields

$$\Psi_t^{\mathrm{LDE}}(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon} \int_0^t \mathrm{e}^{-s\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon \mathrm{e}^{s\mathcal{P}_\varepsilon} v_0\,\mathrm{d}s + \mathrm{e}^{t\mathcal{P}_\varepsilon} \int_0^t \mathrm{e}^{-s\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon \mathrm{e}^{s\mathcal{P}_\varepsilon} \int_0^s \mathrm{e}^{-r\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon v(r)\,\mathrm{d}r\,\mathrm{d}s,$$

which immediately implies (4.20). Finally, (4.21) follows when employing (4.19) with $t = r$ to replace $u(r)$ by $\mathrm{e}^{r\mathcal{P}_\varepsilon}[v_0] + r\mathcal{R}_1^{\mathrm{LDE}}$ in the double integral and using the properties of $\mathcal{L}_\varepsilon$ and $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ once more. □

NL-subproblem

Analyzing the NL-subproblem in (4.12) uses similar techniques. There are, however, some difficulties arising from the nonlinearity. To begin with, for any $t \geq 0$ we define the two different auxiliary operators

$$\Upsilon_t^{\mathrm{NL}} : \left(H^2(\mathbb{R}^3)\right)^4 \longrightarrow \left(H^2(\mathbb{R}^3)\right)^4, \quad \Upsilon_t^{\mathrm{NL}}(v) = -\mathrm{i}\int_0^t \mathrm{e}^{-s\mathcal{P}_\varepsilon}\left[F\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}v\right)\mathrm{e}^{s\mathcal{P}_\varepsilon}v\right]\,\mathrm{d}s, \tag{4.23}$$

and

$$\begin{aligned}\widetilde{\Upsilon}_t^{\mathrm{NL}} :\ & \left(H^2(\mathbb{R}^3)\right)^4 \times C\left([0,t],\left(H^2(\mathbb{R}^3)\right)^4\right) \longrightarrow \left(H^2(\mathbb{R}^3)\right)^4,\\ & \widetilde{\Upsilon}_t^{\mathrm{NL}}(v,w) = -\mathrm{i}\int_0^t \mathrm{e}^{-s\mathcal{P}_\varepsilon}T\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}v, \mathrm{e}^{s\mathcal{P}_\varepsilon}w(s)\right)\,\mathrm{d}s\end{aligned} \tag{4.24}$$

with

$$T(v,w) = |v|^2 w + v^* w v + w^* v v = |v|^2 w + 2\mathrm{Re}(v^* w)v. \tag{4.25}$$

Only in the second argument of $\widetilde{\Upsilon}_t^{\mathrm{NL}}$, we allow for time-dependent functions. Similar to before, we write $\widetilde{\Upsilon}_t^{\mathrm{NL}}(v, w(s))$ instead of $\widetilde{\Upsilon}_t^{\mathrm{NL}}(v, s \mapsto w(s))$, and $\widetilde{\Upsilon}_t^{\mathrm{NL}}(v, w_0)$ for the constant function $w(s) \equiv w_0$, $s \in [0,t]$.

As for the LDE-subproblem, the main purpose of the following lemma is to analyze different expansions of Ψ_t^{NL} based on Υ_t^{NL} and $\widetilde{\Upsilon}^{\mathrm{NL}}$, which is the content of part (iv). However, some technical aspects of Υ_t^{NL} and $\widetilde{\Upsilon}_t^{\mathrm{NL}}$ have to be discussed first.

Lemma 4.5. *(i) For any $t \geq 0$, Υ_t^{NL} and $\widetilde{\Upsilon}_t^{\mathrm{NL}}$ are well-defined. Further, $\widetilde{\Upsilon}_t^{\mathrm{NL}}$ is real-linear in the second component and for any $m \geq 2$, the estimates*

$$\left\|\Upsilon_t^{\mathrm{NL}}(v)\right\|_{H^m} \leq Ct\,\|v\|_{H^m}^3, \qquad v \in \left(H^m(\mathbb{R}^3)\right)^4, \tag{4.26}$$

$$\left\|\widetilde{\Upsilon}_t^{\mathrm{NL}}(v, w(s))\right\|_{H^m} \leq Ct\,\|v\|_{H^m}^2 \sup_{s\in[0,t]}\|w(s)\|_{H^m}, \qquad \begin{aligned} &v \in \left(H^m(\mathbb{R}^3)\right)^4,\\ &w \in C\left([0,t],\left(H^m(\mathbb{R}^3)\right)^4\right)\end{aligned} \tag{4.27}$$

hold for a constant C independent of t, ε, v and w.

(ii) For any $t \geq 0$ and $m \geq 2$, the following estimates concerning $\mathcal{O}^m(t)$ and $\mathcal{O}^m(t^2)$ perturbations of the argument of Υ_t^{NL} hold:

$$\Upsilon_t^{\mathrm{NL}}(v+tw) = \Upsilon_t^{\mathrm{NL}}(v) + \widetilde{\Upsilon}_t^{\mathrm{NL}}(v, tw) + \mathcal{O}^m\left(t^3\right), \tag{4.28}$$

$$\Upsilon_t^{\mathrm{NL}}(v+tw) = \Upsilon_t^{\mathrm{NL}}(v) + \mathcal{O}^m\left(t^2\right), \tag{4.29}$$

$$\Upsilon_t^{\mathrm{NL}}(v+t^2w) = \Upsilon_t^{\mathrm{NL}}(v) + \mathcal{O}^m\left(t^3\right) \tag{4.30}$$

for all $v, w \in \left(H^m(\mathbb{R}^3)\right)^4$.

(iii) For any $t \geq 0$ and $m \geq 2$, the following estimates concerning $\mathcal{O}^m(t)$ and $\mathcal{O}^m(t^2)$ perturbations in the first and second argument of $\widetilde{\Upsilon}_t^{\mathrm{NL}}$, respectively, hold:

$$\widetilde{\Upsilon}_t^{\mathrm{NL}}(v+tz, tw) = \widetilde{\Upsilon}_t^{\mathrm{NL}}(v, tw) + \mathcal{O}^m\left(t^3\right), \tag{4.31}$$

$$\widetilde{\Upsilon}_t^{\mathrm{NL}}(v, w+t^2z) = \widetilde{\Upsilon}_t^{\mathrm{NL}}(v, w) + \mathcal{O}^m\left(t^3\right) \tag{4.32}$$

for all $v, w, z \in \left(H^m(\mathbb{R}^3)\right)^4$.

(iv) Let $v_0 \in \left(H^m(\mathbb{R}^3)\right)^4$ for some $m \geq 2$ and $T > 0$. Assume that for all $\varepsilon \in (0,1)$, the solution $v = v(t)$ of the NL-subproblem from (4.12) exists on the interval $[0,T]$ and remains uniformly bounded in H^m w.r.t. ε and t. Then, for the flow Ψ_t^{NL} of the NL-subproblem, we have

$$\Psi_t^{\mathrm{NL}}(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + t\mathcal{R}_1^{\mathrm{NL}} \tag{4.33}$$

$$\Psi_t^{\mathrm{NL}}(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{NL}}(v_0) + t^2\mathcal{R}_2^{\mathrm{NL}} \tag{4.34}$$

$$\Psi_t^{\mathrm{NL}}(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{NL}}(v_0) + \mathrm{e}^{t\mathcal{P}_\varepsilon} \widetilde{\Upsilon}_t^{\mathrm{NL}}\left(v_0, \Upsilon_s^{\mathrm{NL}}(v_0)\right) + t^3\mathcal{R}_3^{\mathrm{NL}} \tag{4.35}$$

for any $0 \leq t \leq T$ and some remainders $\mathcal{R}_j^{\mathrm{NL}} \in \left(H^m(\mathbb{R}^3)\right)^4$ with $\left\|\mathcal{R}_j^{\mathrm{NL}}\right\|_{H^m} \leq C$, $j = 1,2,3$, for a constant C that depends on v_0, but is independent of t and ε.

Note that the assumptions of part (iv) correspond to Assumption 4.1 (D) if we choose $m = \widehat{m} + 6$, $T = \tau$ and v_0 from (4.15).

Proof. (i) Since $\mathrm{e}^{s\mathcal{P}_\varepsilon}$ is an isometry in H^2 for all $s \in \mathbb{R}$ by Lemma 4.3 and since H^2 is an algebra, we do indeed have $\Upsilon_t^{\mathrm{NL}}(v) \in \left(H^2(\mathbb{R}^3)\right)^4$ for all $v \in \left(H^2(\mathbb{R}^3)\right)^4$ and $\widetilde{\Upsilon}_t^{\mathrm{NL}}(v,w) \in \left(H^2(\mathbb{R}^3)\right)^4$ for all $v \in \left(H^2(\mathbb{R}^3)\right)^4$, $w \in C\left([0,t], \left(H^2(\mathbb{R}^3)\right)^4\right)$, such that both operators are well-defined. The same arguments yield the norm bound (4.26) for Υ_t^{NL}. Further, the map T is real-linear in the second argument by definition. The same thus also holds for $\widetilde{\Upsilon}_t^{\mathrm{NL}}$. Finally, since H^m is an algebra for $m \geq 2$, we have

$$\|T(v, w(s))\|_{H^m} \leq C \|v\|_{H^m}^2 \|w(s)\|_{H^m}, \qquad s \in [0,t]$$

for some constant C. The norm bound (4.27) for $\widetilde{\Upsilon}_t^{\mathrm{NL}}$ thus follows from the definition of $\widetilde{\Upsilon}_t^{\mathrm{NL}}$ and Lemma 4.3.

(ii) Let $\widetilde{v}, \widetilde{w} \in \left(H^m(\mathbb{R}^3)\right)^4$ for some $m \geq 2$ and $t \geq 0$. Then, we have

$$\begin{aligned} F(\widetilde{v} + t\widetilde{w})(\widetilde{v} + t\widetilde{w}) &= (\widetilde{v} + t\widetilde{w})^*(\widetilde{v} + t\widetilde{w})(\widetilde{v} + t\widetilde{w}) \\ &= |\widetilde{v}|^2 \widetilde{v} + t\left(|\widetilde{v}|^2 \widetilde{w} + \widetilde{v}^* \widetilde{w} \widetilde{v} + \widetilde{w}^* \widetilde{v} \widetilde{v}\right) + \mathcal{O}^m\left(t^2\right) \\ &= F(\widetilde{v})\widetilde{v} + T(\widetilde{v}, t\widetilde{w}) + \mathcal{O}^m\left(t^2\right) \end{aligned} \tag{4.36}$$

since H^m is an algebra for $m \geq 2$. This in particular holds for $\widetilde{v} = \mathrm{e}^{s\mathcal{P}_\varepsilon} v$ and $\widetilde{w} = \mathrm{e}^{s\mathcal{P}_\varepsilon} w$ for some $v, w \in \left(H^m(\mathbb{R}^3)\right)^4$ and $s \in [0,t]$. Together with the definition of Υ_t^{NL} and $\widetilde{\Upsilon}_t^{\mathrm{NL}}$ and with Lemma 4.3, this yields the first estimate (4.28). The second and third estimate follow in the same way when the representations

$$F(\widetilde{v} + t\widetilde{w})(\widetilde{v} + t\widetilde{w}) = F(\widetilde{v})\widetilde{v} + \mathcal{O}^m(t) \tag{4.37}$$

or

$$F(\widetilde{v} + t^2\widetilde{w})(\widetilde{v} + t^2\widetilde{w}) = F(\widetilde{v})\widetilde{v} + \mathcal{O}^m\left(t^2\right)$$

are used instead of (4.36).

(iii) For the first estimate, one can use the fact that

$$T(v + tz, tw) = T(v, tw) + \mathcal{O}^m\left(t^2\right)$$

(note that here, the second argument of T itself is already of $\mathcal{O}^m(t)$). Further, the real-linearity of T in the second argument yields

$$T(v, w + t^2 z) = T(v, w) + t^2 T(v, z) = T(v, w) + \mathcal{O}^m\left(t^2\right).$$

Both estimates can then be shown with similar strategies as in (ii).

(iv) Duhamel's formula for the solution v of the NL-subproblem yields

$$v(t) = \Psi_t^{\mathrm{NL}}(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 - \mathrm{i}\mathrm{e}^{t\mathcal{P}_\varepsilon} \int_0^t \mathrm{e}^{-s\mathcal{P}_\varepsilon} \left[F\left(v(s)\right) v(s)\right] \mathrm{d}s, \qquad t \in [0, T]. \tag{4.38}$$

Since H^m is an algebra for $m \geq 2$, (4.33) directly follows.

To obtain (4.34), we would like to use (4.33) with $t = s$ to replace $v(s)$ inside the integral in (4.38). Similar to (4.37), note that for an $\mathcal{O}(s)$ approximation of $F(v(s))v(s)$, one can drop components in $v(s)$ that are of $\mathcal{O}(s)$. More precisely, we have

$$F\left(v(s)\right) v(s) - F\left(\mathrm{e}^{s\mathcal{P}_\varepsilon} v_0\right) \mathrm{e}^{s\mathcal{P}_\varepsilon} v_0 = \mathcal{O}^m(s)$$

for all $s \geq 0$. Together with (4.38) and Lemma 4.3, this yields (4.34).

For the expansion (4.35) of Ψ_t^{NL}, we replace $v(s)$ in the integral of (4.38) by the representation (4.34) obtained just before, which yields

$$\Psi_t^{\mathrm{NL}}(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{NL}} \left(v_0 + \Upsilon_s^{\mathrm{NL}}(v_0) + t^2 \mathrm{e}^{-s\mathcal{P}_\varepsilon} \mathcal{R}_2^{\mathrm{LDE}}\right).$$

First using (4.30) and then (4.28) (note $\Upsilon_s^{\mathrm{NL}}(v_0) = \mathcal{O}^m(s)$ according to (4.26)) implies the final representation (4.35). □

Full NLDE

Similar to the LDE-subproblem and the NL-subproblem, we now derive different expansions of solutions of the full NLDE (4.10). Having defined the operators $\Upsilon_t^{\mathrm{LDE}}$, Υ_t^{NL} and $\widetilde{\Upsilon}_t^{\mathrm{NL}}$ before, those expansions can be stated relatively easy.

For the fixed initial data $u_0 = \psi^\varepsilon(t_n)$ from this section, we assumed that the solution of the NLDE remains uniformly bounded in $H^{\widehat{m}+6}$ for all $\varepsilon \in (0, 1)$ and $t \in [0, T_1]$ in Assumption 4.1. However, we will divide the Strang splitting step into two half steps later. In particular, we also have to consider expansions of the solution of the NLDE with initial data $\Psi_{\frac{\tau}{2}}(u_0)$. If $\tau \leq T_1$, then Assumption 4.1 implies that no matter if $v_0 = u_0$ or $v_0 = \Psi_{\frac{\tau}{2}}(u_0)$, we can be sure that $\Psi_t(v_0)$ is in $H^{\widehat{m}+6}$ for all $t \leq \frac{\tau}{2}$ and that $\|\Psi_t(v_0)\|_{H^{\widehat{m}+6}}$ is uniformly bounded w.r.t. t and ε. Keeping that in mind helps to understand the setting of the next lemma.

Lemma 4.6. *Let Ass. 4.1 (A)-(C) hold. Further, let $t \leq \frac{\tau}{2}$ arbitrary and let $v_0 = u_0$ or $v_0 = \Psi_{\frac{\tau}{2}}(u_0)$. Then, we have*

$$\Psi_t(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + t\mathcal{R}_1^{\mathrm{NLDE}}, \tag{4.39}$$

$$\Psi_t(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}}(v_0) + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{NL}}(v_0) + t^2 \mathcal{R}_2^{\mathrm{NLDE}}, \tag{4.40}$$

$$\begin{aligned}\Psi_t(v_0) = {} & \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}}(v_0) + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{LDE}}(v_0)\right) + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{NL}}(v_0)\right) \\ & + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{NL}}(v_0) + \mathrm{e}^{t\mathcal{P}_\varepsilon} \widetilde{\Upsilon}_t^{\mathrm{NL}} \left(v_0, \Upsilon_s^{\mathrm{NL}}(v_0)\right) + \mathrm{e}^{t\mathcal{P}_\varepsilon} \widetilde{\Upsilon}_t^{\mathrm{NL}} \left(v_0, \Upsilon_s^{\mathrm{LDE}}(v_0)\right) \\ & + t^3 \mathcal{R}_3^{\mathrm{NLDE}},\end{aligned} \tag{4.41}$$

where $\mathcal{R}_j^{\mathrm{NLDE}} \in \left(H^{\widehat{m}+6-2j}(\mathbb{R}^3)\right)^4$ *are remainders with* $\left\|\mathcal{R}_j^{\mathrm{NLDE}}\right\|_{H^{\widehat{m}+6-2j}} \leq C$, $j = 1, 2, 3$, *for some constant* C *that depends on* v_0, *but is independent of* t *and* ε.

Proof. Let $v(s) = \Psi_s(v_0)$, $s \in [0, t]$, be the solution of the NLDE (4.10) with initial data v_0. According to the discussion above, we have $v(s) \in \left(H^{\widehat{m}+6}(\mathbb{R}^3)\right)$ for all $s \in [0, t]$ with uniform norm bound in ε and s. Duhamel's formula yields

$$\Psi_t(v_0) = \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon} \int_0^t \mathrm{e}^{-s\mathcal{P}_\varepsilon} \mathcal{L}_\varepsilon v(s)\, \mathrm{d}s - \mathrm{i}\mathrm{e}^{t\mathcal{P}_\varepsilon} \int_0^t \mathrm{e}^{-s\mathcal{P}_\varepsilon} \left[F(v(s))v(s)\right] \mathrm{d}s. \tag{4.42}$$

Combining the arguments of the proof of Lemma 4.4 (ii) (LDE-subproblem) and Lemma 4.5 (iv) (NL-subproblem) yields the first representation (4.39). Inserting (4.39) for $t = s$ into (4.42) once again and treating the remainder $\mathcal{R}_1^{\mathrm{NLDE}}$ as in the proofs just mentioned also yields the second representation (4.40). Finally, we insert (4.40) for $t = s$ into (4.42). Using the linearity of $\mathcal{L}_\varepsilon$, we obtain

$$\begin{aligned}
\Psi_t(v_0) = {} & \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}}(v_0) + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{LDE}}(v_0)\right) \\
& + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{NL}}(v_0)\right) + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}} \left(s^2 \mathrm{e}^{-s\mathcal{P}_\varepsilon} \mathcal{R}_2^{\mathrm{NLDE}}\right) \\
& + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{NL}} \left(v_0 + \Upsilon_s^{\mathrm{LDE}}(v_0) + \Upsilon_s^{\mathrm{NL}}(v_0) + s^2 \mathrm{e}^{-s\mathcal{P}_\varepsilon} \mathcal{R}_2^{\mathrm{NLDE}}\right).
\end{aligned}$$

Recall that $\mathcal{R}_2^{\mathrm{NLDE}}$ is uniformly bounded in $\left(H^{\widehat{m}+2}(\mathbb{R}^3)\right)^4$. Thus, using the norm bound (4.17) for $\Upsilon_t^{\mathrm{LDE}}$ and the fact that $\mathcal{O}^{\widehat{m}+2}(t^2)$-contributions in the argument of Ψ_t^{NL} lead to $\mathcal{O}^{\widehat{m}+2}(t^3)$ remainders according to (4.30), we find

$$\begin{aligned}
\Psi_t(v_0) = {} & \mathrm{e}^{t\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}}(v_0) + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{LDE}}(v_0)\right) + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{NL}}(v_0)\right) \\
& + \mathrm{e}^{t\mathcal{P}_\varepsilon} \Upsilon_t^{\mathrm{NL}} \left(v_0 + \Upsilon_s^{\mathrm{LDE}}(v_0) + \Upsilon_s^{\mathrm{NL}}(v_0)\right) + \mathcal{O}^{\widehat{m}}\left(t^3\right).
\end{aligned}$$

Finally, (4.28) allows separating the three addends in the argument of Υ_t^{NL}. Since $\Upsilon_s^{\mathrm{LDE}}(v_0) \in \left(H^{\widehat{m}+4}\right)^4$ and $\Upsilon_s^{\mathrm{NL}}(v_0) \in \left(H^{\widehat{m}+6}\right)^4$, this comes at the cost of an additional $\mathcal{O}^{\widehat{m}+4}(t^3)$-remainder. All in all, the last claim (4.41) follows. □

4.3.2 Step 2: Expansions of Lie splitting steps

The Strang splitting step described in (4.14) can be interpreted as two consecutive Lie splitting steps in reversed order. More precisely,

$$u_0 \xrightarrow[\widetilde{\tau}]{\Psi_{\widetilde{\tau}}^{\mathrm{NL}}} u^{①} \xrightarrow[\widetilde{\tau}]{\Psi_{\widetilde{\tau}}^{\mathrm{RO}}} u^{②} \xrightarrow[\widetilde{\tau}]{\Psi_{\widetilde{\tau}}^{\mathrm{LDE}}} u^{③} \quad \text{and} \quad u^{③} \xrightarrow[\widetilde{\tau}]{\Psi_{\widetilde{\tau}}^{\mathrm{LDE}}} u^{④} \xrightarrow[\widetilde{\tau}]{\Psi_{\widetilde{\tau}}^{\mathrm{RO}}} u^{⑤} \xrightarrow[\widetilde{\tau}]{\Psi_{\widetilde{\tau}}^{\mathrm{NL}}} u^{⑥} \tag{4.43}$$

with $\widetilde{\tau} = \frac{\tau}{2}$. In the local error analysis in Section 4.3.3, we will consider the error of each Lie splitting step separately, i.e. we will compare $u^{③}$ to $\Psi_{\widetilde{\tau}}(u_0)$ and $u^{⑥}$ to $\Psi_{\widetilde{\tau}}(u^{③})$, and only afterward combine both errors in a suitable way. This is why we now want to combine the expansions of the flows of the subproblems from Section 4.3.1 to derive expansions of the Lie splitting steps up to terms of order $\mathcal{O}(\widetilde{\tau}^3) = \mathcal{O}(\tau^3)$.

In the following resulting lemmas, we introduce colors that help to keep track of the origin of all resulting terms when several expansions are combined.

Lemma 4.7. *Let Assumption 4.1 hold. Then, we have*

$$u^{③} = \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} u_0 + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{NL}}(u_0) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \widetilde{\Upsilon}_{\widetilde{\tau}}^{\mathrm{NL}} \left(u_0, \Upsilon_s^{\mathrm{NL}}(u_0)\right)$$
$$+ \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}}(u_0) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\Upsilon_{\widetilde{\tau}}^{\mathrm{NL}}(u_0)\right) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{LDE}}(u_0)\right) + \tau^3 \mathcal{R}_1^{\mathrm{Lie}},$$

where $\mathcal{R}_1^{\mathrm{Lie}} \in \left(H^{\widehat{m}}(\mathbb{R}^3)\right)^4$ *with* $\left\|\mathcal{R}_1^{\mathrm{Lie}}\right\|_{H^{\widehat{m}}} \leq C$ *for some constant* C *independent of* τ *and* ε.

Proof. By Assumption 4.1 (D), we know that the solution of the NL-subproblem with initial data u_0 remains uniformly bounded in $H^{\widehat{m}+6}$ over the interval $[0, \widetilde{\tau}] = [0, \frac{\tau}{2}]$. In particular, $u^{①} \in \left(H^{\widehat{m}+6}(\mathbb{R}^3)\right)^4$ with norm bounded independently of ε and τ. Further, Lemma 4.3 then yields the same for $u^{②}$. Thus, the third order expansion (4.21) of Ψ_t^{LDE} gives

$$u^{③} = \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} u^{②} + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}}(u^{②}) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{LDE}}(u^{②})\right) + \widetilde{\tau}^3 \mathcal{R}_3^{\mathrm{LDE}}.$$

Next, we insert $u^{②} = \Psi_{\widetilde{\tau}}^{\mathrm{RO}}(u^{①}) = \mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} u^{①}$ to obtain

$$u^{③} = u^{①} + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} u^{①}\right) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{LDE}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} u^{①}\right)\right) + \widetilde{\tau}^3 \mathcal{R}_3^{\mathrm{LDE}}. \tag{4.44}$$

Finally, we replace $u^{①} = \Psi_{\widetilde{\tau}}^{\mathrm{NL}}(u_0)$ in each addend by the appropriate representation from Lemma 4.5 (iv) which only leads to $\mathcal{O}^{\widehat{m}}(\tau^3)$ remainders. In the first term, we can replace $u^{①}$ by its expansions (4.35) up to third order terms, yielding the purple terms in the claim and the additional $\mathcal{O}^{\widehat{m}+6}(\tau^3)$ remainder $\widetilde{\tau}^3 \mathcal{R}_3^{\mathrm{NL}}$ (which of course also is in $\left(H^{\widehat{m}}(\mathbb{R}^3)\right)^4$). In the second term, we replace $u^{①}$ by its expansion (4.34) up to second order terms and use the linearity of $\Psi_{\widetilde{\tau}}^{\mathrm{LDE}}$ to separate all addends. We obtain

$$\mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} u^{①}\right) = \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}}(v_0) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\Upsilon_{\widetilde{\tau}}^{\mathrm{NL}}(v_0)\right) + \widetilde{\tau}^2 \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} \mathcal{R}_2^{\mathrm{NL}}\right).$$

The first two terms are exactly the green terms in the representation from the claim. Additionally, the uniform $H^{\widehat{m}+6}$-bound of $\mathcal{R}_2^{\mathrm{NL}}$ together with Lemma 4.3 and the norm bound (4.26) of $\Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}}$ imply that the last term overall yields another $\mathcal{O}^{\widehat{m}+4}(\tau^3)$ remainder. Finally, in the blue term in (4.44), we use the expansion (4.33) up to first order terms. Together with the linearity of $\Upsilon_t^{\mathrm{LDE}}$, we obtain

$$\mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{LDE}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} u^{①}\right)\right) = \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{LDE}}(v_0)\right) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{LDE}} \left(\widetilde{\tau} \mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} \mathcal{R}_1^{\mathrm{NL}}\right)\right).$$

The first term is exactly the blue term in the claim, whereas the second term corresponds to another $\mathcal{O}^{\widehat{m}+2}(\tau^3)$ remainder due to (4.18). Overall, the assertion follows. □

When establishing a similar result for the second Lie splitting step in (4.43), we assume for the moment that we would start with the exact solution at time $\widetilde{\tau} = \frac{\tau}{2}$ (cf. Eq. (4.46) and the discussion thereafter). That means we replace $u^{③}$ by $v_0 = u(\frac{\tau}{2})$, where $u(t) = \Psi_t(u_0)$, and define $v^{①}, v^{②}, v^{③}$ by the scheme

$$u\left(\frac{\tau}{2}\right) = v_0 \xrightarrow{\Psi_{\widetilde{\tau}}^{\mathrm{LDE}}} v^{①} \xrightarrow{\Psi_{\widetilde{\tau}}^{\mathrm{RO}}} v^{②} \xrightarrow{\Psi_{\widetilde{\tau}}^{\mathrm{NL}}} v^{③}.$$

In particular, we have $v^{③} = \Psi_{\frac{\tau}{2}}^{\mathrm{NL}} \left(\Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \left(\Psi_{\frac{\tau}{2}}^{\mathrm{LDE}} \left(u\left(\frac{\tau}{2}\right)\right)\right)\right)$.

Lemma 4.8. *Let Assumption 4.1 hold. Then we have*

$$\begin{aligned} v^{③} = {} & \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} v_0 + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}}(v_0) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}} \left(\Upsilon_s^{\mathrm{LDE}}(v_0) \right) \\ & + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{NL}}(v_0) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \widetilde{\Upsilon}_{\widetilde{\tau}}^{\mathrm{NL}} \left(v_0, \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}}(v_0) \right) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \widetilde{\Upsilon}_{\widetilde{\tau}}^{\mathrm{NL}} \left(v_0, \Upsilon_s^{\mathrm{NL}}(v_0) \right) + \tau^3 \mathcal{R}_2^{\mathrm{Lie}} \end{aligned}$$

where $\mathcal{R}_2^{\mathrm{Lie}} \in \left(H^{\widehat{m}}(\mathbb{R}^3)\right)^4$ *with* $\left\| \mathcal{R}_2^{\mathrm{Lie}} \right\|_{H^{\widehat{m}}} \leq C$ *for some constant* C *independent of* τ *and* ε.

Proof. We proceed similarly as in the proof of Lemma 4.7. By Assumption 4.1 (D), we know that the solution of the NL-subproblem with initial data $v^{②} = \Psi_{\widetilde{\tau}}^{\mathrm{RO}} \circ \Psi_{\widetilde{\tau}}^{\mathrm{LDE}} \left(u\left(\frac{\tau}{2}\right) \right)$ remains uniformly bounded on the time interval $[0, \widetilde{\tau}] = [0, \frac{\tau}{2}]$. Thus, we can use the expansion (4.35) of the flow of the NL-subproblem to represent $v^{③}$ based on $v^{②}$. Afterward, we can express $v^{②}$ via $v^{①}$ by $v^{②} = \mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} v^{①}$. We obtain

$$\begin{aligned} v^{③} &= \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} v^{②} + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{NL}}(v^{②}) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \widetilde{\Upsilon}_{\widetilde{\tau}}^{\mathrm{NL}} \left(v^{②}, \Upsilon_s^{\mathrm{NL}}(v^{②}) \right) + \widetilde{\tau}^3 \mathcal{R}_3^{\mathrm{NL}} \\ &= v^{①} + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{NL}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} v^{①} \right) + \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \widetilde{\Upsilon}_{\widetilde{\tau}}^{\mathrm{NL}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} v^{①}, \Upsilon_s^{\mathrm{NL}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} v^{①} \right) \right) + \widetilde{\tau}^3 \mathcal{R}_3^{\mathrm{NL}}. \end{aligned} \tag{4.45}$$

Considering that $v^{①} \in \left(H^{\widehat{m}+6}(\mathbb{R}^3)\right)^4$ (cf. the short discussion at the beginning of the proof of Lemma 4.4 (ii)), the purple terms in the claim follow from the representation (4.21) for $v^{①}$. Further, for the second term in (4.45), we obtain with the representation (4.20) of $v^{①}$ that

$$\mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{NL}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} v^{①} \right) = \mathrm{e}^{\widetilde{\tau}\mathcal{P}_\varepsilon} \Upsilon_{\widetilde{\tau}}^{\mathrm{NL}} \left(v_0 + \Upsilon_{\widetilde{\tau}}^{\mathrm{LDE}}(v_0) + \widetilde{\tau}^2 \mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} \mathcal{R}_2^{\mathrm{LDE}} \right)$$

with a remainder $\mathcal{R}_2^{\mathrm{LDE}}$ that is uniformly bounded in $H^{\widehat{m}+2}$ w.r.t. ε and τ. We know from (4.30) that we can drop the $\mathcal{R}_2^{\mathrm{LDE}}$-part in the argument of $\Upsilon_{\widetilde{\tau}}^{\mathrm{NL}}$ at the price of an $\mathcal{O}^{\widehat{m}+2}(\tau^3)$-remainder. Using (4.17) and (4.28) afterward to separate the remaining arguments of $\Upsilon_{\widetilde{\tau}}^{\mathrm{NL}}$ yields the green terms in the claim together with an $\mathcal{O}^{\widehat{m}+4}(\tau^3)$-remainder.

Finally, inserting the representation (4.19) for $v^{①}$ in both arguments of the blue term in (4.45) yields

$$\widetilde{\Upsilon}_{\widetilde{\tau}}^{\mathrm{NL}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} v^{①}, \Upsilon_s^{\mathrm{NL}} \left(\mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} v^{①} \right) \right) = \widetilde{\Upsilon}_{\widetilde{\tau}}^{\mathrm{NL}} \left(v_0 + \widetilde{\tau} \mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} \mathcal{R}_1^{\mathrm{LDE}}, \Upsilon_s^{\mathrm{NL}} \left(v_0 + \widetilde{\tau} \mathrm{e}^{-\widetilde{\tau}\mathcal{P}_\varepsilon} \mathcal{R}_1^{\mathrm{LDE}} \right) \right).$$

with remainder $\mathcal{R}_1^{\mathrm{LDE}}$ that is uniformly bounded in $H^{\widehat{m}+4}$ w.r.t. ε and τ. According to (4.29), dropping the $\mathcal{R}_1^{\mathrm{LDE}}$-part in the argument of Υ_s^{NL} leads to an $\mathcal{O}^{\widehat{m}+4}(\tau^2)$-remainder in the second argument of $\widetilde{\Upsilon}_{\widetilde{\tau}}^{\mathrm{NL}}$, which in turn leads to an $\mathcal{O}^{\widehat{m}+4}(\tau^3)$-remainder in the end due to (4.32). Further, (4.31) implies that omitting the $\mathcal{R}_1^{\mathrm{LDE}}$-part in the first argument of $\widetilde{\Upsilon}_{\widetilde{\tau}}^{\mathrm{NL}}$ leads to another $\mathcal{O}^{\widehat{m}+4}(\tau^3)$-remainder. Overall, this also explains the blue term in the claim. □

4.3.3 Step 3: Combining the Lie splitting steps

In this subsection, we show how the error of the Strang splitting step (4.14) can be related to the errors of two Lie splitting steps. The latter ones are then analyzed by comparing the expansions of the Lie splitting steps from the previous subsection to the expansion of the exact solution from Subsection 4.3.1.

Lemma 4.9. *Let Assumption 4.1 hold. Further, let $u^{⑥}$ be the result after one splitting step according to the scheme (4.14). Then, for the local error, we have*

$$\Psi_\tau(u_0) - u^{⑥} = \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\mathcal{R}^1_\tau(\mathcal{L}_\varepsilon) + \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon) + \tau^3\mathcal{R}^{loc}$$

with

$$\begin{aligned}
\mathcal{R}^1_\tau(\mathcal{L}_\varepsilon) &= \Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(\Upsilon^{\mathrm{NL}}_s\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0\right)\right) + \widetilde{\Upsilon}^{\mathrm{NL}}_{\frac{\tau}{2}}\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0, \Upsilon^{\mathrm{LDE}}_s\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0\right) - \Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0\right)\right)\\
\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon) &= \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\widetilde{\Upsilon}^{\mathrm{NL}}_{\frac{\tau}{2}}\left(u_0, \Upsilon^{\mathrm{LDE}}_s(u_0)\right) + \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(\Upsilon^{\mathrm{NL}}_s(u_0) - \Upsilon^{\mathrm{NL}}_{\frac{\tau}{2}}(u_0)\right)
\end{aligned}$$

and with a remainder $\mathcal{R}^{loc} \in \left(H^{\widehat{m}}(\mathbb{R}^3)\right)^4$ with $\left\|\mathcal{R}^{loc}\right\|_{H^{\widehat{m}}} \leq C$ for some constant C independent of τ and ε.

Proof. Let $u(s) = \Psi_s(u_0)$, $s \in [0,\tau]$ be the exact solution of the NLDE on the time interval $[0,\tau]$ with initial data u_0. The objective then is to analyze the difference $u(\tau) - u^{⑥}$. We will start by dividing this difference into two parts. For that purpose, we express $u^{⑥}$ and $u(\tau)$ as $u^{⑥} = \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u^{③}\right)\right)\right)$ and $u(\tau) = \Psi_{\frac{\tau}{2}}\left(u\left(\frac{\tau}{2}\right)\right)$. This allows the decomposition

$$\begin{aligned}
u(\tau) - u^{⑥} = {}& \Psi_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right) - \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)\right)\right)\\
&+ \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)\right)\right) - \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u^{③}\right)\right)\right)
\end{aligned} \tag{4.46}$$

The difference in the first line corresponds to the local error made *only in the second half* of the Strang splitting step (4.14), or, in other words, of the second Lie splitting step. Those errors are responsible for the remainders contained in $\mathcal{R}^1_\tau(\mathcal{L}_\varepsilon)$. In the second line, the difference of the arguments themselves is the local error made *only in the first half* of the Strang splitting step (4.14), i.e., in the first Lie splitting step. However, both arguments are first inserted in the flows of the subproblems from the second half of the splitting step, and it has to be analyzed how this affects the error. This will lead to the remainders in $\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon)$.

The proof can thus be divided into two parts accordingly.

Part 1: Error of the second Lie splitting step. We use the expansions up to $\mathcal{O}(\tau^3)$-terms for the exact solution and the Lie splitting step from Lemma 4.6 (applied with $v_0 = u(\frac{\tau}{2})$ and $t = \widetilde{\tau} = \frac{\tau}{2}$) and Lemma 4.8, respectively. Comparing them yields

$$\begin{aligned}
&\Psi_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right) - \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)\right)\right)\\
&\quad= \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\Big(\Upsilon^{\mathrm{NL}}_s\left(u\left(\tfrac{\tau}{2}\right)\right)\Big) + \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\widetilde{\Upsilon}^{\mathrm{NL}}_{\frac{\tau}{2}}\Big(u\left(\tfrac{\tau}{2}\right), \Upsilon^{\mathrm{LDE}}_s\left(u\left(\tfrac{\tau}{2}\right)\right)\Big)\\
&\qquad- \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\widetilde{\Upsilon}^{\mathrm{NL}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right), \Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)\right) + \mathcal{O}^{\widehat{m}}\left(\tau^3\right).
\end{aligned} \tag{4.47}$$

In the next step, $u\left(\frac{\tau}{2}\right)$ can be related to $u(0) = u_0$. To this end, we use the easiest representation of the exact solution given by (4.39), i.e. $u\left(\frac{\tau}{2}\right) = \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0 + \frac{\tau}{2}\mathcal{R}^{\mathrm{NLDE}}_1$ with remainder $\mathcal{R}^{\mathrm{NLDE}}_1$ uniformly bounded in $\left(H^{\widehat{m}+4}(\mathbb{R}^3)\right)^4$. We will now see that this representation is sufficient since the $\mathcal{R}^{\mathrm{NLDE}}_1$-term can be considered as an $\mathcal{O}^{\widehat{m}+4}(\tau)$-perturbation of the arguments which can be omitted at the cost of $\mathcal{O}^{\widehat{m}}(\tau^3)$ remainders: According to (4.29), $\mathcal{O}^{\widehat{m}+4}(\tau)$-perturbations in the arguments of Υ^{NL}_s only induce an $\mathcal{O}^{\widehat{m}+4}(\tau^2)$ remainder. Additionally inserting the result in $\Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}$, using its linearity and the norm bound (4.17) leads to an $\mathcal{O}^{\widehat{m}+2}(\tau^3)$ remainder. Overall, we have

$$\Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\Big(\Upsilon^{\mathrm{NL}}_s\left(u\left(\tfrac{\tau}{2}\right)\right)\Big) = \Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\Big(\Upsilon^{\mathrm{NL}}_s\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0\right)\Big) + \mathcal{O}^{\widehat{m}+2}\left(\tau^3\right).$$

Similar arguments involving (4.17), (4.31) and (4.32) allow replacing $u\left(\frac{\tau}{2}\right)$ by $\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0$ in the other terms in (4.47) at the cost of additional $\mathcal{O}^{\widehat{m}+2}(\tau^3)$ remainders, i.e.,

$$\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\widetilde{\Upsilon}^{\mathrm{NL}}_{\frac{\tau}{2}}\Big(u\left(\tfrac{\tau}{2}\right),\Upsilon^{\mathrm{LDE}}_s\left(u\left(\tfrac{\tau}{2}\right)\right)\Big)=\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\widetilde{\Upsilon}^{\mathrm{NL}}_{\frac{\tau}{2}}\Big(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0,\Upsilon^{\mathrm{LDE}}_s\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0\right)\Big)+\mathcal{O}^{\widehat{m}+2}\Big(\tau^3\Big),$$
$$\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\widetilde{\Upsilon}^{\mathrm{NL}}_{\frac{\tau}{2}}\Big(u\left(\tfrac{\tau}{2}\right),\Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)\Big)=\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\widetilde{\Upsilon}^{\mathrm{NL}}_{\frac{\tau}{2}}\Big(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0,\Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0\right)\Big)+\mathcal{O}^{\widehat{m}+2}\Big(\tau^3\Big).$$

Combining all of the above and using the real-linearity of $\widetilde{\Upsilon}^{\mathrm{NL}}_{\frac{\tau}{2}}$ in the second argument, one obtains

$$\Psi_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)-\Psi^{\mathrm{NL}}_{\frac{\tau}{2}}\Big(\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\Big(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)\Big)\Big)=\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\mathcal{R}^1_\tau(\mathcal{L}_\varepsilon)+\mathcal{O}^{\widehat{m}}\Big(\tau^3\Big). \tag{4.48}$$

Part 2: Propagated error of the first Lie splitting step. Similar to (4.47), one can compare the expansions up to $\mathcal{O}^{\widehat{m}}(\tau^3)$-terms of the exact solution and the first Lie splitting step from Lemma 4.6 (applied with $v_0=u_0$ and $t=\frac{\tau}{2}$) and Lemma 4.7, respectively, to obtain

$$\begin{aligned}u\left(\tfrac{\tau}{2}\right)-u^{③}&=\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\Big(\Upsilon^{\mathrm{NL}}_s\left(u_0\right)\Big)+\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\widetilde{\Upsilon}^{\mathrm{NL}}_{\frac{\tau}{2}}\Big(u_0,\Upsilon^{\mathrm{LDE}}_s\left(u_0\right)\Big)\\&\quad-\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\Upsilon^{\mathrm{LDE}}_{\frac{\tau}{2}}\Big(\Upsilon^{\mathrm{NL}}_{\frac{\tau}{2}}\left(u_0\right)\Big)+\mathcal{O}^{\widehat{m}}\Big(\tau^3\Big)\\&=\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon)+\mathcal{O}^{\widehat{m}}\Big(\tau^3\Big).\end{aligned} \tag{4.49}$$

Since $u_0\in H^{\widehat{m}+6}$, the norm bounds of $\Upsilon^{\mathrm{LDE}}_t$, Υ^{NL}_t and $\widetilde{\Upsilon}^{\mathrm{NL}}_t$ from (4.17), (4.26) and (4.27) yield that $\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon)=\mathcal{O}^{\widehat{m}+2}(\tau^2)$. Thus, (4.49) is equivalent to

$$u\left(\tfrac{\tau}{2}\right)-u^{③}=\tau^2\mathcal{S}_1+\tau^3\mathcal{S}_2\qquad\text{or}\qquad u\left(\tfrac{\tau}{2}\right)=u^{③}+\tau^2\mathcal{S}_1+\tau^3\mathcal{S}_2 \tag{4.50}$$

with $\mathcal{S}_1=\frac{1}{\tau^2}\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon)\in\left(H^{\widehat{m}+2}(\mathbb{R}^3)\right)^4$ and a suitable function $\mathcal{S}_2\in\left(H^{\widehat{m}}(\mathbb{R}^3)\right)^4$, both of them being uniformly bounded in ε and τ. Analyzing the second line of (4.46) thus is equivalent to answering the question of how $\mathcal{O}^{\widehat{m}+2}(\tau^2)$ and $\mathcal{O}^{\widehat{m}}(\tau^3)$-perturbations of the argument affect the result of the Lie splitting step. It would seem natural to use the expansions of the Lie splitting step from Lemma 4.8 to this purpose. This would indeed result in the desired representation. However, the presence of multiple operators of the kind $\Upsilon^{\mathrm{LDE}}_t$ would require additional regularity of $\mathcal{S}_1$ and $\mathcal{S}_2$ that we do not want to invest. This is why we work with the exact flows Ψ^{LDE}_t, Ψ^{RO}_t and Ψ^{NL}_t instead.

We start from the inside, i.e. with the flow of the LDE-subproblem. Its linearity implies

$$\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)-\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u^{③}\right)=\tau^2\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(\mathcal{S}_1\right)+\tau^3\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(\mathcal{S}_2\right).$$

Since solutions of the LDE remain uniformly bounded if the potentials are sufficiently regular, we have $\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(\mathcal{S}_2\right)=\mathcal{O}^{\widehat{m}}(1)$ and $\Psi^{\mathrm{LDE}}_s\left(\mathcal{S}_1\right)=\mathcal{O}^{\widehat{m}+2}(1)$ for all $s\in[0,\frac{\tau}{2}]$. The second fact together with Duhamel's formula yields

$$\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(\mathcal{S}_1\right)=\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\mathcal{S}_1+\int_0^{\frac{\tau}{2}}\mathrm{e}^{(\frac{\tau}{2}-s)\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\Psi^{\mathrm{LDE}}_s\left(\mathcal{S}_1\right)\,\mathrm{d}s=\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\mathcal{S}_1+\mathcal{O}^{\widehat{m}}(\tau).$$

Altogether, we have

$$\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)-\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u^{③}\right)=\tau^2\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\mathcal{S}_1+\tau^3\widetilde{\mathcal{S}}_2$$

for some function $\widetilde{\mathcal{S}}_2$ that has the same properties as $\mathcal{S}_2$. Next, we apply the exact flow of the RO-subproblem from Lemma 4.3 and obtain

$$\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)\right) - \Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u^{③}\right)\right) = \tau^2\mathcal{S}_1 + \tau^3 \mathrm{e}^{-\frac{\tau}{2}\mathcal{P}_\varepsilon}\widetilde{\mathcal{S}}_2. \tag{4.51}$$

Finally, we have to deal with the NL-subproblem. To this end, let $v_0 = \Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)\right)$ and $w_0 = \Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u^{③}\right)\right)$. Eq. (4.51) then becomes

$$v_0 - w_0 = \tau^2\mathcal{S}_1 + \tau^3 \mathrm{e}^{-\frac{\tau}{2}\mathcal{P}_\varepsilon}\widetilde{\mathcal{S}}_2.$$

Additionally, let $v(s) = \Psi^{\mathrm{NL}}_s(v_0)$ and $w(s) = \Psi^{\mathrm{NL}}_s(w_0)$, $s \in [0, \frac{\tau}{2}]$ be the solution of the NL-subproblem with initial data v_0 and w_0, respectively. Both exist and remain uniformly bounded due to Assumption 4.1 (D). In this notation, it remains to analyze $v(\frac{\tau}{2}) - w(\frac{\tau}{2})$. Duhamel's formula, applied to both v and w yields

$$v\left(\tfrac{\tau}{2}\right) - w\left(\tfrac{\tau}{2}\right) = \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\left[v_0 - w_0\right] - \mathrm{i}\int_0^{\frac{\tau}{2}} \mathrm{e}^{(\frac{\tau}{2}-s)\mathcal{P}_\varepsilon}\left[F(v(s))v(s) - F(w(s))w(s)\right]\,\mathrm{d}s. \tag{4.52}$$

The difference between the two nonlinearities can be related to the difference of $v(s)$ and $w(s)$ by introducing mixed terms. Further, using a similar ansatz as in (4.52), but with $\frac{\tau}{2}$ replaced by s, one can check with a Gronwall-type argument that the difference $v(s) - w(s)$ remains proportional to the initial difference $v_0 - w_0$ in the sense that

$$\left\|v(s) - w(s)\right\|_{H^{\widehat{m}}} \leq C\left\|v_0 - w_0\right\|_{H^{\widehat{m}}}, \qquad s \in \left[0, \frac{\tau}{2}\right],$$

for some constant C which depends on τ, but converges to 1 from above when $\tau \to 0$. Considering the additional integral in (4.52) and that $v_0 - w_0 = \mathcal{O}^{\widehat{m}}(\tau^2)$, we finally obtain

$$v\left(\tfrac{\tau}{2}\right) - w\left(\tfrac{\tau}{2}\right) = \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\left[v_0 - w_0\right] + \mathcal{O}^{\widehat{m}}\left(\tau^3\right) = \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\left[\tau^2\mathcal{S}_1\right] + \mathcal{O}^{\widehat{m}}\left(\tau^3\right)$$

Recalling the definition of $v\left(\frac{\tau}{2}\right)$ and $w\left(\frac{\tau}{2}\right)$ and considering that $\mathcal{S}_1 = \frac{1}{\tau^2}\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon)$, this is equivalent to

$$\Psi^{\mathrm{NL}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u\left(\tfrac{\tau}{2}\right)\right)\right)\right) - \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\frac{\tau}{2}}\left(u^{③}\right)\right)\right) = \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon) + \mathcal{O}^{\widehat{m}}\left(\tau^3\right). \tag{4.53}$$

After all, combining (4.46), (4.48) and (4.53) yields the claim. □

4.3.4 Step 4: Analyzing the remainder terms

In Lemma 4.9, we were able to identify all terms that appear in the expansion of the Strang splitting step, but not of the exact solution, and vice versa. This led to the remainders $\mathcal{R}^1_\tau(\mathcal{L}_\varepsilon)$ and $\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon)$, which are both in $\mathcal{O}(\tau^2)$ (for $\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon)$, this was discussed in part 2 of the proof of Lemma 4.9). We are, however, aiming for a better result. This will be achieved by showing that the terms from $\mathcal{R}^1_\tau(\mathcal{L}_\varepsilon)$ cancel with those from $\mathcal{R}^2_\tau(\mathcal{L}_\varepsilon)$ to some extent, which will yield the assertion from Lemma 4.2 in the end.

The crucial strategy will be to replace operators of the form $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ by suitable matrix approximations which will have a different commutative behavior. Establishing and analyzing those approximations requires some preparation, which is the content of the next three lemmas. Afterward, we will finally be able to prove Lemma 4.2.

Lemma 4.10 (Lemma 2.1 in [BMP98]). *Let $m \geq 1$. The projectors $\Pi_\varepsilon^\pm$ allow the following expansion w.r.t. ε:*

$$\Pi_\varepsilon^\pm = \Pi_0^\pm \pm \varepsilon \mathcal{R}^{\mathrm{Proj}}$$

where

$$\Pi_0^+ = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & \\ & & & 0 \end{pmatrix}, \qquad \Pi_0^- = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}$$

and $\mathcal{R}^{\mathrm{Proj}}$ is a uniformly (in ε) bounded operator from $(H^m(\mathbb{R}^3))^4$ to $(H^{m-1}(\mathbb{R}^3))^4$ (which is the same in the "+" and the "-" case).

In all the expansions of the subproblems or the exact solution as well as in the remainders $\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon)$ and $\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon)$ from Lemma 4.9, the projectors $\Pi_\varepsilon^\pm$ mainly appear within the (unbounded) operator $\mathcal{P}_\varepsilon = -\frac{\mathrm{i}}{\varepsilon^2}\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right)$. To ensure that all remainders are uniformly bounded in ε, we always made sure that $\mathcal{P}_\varepsilon$ is kept in the exponential, i.e., only appears in the form

$$\mathrm{e}^{t\mathcal{P}_\varepsilon} = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right)} = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^+ + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^-$$

for some $t \in \mathbb{R}$. The crucial tool not only for the proof of Lemma 4.2, but also later for the construction of an efficient method to solve the nonlinearity-subproblem in (4.12), will be to replace the operators $\Pi_\varepsilon^\pm$ by their limits $\Pi_0^\pm$ within operators of the form $\mathrm{e}^{t\mathcal{P}_\varepsilon}$. In other words, we will approximate $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ by

$$\mathrm{e}^{t\mathcal{P}_0} := \mathrm{e}^{-\mathrm{i}t/\varepsilon^2\left(\Pi_0^+ - \Pi_0^-\right)} = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi_0^+ + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\Pi_0^-. \tag{4.54}$$

Lemma 4.10 immediately implies an $\mathcal{O}(\varepsilon)$-bound for the approximation error. However, the following, crucial Lemma gives an alternative bound which is less obvious.

Lemma 4.11. *Let $m \geq 1$ and $t \in \mathbb{R}$ arbitrary. Then, for all $v \in \left(H^m(\mathbb{R}^3)\right)^4$, we have*

$$\left\| \mathrm{e}^{t\mathcal{P}_\varepsilon} v - \mathrm{e}^{t\mathcal{P}_0} v \right\|_{H^{m-1}} \leq C \min\left\{ \varepsilon, \frac{|t|}{\varepsilon} \right\} \|v\|_{H^m}$$

for a constant C independent of t, ε and v.

Proof. With Lemma 4.10, we obtain the representation

$$\begin{aligned} \mathrm{e}^{t\mathcal{P}_\varepsilon} v = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^+ v + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^- v &= \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\left(\Pi_0^+ + \varepsilon\mathcal{R}^{\mathrm{Proj}}\right) v + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\left(\Pi_0^- - \varepsilon\mathcal{R}^{\mathrm{Proj}}\right) v \\ &= \mathrm{e}^{t\mathcal{P}_0} v + \varepsilon\left(\mathrm{e}^{-\mathrm{i}t/\varepsilon^2} - \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\right)\mathcal{R}^{\mathrm{Proj}} v, \end{aligned}$$

and we know that $\left\|\mathcal{R}^{\mathrm{Proj}} v\right\|_{H^{m-1}} \leq C \|v\|_{H^m}$ for a constant independent of v and ε. The fact that $\mathrm{e}^{\mathrm{i}x} - \mathrm{e}^{-\mathrm{i}x} = 2\mathrm{i}\sin(x)$ for all $x \in \mathbb{R}$ together with the estimates $|\sin(x)| \leq 1$ and $|\sin(x)| < |x|$ yields the assertion. □

Since $\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon)$ and $\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon)$ from Lemma 4.9 are already in $\mathcal{O}(\tau^2)$, Lemma 4.11 implies that using the approximation $\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon} \approx \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_0}$ therein only leads to error terms that are of third order in τ. However, we have to accept one ϵ in the denominator in the worst case. The crucial difference between $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ and $\mathrm{e}^{t\mathcal{P}_0}$ is that the former are pseudo-differential operators, whereas the latter are matrices. Thus, different calculation rules apply, which we will make use of in the proof of Lemma 4.2. Before we do this, we collect some properties of the matrices $\mathrm{e}^{t\mathcal{P}_0}$.

Lemma 4.12. *Let $t \in \mathbb{R}$.*

(i) For the conjugate transpose of $\mathrm{e}^{t\mathcal{P}_0}$, we have $(\mathrm{e}^{t\mathcal{P}_0})^* = \mathrm{e}^{-t\mathcal{P}_0}$. In particular, $\mathrm{e}^{t\mathcal{P}_0}$ is unitary, preserves the Euclidean norm and $(\mathrm{e}^{t\mathcal{P}_0}v)^*\mathrm{e}^{t\mathcal{P}_0}w = v^*w$ holds for all $v, w \in \mathbb{C}^4$.

(ii) For the matrices α_j, $j = 1, 2, 3$ in the magnetic potential, we have $\mathrm{e}^{t\mathcal{P}_0}\alpha_j = \alpha_j\mathrm{e}^{-t\mathcal{P}_0}$.

Proof. (i) The property $(\mathrm{e}^{t\mathcal{P}_0})^* = \mathrm{e}^{-t\mathcal{P}_0}$ follows directly from the definition (4.54) of $\mathrm{e}^{t\mathcal{P}_0}$ when considering that $\Pi_0^{\pm}$ are real-valued diagonal matrices. The remaining properties then are an immediate consequence.

(ii) Let $j \in \{1, 2, 3\}$. We have

$$\Pi_0^+\alpha_j = \begin{pmatrix} I_2 & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_j \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & I_2 \end{pmatrix} = \alpha_j\Pi_0^-$$

where each "0" stands for a 2×2 matrix with all entries being zero. Similarly, we find $\Pi_0^-\alpha_j = \alpha_j\Pi_0^+$. Altogether, the calculation

$$\mathrm{e}^{t\mathcal{P}_0}\alpha_j = \left(\mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi_0^+ + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\Pi_0^-\right)\alpha_j = \alpha_j\left(\mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi_0^- + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\Pi_0^+\right) = \alpha_j\mathrm{e}^{-t\mathcal{P}_0},$$

yields the claim. □

Now, we are finally in the position to prove the local error estimate from Lemma 4.2.

Proof of Lemma 4.2. In Lemma 4.9, we have already established a representation of the local error using the two remainders $\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon)$ and $\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon)$. Now, we analyze those remainders in detail. We start by inserting the definitions of the auxiliary operators $\Upsilon_t^{\mathrm{LDE}}$, Υ_t^{NL} and $\widetilde{\Upsilon}_t^{\mathrm{NL}}$ from (4.16), (4.23) and (4.24). For the second argument of $\widetilde{\Upsilon}_{\frac{\tau}{2}}^{\mathrm{NL}}$ in $\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon)$ and the argument of $\Upsilon_{\frac{\tau}{2}}^{\mathrm{LDE}}$ in $\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon)$, this yields

$$\begin{aligned}
\Upsilon_s^{\mathrm{LDE}}\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0\right) - \Upsilon_{\frac{\tau}{2}}^{\mathrm{LDE}}\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0\right) &= -\int_s^{\frac{\tau}{2}} \mathrm{e}^{-r\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{(r+\frac{\tau}{2})\mathcal{P}_\varepsilon}u_0\,\mathrm{d}r, \\
\Upsilon_s^{\mathrm{NL}}(u_0) - \Upsilon_{\frac{\tau}{2}}^{\mathrm{NL}}(u_0) &= \mathrm{i}\int_s^{\frac{\tau}{2}} \mathrm{e}^{-r\mathcal{P}_\varepsilon}\left[F\left(\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\right)\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\right]\,\mathrm{d}r.
\end{aligned}$$

Thus, using the real-linearity of T, we obtain

$$\begin{aligned}
\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon) &= -\mathrm{i}\int_0^{\frac{\tau}{2}} \mathrm{e}^{-s\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{s\mathcal{P}_\varepsilon}\int_0^s \mathrm{e}^{-r\mathcal{P}_\varepsilon}\left[F\left(\mathrm{e}^{(r+\frac{\tau}{2})\mathcal{P}_\varepsilon}u_0\right)\mathrm{e}^{(r+\frac{\tau}{2})\mathcal{P}_\varepsilon}u_0\right]\,\mathrm{d}r\,\mathrm{d}s \\
&\quad + \mathrm{i}\int_0^{\frac{\tau}{2}} \mathrm{e}^{-s\mathcal{P}_\varepsilon}T\left(\mathrm{e}^{(s+\frac{\tau}{2})\mathcal{P}_\varepsilon}u_0, \mathrm{e}^{s\mathcal{P}_\varepsilon}\int_s^{\frac{\tau}{2}} \mathrm{e}^{-r\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{(r+\frac{\tau}{2})\mathcal{P}_\varepsilon}u_0\,\mathrm{d}r\right)\,\mathrm{d}s, \\
\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon) &= -\mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}} \mathrm{e}^{-s\mathcal{P}_\varepsilon}T\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}u_0, \mathrm{e}^{s\mathcal{P}_\varepsilon}\int_0^s \mathrm{e}^{-r\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\,\mathrm{d}r\right)\,\mathrm{d}s \\
&\quad + \mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}} \mathrm{e}^{-s\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{s\mathcal{P}_\varepsilon}\int_s^{\frac{\tau}{2}} \mathrm{e}^{-r\mathcal{P}_\varepsilon}\left[F\left(\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\right)\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\right]\,\mathrm{d}r\,\mathrm{d}s.
\end{aligned}$$

The goal now is to exploit Lemma 4.11 in order to identify terms in $\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon)$ and $\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon)$ that (essentially) cancel each other. We start by analyzing the nonlinear functions F and T. If $v \in (H^{m+1}(\mathbb{R}^3))^4$ for some $m \geq 2$, then Lemma 4.11 yields

$$\left\|F\left(\mathrm{e}^{t\mathcal{P}_\varepsilon}v\right)\mathrm{e}^{t\mathcal{P}_\varepsilon}v - F\left(\mathrm{e}^{t\mathcal{P}_0}v\right)\mathrm{e}^{t\mathcal{P}_0}v\right\|_{H^m} \leq C\min\left\{\varepsilon, \frac{t}{\varepsilon}\right\}\|v\|_{H^{m+1}}$$

for all $t \geq 0$ and a constant C independent of t and ε. Further, using the fact that the matrix $\mathrm{e}^{t\mathcal{P}_0}$ preserves the Euclidean norm and commutes with scalars, we obtain

$$F\left(\mathrm{e}^{t\mathcal{P}_0}v\right)\mathrm{e}^{t\mathcal{P}_0}v = F\left(v\right)\mathrm{e}^{t\mathcal{P}_0}v = \mathrm{e}^{t\mathcal{P}_0}F\left(v\right)v.$$

Next, we replace the matrix $\mathrm{e}^{t\mathcal{P}_0}$ by the operator $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ again. Lemma 4.11 then gives

$$\left\|F\left(\mathrm{e}^{t\mathcal{P}_\varepsilon}u_0\right)\mathrm{e}^{t\mathcal{P}_\varepsilon}u_0 - \mathrm{e}^{t\mathcal{P}_\varepsilon}\left[F\left(u_0\right)u_0\right]\right\| \leq C\min\left\{\varepsilon, \frac{t}{\varepsilon}\right\}\|v\|_{H^{m+1}}. \tag{4.55}$$

Further, recall that $T(v,w) = |v|^2 w + v^* w v + w^* v v$. Thus, if $v \in (H^{m+1}(\mathbb{R}^3))^4$ and $w \in (H^{m+1}(\mathbb{R}^3))^4$ for some $m \geq 2$, Lemma 4.11 yields

$$\left\|T\left(\mathrm{e}^{t\mathcal{P}_\varepsilon}v, \mathrm{e}^{t\mathcal{P}_\varepsilon}w\right) - T\left(\mathrm{e}^{t\mathcal{P}_0}v, \mathrm{e}^{t\mathcal{P}_0}w\right)\right\|_{H^m} \leq C\min\left\{\varepsilon, \frac{t}{\varepsilon}\right\}\|v\|_{H^{m+1}}^2\|w\|_{H^{m+1}}$$

for all $t \geq 0$ and a constant C independent of t and ε. With the properties from Lemma 4.12 and the fact that matrices commute with scalars, we obtain

$$T\left(\mathrm{e}^{t\mathcal{P}_0}v, \mathrm{e}^{t\mathcal{P}_0}w\right) = \mathrm{e}^{t\mathcal{P}_0}T(v,w).$$

Again, we can replace $\mathrm{e}^{t\mathcal{P}_0}$ by $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ using Lemma 4.11, which yields

$$\left\|T\left(\mathrm{e}^{t\mathcal{P}_\varepsilon}v, \mathrm{e}^{t\mathcal{P}_\varepsilon}w\right) - \mathrm{e}^{t\mathcal{P}_\varepsilon}T\left(v,w\right)\right\|_{H^m} \leq C\min\left\{\varepsilon, \frac{t}{\varepsilon}\right\}\|v\|_{H^{m+1}}^2\|w\|_{H^{m+1}}. \tag{4.56}$$

We now want to use both (4.55) and (4.56) for $\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon)$ and $\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon)$. Since $u_0 \in (H^{\widehat{m}+6}(\mathbb{R}^3))^4$ by assumption, we can use (4.55) with $m = \widehat{m}+5$ and with $t = r + \frac{\tau}{2}$ in $\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon)$ and $t = r$ in $\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon)$. Considering the two additional integrals and that the operator $\mathcal{L}_\varepsilon$ is uniformly bounded in ε at the cost of two spatial derivatives, this yields an $\mathcal{O}^{\widehat{m}+3}(\tau^2\min\{\varepsilon, \frac{\tau}{\varepsilon}\})$ remainder. Further, using similar reasons, one can easily see that the first argument of T in $\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon)$ and $\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon)$ is in $(H^{\widehat{m}+6}(\mathbb{R}^3))^4$ and the second one is in $(H^{\widehat{m}+4}(\mathbb{R}^3))^4$ with norm of $\mathcal{O}(\tau)$. Thus, (4.56) can be applied with $m = \widehat{m}+3$ and $t = s$ in both $\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon)$ and $\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon)$, yielding another $\mathcal{O}^{\widehat{m}+3}(\tau^2\min\{\varepsilon, \frac{\tau}{\varepsilon}\})$ remainder. Overall, we obtain

$$\begin{aligned}
\mathcal{R}_\tau^1(\mathcal{L}_\varepsilon) &= \widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_\varepsilon) + \mathcal{O}^{\widehat{m}+3}\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right),\\
\mathcal{R}_\tau^2(\mathcal{L}_\varepsilon) &= \widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_\varepsilon) + \mathcal{O}^{\widehat{m}+3}\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right)
\end{aligned} \tag{4.57}$$

where

$$\begin{aligned}
\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_\varepsilon) &= -\mathrm{i}\int_0^{\frac{\tau}{2}} \mathrm{e}^{-s\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{s\mathcal{P}_\varepsilon}\int_0^s \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\left[F\left(u_0\right)u_0\right]\mathrm{d}r\,\mathrm{d}s\\
&\quad + \mathrm{i}\int_0^{\frac{\tau}{2}} T\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0, \int_s^{\frac{\tau}{2}} \mathrm{e}^{-r\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{(r+\frac{\tau}{2})\mathcal{P}_\varepsilon}u_0\,\mathrm{d}r\right)\mathrm{d}s\\
&= -\mathrm{i}\int_0^{\frac{\tau}{2}} s\mathrm{e}^{-s\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{(s+\frac{\tau}{2})\mathcal{P}_\varepsilon}\left[F\left(u_0\right)u_0\right]\mathrm{d}s\\
&\quad + \mathrm{i}\int_0^{\frac{\tau}{2}} T\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0, \int_s^{\frac{\tau}{2}} \mathrm{e}^{-r\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{(r+\frac{\tau}{2})\mathcal{P}_\varepsilon}u_0\,\mathrm{d}r\right)\mathrm{d}s,\\
\widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_\varepsilon) &= -\mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}} T\left(u_0, \int_0^s \mathrm{e}^{-r\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\,\mathrm{d}r\right)\mathrm{d}s\\
&\quad + \mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}} \mathrm{e}^{-s\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon\mathrm{e}^{s\mathcal{P}_\varepsilon}\int_s^{\frac{\tau}{2}} F\left(u_0\right)u_0\,\mathrm{d}r\,\mathrm{d}s
\end{aligned} \tag{4.58}$$

$$= -\mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}} T\left(u_0, \int_0^s \mathrm{e}^{-r\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon \mathrm{e}^{r\mathcal{P}_\varepsilon} u_0 \,\mathrm{d}r\right)\mathrm{d}s$$
$$+\mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}} \left(\frac{\tau}{2}-s\right)\mathrm{e}^{-s\mathcal{P}_\varepsilon}\mathcal{L}_\varepsilon \mathrm{e}^{s\mathcal{P}_\varepsilon}\left[F\left(u_0\right)u_0\right]\mathrm{d}s. \tag{4.59}$$

Before we continue, we divide the operator $\mathcal{L}_\varepsilon$ from (4.9) into $\mathcal{L}_\varepsilon = \mathcal{L}_{\mathcal{D}_\varepsilon} + \mathcal{L}_V + \mathcal{L}_A$ with

$$\mathcal{L}_{\mathcal{D}_\varepsilon} = -\mathrm{i}\mathcal{D}_\varepsilon\left(\Pi_\varepsilon^+ - \Pi_\varepsilon^-\right), \qquad \mathcal{L}_V = -\mathrm{i}V(x), \qquad \mathcal{L}_A = \mathrm{i}\sum_{j=1}^3 A_j(x)\alpha_j.$$

The reason for this distinction is their different commutative behavior with regard to the operator $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ or the matrix $\mathrm{e}^{t\mathcal{P}_0}$: $\mathcal{L}_{\mathcal{D}_\varepsilon}$ is a pseudo-differential operator which commutes with $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ (recall that $\mathcal{D}_\varepsilon$ corresponds to multiplication with a scalar in Fourier space). $\mathcal{L}_V$ is a scalar-valued function and thus commutes with $\mathrm{e}^{t\mathcal{P}_0}$. However, the matrix-valued function $\mathcal{L}_A$ commutes neither with $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ nor with $\mathrm{e}^{t\mathcal{P}_0}$. Since T is additive in the second argument, we can divide $\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_\varepsilon)$ and $\widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_\varepsilon)$ accordingly as

$$\begin{aligned}\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_\varepsilon) &= \widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_{\mathcal{D}_\varepsilon}) + \widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_V) + \widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_A),\\ \widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_\varepsilon) &= \widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_{\mathcal{D}_\varepsilon}) + \widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_V) + \widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_A).\end{aligned} \tag{4.60}$$

In the rest of the proof, we will analyze the $\mathcal{L}_{\mathcal{D}_\varepsilon}$, $\mathcal{L}_V$ and $\mathcal{L}_A$ parts separately.

Part 1: $\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_{\mathcal{D}_\varepsilon})$ and $\widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_{\mathcal{D}_\varepsilon})$. Since $\mathrm{e}^{t\mathcal{P}_\varepsilon}$ and $\mathcal{L}_{\mathcal{D}_\varepsilon}$ commute, we obtain from (4.58) and (4.59) with $\mathcal{L}_\varepsilon$ replaced by $\mathcal{L}_{\mathcal{D}_\varepsilon}$ that

$$\begin{aligned}\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_{\mathcal{D}_\varepsilon}) &= -\mathrm{i}\int_0^{\frac{\tau}{2}} s\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\mathcal{L}_{\mathcal{D}_\varepsilon}\left[F\left(u_0\right)u_0\right]\mathrm{d}s + \mathrm{i}\int_0^{\frac{\tau}{2}} T\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0, \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_s^{\frac{\tau}{2}}\mathcal{L}_{\mathcal{D}_\varepsilon}u_0\,\mathrm{d}r\right)\mathrm{d}s\\ &= -\mathrm{i}\int_0^{\frac{\tau}{2}} s\,\mathrm{d}s\,\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\mathcal{L}_{\mathcal{D}_\varepsilon}\left[F\left(u_0\right)u_0\right] + \mathrm{i}\int_0^{\frac{\tau}{2}} \frac{\tau}{2}-s\,\mathrm{d}s\,\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}T\left(u_0, \mathcal{L}_{\mathcal{D}_\varepsilon}u_0\right)\\ &\quad + \mathcal{O}^{\widehat{m}+3}\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right),\\ \widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_{\mathcal{D}_\varepsilon}) &= -\mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}} T\left(u_0, \int_0^s \mathcal{L}_{\mathcal{D}_\varepsilon}u_0\,\mathrm{d}r\right)\mathrm{d}s + \mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}}\left(\frac{\tau}{2}-s\right)\mathcal{L}_{\mathcal{D}_\varepsilon}\left[F\left(u_0\right)u_0\right]\mathrm{d}s\\ &= -\mathrm{i}\int_0^{\frac{\tau}{2}} s\,\mathrm{d}s\,\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}T\left(u_0, \mathcal{L}_{\mathcal{D}_\varepsilon}u_0\right) + \mathrm{i}\int_0^{\frac{\tau}{2}} \frac{\tau}{2}-s\,\mathrm{d}s\,\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\mathcal{L}_{\mathcal{D}_\varepsilon}\left[F\left(u_0\right)u_0\right].\end{aligned}$$

Here, we used (4.56) once more for $\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_{\mathcal{D}_\varepsilon})$ (with $m = \widehat{m}+3$ and $t = \frac{\tau}{2}$), yielding another remainder term. Further, we used the real-linearity of T in the second argument for both terms. Since

$$\int_0^{\frac{\tau}{2}} s\,\mathrm{d}s = \frac{1}{8}\tau^2 = \int_0^{\frac{\tau}{2}} \frac{\tau}{2}-s\,\mathrm{d}s, \tag{4.61}$$

all terms in $\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_{\mathcal{D}_\varepsilon})$ apart from the remainder appear in $\widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_{\mathcal{D}_\varepsilon})$ with opposite sign. Thus,

$$\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_{\mathcal{D}_\varepsilon}) + \widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_{\mathcal{D}_\varepsilon}) = \mathcal{O}^{\widehat{m}+3}\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right). \tag{4.62}$$

Since $\mathcal{R}_\tau^1(\mathcal{L}_{\mathcal{D}_\varepsilon})$ and $\mathcal{R}_\tau^2(\mathcal{L}_{\mathcal{D}_\varepsilon})$ originated from the errors in the first and the second Lie splitting step, respectively, this means that the $\mathcal{O}(\tau^2)$ errors from the first Lie splitting step cancel with those of the second one up to $\mathcal{O}^{\widehat{m}+3}(\tau^2\min\{\varepsilon, \frac{\tau}{\varepsilon}\})$ remainders.

Part 2: $\widetilde{\mathcal{R}}^1_\tau(\mathcal{L}_V)$ and $\widetilde{\mathcal{R}}^2_\tau(\mathcal{L}_V)$. Next, we consider (4.58) and (4.59) with the scalar-valued function $\mathcal{L}_V = -\mathrm{i}V(x)$ instead of the operator $\mathcal{L}_\varepsilon$. We first note that for $v \in (H^{\widehat{m}+6}(\mathbb{R}^3))^4$, Lemma 4.11 together with the regularity assumption on V implies

$$\left\| \mathrm{e}^{t_1\mathcal{P}_\varepsilon} \mathcal{L}_V \mathrm{e}^{t_2\mathcal{P}_\varepsilon} v - \mathrm{e}^{t_1\mathcal{P}_0} \mathcal{L}_V \mathrm{e}^{t_2\mathcal{P}_0} v \right\|_{H^{\widehat{m}+5}} \leq C \min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\} \|v\|_{H^{\widehat{m}+6}}$$

for all $t_1, t_2 \in \mathbb{R}$ with $|t_1|, |t_2| \leq \tau$ and a constant C independent of τ and ε. Considering that $\mathcal{L}_V$ commutes with $\mathrm{e}^{t\mathcal{P}_0}$ for any $t \in \mathbb{R}$ and using Lemma 4.11 in the reverse direction, we have

$$\left\| \mathrm{e}^{t_1\mathcal{P}_\varepsilon} \mathcal{L}_V \mathrm{e}^{t_2\mathcal{P}_\varepsilon} v - \mathrm{e}^{(t_1+t_2)\mathcal{P}_\varepsilon} \mathcal{L}_V v \right\|_{H^{\widehat{m}+5}} \leq C \min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\} \|v\|_{H^{\widehat{m}+6}}.$$

Together with the surrounding integrals in (4.58) and (4.59), we obtain

$$\begin{aligned}
\widetilde{\mathcal{R}}^1_\tau(\mathcal{L}_V) &= -\mathrm{i}\int_0^{\frac{\tau}{2}} s\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon} \mathcal{L}_V \left[F\left(u_0\right) u_0\right] \mathrm{d}s + \mathrm{i}\int_0^{\frac{\tau}{2}} T\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon} u_0, \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon} \int_s^{\frac{\tau}{2}} \mathcal{L}_V u_0 \,\mathrm{d}r\right) \mathrm{d}s \\
&\quad + \mathcal{O}^{\widehat{m}+5}\left(\tau^2 \min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right) \\
&= -\mathrm{i}\int_0^{\frac{\tau}{2}} s\,\mathrm{d}s\, \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon} \mathcal{L}_V \left[F\left(u_0\right) u_0\right] + \mathrm{i}\int_0^{\frac{\tau}{2}} \frac{\tau}{2} - s\,\mathrm{d}s\, \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon} T\left(u_0, \mathcal{L}_V u_0\right) \\
&\quad + \mathcal{O}^{\widehat{m}+5}\left(\tau^2 \min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right), \\
\widetilde{\mathcal{R}}^2_\tau(\mathcal{L}_V) &= -\mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon} \int_0^{\frac{\tau}{2}} T\left(u_0, \int_0^s \mathcal{L}_V u_0 \,\mathrm{d}r\right) \mathrm{d}s + \mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon} \int_0^{\frac{\tau}{2}} \left(\frac{\tau}{2} - s\right) \mathcal{L}_V \left[F\left(u_0\right) u_0\right] \mathrm{d}s \\
&\quad + \mathcal{O}^{\widehat{m}+5}\left(\tau^2 \min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right) \\
&= -\mathrm{i}\int_0^{\frac{\tau}{2}} s\,\mathrm{d}s\, \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon} T\left(u_0, \mathcal{L}_V u_0\right) + \mathrm{i}\int_0^{\frac{\tau}{2}} \frac{\tau}{2} - s\,\mathrm{d}s\, \mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon} \mathcal{L}_V \left[F\left(u_0\right) u_0\right] \\
&\quad + \mathcal{O}^{\widehat{m}+5}\left(\tau^2 \min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right),
\end{aligned}$$

where we again used (4.56) for $\widetilde{\mathcal{R}}^1_\tau(\mathcal{L}_V)$. As before, with (4.61), we obtain

$$\widetilde{\mathcal{R}}^1_\tau(\mathcal{L}_V) + \widetilde{\mathcal{R}}^2_\tau(\mathcal{L}_V) = \mathcal{O}^{\widehat{m}+5}\left(\tau^2 \min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right). \tag{4.63}$$

Part 3: $\widetilde{\mathcal{R}}^1_\tau(\mathcal{L}_A)$ and $\widetilde{\mathcal{R}}^2_\tau(\mathcal{L}_A)$. Finally, we look at (4.58) and (4.59) with the matrix-valued function $\mathcal{L}_A = \mathrm{i}\sum_{j=1}^3 A_j(x)\alpha_j$ instead of the operator $\mathcal{L}_\varepsilon$. As in the $\mathcal{L}_V$-case, we obtain

$$\left\| \mathrm{e}^{t_1\mathcal{P}_\varepsilon} \mathcal{L}_A \mathrm{e}^{t_2\mathcal{P}_\varepsilon} v - \mathrm{e}^{t_1\mathcal{P}_0} \mathcal{L}_A \mathrm{e}^{t_2\mathcal{P}_0} v \right\|_{H^{\widehat{m}+5}} \leq C \min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\} \|v\|_{H^{\widehat{m}+6}}$$

for $v \in (H^{\widehat{m}+6}(\mathbb{R}^3))^4$ and for all $t_1, t_2 \in \mathbb{R}$ with $|t_1|, |t_2| \leq \tau$. However, $\mathcal{L}_A$ and $\mathrm{e}^{t\mathcal{P}_0}$ do not commute for any $t \neq 0$. Instead, Lemma 4.12 (ii) yields

$$\mathcal{L}_A \mathrm{e}^{t\mathcal{P}_0} = \mathrm{e}^{-t\mathcal{P}_0} \mathcal{L}_A \tag{4.64}$$

for all $t \in \mathbb{R}$. This in particular implies $\mathrm{e}^{t_1\mathcal{P}_0} \mathcal{L}_A \mathrm{e}^{t_2\mathcal{P}_0} v = \mathrm{e}^{(t_1-t_2)\mathcal{P}_0} \mathcal{L}_A v$, and thus

$$\left\| \mathrm{e}^{t_1\mathcal{P}_\varepsilon} \mathcal{L}_A \mathrm{e}^{t_2\mathcal{P}_\varepsilon} v - \mathrm{e}^{(t_1-t_2)\mathcal{P}_0} \mathcal{L}_A v \right\|_{H^{\widehat{m}+5}} \leq C \min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\} \|v\|_{H^{\widehat{m}+6}}.$$

Applying this for $v = u_0$ and for $v = F(u_0)u_0$ in (4.58) and (4.59) gives

$$\begin{aligned}
\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_A) &= -\mathrm{i}\int_0^{\frac{\tau}{2}} s\mathrm{e}^{-(2s+\frac{\tau}{2})\mathcal{P}_0}\mathcal{L}_A\left[F\left(u_0\right)u_0\right]\,\mathrm{d}s \\
&\quad + \mathrm{i}\int_0^{\frac{\tau}{2}} T\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}u_0, \int_s^{\frac{\tau}{2}} \mathrm{e}^{-(2r+\frac{\tau}{2})\mathcal{P}_0}\mathcal{L}_A u_0\,\mathrm{d}r\right)\,\mathrm{d}s + \mathcal{O}^{\widehat{m}+5}\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right) \\
&= -\mathrm{i}\int_0^{\frac{\tau}{2}} s\mathrm{e}^{-(2s+\frac{\tau}{2})\mathcal{P}_0}\,\mathrm{d}s\,\mathcal{L}_A\left[F\left(u_0\right)u_0\right] \\
&\quad + \mathrm{i}\int_0^{\frac{\tau}{2}}\int_s^{\frac{\tau}{2}} T\left(\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_0}u_0, \mathrm{e}^{-(2r+\frac{\tau}{2})\mathcal{P}_0}\mathcal{L}_A u_0\right)\mathrm{d}r\,\mathrm{d}s + \mathcal{O}^{\widehat{m}+5}\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right), \qquad (4.65) \\
\widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_A) &= -\mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}} T\left(u_0, \int_0^s \mathrm{e}^{-2r\mathcal{P}_0}\mathcal{L}_A u_0\,\mathrm{d}r\right)\,\mathrm{d}s \\
&\quad + \mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}}\left(\frac{\tau}{2}-s\right)\mathrm{e}^{-2s\mathcal{P}_0}\mathcal{L}_A\left[F\left(u_0\right)u_0\right]\,\mathrm{d}s + \mathcal{O}^{\widehat{m}+5}\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right) \\
&= -\mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}}\int_0^s T\left(u_0, \mathrm{e}^{-2r\mathcal{P}_0}\mathcal{L}_A u_0\right)\mathrm{d}r\,\mathrm{d}s \\
&\quad + \mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\int_0^{\frac{\tau}{2}}\left(\frac{\tau}{2}-s\right)\mathrm{e}^{-2s\mathcal{P}_0}\,\mathrm{d}s\,\mathcal{L}_A\left[F\left(u_0\right)u_0\right] + \mathcal{O}^{\widehat{m}+5}\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right) \qquad (4.66)
\end{aligned}$$

where we also replaced $\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}$ by $\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_0}$ in the first argument of T in $\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_A)$. To analyze (4.65) and (4.66) further, we need to take a detailed look at terms of the form $T\left(\mathrm{e}^{t_1\mathcal{P}_0}u_0, \mathrm{e}^{t_2\mathcal{P}_0}\mathcal{L}_A u_0\right)$ for any $t_1, t_2 \in \mathbb{R}$. The definition of T, cf. (4.25), together with the properties from Lemma 4.12 (i) yields

$$\begin{aligned}
T\left(\mathrm{e}^{t_1\mathcal{P}_0}u_0, \mathrm{e}^{t_2\mathcal{P}_0}\mathcal{L}_A u_0\right) &= \left|\mathrm{e}^{t_1\mathcal{P}_0}u_0\right|^2 \mathrm{e}^{t_2\mathcal{P}_0}\mathcal{L}_A u_0 + 2\mathrm{Re}\left(\left(\mathrm{e}^{t_1\mathcal{P}_0}u_0\right)^* \mathrm{e}^{t_2\mathcal{P}_0}\mathcal{L}_A u_0\right)\mathrm{e}^{t_1\mathcal{P}_0}u_0 \\
&= \mathrm{e}^{t_2\mathcal{P}_0}\mathcal{L}_A\left[F(u_0)u_0\right] + 2\mathrm{Re}\left(u_0^*\mathrm{e}^{(t_2-t_1)\mathcal{P}_0}\mathcal{L}_A u_0\right)\mathrm{e}^{t_1\mathcal{P}_0}u_0.
\end{aligned}$$

Since $\mathcal{L}_A = \mathrm{i}\sum_{j=1}^3 A_j(x)\alpha_j$ by definition and since the matrices α_j are Hermitian, the matrix $\mathcal{L}_A$ is skew-Hermitian. Additionally using Lemma 4.12 (i) and (4.64), we obtain

$$\left(\mathrm{e}^{(t_2-t_1)\mathcal{P}_0}\mathcal{L}_A\right)^* = (\mathcal{L}_A)^*\left(\mathrm{e}^{(t_2-t_1)\mathcal{P}_0}\right)^* = -\mathcal{L}_A\mathrm{e}^{-(t_2-t_1)\mathcal{P}_0} = -\mathrm{e}^{(t_2-t_1)\mathcal{P}_0}\mathcal{L}_A.$$

This means that the matrix $\mathrm{e}^{(t_2-t_1)\mathcal{P}_0}\mathcal{L}_A$ is also skew-Hermitian, which in turns implies that

$$\mathrm{Re}\left(u_0^*\mathrm{e}^{(t_2-t_1)\mathcal{P}_0}\mathcal{L}_A u_0\right) = 0.$$

Overall, we find

$$T\left(\mathrm{e}^{t_1\mathcal{P}_0}u_0, \mathrm{e}^{t_2\mathcal{P}_0}\mathcal{L}_A u_0\right) = \mathrm{e}^{t_2\mathcal{P}_0}\mathcal{L}_A\left[F(u_0)u_0\right].$$

This can be used with $t_1 = \frac{\tau}{2}, t_2 = -(2r+\frac{\tau}{2})$ in (4.65) and with $t_1 = 0, t_2 = -2r$ in (4.66) to obtain

$$\begin{aligned}
\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_A) &= -\mathrm{i}\left(\int_0^{\frac{\tau}{2}} s\mathrm{e}^{-(2s+\frac{\tau}{2})\mathcal{P}_0}\,\mathrm{d}s - \int_0^{\frac{\tau}{2}}\int_s^{\frac{\tau}{2}} \mathrm{e}^{-(2r+\frac{\tau}{2})\mathcal{P}_0}\,\mathrm{d}r\,\mathrm{d}s\right)\mathcal{L}_A\left[F\left(u_0\right)u_0\right] \\
&\quad + \mathcal{O}^{\widehat{m}+5}\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right),
\end{aligned}$$

$$\widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_A) = -\mathrm{i}\mathrm{e}^{\frac{\tau}{2}\mathcal{P}_\varepsilon}\left(\int_0^{\frac{\tau}{2}}\int_0^s \mathrm{e}^{-2r\mathcal{P}_0}\,\mathrm{d}r\,\mathrm{d}s - \int_0^{\frac{\tau}{2}}\left(\frac{\tau}{2}-s\right)\mathrm{e}^{-2s\mathcal{P}_0}\,\mathrm{d}s\right)\mathcal{L}_A\left[F\left(u_0\right)u_0\right] + \mathcal{O}^{\widehat{m}+5}\left(\tau^2\min\left\{\varepsilon,\frac{\tau}{\varepsilon}\right\}\right).$$

Since one can check that

$$\int_0^{\frac{\tau}{2}} s\mathrm{e}^{-2s\mathcal{P}_0}\,\mathrm{d}s = \frac{\tau^2}{4}\mathrm{e}^{-\tau\mathcal{P}_0}\varphi_2(\tau\mathcal{P}_0) = \int_0^{\frac{\tau}{2}}\int_s^{\frac{\tau}{2}} \mathrm{e}^{-2r\mathcal{P}_0}\,\mathrm{d}r\,\mathrm{d}s,$$
$$\int_0^{\frac{\tau}{2}}\int_0^s \mathrm{e}^{-2r\mathcal{P}_0}\,\mathrm{d}r\,\mathrm{d}s = \frac{\tau^2}{4}\varphi_2(-\tau\mathcal{P}_0) = \int_0^{\frac{\tau}{2}}\left(\frac{\tau}{2}-s\right)\mathrm{e}^{-2s\mathcal{P}_0}\,\mathrm{d}s,$$

we finally obtain

$$\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_A) = \mathcal{O}^{\widehat{m}+5}\left(\tau^2\min\left\{\varepsilon,\frac{\tau}{\varepsilon}\right\}\right), \qquad \widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_A) = \mathcal{O}^{\widehat{m}+5}\left(\tau^2\min\left\{\varepsilon,\frac{\tau}{\varepsilon}\right\}\right). \tag{4.67}$$

Note that in contrast to parts 1 and 2, we could consider $\widetilde{\mathcal{R}}_\tau^1(\mathcal{L}_A)$ and $\widetilde{\mathcal{R}}_\tau^2(\mathcal{L}_A)$ separately here. This means that for the magnetic potential part of $\mathcal{L}_\varepsilon$, there are actually no $\mathcal{O}(\tau^2)$ error terms from the individual Lie splitting steps.

After all, Eq. (4.67) together with (4.57), (4.60), (4.62) and (4.63) as well as Lemma 4.9 yield the claim. □

4.3.5 Numerical experiment

To validate the local splitting error estimate from Lemma 4.2, we conduct a numerical experiment where we choose various step sizes τ and three different values of ε, and we observe the error between the result obtained after applying *one* step of the splitting scheme (4.14) with step size τ on the one hand side and the exact solution at time $t = \tau$ on the other hand side. Since we can neither solve the full NLDE nor the LDE- and the NL-subproblems exactly, we approximate each of its solution with MATLAB's `ode45`-solver using very small tolerances. The results can be considered as "exact", in the sense that the overall error is dominated by the (local) splitting error. As in Sections 2.4 and 3.5.1, we switch to the NLDE in one space dimension for the experiment, and we use the same initial data and potentials. Since $H^1(\mathbb{R})$ is an algebra, it is sufficient to choose $\widehat{m} = 1$ in Assumption 4.1. Consequently, the error is measured in the H^1-norm. The results are shown in Figure 4.2.

To understand the consistency of the error bound with the observed error, first note that for the right-hand side of the local error estimate from Lemma 4.2, we have

$$\min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\} = \begin{cases} \tau^3, & \varepsilon < \tau, \\ \tau^2\varepsilon, & \varepsilon^2 < \tau \leq \varepsilon, \\ \frac{\tau^3}{\varepsilon}, & \tau \leq \varepsilon^2. \end{cases}$$

In particular, for $\tau > \varepsilon$, we obtain a local error bound that is of third order in τ uniformly in ε, which is what we observe in Figure 4.2 by a comparison with the black, dash-dotted reference line. For $\varepsilon^2 < \tau \leq \varepsilon$, a local error proportional to $\tau^2\varepsilon$ is expected. The dotted reference lines in Figure 4.2, which are of the form $C_3\tau^2\varepsilon$ for a joint constant C_3, reveal that indeed, the error can be capped by said bound in this step size regime. However, for most step sizes $\varepsilon^2 < \tau \leq \varepsilon$, a better, but irregular error behavior is actually observed. Finally, for step sizes $\tau \leq \varepsilon^2$, Lemma 4.2 yields an $\mathcal{O}\left(\frac{\tau^3}{\varepsilon}\right)$ local error bound. This is exactly what we see with the help of the dashed reference lines in Figure 4.2, which are of the form $C_2\frac{\tau^3}{\varepsilon}$ with a constant C_2 that is the same for all three values of ε depicted.

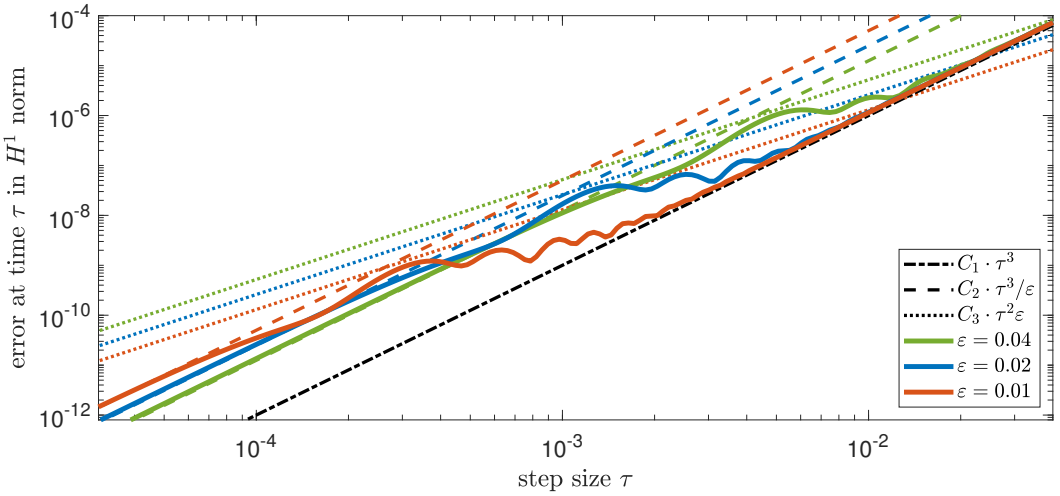

Figure 4.2: Local error in H^1 of the splitting scheme (4.14) in dependency of the time step size τ for three different values of ε. Note that the dashed third order reference lines all use the same constant C_2, and the dotted second order reference lines the same constant C_3.

4.4 Solving the subproblems and final method

So far, we assumed that all three subproblems in (4.12) can be solved exactly, which, however, is not the case for the LDE- and the NL-subproblem. In this section, we discuss how the solutions of these subproblems can be approximated. Since we know from Lemma 4.2 that the local splitting error itself is in $\mathcal{O}^{\widehat{m}}\Big(\min\Big\{\frac{\tau^3}{\varepsilon}, \max\{\tau^2\varepsilon, \tau^3\}\Big\}\Big)$, we aim for an accuracy of the same size for each subproblem. As for the NPI-2 method from Section 3.3.1, the key strategy is to iterate Duhamel's formula and then integrate all oscillatory parts exactly, but approximate slowly varying parts. However, in contrast to Section 3.3.1, having split the NLDE into several subproblems brings some significant advantages. The LDE-subproblem is linear, such that the number of terms does not increase dramatically for each additional iteration of Duhamel's formula. Furthermore, the NL-subproblem only contains the dominant part $\mathcal{P}_\varepsilon$ of the differential operator $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon$ and no potentials. It turns out that this leads to special properties of solutions of the NL-subproblem which yield major simplifications in the integrals of Duhamel's formula. All in all, the solutions of both subproblems can be approximated efficiently.

We first discuss the NL-subproblem and then the LDE-subproblem in Subsections 4.4.1 and 4.4.2, before combining both results to state the final time integrator in Subsection 4.4.3. As in Section 4.3.1, we will analyze the approximation error in H^m for a generic value of m when talking about the NL-subproblem, whereas we chose the particular value $m = \widehat{m}$ from Assumption 4.1 for the LDE-subproblem.

4.4.1 The nonlinearity-subproblem

For the nonlinearity-subproblem, we assume that we start with initial data $u_0 \in \big(H^{m+1}(\mathbb{R}^3)\big)^4$ for some $m \geq 2$, and that the solution with said initial data exists over the whole time interval $[0, \tau]$ and remains uniformly bounded in H^{m+1} w.r.t. ε and t. This is especially fulfilled with $m = \widehat{m}$ in the setting of Assumption 4.1. We already established the expansion

$$\Psi_\tau^{\mathrm{NL}}(u_0) = \mathrm{e}^{\tau\mathcal{P}_\varepsilon}u_0 + \mathrm{e}^{\tau\mathcal{P}_\varepsilon}\Upsilon_\tau^{\mathrm{NL}}(u_0) + \mathrm{e}^{\tau\mathcal{P}_\varepsilon}\widetilde{\Upsilon}_\tau^{\mathrm{NL}}\Big(u_0, \Upsilon_s^{\mathrm{NL}}(u_0)\Big) + \mathcal{O}^{m+1}\Big(\tau^3\Big)$$

in Lemma 4.5 (iv). Inserting the definition of Υ_t^{NL} and $\widetilde{\Upsilon}_t^{\mathrm{NL}}$ gives

$$\begin{aligned}\Psi_\tau^{\mathrm{NL}}(u_0) = {} & \mathrm{e}^{\tau\mathcal{P}_\varepsilon}u_0 - \mathrm{i}\mathrm{e}^{\tau\mathcal{P}_\varepsilon}\int_0^\tau \mathrm{e}^{-s\mathcal{P}_\varepsilon}\left[F\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}u_0\right)\mathrm{e}^{s\mathcal{P}_\varepsilon}u_0\right]\mathrm{d}s \\ & - \mathrm{i}\mathrm{e}^{\tau\mathcal{P}_\varepsilon}\int_0^\tau \mathrm{e}^{-s\mathcal{P}_\varepsilon}T\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}u_0, -\mathrm{i}\mathrm{e}^{s\mathcal{P}_\varepsilon}\int_0^s \mathrm{e}^{-r\mathcal{P}_\varepsilon}\left[F\left(\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\right)\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\right]\mathrm{d}r\right)\mathrm{d}s \\ & + \mathcal{O}^{m+1}\left(\tau^3\right). \end{aligned} \tag{4.68}$$

If we omit the remainders, then this representation is obviously explicit since it only depends on the initial value u_0. Furthermore, as $\mathrm{e}^{t\mathcal{P}_\varepsilon} = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^+ + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^-$, the integration variables s and r only appear within scalar-valued, space-independent functions. In the integrals, those functions can thus be separated from all operators. All in all, this implies that the representation can indeed be computed analytically for given u_0. On top of that, it is a uniform third order in τ approximation to the exact solution $\Psi_\tau^{\mathrm{NL}}(u_0)$. This is exactly what we aim for in this section. However, this representation is fairly complicated, in particular due to the composition of the nonlinearities in the second integral. Additionally, the fact that both applications of the projectors and products of space-dependent functions appear multiple times implies that the representation is expensive to compute numerically (after a suitable space discretization) since it requires several Fourier transforms to switch between Fourier and physical space. This is why we aim for a simpler representation.

To this purpose, we can make use of the approximation $\mathrm{e}^{t\mathcal{P}_\varepsilon} \approx \mathrm{e}^{t\mathcal{P}_0}$ again in the second integral. This approximation in particular allowed deriving the estimates (4.55) and (4.56). Using the former one first with $t = r$ (and considering the two surrounding integrals) and the latter one afterward with $t = s$ (and considering the surrounding integral and that the second argument of T is of $\mathcal{O}^{m+1}(\tau)$), we obtain

$$\begin{aligned}&\int_0^\tau \mathrm{e}^{-s\mathcal{P}_\varepsilon}T\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}u_0, -\mathrm{i}\mathrm{e}^{s\mathcal{P}_\varepsilon}\int_0^s \mathrm{e}^{-r\mathcal{P}_\varepsilon}\left[F\left(\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\right)\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\right]\mathrm{d}r\right)\mathrm{d}s \\ &\quad = \int_0^\tau T\left(u_0, -\mathrm{i}\int_0^s F\left(u_0\right)u_0\,\mathrm{d}r\right)\mathrm{d}s + \mathcal{O}^m\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right).\end{aligned}$$

Further, the definition (4.25) of T yields

$$\begin{aligned}T\left(u_0, -\mathrm{i}\int_0^s F\left(u_0\right)u_0\,\mathrm{d}r\right) &= sT\left(u_0, -\mathrm{i}\left|u_0\right|^2 u_0\right) \\ &= s\left(-\mathrm{i}\left|u_0\right|^2\left|u_0\right|^2 u_0 + 2\mathrm{Re}\left(-\mathrm{i}\left|u_0\right|^2 u_0^* u_0\right)\right) \\ &= -\mathrm{i}s\left|u_0\right|^4 u_0,\end{aligned}$$

such that we obtain the representation

$$\begin{aligned}&\int_0^\tau \mathrm{e}^{-s\mathcal{P}_\varepsilon}T\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}u_0, -\mathrm{i}\mathrm{e}^{s\mathcal{P}_\varepsilon}\int_0^s \mathrm{e}^{-r\mathcal{P}_\varepsilon}\left[F\left(\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\right)\mathrm{e}^{r\mathcal{P}_\varepsilon}u_0\right]\mathrm{d}r\right)\mathrm{d}s \\ &\quad = -\mathrm{i}\frac{\tau^2}{2}\left|u_0\right|^4 u_0 + \mathcal{O}^m\left(\tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right).\end{aligned}$$

This simplified the second integral in (4.68) immensely. Overall, we have

$$\begin{aligned}\Psi_\tau^{\mathrm{NL}}(u_0) &= \Phi_\tau^{\mathrm{NL}}(u_0) + \mathcal{O}^m\left(\max\left\{\tau^3, \tau^2\min\left\{\varepsilon, \frac{\tau}{\varepsilon}\right\}\right\}\right) \\ &= \Phi_\tau^{\mathrm{NL}}(u_0) + \mathcal{O}^m\left(\min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\}\right)\end{aligned}$$

where we define Φ_τ^{NL} to be the numerical flow of the nonlinearity-subproblem, given by

$$\Phi_\tau^{\mathrm{NL}}(u) = \mathrm{e}^{\tau\mathcal{P}_\varepsilon}u - \mathrm{i}\mathrm{e}^{\tau\mathcal{P}_\varepsilon}\int_0^\tau \mathrm{e}^{-s\mathcal{P}_\varepsilon}\left[F\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}u\right)\mathrm{e}^{s\mathcal{P}_\varepsilon}u\right]\mathrm{d}s - \frac{\tau^2}{2}\mathrm{e}^{\tau\mathcal{P}_\varepsilon}|u|^4\,u. \tag{4.69}$$

Using (4.55) in the remaining integral as well is not a good idea, since there is only one surrounding integral, such that the local error order w.r.t. τ would be reduced. However, computing the remaining integral, and thus applying the whole operator Φ_τ^{NL}, does not cause any problems and, in particular, is not very expensive from a numerical point of view. To understand this, we present a different representation of Φ_τ^{NL}. First, we decompose

$$\Phi_\tau^{\mathrm{NL}}(u) = \Pi_\varepsilon^+\left[\Phi_\tau^{\mathrm{NL}}(u)\right] + \Pi_\varepsilon^-\left[\Phi_\tau^{\mathrm{NL}}(u)\right]. \tag{4.70}$$

For each component, using $\Pi_\varepsilon^\pm \mathrm{e}^{t\mathcal{P}_\varepsilon} = \Pi_\varepsilon^\pm\left[\mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^+ + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^-\right] = \mathrm{e}^{\mp\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^\pm$, we have

$$\begin{aligned}
\Pi_\varepsilon^\pm\left[\Phi_\tau^{\mathrm{NL}}(u)\right] &= \mathrm{e}^{\mp\mathrm{i}\tau/\varepsilon^2}\Pi_\varepsilon^\pm[u] - \mathrm{i}\mathrm{e}^{\mp\mathrm{i}\tau/\varepsilon^2}\Pi_\varepsilon^\pm\left[\int_0^\tau \mathrm{e}^{\pm\mathrm{i}s/\varepsilon^2}F\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}u\right)\mathrm{e}^{s\mathcal{P}_\varepsilon}u\,\mathrm{d}s\right] \\
&\quad - \frac{\tau^2}{2}\mathrm{e}^{\mp\mathrm{i}\tau/\varepsilon^2}\Pi_\varepsilon^\pm\left[|u|^4\,u\right] \\
&= \mathrm{e}^{\mp\mathrm{i}\tau/\varepsilon^2}\left(\Pi_\varepsilon^\pm[u] - \Pi_\varepsilon^\pm\left[\mathrm{i}\int_0^\tau \mathrm{e}^{\pm\mathrm{i}s/\varepsilon^2}F\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}u\right)\mathrm{e}^{s\mathcal{P}_\varepsilon}u\,\mathrm{d}s + \frac{\tau^2}{2}|u|^4\,u.\right]\right).
\end{aligned}$$

Introducing $u_+ = \Pi_\varepsilon^+[u]$, $u_- = \Pi_\varepsilon^-[u]$, we can compute

$$\left|\mathrm{e}^{-\mathrm{i}s/\varepsilon^2}u_+ + \mathrm{e}^{\mathrm{i}s/\varepsilon^2}u_-\right|^2 = |u_+|^2 + |u_-|^2 + \mathrm{e}^{2\mathrm{i}s/\varepsilon^2}(u_+)^*u_- + \mathrm{e}^{-2\mathrm{i}s/\varepsilon^2}(u_-)^*u_+$$

and thus

$$\begin{aligned}
F\left(\mathrm{e}^{s\mathcal{P}_\varepsilon}u\right)\mathrm{e}^{s\mathcal{P}_\varepsilon}u &= \left|\mathrm{e}^{-\mathrm{i}s/\varepsilon^2}u_+ + \mathrm{e}^{\mathrm{i}s/\varepsilon^2}u_-\right|^2\left(\mathrm{e}^{-\mathrm{i}s/\varepsilon^2}u_+ + \mathrm{e}^{\mathrm{i}s/\varepsilon^2}u_-\right) \\
&= \mathrm{e}^{-\mathrm{i}s/\varepsilon^2}\left(\left(|u_+|^2 + |u_-|^2\right)u_+ + (u_-)^*u_+u_-\right) + \mathrm{e}^{-3\mathrm{i}s/\varepsilon^2}(u_-)^*u_+u_+ \\
&\quad + \mathrm{e}^{\mathrm{i}s/\varepsilon^2}\left(\left(|u_+|^2 + |u_-|^2\right)u_- + (u_+)^*u_-u_+\right) + \mathrm{e}^{3\mathrm{i}s/\varepsilon^2}(u_+)^*u_-u_-.
\end{aligned}$$

Finally, we arrive at

$$\begin{aligned}
\Pi_\varepsilon^\pm\left[\Phi_\tau^{\mathrm{NL}}(u)\right] = \mathrm{e}^{\mp\mathrm{i}\tau/\varepsilon^2}\Bigg(u_\pm - \Pi_\varepsilon^\pm\Bigg[&\mathrm{i}\int_0^\tau \mathrm{e}^{(\pm1-1)\mathrm{i}s/\varepsilon^2}\,\mathrm{d}s\left(\left(|u_+|^2 + |u_-|^2\right)u_+ + (u_-)^*u_+u_-\right) \\
&+ \mathrm{i}\int_0^\tau \mathrm{e}^{(\pm1-3)\mathrm{i}s/\varepsilon^2}\,\mathrm{d}s\,(u_-)^*u_+u_+ \\
&+ \mathrm{i}\int_0^\tau \mathrm{e}^{(\pm1+1)\mathrm{i}s/\varepsilon^2}\,\mathrm{d}s\left(\left(|u_+|^2 + |u_-|^2\right)u_- + (u_+)^*u_-u_+\right) \\
&+ \mathrm{i}\int_0^\tau \mathrm{e}^{(\pm1+3)\mathrm{i}s/\varepsilon^2}\,\mathrm{d}s\,(u_+)^*u_-u_- \\
&+ \frac{\tau^2}{2}|u|^4\,u\Bigg]\Bigg).
\end{aligned} \tag{4.71}$$

All remaining integrals can easily be computed. Now, for a moment, assume that we know the Fourier representation of u_+ and u_- from the previous (sub)step and that we are seeking the Fourier representation of the two eigenspace components $\Pi_\varepsilon^\pm\left[\Phi_\tau^{\mathrm{NL}}(u)\right]$ of $\Phi_\tau^{\mathrm{NL}}(u)$ (see Remark 4.15 for a corresponding discussion). Then, the remarkable thing about this representation is that only two inverse Fourier transforms and two Fourier transforms are required, namely to translate both u_+ and u_- into physical space, and to translate the functions in the square brackets into Fourier space such that the projectors can be applied, respectively. We summarize the results in the following

Corollary 4.13. *Let $u_0 \in (H^{m+1}(\mathbb{R}^3))^4$ for some $m \geq 2$ and let $\tau > 0$. Assume that for all $\varepsilon \in (0,1)$, the solution $u(t) = \Psi_t^{\mathrm{NL}}(u_0)$ of the NL-subproblem from (4.12) exists on the interval $[0,\tau]$ and remains uniformly bounded w.r.t. ε and t. Then, for the numerical flow Φ_τ^{NL} of the nonlinearity-subproblem, given either by (4.69) or by (4.70) together with (4.71), we have*

$$\left\| \Psi_\tau^{\mathrm{NL}}(u_0) - \Phi_\tau^{\mathrm{NL}}(u_0) \right\|_{H^m} \leq C \min\left\{ \frac{\tau^3}{\varepsilon}, \max\left\{ \tau^2 \varepsilon, \tau^3 \right\} \right\}$$

for some constant C independent of τ and ε.

4.4.2 The LDE-subproblem

For the LDE-subproblem, we also already established an $\mathcal{O}(\tau^3)$ expansion in Lemma 4.4, which helped us to analyze the splitting error in Section 4.3. To construct this expansion, we always kept the dominating part $\mathcal{P}_\varepsilon$ of the differential operator $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon$ in the exponent of the evolutionary operator in Duhamel's formula, whereas the bounded operator $-\mathrm{i}\mathcal{D}_\varepsilon$ is considered as part of the inhomogeneity. Application of $\mathcal{D}_\varepsilon$ comes with a loss of spatial regularity, however. Since for the stability of the resulting method, we want to avoid this wherever possible, we consider different expansions here where the full operator $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon$ is taken to the exponential in Duhamel's formula. Thus, in contrast to (4.12), we write the LDE-subproblem as

$$\partial_t \psi^{\mathrm{LDE}} = -\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi^{\mathrm{LDE}} - \mathrm{i}W\psi^{\mathrm{LDE}}.$$

We assume that Assumption 4.1 holds (i.e., the same assumptions that were required for the local error bound of the splitting step). In particular, we assume that we start with initial data $u_0 \in (H^{\widehat{m}+6}(\mathbb{R}^3))^4$. Further, let $u(t) = \Psi_t^{\mathrm{LDE}}(u_0)$, $t \in [0,\tau]$, be the exact solution for said initial data. Then, Duhamel's formula yields

$$u(t) = \mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\mathcal{T}_\varepsilon} u_0 - \mathrm{i}\int_0^t \mathrm{e}^{-\frac{\mathrm{i}(t-s)}{\varepsilon^2}\mathcal{T}_\varepsilon} \left[W u(s) \right] \mathrm{d}s \tag{4.72}$$

for all $t \in [0,\tau]$. From the regularity of the potentials and the fact that solutions of the LDE remain uniformly bounded, we directly obtain

$$u(t) = \mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\mathcal{T}_\varepsilon} u_0 + \mathcal{O}^{\widehat{m}+6}(t)\,.$$

Inserting this into (4.72) once again, with t replaced by s, yields

$$u(t) = \mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\mathcal{T}_\varepsilon} u_0 - \mathrm{i}\int_0^t \mathrm{e}^{-\frac{\mathrm{i}(t-s)}{\varepsilon^2}\mathcal{T}_\varepsilon} \left[W \mathrm{e}^{-\frac{\mathrm{i}s}{\varepsilon^2}\mathcal{T}_\varepsilon} u_0 \right] \mathrm{d}s + \mathcal{O}^{\widehat{m}+6}\left(t^2\right).$$

Finally, taking $t = \tau$ in (4.72) and inserting the previous representation with t replaced by s inside the integral, we find

$$\begin{aligned} u(\tau) = \mathrm{e}^{-\frac{\mathrm{i}\tau}{\varepsilon^2}\mathcal{T}_\varepsilon} u_0 &- \mathrm{i}\int_0^\tau \mathrm{e}^{-\frac{\mathrm{i}(\tau-s)}{\varepsilon^2}\mathcal{T}_\varepsilon} \left[W \mathrm{e}^{-\frac{\mathrm{i}s}{\varepsilon^2}\mathcal{T}_\varepsilon} u_0 \right] \mathrm{d}s \\ &- \int_0^\tau \mathrm{e}^{-\frac{\mathrm{i}(\tau-s)}{\varepsilon^2}\mathcal{T}_\varepsilon} \left[W \int_0^s \mathrm{e}^{-\frac{\mathrm{i}(s-r)}{\varepsilon^2}\mathcal{T}_\varepsilon} \left[W \mathrm{e}^{-\frac{\mathrm{i}r}{\varepsilon^2}\mathcal{T}_\varepsilon} u_0 \right] \mathrm{d}r \right] \mathrm{d}s + \mathcal{O}^{\widehat{m}+6}\left(\tau^3\right). \end{aligned} \tag{4.73}$$

All s- or r-dependent operators cannot be combined due to the potential W in between them, such that the integrals cannot be computed analytically. Thus, it remains to approximate

both integrals appropriately. To that purpose, we replace the slowly varying part of operators of the form $\mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\mathcal{T}_\varepsilon}$ by suitable Taylor approximations similar as for the NPI-2 method from Section 3.3.1. More precisely, we use the decomposition (4.2) together with the approximations of $\mathrm{e}^{\mathrm{i}t\mathcal{D}_\varepsilon}$ from Lemma 3.2. For any $m \in \mathbb{N}_0$, combining (4.2) with the first approximation $\mathrm{e}^{\mathrm{i}t\mathcal{D}_\varepsilon}u \approx u$ yields

$$\mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\mathcal{T}_\varepsilon}u = \left(\mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}}\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}t}{\varepsilon^2}}\Pi_\varepsilon^-\right)u + \mathcal{O}^m(t) = \mathrm{e}^{t\mathcal{P}_\varepsilon}u + \mathcal{O}^m(t) \tag{4.74}$$

for $u \in \left(H^{m+2}(\mathbb{R}^3)\right)^4$ and $t \in [0,\tau]$, whereas the second approximation $\mathrm{e}^{\mathrm{i}t\mathcal{D}_\varepsilon}u \approx \mathrm{Id} + \mathrm{i}t\mathcal{D}_\varepsilon$ gives

$$\mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\mathcal{T}_\varepsilon}u = \left(\mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}}(\mathrm{Id} - \mathrm{i}t\mathcal{D}_\varepsilon)\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}t}{\varepsilon^2}}(\mathrm{Id} + \mathrm{i}t\mathcal{D}_\varepsilon)\Pi_\varepsilon^-\right)u + \mathcal{O}^m\left(t^2\right) \tag{4.75}$$

for $u \in \left(H^{m+4}(\mathbb{R}^3)\right)^4$.

Using the second approximation (4.75) with $t = s$ and $m = \widehat{m} + 2$ in the first integral in (4.73) and considering the assumptions on u_0 and the potentials, we obtain

$$\begin{aligned}\int_0^\tau \mathrm{e}^{-\frac{\mathrm{i}(\tau-s)}{\varepsilon^2}\mathcal{T}_\varepsilon}\left[W\mathrm{e}^{-\frac{\mathrm{i}s}{\varepsilon^2}\mathcal{T}_\varepsilon}u_0\right]\mathrm{d}s = &\int_0^\tau \mathrm{e}^{-\frac{\mathrm{i}(\tau-s)}{\varepsilon^2}\mathcal{T}_\varepsilon}\left[W\left(\mathrm{e}^{-\frac{\mathrm{i}s}{\varepsilon^2}}\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}s}{\varepsilon^2}}\Pi_\varepsilon^-\right)u_0\right]\mathrm{d}s\\ &+ \mathrm{i}\int_0^\tau s\mathrm{e}^{-\frac{\mathrm{i}(\tau-s)}{\varepsilon^2}\mathcal{T}_\varepsilon}\left[W\left(-\mathrm{e}^{-\frac{\mathrm{i}s}{\varepsilon^2}}\mathcal{D}_\varepsilon\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}s}{\varepsilon^2}}\mathcal{D}_\varepsilon\Pi_\varepsilon^-\right)u_0\right]\mathrm{d}s\\ &+ \mathcal{O}^{\widehat{m}+2}\left(\tau^3\right).\end{aligned}$$

The additional factor s in the second integral therein allows using the first approximation (4.74) with $t = \tau - s$ afterward. The same approximation can also be used for the second integral in (4.73), namely with $t = r$, $t = s - r$ and $t = \tau - s$, respectively. Each application comes at the cost of two spatial derivatives, which is why the assumption $u_0 \in \left(H^{\widehat{m}+6}(\mathbb{R}^3)\right)^4$ is necessary. Overall, we find

$$u(\tau) = \mathrm{e}^{-\frac{\mathrm{i}\tau}{\varepsilon^2}\mathcal{T}_\varepsilon}u_0 - \mathrm{i}\mathcal{I}_1(u_0) + \mathcal{I}_2(u_0) - \mathcal{I}_3(u_0) + \mathcal{O}^{\widehat{m}}\left(\tau^3\right)$$

with

$$\begin{aligned}\mathcal{I}_1(u) &= \int_0^\tau \mathrm{e}^{-\frac{\mathrm{i}(\tau-s)}{\varepsilon^2}\mathcal{T}_\varepsilon}\left[W\left(\mathrm{e}^{-\frac{\mathrm{i}s}{\varepsilon^2}}\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}s}{\varepsilon^2}}\Pi_\varepsilon^-\right)u\right]\mathrm{d}s,\\ \mathcal{I}_2(u) &= \int_0^\tau s\mathrm{e}^{(\tau-s)\mathcal{P}_\varepsilon}\left[W\left(-\mathrm{e}^{-\frac{\mathrm{i}s}{\varepsilon^2}}\widetilde{\mathcal{D}_\varepsilon}\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}s}{\varepsilon^2}}\widetilde{\mathcal{D}_\varepsilon}\Pi_\varepsilon^-\right)u\right]\mathrm{d}s,\\ \mathcal{I}_3(u) &= \int_0^\tau \mathrm{e}^{(\tau-s)\mathcal{P}_\varepsilon}\left[W\int_0^s\left(\mathrm{e}^{-\frac{\mathrm{i}(s-r)}{\varepsilon^2}}\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}(s-r)}{\varepsilon^2}}\Pi_\varepsilon^-\right)\left[W\left(\mathrm{e}^{-\frac{\mathrm{i}r}{\varepsilon^2}}\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}r}{\varepsilon^2}}\Pi_\varepsilon^-\right)u\right]\mathrm{d}r\right]\mathrm{d}s.\end{aligned} \tag{4.76}$$

Note that for stability reasons, we replaced $\mathcal{D}_\varepsilon$ by the filtered version $\widetilde{\mathcal{D}_\varepsilon} = \frac{\sin(\tau\mathcal{D}_\varepsilon)}{\tau}$ that was already used in Sections 2.3.1 and 3.3.1. Now, in each of the three integrals, only one operator that depends on the integration variable appears. Apart from that, all integration variables only appear within scalar functions that can be commuted to an arbitrary position. This allows to compute all three integrals analytically, which is why we define the numerical flow of the LDE-subproblem to be

$$\Phi_\tau^{\mathrm{LDE}}(u) = \mathrm{e}^{-\frac{\mathrm{i}\tau}{\varepsilon^2}\mathcal{T}_\varepsilon}u - \mathrm{i}\mathcal{I}_1(u) + \mathcal{I}_2(u) - \mathcal{I}_3(u). \tag{4.77}$$

Again, in order to ensure that the splitting ansatz yields an efficiency gain, we need to take a look at the computational costs for each application of the numerical flow. In particular, we

want to avoid unnecessary Fourier transforms. This is why we consider a different formulation of Φ_τ^{LDE}. As in the NL-subproblem, we divide the numerical flow

$$\Phi_\tau^{\mathrm{LDE}}(u) = \Pi_\varepsilon^+ \left[\Phi_\tau^{\mathrm{LDE}}(u)\right] + \Pi_\varepsilon^- \left[\Phi_\tau^{\mathrm{LDE}}(u)\right] \tag{4.78}$$

into its two eigenspace components, set $u_\pm = \Pi_\varepsilon^\pm [u]$ and make use of $\Pi_\varepsilon^\pm \mathrm{e}^{t\mathcal{P}_\varepsilon} = \mathrm{e}^{\mp \mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^\pm$ as well as $\Pi_\varepsilon^\pm \mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\mathcal{T}_\varepsilon} = \mathrm{e}^{\mp \mathrm{i}t/\varepsilon^2}\mathrm{e}^{\mp \mathrm{i}t\mathcal{D}_\varepsilon}\Pi_\varepsilon^\pm$ for any $t \in \mathbb{R}$. From the definition (4.77) of the numerical flow, we obtain

$$\Pi_\varepsilon^\pm \left[\Phi_\tau^{\mathrm{LDE}}(u)\right] = \mathrm{e}^{\mp \mathrm{i}\tau/\varepsilon^2}\mathrm{e}^{\mp \mathrm{i}\tau\mathcal{D}_\varepsilon} u_\pm - \mathrm{i}\Pi_\varepsilon^\pm [\mathcal{I}_1(u)] + \Pi_\varepsilon^\pm [\mathcal{I}_2(u)] - \Pi_\varepsilon^\pm [\mathcal{I}_3(u)]\,. \tag{4.79}$$

For the eigenspace components of the integrals $\mathcal{I}_1$ and $\mathcal{I}_2$, we observe

$$\begin{aligned}
\Pi_\varepsilon^\pm [\mathcal{I}_1(u)] &= \mathrm{e}^{\mp \mathrm{i}\tau/\varepsilon^2}\Pi_\varepsilon^\pm \left[\int_0^\tau \mathrm{e}^{\mathrm{i}(\pm 1-1)s/\varepsilon^2}\mathrm{e}^{\mp \mathrm{i}(\tau-s)\mathcal{D}_\varepsilon}\,\mathrm{d}s\,[Wu_+]\right. \\
&\qquad \left. + \int_0^\tau \mathrm{e}^{\mathrm{i}(\pm 1+1)s/\varepsilon^2}\mathrm{e}^{\mp \mathrm{i}(\tau-s)\mathcal{D}_\varepsilon}\,\mathrm{d}s\,[Wu_-]\right], \\
\Pi_\varepsilon^\pm [\mathcal{I}_2(u)] &= \mathrm{e}^{\mp \mathrm{i}\tau/\varepsilon^2}\Pi_\varepsilon^\pm \left[-\int_0^\tau s\mathrm{e}^{\mathrm{i}(\pm 1-1)s/\varepsilon^2}\,\mathrm{d}s W\widetilde{\mathcal{D}_\varepsilon}u_+ + \int_0^\tau s\mathrm{e}^{\mathrm{i}(\pm 1+1)s/\varepsilon^2}\,\mathrm{d}s W\widetilde{\mathcal{D}_\varepsilon}u_-\right].
\end{aligned} \tag{4.80}$$

As a preparation for the last integral $\mathcal{I}_3$, we compute

$$\begin{aligned}
&W\int_0^s \left(\mathrm{e}^{-\frac{\mathrm{i}(s-r)}{\varepsilon^2}}\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}(s-r)}{\varepsilon^2}}\Pi_\varepsilon^-\right)\left[W\left(\mathrm{e}^{-\frac{\mathrm{i}r}{\varepsilon^2}}\Pi_\varepsilon^+ + \mathrm{e}^{\frac{\mathrm{i}r}{\varepsilon^2}}\Pi_\varepsilon^-\right)u\right]\mathrm{d}r \\
&\quad = s\mathrm{e}^{-\mathrm{i}s/\varepsilon^2}W\Pi_\varepsilon^+ [Wu_+] + \mathrm{e}^{-\mathrm{i}s/\varepsilon^2}\int_0^s \mathrm{e}^{2\mathrm{i}r/\varepsilon^2}\,\mathrm{d}r\,W\Pi_\varepsilon^+ [Wu_-] \\
&\qquad + \mathrm{e}^{\mathrm{i}s/\varepsilon^2}\int_0^s \mathrm{e}^{-2\mathrm{i}r/\varepsilon^2}\,\mathrm{d}r\,W\Pi_\varepsilon^- [Wu_+] + s\mathrm{e}^{\mathrm{i}s/\varepsilon^2}W\Pi_\varepsilon^- [Wu_-]\,,
\end{aligned}$$

which then yields

$$\begin{aligned}
\Pi_\varepsilon^\pm [\mathcal{I}_3(u)] = \mathrm{e}^{\mp \mathrm{i}\tau/\varepsilon^2}\Pi_\varepsilon^\pm \Bigg[&\int_0^\tau s\mathrm{e}^{\mathrm{i}(\pm 1-1)s/\varepsilon^2}\,\mathrm{d}s\,W\Pi_\varepsilon^+ [Wu_+] \\
&+ \int_0^\tau \mathrm{e}^{\mathrm{i}(\pm 1-1)s/\varepsilon^2}\int_0^s \mathrm{e}^{2\mathrm{i}r/\varepsilon^2}\,\mathrm{d}r\,\mathrm{d}s\,W\Pi_\varepsilon^+ [Wu_-] \\
&+ \int_0^\tau s\mathrm{e}^{\mathrm{i}(\pm 1+1)s/\varepsilon^2}\int_0^s \mathrm{e}^{-2\mathrm{i}r/\varepsilon^2}\,\mathrm{d}r\,\mathrm{d}s\,W\Pi_\varepsilon^- [Wu_+] \\
&+ \int_0^\tau s\mathrm{e}^{\mathrm{i}(\pm 1+1)s/\varepsilon^2}\,\mathrm{d}s\,W\Pi_\varepsilon^- [Wu_-]\Bigg].
\end{aligned}$$

The integrals $\mathcal{I}_2$ and $\mathcal{I}_3$ can be combined and the potential W can be factorized, such that we finally obtain

$$\begin{aligned}
\Pi_\varepsilon^\pm [\mathcal{I}_2(u) - \mathcal{I}_3(u)] = -\mathrm{e}^{\mp \mathrm{i}\tau/\varepsilon^2}\Pi_\varepsilon^\pm \Bigg[W\Bigg(&\int_0^\tau s\mathrm{e}^{\mathrm{i}(\pm 1-1)s/\varepsilon^2}\,\mathrm{d}s\,\left(\Pi_\varepsilon^+ [Wu_+] + \widetilde{\mathcal{D}_\varepsilon}u_+\right) \\
&+ \int_0^\tau \mathrm{e}^{\mathrm{i}(\pm 1-1)s/\varepsilon^2}\int_0^s \mathrm{e}^{2\mathrm{i}r/\varepsilon^2}\,\mathrm{d}r\,\mathrm{d}s\,\Pi_\varepsilon^+ [Wu_-] \\
&+ \int_0^\tau s\mathrm{e}^{\mathrm{i}(\pm 1+1)s/\varepsilon^2}\int_0^s \mathrm{e}^{-2\mathrm{i}r/\varepsilon^2}\,\mathrm{d}r\,\mathrm{d}s\,\Pi_\varepsilon^- [Wu_+] \\
&+ \int_0^\tau s\mathrm{e}^{\mathrm{i}(\pm 1+1)s/\varepsilon^2}\,\mathrm{d}s\,\left(\Pi_\varepsilon^- [Wu_-] - \widetilde{\mathcal{D}_\varepsilon}u_-\right)\Bigg)\Bigg].
\end{aligned} \tag{4.81}$$

This representation reduced the number of Fourier transforms as much as possible. As in Section 4.4.1, we assume that the Fourier representation of u_+ and u_- is known from the previous (sub)step, cf. Remark 4.15. In order to compute the products Wu_+ and Wu_- that appear in both $\mathcal{I}_1$ and $\mathcal{I}_2 - \mathcal{I}_3$, we need u_+ and u_- in physical space, which requires two inverse Fourier transforms. The result is required in Fourier space, such that two Fourier transforms have to be performed. This then allows computing the Fourier representation of $\Pi_\varepsilon^\pm[\mathcal{I}_1(u)]$. In the difference $\Pi_\varepsilon^\pm[\mathcal{I}_2(u) - \mathcal{I}_3(u)]$, however, another two inverse Fourier transforms of the factors that are multiplied with W (which differ in the "+" and the "-" case) are required, and two Fourier transforms immediately afterward. Thus, all in all, eight Fourier transforms are necessary for the Fourier representation of both eigenspace components of $\Phi_\tau^{\mathrm{LDE}}(u)$ in (4.79).

All considerations from this subsection lead to the following

Corollary 4.14. *Let Assumption 4.1 (A) and (B) hold and let $\tau > 0$. Then, for the numerical flow Φ_τ^{LDE} of the LDE-subproblem, given either by (4.77) and (4.76), or by (4.78) - (4.81), we have*

$$\left\| \Psi_\tau^{\mathrm{LDE}}(u_0) - \Phi_\tau^{\mathrm{LDE}}(u_0) \right\|_{H^{\widehat{m}}} \leq C\tau^3$$

for some constant C independent of τ and ε.

4.4.3 Final time integrator

After we have discussed the splitting ansatz in Section 4.2 and the approximation of the subproblems in the previous subsections, we are now in the position to state the final time integrator. To that purpose, we mimic the scheme (4.13), but replace the exact flows of the LDE- and the NL-subproblem by the corresponding numerical flows. The RO-subproblem, on the other hand, can be solved exactly, so that we can indeed utilize the exact flow. Thus, the approximations $\psi^n \approx \psi^\varepsilon(t_n)$ to the exact solution of the NLDE at time t_n are obtained by the iteration

$$\psi^{n+1} = \Phi_\tau\left(\psi^n\right), \qquad n = 0, 1, \ldots \tag{4.82}$$

with the numerical flow

$$\Phi_\tau(u) = \Phi_{\frac{\tau}{2}}^{\mathrm{NL}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_\tau^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(u). \tag{4.83}$$

In the following, we will refer to this method as *oscillation-rewinding splitting method* (ORSM) for the nonlinear Dirac equation. The rest of the chapter is devoted to a detailed analysis of this method.

Remark 4.15. *Solving the RO-subproblem with initial data u means computing $\mathrm{e}^{t\mathcal{P}_\varepsilon}u = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^+ u + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\Pi_\varepsilon^- u$ for suitable $t \in \mathbb{R}$. The projectors therein correspond to multiplication with a matrix in Fourier space. Thus, either the representation of u in Fourier space or the knowledge of the eigenspace components $u_\pm = \Pi_\varepsilon^\pm[u]$ is required. Since the last step in the numerical flows Φ_t^{NL} and Φ_t^{LDE} of the subproblems also involves applying the projectors, cf. (4.71) or (4.78)-(4.81), the most efficient strategy is to start and end each subproblem with the Fourier representation of both eigenspace components. As we have discussed before, computing Φ_t^{NL} or Φ_t^{LDE} then requires 4 or 8 Fourier transforms, respectively. Thus, applying the latter one is more expensive, which is why we chose the order of the subproblems in such a way that the flow Φ_t^{LDE} of the LDE-subproblem only has to be applied once per time step. The total number of Fourier transforms for one step of the ORSM therefore amounts to 16.*

In contrast to that, each step of the TSFP scheme requires two Fourier transforms if only the final approximation is of interest, cf. Eq. (4.4) and the short discussion afterward. This is why we expect each time step of our method to be roughly eight times as expensive as a classical Strang splitting step. However, this disadvantage is more than compensated for by the better convergence behavior of our method, as will be discussed in Sections 4.5 and 4.6.

Remark 4.16. *A similar method can be derived for time-dependent potentials $W = W(t,x)$. In this case, the same decomposition (4.12) of the NLDE as in the time-independent case is used. Note that the right-hand side of the LDE-subproblem then is no longer autonomous. Nevertheless, one can extend the analysis of the local (Strang) splitting error from Section 4.3 to time-dependent potentials. To that purpose, for fixed $t \geq 0$ and arbitrary $s \in [0,t]$, one can replace evaluations $W(t+s,x)$ of the potentials in Duhamel's formula for the LDE-subproblem or the full NLDE by the Taylor expansions*

$$W(t+s,x) = W(t,x) + \mathcal{O}(s)\,, \qquad W(t+s,x) = W(t,x) + s\partial_t W(t,x) + \mathcal{O}\Big(s^2\Big) \tag{4.84}$$

(depending on whether the evaluations are surrounded by two integrals or one). This yields similar expansions of the flow of the LDE-subproblem or the full NLDE as in Subsection 4.3.1. They can then be combined to expansions of Lie splitting steps, and the local splitting error can be analyzed in the same manner as in Subsections 4.3.2-4.3.4. Furthermore, those Taylor expansions can also be used to construct a scheme to approximate solutions of the LDE-subproblem. Of course, sufficient temporal regularity of the potential is required for (4.84).

Remark 4.17. *The interpretation of the splitting ansatz from Section 4.2 also suggest another splitting approach: Could one even rewind the full operator $\mathcal{T}_\varepsilon$ instead of just the dominating part? This would result in the splitting*

$$\begin{aligned}
\partial_t \psi^{\mathrm{LDE}} &= -\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi^{\mathrm{LDE}} - \mathrm{i}W\psi^{\mathrm{LDE}},\\
\partial_t \psi^{\mathrm{RO}} &= \frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi^{\mathrm{RO}},\\
\partial_t \psi^{\mathrm{NL}} &= -\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi^{\mathrm{NL}} - \mathrm{i}F(\psi^{\mathrm{NL}})\psi^{\mathrm{NL}}
\end{aligned} \tag{4.85}$$

of the NLDE instead of (4.12). Indeed, with a similar procedure as in Section 4.3, one can obtain the same local error result as in Lemma 4.2. Furthermore, the RO-subproblem can still be solved exactly, cf. (4.2), and the LDE-subproblem is identical to the one in (4.12), such that its solution can be approximated in the same way. However, in the NL-subproblem, the full operator $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon$ appears instead of just the dominating part $\mathcal{P}_\varepsilon$. When Duhamel's formula is iterated for the NL-subproblem, finding a computable approximation of the integrals requires the same Taylor approximations of the operator $\mathrm{e}^{-\frac{\mathrm{i}t}{\varepsilon^2}\mathcal{T}_\varepsilon}$ that we used in the LDE-subproblem. However, those Taylor expansions lead to an increased number of terms and, as a consequence, more necessary Fourier transforms due to the appearance of the operator $\mathcal{D}_\varepsilon$ at multiple locations. In particular, the benefits of the NL-subproblem from (4.85) over the full NLDE are only limited, whereas the splitting ansatz (4.12) allowed for considerable simplifications when iterating Duhamel's formula for the NL-subproblem.

4.5 Global error analysis

The goal of this section is to derive a global error bound for the ORSM (4.82). As usual, this is achieved by first deriving a local error bound and then combining it with a stability estimate. There are two different sources for (local) errors, namely the splitting of the full PDE into

several subproblems and the approximation of the flows of the subproblems by numerical schemes. Both errors have been analyzed separately in Sections 4.3 and 4.4, respectively. However, for a local error bound for the full method (4.82), one has to keep in mind that the latter errors are propagated by the subsequent subproblem-flows in (4.83). Thus, stability estimates for the subproblems are already required in the local error analysis. The same estimates also yield a stability estimate for the full method. This is why we will first discuss stability in this section, and afterward the local error. Finally, all results are combined to obtain the desired global error estimate.

Throughout this section, we will make the technical assumption $\tau \leq 1$, such that the estimate $\tau^2 \leq \tau$ holds. Although this is not a strong restriction anyway, it could also be replaced by the bound $\tau \leq \tau_0$ for an arbitrary $\tau_0 > 1$. All constants would then additionally contain the factor τ_0.

4.5.1 Stability

Here, we derive stability estimates for the numerical flows of the NL- and the LDE-subproblem, and of the full ORSM (4.82). Note that the flow of the LDE subproblem is linear, so that the notion of stability simplifies. As in Subsections 4.3.1 and 4.4, we let $m \geq 2$ arbitrary for the NL-subproblem, but chose $m = \widehat{m}$ for the LDE-subproblem and the ORSM.

Lemma 4.18. *Let $0 < \tau \leq 1$.*

(i) Let $m \geq 2$ and let Φ_τ^{NL} be the numerical flow (4.69) of the NL-subproblem. Then, we have the uniform bound

$$\left\|\Phi_\tau^{\mathrm{NL}}(v)\right\|_{H^m} \leq C, \qquad v \in \left(H^m(\mathbb{R}^3)\right)^4 \tag{4.86}$$

for some constant that depends on $\|v\|_{H^m}$, but not on τ and ε. Further, the stability estimate

$$\left\|\Phi_\tau^{\mathrm{NL}}(v) - \Phi_\tau^{\mathrm{NL}}(w)\right\|_{H^m} \leq (1 + C\tau)\,\|v - w\|_{H^m}\,, \qquad v, w \in \left(H^m(\mathbb{R}^3)\right)^4, \tag{4.87}$$

holds for some constant C that depends on $\|v\|_{H^m}$ and $\|w\|_{H^m}$, but not on τ and ε.

(ii) Let Assumption 4.1 (A) hold and let Φ_τ^{LDE} be the numerical flow (4.77) of the LDE-subproblem. Then, for $v \in \left(H^{\widehat{m}}(\mathbb{R}^3)\right)^4$, we have the uniform bound and the stability estimate

$$\left\|\Phi_\tau^{\mathrm{LDE}}(v)\right\|_{H^{\widehat{m}}} \leq C\,\|v\|_{H^{\widehat{m}}}\,, \qquad \left\|\Phi_\tau^{\mathrm{LDE}}(v)\right\|_{H^{\widehat{m}}} \leq (1 + C\tau)\,\|v\|_{H^{\widehat{m}}} \tag{4.88}$$

for some constant C independent of v, τ and ε.

(iii) Let Assumption 4.1 (A) hold and let Φ_τ be the numerical flow (4.83) of the ORSM. Then, for $v, w \in \left(H^{\widehat{m}}(\mathbb{R}^3)\right)^4$, the stability estimate

$$\|\Phi_\tau(v) - \Phi_\tau(w)\|_{H^{\widehat{m}}} \leq (1 + C_S\tau)\,\|v - w\|_{H^{\widehat{m}}}$$

holds for some constant C_S that depends on $\|v\|_{H^{\widehat{m}}}$ and $\|w\|_{H^{\widehat{m}}}$, but not on τ and ε.

Proof. (i) We first prove the stability estimate. To that purpose, consider the definition of Φ_τ^{NL} given by (4.69). Since $\mathrm{e}^{\tau\mathcal{P}_\varepsilon}$ is linear and an isometry according to Lemma 4.3, we know that

$$\left\|\mathrm{e}^{\tau\mathcal{P}_\varepsilon} v - \mathrm{e}^{\tau\mathcal{P}_\varepsilon} w\right\|_{H^{\widehat{m}}} = \|v - w\|_{H^{\widehat{m}}}\,.$$

Further, using a decomposition of the form (3.56) with u, v, w replaced by $\mathrm{e}^{s\mathcal{P}_\varepsilon} v$ and $\widetilde{u}, \widetilde{v}, \widetilde{w}$ by $\mathrm{e}^{s\mathcal{P}_\varepsilon} w$ together with the fact that H^m is an algebra for $m \geq 2$, one easily obtains

$$\left\| F\left(\mathrm{e}^{s\mathcal{P}_\varepsilon} v\right) \mathrm{e}^{s\mathcal{P}_\varepsilon} v - F\left(\mathrm{e}^{s\mathcal{P}_\varepsilon} w\right) \mathrm{e}^{s\mathcal{P}_\varepsilon} w \right\|_{H^m} \leq C \left\| v - w \right\|_{H^m}$$

for some constant C that depends on $\|v\|_{H^m}$ and $\|w\|_{H^m}$. Similarly, we find

$$\left\| |v|^4 v - |w|^4 w \right\|_{H^m} \leq C \left\| v - w \right\|_{H^m}.$$

Combining all equations yields (4.87). The uniform bound (4.86) then follows by setting $w = 0$ in (4.87) and using $\tau \leq 1$.

(ii) Again, we start with the stability estimate. Recall the representation (4.77) and (4.76) of the flow Φ_τ^{LDE} and the integrals $\mathcal{I}_1$, $\mathcal{I}_2$ and $\mathcal{I}_3$ contained therein. Since $\mathrm{e}^{-\frac{it}{\varepsilon^2}\mathcal{T}_\varepsilon}$ is a unitary operator in $H^{\widehat{m}}$ for all $t \in \mathbb{R}$, we initially get that

$$\left\| \Phi_\tau^{\mathrm{LDE}}(v) \right\|_{H^{\widehat{m}}} \leq \|v\|_{H^{\widehat{m}}} + \|\mathcal{I}_1(v)\|_{H^{\widehat{m}}} + \|\mathcal{I}_2(v)\|_{H^{\widehat{m}}} + \|\mathcal{I}_3(v)\|_{H^{\widehat{m}}}.$$

Furthermore, the regularity of the potential W from Assumption 4.1 (A) together with the fact that the projectors are isometries yield

$$\|\mathcal{I}_1(v)\|_{H^{\widehat{m}}} \leq C\tau \|v\|_{H^{\widehat{m}}}, \qquad \|\mathcal{I}_3(v)\|_{H^{\widehat{m}}} \leq C\tau^2 \|v\|_{H^{\widehat{m}}}.$$

Additionally using the estimate (3.24) for the filtered operator $\widetilde{\mathcal{D}_\varepsilon}$ and considering the additional factor of s in the integrand of $\mathcal{I}_2$, we finally obtain

$$\|\mathcal{I}_2(v)\|_{H^{\widehat{m}}} \leq C\tau \|v\|_{H^{\widehat{m}}},$$

such that the second estimate in (4.88) follows. The first estimate is then trivially obtained from the first one by using $\tau \leq 1$.

(iii) Let $v, w \in \left(H^{\widehat{m}}(\mathbb{R}^3)\right)^4$. Then, (4.87) yields

$$\left\| \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(v) - \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(w) \right\|_{H^{\widehat{m}}} \leq (1 + C_1\tau) \left\| v - w \right\|_{H^{\widehat{m}}}$$

for a constant C_1 dependent on $\|v\|_{H^m}$ and $\|w\|_{H^m}$. The fact that Ψ_t^{RO} is linear and is an isometry in $H^{\widehat{m}}$ for all $t \in \mathbb{R}$ then implies

$$\left\| \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(v) - \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(w) \right\|_{H^{\widehat{m}}} \leq (1 + C_1\tau) \left\| v - w \right\|_{H^{\widehat{m}}}.$$

Next, the linearity of Φ_τ^{LDE} together with the stability estimate from (4.88) gives

$$\left\| \Phi_\tau^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(v) - \Phi_\tau^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(w) \right\|_{H^{\widehat{m}}} \leq (1 + C_1\tau)(1 + C_2\tau) \left\| v - w \right\|_{H^{\widehat{m}}}$$

for a constant C_2 independent of τ, ε, v and w. Again using the properties of Ψ_t^{RO} yields

$$\begin{aligned} &\left\| \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_\tau^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(v) - \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_\tau^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(w) \right\|_{H^{\widehat{m}}} \\ &\qquad \leq (1 + C_1\tau)(1 + C_2\tau) \left\| v - w \right\|_{H^{\widehat{m}}}. \end{aligned}$$

Then, the stability estimate (4.87) gives

$$\begin{aligned}
&\left\|\Phi_{\frac{\tau}{2}}^{\mathrm{NL}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\tau}^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(v) - \Phi_{\frac{\tau}{2}}^{\mathrm{NL}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\tau}^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(w)\right\|_{H^{\widehat{m}}} \\
&\quad \leq (1 + C_3\tau) \left\|\Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\tau}^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(v) - \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\tau}^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(w)\right\|_{H^{\widehat{m}}} \\
&\quad \leq (1 + C_1\tau)(1 + C_2\tau)(1 + C_3\tau) \left\|v - w\right\|_{H^{\widehat{m}}}.
\end{aligned}$$

The constant C_3 therein depends on the norm of both arguments of $\Phi_{\frac{\tau}{2}}^{\mathrm{NL}}$, i.e. on

$$\left\|\Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\tau}^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(v)\right\|_{H^{\widehat{m}}} \qquad \text{and} \qquad \left\|\Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\tau}^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\frac{\tau}{2}}^{\mathrm{NL}}(w)\right\|_{H^{\widehat{m}}}. \tag{4.89}$$

In particular, since all flows depend on τ and ε, the same holds for C_3. However, the uniform bounds from (4.86) and (4.88) imply that both norms in (4.89) can be uniformly bounded w.r.t. τ and ε, such that C_3 can be chosen independently of ε and τ (but dependent on $\|v\|_{H^{\widehat{m}}}$ and $\|w\|_{H^{\widehat{m}}}$). Finally, recognizing that multiple factors of the form $(1 + C\tau)$ with $\tau \leq 1$ lead to a factor of the same form again, only with a different constant C, yields the assertion. □

4.5.2 Local error

The bounds for the local splitting error and for the local error of the schemes approximating solutions of the subproblems from Sections 4.3 and 4.4, respectively, can now be combined with the stability estimates from the previous subsection to obtain a local error bound for the ORSM.

Lemma 4.19. *Let Assumption 4.1 hold and assume $\tau \leq 1$ in addition. Further, let Φ_τ be the numerical flow of the ORSM from (4.83) and let Ψ_τ be the exact flow of the NLDE. Then, the local error estimate*

$$\left\|\Psi_\tau(u_0) - \Phi_\tau(u_0)\right\|_{H^{\widehat{m}}} \leq C_L \min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\}$$

holds for some constant C_L independent of τ and ε.

Proof. We divide the local error of the ORSM into the splitting error and the error introduced by replacing the exact flows of the subproblems by the corresponding numerical flows. To this purpose, let

$$u^{\textcircled{6}} = \Psi_{\frac{\tau}{2}}^{\mathrm{NL}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Psi_{\tau}^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{NL}}(u_0)$$

be the result of the splitting ansatz using exact flows of the subproblems as in (4.14) (with the two half steps of the LDE-subproblem combined to one full step). Then, we can write

$$\Psi_\tau(u_0) - \Phi_\tau(u_0) = \Psi_\tau(u_0) - u^{\textcircled{6}} + u^{\textcircled{6}} - \Phi_\tau(u_0). \tag{4.90}$$

From Lemma 4.2, we know that the bound

$$\left\|\Psi_\tau(u_0) - u^{\textcircled{6}}\right\|_{H^{\widehat{m}}} \leq C \min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\} \tag{4.91}$$

holds for the local splitting error, such that it remains to analyze the second difference in (4.90). To this end, we introduce the two auxiliary values

$$v^{\textcircled{6}} = \Phi_{\frac{\tau}{2}}^{\mathrm{NL}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Psi_{\tau}^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{NL}}(u_0), \qquad w^{\textcircled{6}} = \Phi_{\frac{\tau}{2}}^{\mathrm{NL}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Phi_{\tau}^{\mathrm{LDE}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{RO}} \circ \Psi_{\frac{\tau}{2}}^{\mathrm{NL}}(u_0),$$

where *some* of the exact flows are replaced by numerical flows. We then divide

$$u^{⑥} - \Phi_\tau(u_0) = \; u^{⑥} - v^{⑥} \; + \; v^{⑥} - w^{⑥} \; + \; w^{⑥} - \Phi_\tau(u_0), \tag{4.92}$$

and consider all three differences separately. In each of them, exactly one of the flows differs. First, with $u^{⑤} = \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{LDE}}_{\tau} \circ \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}(u_0)$, we have

$$u^{⑥} - v^{⑥} = \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}(u^{⑤}) - \Phi^{\mathrm{NL}}_{\frac{\tau}{2}}(u^{⑤}). \tag{4.93}$$

Since the solution of the NL-subproblem with initial data $u^{⑤}$ remains uniformly bounded in $H^{\widehat{m}+6}$ over the time interval $[0, \frac{\tau}{2}]$ by Assumption 4.1 (D), we can apply the local error estimate from Corollary 4.13 to obtain

$$\|u^{⑥} - v^{⑥}\|_{H^{\widehat{m}}} \leq C \min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\}.$$

In fact, we could even use the $H^{\widehat{m}+5}$-norm on the left-hand side, but $H^{\widehat{m}}$ is sufficient for our purposes. For the second difference in (4.92), we introduce $u^{②} = \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}(u_0)$, such that

$$v^{⑥} - w^{⑥} = \Phi^{\mathrm{NL}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{LDE}}_{\tau}(u^{②}) - \Phi^{\mathrm{NL}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Phi^{\mathrm{LDE}}_{\tau}(u^{②}).$$

Again, Assumption 4.1 (D) guarantees that $\Psi^{\mathrm{NL}}_{\frac{\tau}{2}}(u_0)$ is in $H^{\widehat{m}+6}$ with uniform norm bound w.r.t. ε and τ. The same then trivially holds for $u^{②}$. Thus, with the local error estimate from Corollary 4.14, we arrive at

$$\left\|\Psi^{\mathrm{LDE}}_{\tau}(u^{②}) - \Phi^{\mathrm{LDE}}_{\tau}(u^{②})\right\|_{H^{\widehat{m}}} \leq C\tau^3$$

and thus

$$\left\|\Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{LDE}}_{\tau}(u^{②}) - \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Phi^{\mathrm{LDE}}_{\tau}(u^{②})\right\|_{H^{\widehat{m}}} = \left\|\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}\left(\Psi^{\mathrm{LDE}}_{\tau}(u^{②}) - \Phi^{\mathrm{LDE}}_{\tau}(u^{②})\right)\right\|_{H^{\widehat{m}}} \leq C\tau^3.$$

Then, we can then apply the stability estimate of the NL-subproblem from Lemma 4.18 (i) with $u = \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{LDE}}_{\tau}(u^{②})$ and $v = \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Phi^{\mathrm{LDE}}_{\tau}(u^{②})$ to find

$$\|v^{⑥} - w^{⑥}\|_{H^{\widehat{m}}} \leq (1 + C\tau)\left\|\Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{LDE}}_{\tau}(u^{②}) - \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Phi^{\mathrm{LDE}}_{\tau}(u^{②})\right\|_{H^{\widehat{m}}} \leq C\tau^3. \tag{4.94}$$

Finally, for the third difference in (4.92), we first note that

$$\left\|\Psi^{\mathrm{NL}}_{\frac{\tau}{2}}(u_0) - \Phi^{\mathrm{NL}}_{\frac{\tau}{2}}(u_0)\right\|_{H^{\widehat{m}}} \leq C \min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\}$$

thanks to Assumption 4.1 (D) together with Corollary 4.13. The same holds after applying the flow $\Psi^{\mathrm{RO}}_{\frac{\tau}{2}}$ of the RO-subproblem to both arguments, since it is linear and an isometry. The stability estimate of the LDE-subproblem from Lemma 4.18 (ii) then gives

$$\begin{aligned}&\left\|\Phi^{\mathrm{LDE}}_{\tau} \circ \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}(u_0) - \Phi^{\mathrm{LDE}}_{\tau} \circ \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Phi^{\mathrm{NL}}_{\frac{\tau}{2}}(u_0)\right\|_{H^{\widehat{m}}} \\ &\quad \leq (1 + C\tau)\left\|\Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Psi^{\mathrm{NL}}_{\frac{\tau}{2}}(u_0) - \Psi^{\mathrm{RO}}_{\frac{\tau}{2}} \circ \Phi^{\mathrm{NL}}_{\frac{\tau}{2}}(u_0)\right\|_{H^{\widehat{m}}} \leq C \min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\}.\end{aligned}$$

Treating the RO-subproblem as before and applying the stability estimate of the NL-subproblem afterward implies

$$\|w^{⑥} - \Phi_{u_0}\|_{H^{\widehat{m}}} \leq C \min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\}. \tag{4.95}$$

Combining (4.90)-(4.95) and using triangle inequality gives the desired result. □

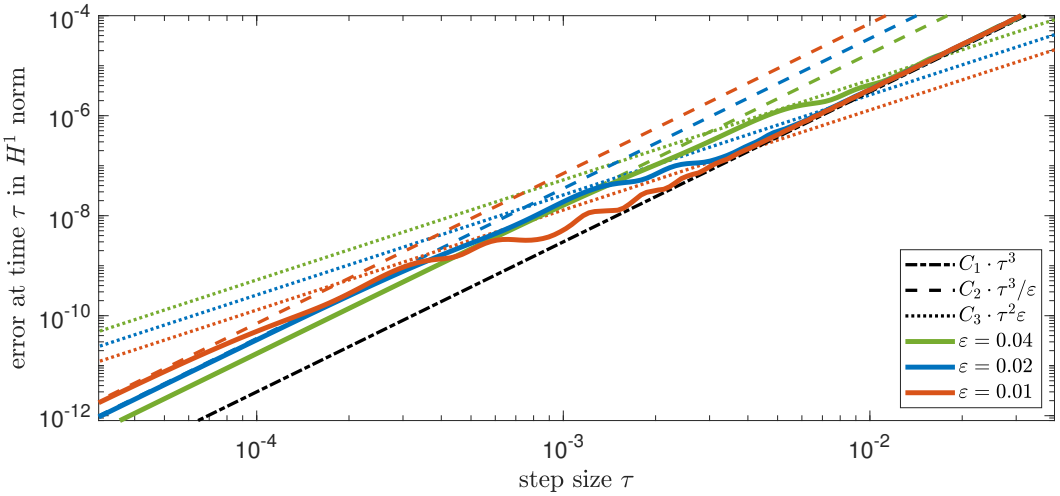

Figure 4.3: Local error in H^1 of the ORSM in dependency of the time step size τ for three different values of ε. Note that the dashed third order reference lines all use the same constant C_2, and the dotted second order reference lines the same constant C_3.

Before we combine Lemmas 4.18 and 4.19 to obtain a global error estimate, we repeat the numerical experiment from Section 4.3.5, in which we observed the local error, but now for the final splitting scheme (4.82). This means that the NL- and the LDE-subproblems are now approximated with the numerical methods from Sections 4.4.1 and 4.4.2, respectively, instead of solving them (almost) exactly using a very fine discretization. Comparing the results in Figure 4.3 with those from Figure 4.2 shows that this barely affects the error behavior. For $\tau > \varepsilon$ or $\tau \leq \varepsilon^2$, both figures essentially correspond. Only the constants C_1 and C_3 have been slightly modified, implying that the error constants are a little different. For some step sizes $\varepsilon^2 < \tau \leq \varepsilon$, smaller errors are observed in Figure 4.2. Nevertheless, the error is still capped by the same reference lines in this regime (even with the same constant C_2 in both figures), which confirms the estimate from Lemma 4.19.

4.5.3 Global error

A bound for the global error of the ORSM can now be obtained from the local error bound together with the stability estimate without any major difficulties. Before doing so, we have to make suitable assumptions.

In the previous sections, we always chose a generic function u_0 as initial data, for which we made Assumption 4.1. Now, we switch to the NLDE (1.2) on an interval $[0, T]$ with initial data $\psi^\varepsilon(0, x) = \psi^{\text{init}}(x)$, such that we have to formulate a corresponding assumption.

Assumption 4.20. *Let $T > 0$, $\widehat{m} \geq 2$ and let Assumptions 4.1 (A) on the potentials hold. Further, assume the following:*

(A) For all $\varepsilon \in (0, 1)$, the NLDE (1.2) with initial data $\psi^\varepsilon(0, x) = \psi^{\text{init}}(x)$ admits a solution ψ^ε on the time interval $[0, T]$ that remains uniformly bounded in $H^{\widehat{m}+6}$ w.r.t. ε and t.

(B) For all $t_0, t_1 \geq 0$ with $t_0 + t_1 \leq T$ and all $\varepsilon \in (0, 1)$, the NL-subproblem with initial data $\psi^\varepsilon(t_0)$ or $\Psi^{\text{RO}}_{t_1} \circ \Psi^{\text{LDE}}_{t_1}(\psi^\varepsilon(t_0))$ admits a solution on the time interval $[0, t_1]$ that remains uniformly bounded in $H^{\widehat{m}+6}$ w.r.t. ε and t, and the same holds on the interval $[0, \frac{t_1}{2}]$ for the initial data $\Psi^{\text{NL}}_{t_1/2} \circ \Psi^{\text{RO}}_{t_1/2} \circ \Psi^{\text{LDE}}_{t_1} \circ \Psi^{\text{RO}}_{t_1/2} \circ \Psi^{\text{LDE}}_{t_1/2}(\psi^\varepsilon(t_0))$.

In fact, if the initial data is in $H^{\widehat{m}+6}$, then we know from Theorem 2.2 that part (A) is fulfilled at least for some $T > 0$. Starting from the uniform bounds for ψ^ε, one could then additionally prove that (B) is fulfilled for sufficiently small T by standard fixed point arguments applied to all subproblems involved. The assumption from part (B) is required such that we can apply the local error bound from Lemma 4.19 with $u_0 = \psi^\varepsilon(t_\ell)$ being the exact solution at any time point $t_\ell \in [0, T]$.

On top of that, we need to make an assumption on the boundedness of the numerical approximations starting from the exact solution at any time point t_ℓ, similar as in the proof of Theorem 2.10. In order to do this, we recursively define the numerical flow over n successive time steps by $\Phi_\tau^n = \Phi_\tau \circ \Phi_\tau^{n-1}$, $n \in \mathbb{N}$, and $\Phi_\tau^0 = Id$.

Assumption 4.21. *There is a constant $\tau_0 > 0$ independent of ε such that for all $\tau \leq \tau_0$, we have*

$$\max_{\substack{n,\ell=0,\dots,\lfloor T/\tau \rfloor \\ n+\ell \leq \lfloor T/\tau \rfloor}} \left\| \Phi_\tau^n \left(\psi^\varepsilon(t_\ell) \right) \right\|_{H^{\widehat{m}}} \leq C$$

for some constant C independent of τ and ε.

This assumption could be proven by a standard bootstrapping argument. As in the proof of Theorem 2.10, we refer to [Lub08] and [JMS17]. However, note that unlike in said proof, no additional stability and local error estimate is necessary. The reason for this is that we assumed $\widehat{m} \geq 2$, such that $H^{\widehat{m}}(\mathbb{R}^3)$ is an algebra, which led to the fact that the constant C_S in Lemma 4.18 (iii) only depends on the $H^{\widehat{m}}$-norm of the functions involved, but not on the norm of higher-order Sobolev spaces.

With those assumptions, we can now state and prove a global error bound for the ORSM.

Theorem 4.22. *Let Assumptions 4.20 and 4.21 hold and let τ_0 be the constant from the latter. Further, let $0 < \varepsilon < 1$ and $\tau \leq \tau_0$. Then, for the numerical approximations ψ^n of the ORSM (4.82) applied with step size τ, the global error bound*

$$\left\| \psi^\varepsilon(t_n) - \psi^n \right\|_{H^{\widehat{m}}} \leq C \min \left\{ \frac{\tau^2}{\varepsilon}, \max \left\{ \tau\varepsilon, \tau^2 \right\} \right\} \tag{4.96}$$

holds for some constant C independent of ε, τ and n.

Proof. The proof uses a Lady Windermere's fan argument, similar as in the proof of Theorem 2.10. To begin with, we can decompose the global error as

$$\begin{aligned} \left\| \psi^\varepsilon(t_n) - \psi^n \right\|_{H^{\widehat{m}}} &= \left\| \Phi_\tau^0 \left(\psi^\varepsilon(t_n) \right) - \Phi_\tau^n \left(\psi^\varepsilon(0) \right) \right\|_{H^{\widehat{m}}} \\ &\leq \sum_{k=0}^{n-1} \left\| \Phi_\tau^k \left(\psi^\varepsilon(t_{n-k}) \right) - \Phi_\tau^{k+1} \left(\psi^\varepsilon(t_{n-k-1}) \right) \right\|_{H^{\widehat{m}}} \end{aligned}$$

for $n = 1, \dots, \lfloor T/\tau \rfloor$. We now apply the stability estimate from Lemma 4.18 (iii) k times in each addend. In each application, the constant C_S therein depends on the norm of the two arguments involved, i.e. on $\left\| \Phi_\tau^j \left(\psi^\varepsilon(t_{n-k}) \right) \right\|_{H^{\widehat{m}}}$ and $\left\| \Phi_\tau^{j+1} \left(\psi^\varepsilon(t_{n-k-1}) \right) \right\|_{H^{\widehat{m}}}$, $j = k-1, \dots, 0$. However, according to Assumption 4.21, all those norms are uniformly bounded, such that

we can always choose the same constant C_S in the stability estimate. We thus obtain

$$\begin{aligned}\left\|\psi^{\varepsilon}(t_n)-\psi^n\right\|_{H^{\widehat{m}}} &\leq \sum_{k=0}^{n-1}(1+C_S\tau)^k \left\|\psi^{\varepsilon}(t_{n-k})-\Phi_\tau\left(\psi^{\varepsilon}(t_{n-k-1})\right)\right\|_{H^{\widehat{m}}} \\ &= \sum_{k=0}^{n-1}(1+C_S\tau)^k \left\|\Psi_\tau\left(\psi^{\varepsilon}(t_{n-k-1})\right)-\Phi_\tau\left(\psi^{\varepsilon}(t_{n-k-1})\right)\right\|_{H^{\widehat{m}}}\end{aligned}$$

Next, Assumption 4.20 enables us to apply the local error estimate from Lemma 4.19 with $u_0 = \psi^{\varepsilon}(t_{n-k-1})$. This yields

$$\left\|\psi^{\varepsilon}(t_n)-\psi^n\right\|_{H^{\widehat{m}}} \leq \sum_{k=0}^{n-1}(1+C_S\tau)^k C_L \min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\}.$$

Since

$$(1+C_S\tau)^k = \left(1+C_S\frac{t_k}{k}\right)^k \leq \mathrm{e}^{C_S t_k} \leq \mathrm{e}^{C_S T} \qquad \text{and} \qquad n\tau = t_n \leq T,$$

the estimate

$$\begin{aligned}\left\|\psi^{\varepsilon}(t_n)-\psi^n\right\|_{H^{\widehat{m}}} &\leq n\mathrm{e}^{C_S T} C_L \min\left\{\frac{\tau^3}{\varepsilon}, \max\left\{\tau^2\varepsilon, \tau^3\right\}\right\} \\ &\leq T\mathrm{e}^{C_S T} C_L \min\left\{\frac{\tau^2}{\varepsilon}, \max\left\{\tau\varepsilon, \tau^2\right\}\right\}\end{aligned}$$

follows, which yields the claim. □

Since the minimum in the right-hand side of (4.96) is at most $\frac{\tau^2}{\varepsilon}$, Theorem 4.22 implies that the ORSM is second-order convergent in the time step size, but the error constant involves the factor ε in the denominator. This means that the error constant grows linearly for decreasing ε. However, if Strang splitting is applied to the classical decomposition (4.1) of the NLDE, then even in the best case $\tau \leq \varepsilon^2$ the error constant increases quadratically with decreasing ε, as discussed in Section 4.1. The ORSM thus gives a significant improvement over the TSFP scheme.

On top of that, Theorem 4.22 predicts an even smaller error in some step sizes regimes. To understand this, note that for the minimum in the right-hand side of (4.96), we have

$$\min\left\{\frac{\tau^2}{\varepsilon}, \max\left\{\tau\varepsilon, \tau^2\right\}\right\} = \begin{cases}\tau^2, & \varepsilon < \tau, \\ \tau\varepsilon, & \varepsilon^2 < \tau \leq \varepsilon, \\ \frac{\tau^2}{\varepsilon}, & \tau \leq \varepsilon^2.\end{cases} \tag{4.97}$$

This means that for step sizes $\tau > \varepsilon$, the error of the ORSM is proportional to τ^2 with a constant that does *not* grow with decreasing ε. For $\varepsilon^2 < \tau \leq \varepsilon$, there is still some improvement compared to the $\frac{\tau^2}{\varepsilon}$ bound since $\tau\varepsilon = \frac{\tau}{\varepsilon}\varepsilon^2 < \frac{\tau^2}{\varepsilon}$. This improvement gets smaller the closer τ is to ε^2. Both facts are especially worth mentioning since the classical TSFP scheme shows a very irregular error behavior for $\tau > \varepsilon^2$, cf. Figure 4.1. In particular, the error of the TSFP scheme seems to be of $\mathcal{O}(1)$ in the worst case.

Remark 4.23. *In Theorem 4.22, we assumed that the exact solution of the NLDE and the potentials are in $H^{\widehat{m}+6}$ for some $\widehat{m} \geq 2$. Those assumptions then allowed deriving a*

global error bound in $H^{\widehat{m}}$. In contrast to that, for the EEMR and the NRNPI schemes from Chapters 2 and 3, we analyzed the global error in L^2. Here, we only made the significantly less strict assumption that the exact solution and the potentials are in H^4. According to [Bao+16b], the same regularity is also required for an L^2 error bound of the TSFP scheme.

We conjecture, however, that the assumption $\widehat{m} \geq 2$ could be avoided in the sense that a global error bound in L^2 with the same right-hand side as (4.96) can be proven if the exact solution and the potentials are in H^6. To do this, one would have to derive a local error bound and a stability estimate in L^2 based on estimates of the form (2.17) and (2.18), similar as in the previous chapters. Since the constant in the stability estimate would then depend on the H^2-norms of the functions involved, the uniform boundedness of the numerical approximations in H^2 for all ε and all step sizes τ below an ε-independent threshold τ_0 would be required, as in Eq. (2.48) or in Assumption 3.10. This bound could be proven in the same way as (2.48). Since the procedure is identical as in the previous chapters, we refrained from doing so here. Instead, we only presented the error analysis in $H^{\widehat{m}}$, $\widehat{m} \geq 2$, where the algebra property makes things easier.

4.6 Numerical experiments

To close this chapter, we validate the global error bound of the ORSM from Theorem 4.22 in a numerical experiment. We will see that in many cases, the error is even smaller than one would expect from the theorem. Apart from that, we observe the efficiency of the new splitting scheme in this section, in particular compared to the TSFP scheme (4.4). Furthermore, we take a brief look at Lie splitting applied to the classical or the new splitting, i.e. (4.1) or (4.12), of the NLDE.

All experiments are carried out on the 1D-version of the NLDE from Sections 2.4 and 3.5.1, for which the splitting approach and the approximation of solutions of the subproblems, including the error analysis, can be conducted in the same way as in the 3D-case. The only difference is that in Assumption 4.20, we can replace the condition $\widehat{m} \geq 2$ by $\widehat{m} \geq 1$, since this is sufficient for $H^{\widehat{m}}(\mathbb{R})$ being an algebra. We will also use the same strategy for the truncation of the domain and for space discretization as in the aforementioned sections, with the same number of gird points $2M = 256$. Further, we employ identical data. In all plots, we observe the error at time $T = 1$ of approximations obtained via the methods described in the previous sections compared to reference solutions that are computed on the same spatial grid with MATLAB's `ode45`-solver applied with very small tolerances.

4.6.1 Accuracy

In the first experiment, we observe the H^1-error of the ORSM in dependency of the step size τ. For a periodic function $v \in \left(H^m(\mathbb{T}([a,b]))\right)^2$ with $\mathbb{T}([a,b]) = \mathbb{R}/(b-a)\mathbb{Z}$, the H^m-norm of v is approximated by

$$\|v\|_{H^m} \approx \sqrt{\sum_{k=-M}^{M} \left(1 + \left(\frac{2\pi k}{b-a}\right)^2\right)^m |\widehat{v}_k|_2^2},$$

where $\widehat{v}_k$, $k \in \mathbb{Z}$, are the Fourier coefficient vectors of v. The results for three different values of ε are depicted in Figure 4.4 in logarithmic axis. The results indeed obey the error bound from Theorem 4.22, but there are even many cases where the error is smaller than expected. To understand this, let us consider the different step size regimes from (4.97) one after the other.

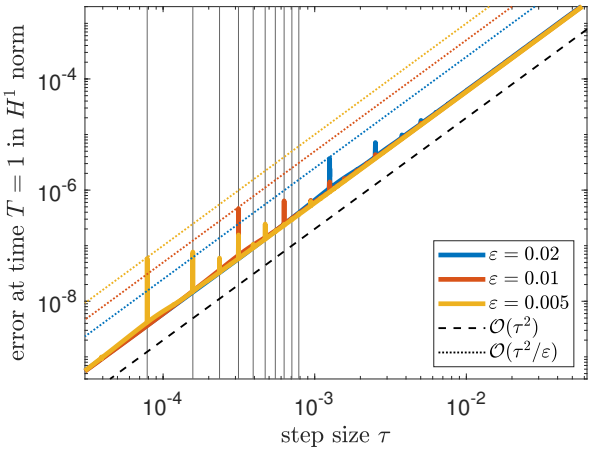

Figure 4.4: H^1-error of the ORSM at time $T = 1$ in dependency of the time step size τ for three different values of ε. The dotted reference lines are of the form $C\frac{\tau^2}{\varepsilon}$ for a joint constant C. The vertical lines mark the step sizes $\tau = k\pi\varepsilon^2$, $k = 1, \dots, 10$ for the value $\varepsilon = 0.005$.

For $\tau > \varepsilon$, the results correspond to the assertion from Theorem 4.22. An error proportional to τ^2 can be observed, as a comparison to the dashed, black, second-order reference line shows. The error for the different values of ε cannot be distinguished, confirming the independence of the error constant of ε.

Unexpectedly, the same holds for most step sizes in the regime $\varepsilon^2 < \tau \leq \varepsilon$. Only for some unfavorable step sizes, very thin peaks appear. The value of those unfavorable step sizes can easily be identified from the plot. They are the multiples of $\pi\varepsilon^2$, as the vertical lines reveal for the smallest of the three values of ε. Similar step sizes were identified as resonant step sizes for the NRNPI-scheme from Chapter 3, cf. Eq. (3.46). Since the value of those step sizes is known, it is no problem to avoid them. But even for those unfavorable step sizes, the error does not grow arbitrarily large. Instead, the height of the furthermost left peak for each value of ε (corresponding to the step size $\tau = \pi\varepsilon^2$) is $C\frac{\tau^2}{\varepsilon}$ for a constant C independent of ε. This is confirmed by the colored, dotted reference lines. Those lines all have the form $C\frac{\tau^2}{\varepsilon}$ for a joint constant C, and they "touch" the furthermost left peak at its largest value. All other peaks stay below those reference lines, which is what we would expect from Theorem 4.22 together with Eq. (4.97). Similarly, for step sizes $\tau \leq \varepsilon^2$ (i.e., further left than the furthermost left peak), the error is of order $\mathcal{O}(\tau^2)$ independently of ε.

Since the uniformity of the error for step sizes in the regimes $\tau \leq \varepsilon^2$ or $\varepsilon^2 < \tau \leq \varepsilon$, but not close to the values $k\pi\varepsilon^2$, $k \in \mathbb{N}$, was not observed in the local error plots in Figures 4.2 or 4.3, this improved error behavior seems to be due to nonresonance effects in the error accumulation, possibly similar as in Chapter 3. To understand this, a detailed analysis of the structure of the local error terms that are in $\mathcal{O}\left(\frac{\tau^3}{\varepsilon}\right)$ would be required. The source of those error terms is the approximation from Lemma 4.11. As an alternative to the bound established in the lemma, one can deduce the representation

$$\mathrm{e}^{t\mathcal{P}_\varepsilon}v - \mathrm{e}^{t\mathcal{P}_0}v = -2\mathrm{i}\varepsilon \sin\left(\frac{t}{\varepsilon^2}\right)\mathcal{R}^{\mathrm{Proj}}v, \qquad v \in \left(H^m(\mathbb{R}^3)\right)^4$$

of the error from its proof. What this representation implies for the structure of the $\mathcal{O}\left(\frac{\tau^3}{\varepsilon}\right)$ local error terms and thus what the exact reason for the improved global error is, however, remains an open research question.

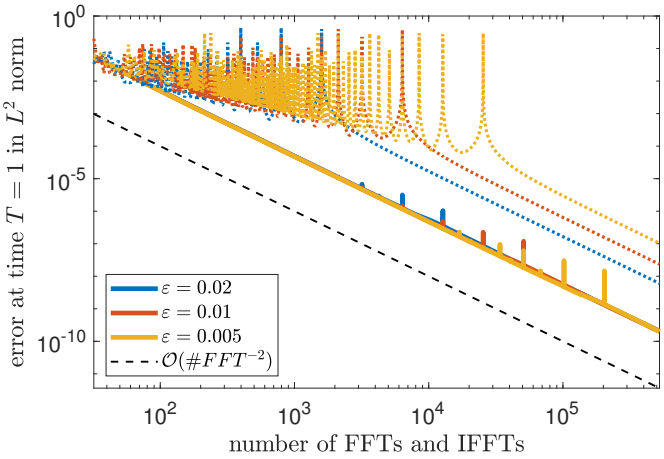

Figure 4.5: L^2-error at time $T = 1$ of the ORSM (solid lines) and of the TSFP scheme (dotted lines) in dependency of the total number of discrete Fourier transforms required in the course of all time steps.

Overall, the accuracy of the ORSM for a fixed step size τ is far superior to that of the TSFP. However, one has to keep in mind that each time step of the former scheme is more expensive than a time step of the latter. Nevertheless, a large efficiency gain remains, as we will discuss in the next subsection.

The remaining experiments all include comparisons of the ORSM to other methods. For most of those methods, bounds of the L^2-error have been studied. This is why from now on, we will always measure the error in L^2 (instead of, e.g., H^1 as above). Of course, the error bound in $H^{\widehat{m}}$ from Theorem 4.22 trivially implies the same bound for the error in L^2.

4.6.2 Efficiency

Here, we want to observe if the improved accuracy of the ORSM compared to the TSFP indeed yields an efficiency gain, i.e. if better accuracies can be achieved for fixed computation times. A fair comparison of the efficiency of different methods is difficult since the runtime of a numerical method heavily depends on the implementation (e.g. avoiding unnecessary computations, vectorization and parallelization of operations, ...). However, after space discretization, the most expensive operations that have to be carried out for computing a time step of any method discussed in this work are (discrete) Fourier transforms and inverse Fourier transforms. Thus, an alternative approach to assess efficiency of the different methods is to observe the number of discrete Fourier transforms required. For a single time step of the ORSM or the TSFP scheme, this number has been discussed in Remark 4.15.

In the next numerical experiment, both methods are applied for several different step sizes. In each application, the error at time $T = 1$ is observed and the total number of Fourier transforms for all time steps required to reach time $T = 1$ is counted. The results are depicted in Figure 4.5. Since the number of Fourier transforms is proportional to the number of steps N, and thus inversely proportional to the step size τ, the error of the ORSM is in $\mathcal{O}(\#FFT^{-2})$ uniformly in ε apart from the peaks corresponding to unfavorable step sizes (see also the black reference line). For the TSFP scheme, we again have to distinguish the cases $\tau \leq \varepsilon^2$ (corresponding to a large number of time steps and thus of Fourier transforms) or $\tau > \varepsilon^2$ (corresponding to small FFT numbers). In the first case, the error again decreases quadratically with increasing number of FFTs, but with an error constant that is proportional

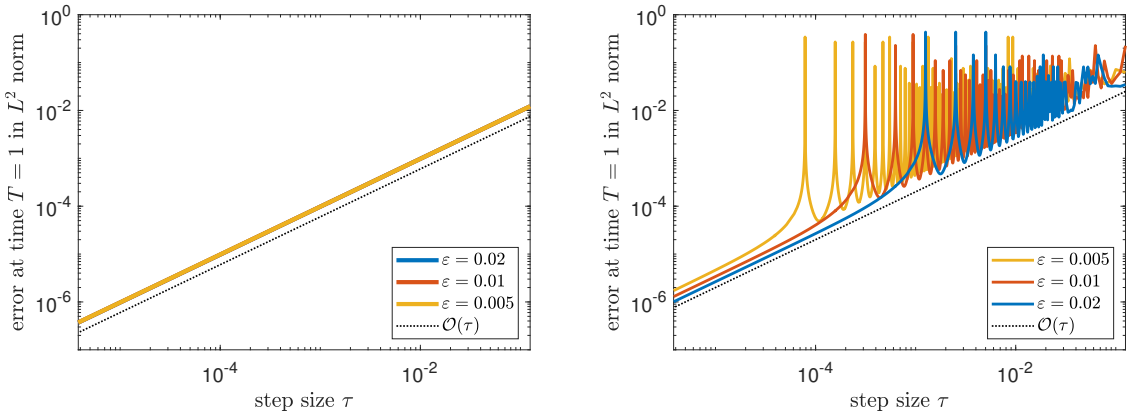

Figure 4.6: L^2-error at time $T = 1$ in dependency of the step size τ for Lie splitting applied to the new splitting (4.12) (left) or the classical splitting (4.1) (right) of the NLDE.

to $\frac{1}{\varepsilon^2}$. In contrast to that, one can again see the irregular error behavior in the second case. The plot shows that in all cases, the ORSM is clearly more efficient for all three values of ε depicted. Even though each of its time steps requires more Fourier transforms, it achieves better accuracies for a fixed number of FFTs. This also holds at those points where peaks appear due to unfavorable step sizes, but the largest efficiency gain is of course obtained for step sizes not too close to them. Since the error constant of the TSFP scheme is proportional to $\frac{1}{\varepsilon^2}$ (in the step size regime $\tau \leq \varepsilon^2$), the efficiency gain is particularly large for small values of ε.

4.6.3 Lie splitting

As supplementary information, we briefly discuss what error behavior one could expect if Lie splitting instead of Strang splitting was applied to the new splitting (4.12) of the NLDE. In the proof of Lemma 4.9, we have seen how the local splitting error of Strang splitting can be related to the error of Lie splitting steps (with different orders of the subproblems), and we have analyzed the latter, cf. (4.47) and (4.49). In particular, this analysis directly yields that the local error of Lie splitting steps is of $\widehat{\mathcal{O}^m}(\tau^2)$ uniformly in ε, and approximating the projectors $\Pi_\varepsilon^\pm$ by the matrices $\Pi_0^\pm$ is not necessary. Globally, one would thus expect uniform first order convergence if the subproblems could be solved exactly. This is confirmed by the left panel of Figure 4.6. Here, Lie splitting is applied to the splitting (4.12). When doing so, the solutions of the LDE- and the NL-subproblems are approximated by MATLAB's `ode45`-solver with very small tolerances, such that the approximations can be considered as exact. For comparison, Lie splitting is also applied to the classical splitting (4.1) of the NLDE in the right panel of Figure 4.6. As for Strang splitting, a very irregular error behavior is observed for step sizes $\tau > \varepsilon^2$. For $\tau \leq \varepsilon^2$, linear convergence is observed, with an error constant that seems to increase only slightly with decreasing ε.

Chapter 5

Conclusion and outlook

This thesis addressed the construction of time integration schemes for the NLDE in the nonrelativistic limit regime. Three novel methods have been presented. The EEMR from Chapter 2 allows approximating solutions of the NLDE with accuracies up to $\mathcal{O}(\varepsilon^2)$ very efficiently. However, since it only approximates solutions of the semi-nonrelativistic limit system, it cannot achieve better accuracies. If an error of $\mathcal{O}(\varepsilon^2)$ is not sufficient, the more sophisticated NRNPI or ORSM schemes have to be employed. For the NRNPI from Chapter 3, we proved that the error is proportional to τ^2 for nonresonant step sizes $\tau \geq \pi\varepsilon^2/4$ and to $\tau\varepsilon^2$ for smaller step sizes. In particular, in the former step size regime, it has the same accuracy as the NPI-2 scheme, even though many terms from the flow of the NPI-2 scheme were simply discarded. In numerical experiments, we observed that this can indeed bring a significant efficiency gain. Finally, we proposed the ORSM scheme in Chapter 4. This scheme was based on a splitting of the NLDE into several subproblems. We have seen that approximations of solutions of those subproblems can be obtained far more efficiently than of the full NLDE. Furthermore, we have analyzed the splitting error and obtained an $\mathcal{O}\left(\min\left\{\frac{\tau^2}{\varepsilon}, \max\left\{\tau\varepsilon, \tau^2\right\}\right\}\right)$ error bound after all. The numerical experiments suggested that the error is even in $\mathcal{O}(\tau^2)$ for all τ and ε if some resonant step sizes are avoided.

The accuracy of all three methods in dependency of the step size and of the number of (inverse) Fourier transforms conducted is compared in Figures 5.1 and 5.2, respectively. This

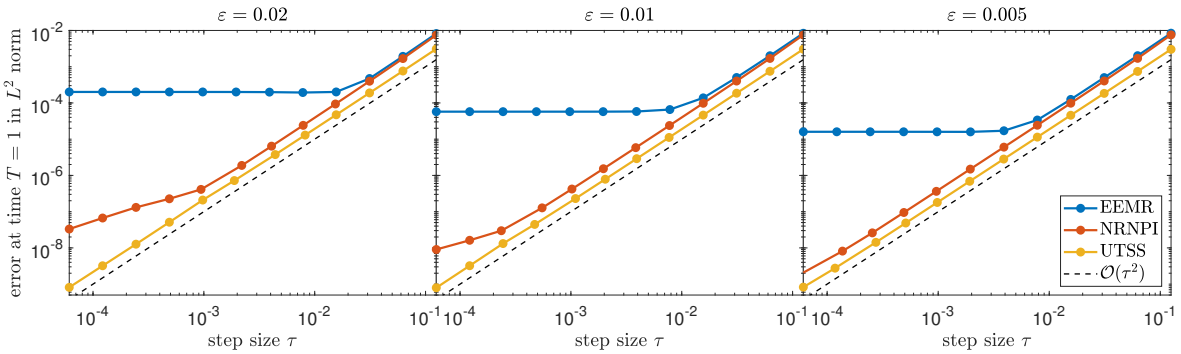

Figure 5.1: L^2-error of the EEMR (blue), the NRNPI (red) and the ORSM (yellow) at time $T = 1$ in dependency of the step size τ for $\varepsilon = 0.02$ (left), $\varepsilon = 0.01$ (middle) and $\varepsilon = 0.005$ (right). Only optimal step sizes were used for the NRNPI, and resonant step sizes were avoided for the ORSM.

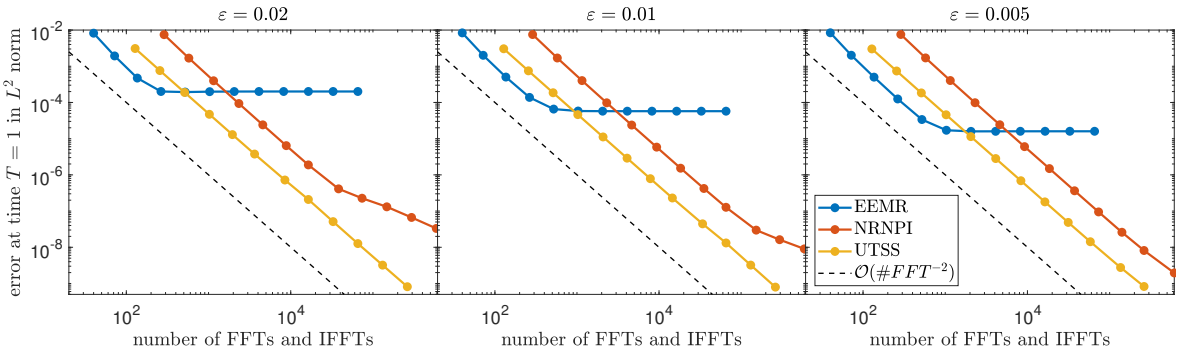

Figure 5.2: As Figure 5.1, but with the error depicted in dependency of the total number of discrete Fourier transforms required in the course of all time steps

not only summarizes the results of all chapters, but also facilitates the choice of an appropriate method for users. In both figures, the three methods are distinguished by different colors, and the results are depicted for three different values of ε in the columns. The NRNPI has only been applied with optimal step sizes, and for the ORSM, resonant step sizes have been avoided.

In Figure 5.1, one can see that for large step sizes $\tau \geq \varepsilon$, all three methods achieve roughly the same accuracy. This is what one would expect from the error analysis. The error constant of the ORSM seems to be slightly smaller than of the other two methods. Nevertheless, thanks to the very simple iteration procedure, the EEMR is the most efficient of all three schemes in this regime, as a look at Figure 5.2 confirms. For step sizes $\varepsilon < \tau \leq \varepsilon^2$ (up to some constants), from the theory we would expect the NRNPI to overtake the ORSM in terms of efficiency at some point (under the assumption that resonant step sizes are avoided), as we were only able to prove an $\mathcal{O}(\tau\varepsilon)$ error bound for the ORSM in this regime, cf. (4.97). However, since in this numerical experiment, an error proportional to τ^2 is in fact observed for the ORSM and since the splitting approach provides significant benefits for the computational work required in each time step, the ORSM is the most efficient in this step size regime. This also holds for step sizes $\tau < \varepsilon^2$. Here, the ORSM is the only scheme that is second order convergent in τ. The fact that the expected factor of ε in the denominator of the error bound does not seem to appear in practice further enhances the efficiency gain of the ORSM.

In Figure 5.2, the ORSM is always more efficient than the NRNPI. On top of that, the construction of the NRNPI required first deriving the full NPI-2 scheme, and even though the numerical flow of the latter has been simplified substantially, the numerical flow of the NRNPI is still rather complicated. This makes implementation and debugging of the NRNPI difficult. In contrast to that, the splitting approach used in the ORSM is easily explained, and the numerical flows used to approximate the subproblems are comparably simple. This suggests that the ORSM is in every respect superior to the NRNPI scheme. However, one has to keep in mind that the improved error behavior (compared to the error bound) of the ORSM is not always guaranteed, as it has so far not been explained analytically. In theory, there might be data for which the NRNPI is in fact more efficient than the ORSM in certain step size regimes. Furthermore, to establish our error bounds, stronger regularity assumptions (in particular on the initial data and on the potentials) have been made for the ORSM than for the NRNPI.

We believe that the improved accuracy that has been observed for the ORSM is systematic. Proving this must be an important goal for future research considering the other favorable

properties of the ORSM. On top of that, a new, special technique of splitting a PDE into several subproblems, namely to include certain terms in all subproblems and to "rewind" them in between, has been used for the construction of the ORSM. This raises the question whether this strategy can also bring benefits for PDEs other than the NLDE. Exploring this is another interesting topic to work on.

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