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Tobias Jahnke, Michael Kirn

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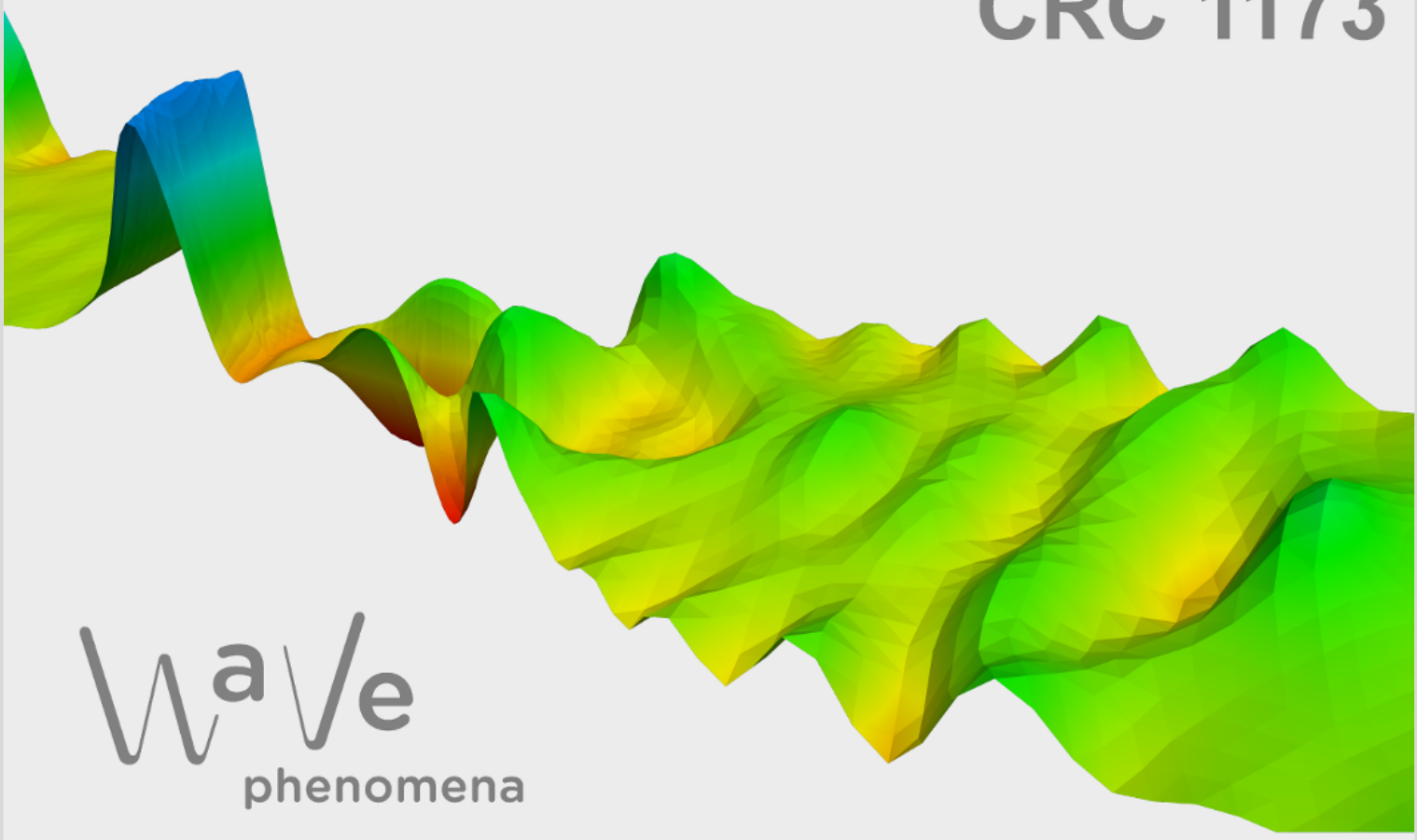

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Employing nonresonant step sizes for time integration of highly oscillatory nonlinear Dirac equations*

Tobias Jahnke† Michael Kirn†

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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. In [10], 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 non-resonant 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.

Keywords: nonlinear Dirac equation, nonrelativistic limit regime, highly oscillatory problems, time integration, error bounds, resonances.

AMS subject classifications: 35Q41 - 65M12 - 65M15.

1 Introduction

One of the most important partial differential equations (PDE) in particle physics is the Dirac equation, which represents a well-established model for relativistic dynamics of electrons, protons, neutrons, and other spin-1/2 particles in an external electromagnetic field [12, 23]. In order to include effects related to self-interaction of particles and other phenomena, nonlinear versions have been introduced in [14, 21, 22, 24]. After a proper nondimensionalization, nonlinear Dirac equations involve a parameter $\varepsilon > 0$ inversely proportional to the speed of light; cf. [1]. In the nonrelativistic limit regime, this parameter is very

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†Karlsruher Institut für Technologie, Fakultät für Mathematik, Institut für Angewandte und Numerische Mathematik, Englerstr. 2, D-76131 Karlsruhe, tobias.jahnke@kit.edu, michael.kirn@kit.edu

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 [1] 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 $\mathcal{O}\big(\varepsilon^2\big)$ 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 [9]. For this purpose, we proposed the *explicit exponential midpoint rule (EEMR)* in [16], which is a second-order integrator and consequently yields a total accuracy of $\mathcal{O}\big(\varepsilon^2 + \tau^2\big)$. For very small step sizes $\tau < \varepsilon^2$, better accuracies can be achieved with the *multiscale time integrator pseudospectral method* from [7], which has an error of $\mathcal{O}\big(\min\{\tau^2 + \varepsilon^2, \tau^2/\varepsilon^2\}\big)$. 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 [2]. 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. Unfortunately, the analysis in [2] is based on the assumption that there is no magnetic field.

Two second-order uniformly accurate methods were proposed in [19] and [10]. In [19], the authors devise an approach which allows them to replace the highly oscillatory Dirac equation 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 [10], uniformly accurate *nested Picard iterative integrators (NPI)* of first and second order are 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 [10]). 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 [10]). 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 construction is carried out for the transformed form of the nonlinear Dirac equation introduced in [9]. 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 $\mathcal{O}\big(\tau^2\big)$ 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 [2, 5, 13, 15, 18, 17]. 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 equation in the nonrelativistic limit regime. We recall the transformation of variables from [9] 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. In Section 4, we present a rigorous error analysis for the NRNPI. Our main results are the global error bounds in Theorem 4.5 and Corollary 4.7. In particular, we show why cancellation effects yield a limited error accumulation for nonresonant step sizes. To keep the focus on the essentials, the proofs of a number of auxiliary results are postponed to Section 6. In Section 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.

2 Problem setting

2.1 Nonlinear Dirac equations in the nonrelativistic limit regime

In the nonlinear Dirac equations (NLDE), the complex-valued vector wave function $\psi = \psi(t,x) \in \mathbb{C}^4$ is modeled by the partial differential equation

$$\partial_t \psi = -\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon \psi - \mathrm{i}W\psi - \mathrm{i}F(\psi)\psi, \qquad x \in \mathbb{R}^3, \quad t > 0, \tag{2.1}$$

together with the initial data $\psi(0,x) = \psi^0(x)$ for some $\mathbb{C}^4$-valued function ψ^0. The solution ψ of (2.1) 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

$$\mathcal{T}_\varepsilon = -\mathrm{i}\sum_{j=1}^{3} \varepsilon\alpha_j\partial_j + \beta, \qquad W(t,x) = V(t,x)I_4 - \sum_{j=1}^{3} A_j(t,x)\alpha_j. \tag{2.2}$$

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

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

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 describes self-interaction of Dirac fermions; see, e.g., [14, 21, 22, 24] and the references in [1, 2, 7, 10, 19]. 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 $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon\psi$ of (2.1) causes oscillations in time with frequency of $\mathcal{O}\big(\varepsilon^{-2}\big)$. 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.

2.2 Function spaces and assumptions

Throughout, the Fourier transform of $u \in L^2(\mathbb{R}^3)$ or $u \in \big(L^2(\mathbb{R}^3)\big)^4$ 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 $\big(H^m(\mathbb{R}^3)\big)^4$ 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 (2.1) into two components, we further define the space

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

for tuples $u = (u_{-1}, u_{+1})$ of two functions $u_{-1}, u_{+1} \in \big(H^m(\mathbb{R}^3)\big)^4$, 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 $\mathbf{H^0} = \big(L^2(\mathbb{R}^3)\big)^4 \times \big(L^2(\mathbb{R}^3)\big)^4$, 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, let us collect some important Sobolev inequalities that we will use frequently. There is a constant $C_S > 0$ such that

$$\|uv\|_{H^2} \leq C_S \|u\|_{H^2} \|v\|_{H^2}, \qquad u \in H^2(\mathbb{R}^3),\ v \in H^2(\mathbb{R}^3) \tag{2.3}$$

$$\|uv\|_{L^2} \leq C_S \|u\|_{L^2} \|v\|_{H^2}, \qquad u \in L^2(\mathbb{R}^3),\ v \in H^2(\mathbb{R}^3) \tag{2.4}$$

In both cases, one of the functions may also be $\mathbb{C}^4$-valued. Further, we have

$$\|u^*v\|_{H^2} \leq C_S \|u\|_{H^2} \|v\|_{H^2}, \qquad u \in \big(H^2(\mathbb{R}^3)\big)^4,\ v \in \big(H^2(\mathbb{R}^3)\big)^4 \tag{2.5}$$

$$\|u^*v\|_{L^2} \leq C_S \|u\|_{L^2} \|v\|_{H^2}, \qquad u \in \big(L^2(\mathbb{R}^3)\big)^4,\ v \in \big(H^2(\mathbb{R}^3)\big)^4. \tag{2.6}$$

All inequalities follow from the fact that $H^m(\mathbb{R}^3)$ is an algebra for $m \geq 2$ and from the Sobolev embedding $H^2(\mathbb{R}^3) \subset L^\infty(\mathbb{R}^3)$.

The following assumptions regarding regularity of the initial data and the potential W (determined by V and A_j via (2.2)) are crucial in the construction of our methods and will thus be made henceforth.

Assumption 2.1. *Let $0 < T < \infty$ be an arbitrary fixed time. We assume that*

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

and that there is a constant $M_{\mathrm{ex}} > 0$ independent of ε such that for the exact solution ψ of (2.1), we have

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

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 $V, A_j \in L^\infty\big([0,\widetilde{T}], H^4(\mathbb{R}^3)\big)$ for some $\widetilde{T} > T$ and if $\psi^0 \in H^4(\mathbb{R}^3)$, see [9, Theorem 2.1].

Assumption (A) together with the inequalities (2.3)–(2.6) yields the existence of some constant $C_W > 0$ such that for all $t \in [0,T]$, we have

$$\begin{aligned} \|W(t,\cdot)u\|_{L^2} &\leq C_W \|u\|_{L^2}, \quad u \in \big(L^2(\mathbb{R}^3)\big)^4, \\ \|W(t,\cdot)u\|_{H^2} &\leq C_W \|u\|_{H^2}, \quad u \in \big(H^2(\mathbb{R}^3)\big)^4. \end{aligned} \tag{2.7}$$

2.3 Transformed Dirac equations

Whilst the uniform boundedness of solutions in (B) is a reasonable assumption, the time derivative of a solution is unbounded w.r.t. ε due to the term $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon\psi$ on the right-hand side of (2.1). In this subsection, we introduce a transformation of variables proposed in [9] 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 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 [9] is based on the decomposition

$$\mathcal{T}_\varepsilon = \Lambda_\varepsilon \Pi^\varepsilon_{-1} - \Lambda_\varepsilon \Pi^\varepsilon_{+1} \tag{2.8}$$

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

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

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 (2.8) is obtained by performing an eigenspace decomposition in Fourier space, see [4, Eq. (1.22)] and [9, Section 2]. It was shown in [4] 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 $\left\|\Pi^\varepsilon_{\mp 1}\right\| = 1$.

The decomposition (2.8) allows to filter out the main part of the temporal oscillations in a solution ψ of the NLDE (2.1). This is achieved by introducing two new functions ϕ_{-1} and ϕ_{+1} defined by

$$\phi_{-1}(t,x) = \mathrm{e}^{\mathrm{i}t/\varepsilon^2} \Pi^\varepsilon_{-1}\left[\psi(t,x)\right], \qquad \phi_{+1}(t,x) = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2} \Pi^\varepsilon_{+1}\left[\psi(t,x)\right] \tag{2.9}$$

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

$$\sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T]} \|\phi_{-1}(t)\|_{H^4} \leq M_{\mathrm{ex}}, \qquad \sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T]} \|\phi_{+1}(t)\|_{H^4} \leq M_{\mathrm{ex}}. \tag{2.10}$$

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

$$\psi(t) = \mathrm{e}^{-\mathrm{i}t/\varepsilon^2}\phi_{-1}(t) + \mathrm{e}^{\mathrm{i}t/\varepsilon^2}\phi_{+1}(t) = \sum_{j\in\{-1,+1\}} \mathrm{e}^{j\mathrm{i}t/\varepsilon^2}\phi_j(t). \tag{2.11}$$

Derivating (2.9) w.r.t. time and inserting the Dirac equation (2.1) yields the PDEs

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

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

$$\partial_t \phi_\sigma = \sigma \mathrm{i}\mathcal{D}_\varepsilon \phi_\sigma - \mathrm{i}\mathrm{e}^{-\sigma \mathrm{i}t/\varepsilon^2}\Pi_\sigma^\varepsilon\left[W\psi\right] - \mathrm{i}\mathrm{e}^{-\sigma \mathrm{i}t/\varepsilon^2}\Pi_\sigma^\varepsilon\left[|\psi|^2\psi\right], \qquad \sigma \in \{-1,+1\}. \tag{2.12}$$

By expanding the product, we can represent the nonlinearity through ϕ as

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

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 in the potential-term of (2.12), we obtain the *transformed Dirac equations*

$$\begin{aligned}\partial_t \phi_\sigma = \sigma \mathrm{i}\mathcal{D}_\varepsilon\phi_\sigma &- \mathrm{i}\sum_{j\in\{-1,1\}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2}\Pi_\sigma^\varepsilon\left[W\phi_j\right]\\ &- \mathrm{i}\sum_{\substack{j=-3\\ j\text{ odd}}}^{3}\sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2}\Pi_\sigma^\varepsilon\left[(\phi_{-j_1})^*\phi_{j_2}\phi_{j_3}\right], \qquad \sigma\in\{-1,+1\}.\end{aligned} \tag{2.13}$$

In contrast to the operator $-\frac{\mathrm{i}}{\varepsilon^2}\mathcal{T}_\varepsilon$ in (2.1), the leading differential operator $\mathcal{D}_\varepsilon$ in (2.13) 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. [9]. More precisely, it fulfills the estimate

$$\left\|\mathcal{D}_\varepsilon u\right\|_{H^m} \leq \frac{1}{2}\left\|u\right\|_{H^{m+2}}, \qquad u \in \left(H^{m+2}(\mathbb{R}^3)\right), \tag{2.14}$$

see [16, Eq. (2.8)]. Thus, Assumption 2.1 implies that the first time derivative of ϕ_{-1} and ϕ_{+1} is uniformly bounded in H^2 w.r.t. ε, i.e. for $\sigma \in \{-1,+1\}$ we have

$$\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\left\|\partial_t\phi_\sigma(t)\right\|_{H^2} \leq C_D \tag{2.15}$$

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 (2.13), one can clearly recognize the origin of each term. However, the double sum makes it somewhat complicated. An alternative representation of the PDEs for ϕ_{-1} and ϕ_{+1} can be obtained by sorting the terms in (2.13) according to the arguments in the exponential functions. For example, in the equation for ϕ_{-1}, i.e. $\sigma = -1$ in (2.13),

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 (2.13), this is

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

because for $\sigma=-1$ and $j=+1$ the summand is $\mathrm{e}^{2\mathrm{i}t/\varepsilon^2}\Pi^{\varepsilon}_{-1}\left[W\phi_{+1}\right]$. 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

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

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

$$\begin{aligned}
\partial_t\phi_\sigma = \sigma\mathrm{i}\mathcal{D}_\varepsilon\phi_\sigma &- \mathrm{i}\mathrm{e}^{-4\sigma\mathrm{i}t/\varepsilon^2}\Pi^{\varepsilon}_{\sigma}\left[(\phi_\sigma)^*\phi_{-\sigma}\phi_{-\sigma}\right]\\
&- \mathrm{i}\mathrm{e}^{-2\sigma\mathrm{i}t/\varepsilon^2}\left(\Pi^{\varepsilon}_{\sigma}\left[W\phi_{-\sigma}\right]+\Pi^{\varepsilon}_{\sigma}\left[\left(|\phi_{-1}|^2+|\phi_{+1}|^2\right)\phi_{-\sigma}+(\phi_\sigma)^*\phi_{-\sigma}\phi_\sigma\right]\right)\\
&- \mathrm{i}\qquad\quad\left(\Pi^{\varepsilon}_{\sigma}\left[W\phi_{\sigma}\right]+\Pi^{\varepsilon}_{\sigma}\left[\left(|\phi_{-1}|^2+|\phi_{+1}|^2\right)\phi_{\sigma}+(\phi_{-\sigma})^*\phi_\sigma\phi_{-\sigma}\right]\right)\\
&- \mathrm{i}\mathrm{e}^{+2\sigma\mathrm{i}t/\varepsilon^2}\Pi^{\varepsilon}_{\sigma}\left[(\phi_{-\sigma})^*\phi_\sigma\phi_\sigma\right].
\end{aligned}\tag{2.16}$$

This can be written in the more compact representation

$$\partial_t\phi_\sigma = \sigma\mathrm{i}\mathcal{D}_\varepsilon\phi_\sigma + \sum_{\substack{p=-4\\ p\text{ even}}}^{2}\mathrm{e}^{p\sigma\mathrm{i}t/\varepsilon^2}G^{(p)}_\sigma(\phi)[\phi], \qquad \sigma\in\{-1,+1\},\tag{2.17}$$

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 $G^{(p)}_\sigma(u)$ are defined by

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

for $v=(v_{-1},v_{+1})\in\mathbf{L^2}$. The linearity of the projectors $\Pi^{\varepsilon}_{\mp1}$ and the estimates (2.3)-(2.7) imply that for every $u\in\mathbf{H^2}$, $G^{(p)}_\sigma(u)$ 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 $G^{(p)}_\sigma$ with argument $\phi(t)$, which are applied to the same function $\phi(t)$. In short, we consider $G^{(p)}_\sigma(\phi(t))[\phi(t)]$ where $\phi(t)=(\phi_{-1}(t),\phi_{+1}(t))$ is a solution of (2.13) (or, equivalently, (2.17)) at some time $t\geq 0$. In this case, we just write $G^{(p)}_\sigma(t)$ to increase readability. However, in our error analysis, the distinction between the argument of $G^{(p)}_\sigma$ and the function to which it is applied to will be crucial.

The representation (2.17) is the most compact form to write the PDEs for ϕ_σ, 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 (2.13) 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. Nevertheless, the representation in (2.13) is more involved due to the distinction between the potential and the nonlinearity parts and the more complicated composition of the exponents. When constructing our numerical methods, we will use both representations to make the best possible use of their individual advantages.

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 (2.13) or (2.17) and will therefore yield approximations

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

with $t_n = n\tau$ for $n = 0, 1, 2, ...$ and a step size $\tau > 0$. The relation (2.11) between ϕ and ψ can then be used to construct approximations $\psi^n \approx \psi(t_n)$ by

$$\psi^n := \mathrm{e}^{-\mathrm{i}t_n/\varepsilon^2}\phi_{-1}^n + \mathrm{e}^{\mathrm{i}t_n/\varepsilon^2}\phi_{+1}^n, \qquad n = 0, 1, \ldots. \tag{3.1}$$

Since

$$\begin{aligned}\|\psi^n - \psi(t_n)\|_{L^2} &= \left\|\mathrm{e}^{-\mathrm{i}t_n/\varepsilon^2}\left(\phi_{-1}^n - \phi_{-1}(t_n)\right) + \mathrm{e}^{\mathrm{i}t_n/\varepsilon^2}\left(\phi_{+1}^n - \phi_{+1}(t_n)\right)\right\|_{L^2} \\ &\le \left\|\phi_{-1}^n - \phi_{-1}(t_n)\right\|_{L^2} + \left\|\phi_{+1}^n - \phi_{+1}(t_n)\right\|_{L^2} = \left|\!\left|\!\left|\phi^n - \phi(t_n)\right|\!\right|\!\right|_{\mathbf{L^2}}, \end{aligned} \tag{3.2}$$

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 [10]. However, we formulate the method in the transformed variables (ϕ_{-1}, ϕ_{+1}) instead of the original variable ψ. 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.

3.1 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 equation* (2.13) 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 [10] and for oscillatory Klein-Gordon equations also in, e.g., [3, 6, 25, 11].

Duhamel's formula for (2.13) yields the representation

$$\begin{aligned}\phi_\sigma(t_n+\tau) &= \mathrm{e}^{\sigma \mathrm{i}\tau\mathcal{D}_\varepsilon}\phi_\sigma(t_n) - \mathrm{i}\sum_{j\in\{-1,1\}}\int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon}\mathrm{e}^{\mathrm{i}(j-\sigma)(t_n+s)/\varepsilon^2}\Pi_\sigma^\varepsilon\left[W\phi_j(t_n+s)\right]\mathrm{d}s \\ &\quad - \mathrm{i}\sum_{\substack{j=-3\\ j\text{ odd}}}^{3}\sum_{\substack{J\in\mathcal{J}\\ \#J=j}}\int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon}\mathrm{e}^{\mathrm{i}(j-\sigma)(t_n+s)/\varepsilon^2}\Pi_\sigma^\varepsilon\left[\phi_{-j_1}(t_n+s)^*\phi_{j_2}(t_n+s)\phi_{j_3}(t_n+s)\right]\mathrm{d}s\end{aligned} \tag{3.3}$$

for the solution ϕ_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 $\mathcal{O}\big(\tau^3\big)$ by an expression where the unknown solution $\phi_{\mp1}$ is only evaluated at the current time t_n. The first step to achieve this is to construct a sufficiently accurate approximation to $\phi_{-1}(t_n+s)$ and $\phi_{+1}(t_n+s)$ 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 (3.3) and compute all remaining oscillatory integrals analytically.

3.1.1 Step 1: approximation of $\phi_{\mp1}(t_n+s)$

In order to approximate $\phi_{\mp1}(t_n+s)$, we apply Duhamel's formula again, but this time to the representation (2.17) of the PDEs for ϕ_σ. This yields

$$\phi_\sigma(t_n+s) = \mathrm{e}^{\sigma\mathrm{i}s\mathcal{D}_\varepsilon}\phi_\sigma(t_n) + \sum_{\substack{p=-4\\ p\text{ even}}}^{2}\int_0^s \mathrm{e}^{\sigma\mathrm{i}(s-r)\mathcal{D}_\varepsilon}\mathrm{e}^{p\sigma\mathrm{i}(t_n+r)/\varepsilon^2}G_\sigma^{(p)}(t_n+r)\,\mathrm{d}r. \tag{3.4}$$

Thanks to (2.15), we have

$$\phi_\sigma(t_n+r) = \phi_\sigma(t_n) + \mathcal{O}(r)\,, \qquad r>0 \tag{3.5}$$

for $\sigma\in\{-1,+1\}$. Using (3.5) 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

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

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 (3.4) produces an error of $\mathcal{O}\big(s^2\big)$. Further, we can use the following

Lemma 3.1. *For any $s \in \mathbb{R}$, we have*

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

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

Using the first estimate inside and the second estimate outside the integrals in (3.4), we overall obtain

$$\phi_\sigma(t_n + s) = \phi_\sigma(t_n) + \sigma \mathrm{i}s\mathcal{D}_\varepsilon \phi_\sigma(t_n) + \sum_{\substack{p=-4 \\ p \text{ even}}}^{2} \int_0^s \mathrm{e}^{p\sigma \mathrm{i}(t_n + r)/\varepsilon^2} \, \mathrm{d}r \, G_\sigma^{(p)}(t_n) + \mathcal{O}\big(s^2\big). \tag{3.6}$$

3.1.2 Step 2: filtered operator

Whilst the order of accuracy in (3.6) 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. (2.14). 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 [8, 10]. The filtered operator $\widehat{\mathcal{D}_\varepsilon}(\tau)$ has the properties that

$$\left\| \widehat{\mathcal{D}_\varepsilon}(\tau) u \right\|_{H^m} \leq \frac{1}{\tau} \left\| u \right\|_{H^m}, \qquad u \in \left(H^m(\mathbb{R}^3)\right)^4, \tag{3.7}$$

$$\left\| \widehat{\mathcal{D}_\varepsilon}(\tau) u \right\|_{H^m} \leq \frac{1}{2} \left\| u \right\|_{H^{m+2}}, \qquad u \in \left(H^{m+2}(\mathbb{R}^3)\right)^4 \tag{3.8}$$

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

$$\left\| \left(\mathcal{D}_\varepsilon - \widehat{\mathcal{D}_\varepsilon}(\tau) \right) u \right\|_{L^2} \leq \frac{\tau}{2} \left\| u \right\|_{H^4} \tag{3.9}$$

for all $u \in \left(H^4(\mathbb{R}^3)\right)^4$ (see [8, Proof of Lemma 3.2]). Since the exact solution is assumed to be in H^4, property (3.9) implies that replacing $\mathcal{D}_\varepsilon$ by $\widehat{\mathcal{D}_\varepsilon}$ in (3.6) introduces an $\mathcal{O}(s\tau)$ error, which is unproblematic in view of the error order we want to achieve. Further, combining the term $\sigma \mathrm{i}s\widehat{\mathcal{D}_\varepsilon}(\tau)\phi_\sigma(t_n)$ with $G_\sigma^{(0)}(t_n) = G_\sigma^{(0)}(\phi(t_n))[\phi(t_n)]$ motivates the definition of the operators $\widehat{G}_\sigma^{(p)}(u)$ for each $u = (u_{-1}, u_{+1}) \in \mathbf{H^2}$ by

$$\begin{aligned} \widehat{G}_\sigma^{(0)}(u)[v] &:= G_\sigma^{(0)}(u)[v] + \sigma \mathrm{i} \widehat{\mathcal{D}_\varepsilon}(\tau) v_\sigma, \\ \widehat{G}_\sigma^{(p)}(u)[v] &:= G_\sigma^{(p)}(u)[v], \qquad p \in \{-4, -2, 2\} \end{aligned} \tag{3.10}$$

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

$$\phi_\sigma(t_n + s) = \phi_\sigma(t_n) + \sum_{\substack{p=-4 \\ p \text{ even}}}^{2} \int_0^s \mathrm{e}^{p\sigma \mathrm{i}(t_n+r)/\varepsilon^2} \,\mathrm{d}r\, \widehat{G}_\sigma^{(p)}(t_n) + \mathcal{O}\big(s^2 + s\tau\big)\,, \tag{3.11}$$

where we wrote $\widehat{G}_\sigma^{(p)}(t_n)$ instead of $\widehat{G}_\sigma^{(p)}(\phi(t_n))[\phi(t_n)]$ similar to before. Property (3.7) 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 6.1 in Section 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. (3.11) can equivalently be expressed as

$$\phi_\sigma(t_n + s) = \phi_\sigma(t_n) + \sum_{\substack{p=-4 \\ p \text{ even}}}^{2} \mathrm{e}^{p\sigma \mathrm{i} t_n/\varepsilon^2} s\varphi_1(p\sigma \mathrm{i} s/\varepsilon^2) \widehat{G}_\sigma^{(p)}(t_n) + \mathcal{O}\big(s^2 + s\tau\big)\,. \tag{3.12}$$

3.1.3 Step 3: Approximating the integrals in (3.3)

Eq. (3.12) can now be inserted into (3.3). At this point, it becomes clear why we established two different representations of the PDEs for ϕ_σ: We would like our $\mathcal{O}\big(s^2\big)$-approximation of $\phi_\sigma(t_n + s)$ to be as simple as possible, which was achieved by using the representation (2.17). When inserting (3.12) into (3.3), however, the similar structure of all terms provided by representation (2.13) 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 (3.12) into the nonlinearity in (3.3), this gives rise to a number of $\mathcal{O}\big(s^2\big)$ terms which lead to a total error of $\mathcal{O}\big(\tau^3\big)$. After all, we can express each component of the exact solution $\phi = (\phi_{-1}, \phi_{+1})$ at time $t_n + \tau$ as

$$\phi_\sigma(t_n + \tau) = \mathrm{e}^{\sigma \mathrm{i} \tau \mathcal{D}_\varepsilon} \phi_\sigma(t_n) - \mathrm{i} I_\sigma^1(t_n, \phi(t_n)) - \mathrm{i} I_\sigma^2(t_n, \phi(t_n)) + \mathcal{O}\big(\tau^3\big)\,, \tag{3.13}$$

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

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

for $t \geq 0$ and $u = (u_{-1}, u_{+1}) \in \mathbf{H^2}$, such that $I_\sigma^1(t_n, \phi(t_n))$ is the $\mathcal{O}(\tau^3)$-approximation to the integrals in (3.3) containing products with the potential W. Further, I_σ^2 is given by

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

which means that $I_\sigma^2(t_n, \phi(t_n))$ is the $\mathcal{O}(\tau^3)$-approximation to the integrals in (3.3) accounting for the nonlinearity. The integrals in I_σ^1 and I_σ^2 do no longer involve the exact solution ϕ. Instead, they are operators that can be computed and applied analytically. For $\delta, \zeta \in \mathbb{Z}$, we have

$$
\begin{aligned}
\mathcal{A}_\sigma(\delta) &:= \int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon} \mathrm{e}^{\mathrm{i}\delta s/\varepsilon^2}\,\mathrm{d}s = \tau \mathrm{e}^{\mathrm{i}\delta\tau/\varepsilon^2} \varphi_1\big(\mathrm{i}\tau(\sigma\mathcal{D}_\varepsilon - \delta/\varepsilon^2 \mathrm{Id})\big), \\
\mathcal{B}_\sigma(\delta,\zeta) &:= \int_0^\tau \mathrm{e}^{\sigma\mathrm{i}(\tau-s)\mathcal{D}_\varepsilon} s \mathrm{e}^{\mathrm{i}\delta s/\varepsilon^2} \varphi_1(\zeta \mathrm{i}s/\varepsilon^2)\,\mathrm{d}s \qquad (3.14)\\
&= \begin{cases} \mathrm{i}\tau\frac{\varepsilon^2}{\zeta} \mathrm{e}^{\mathrm{i}\tau\delta/\varepsilon^2} \left(\varphi_1\big(\mathrm{i}\tau(\sigma\mathcal{D}_\varepsilon - \frac{\delta}{\varepsilon^2}\mathrm{Id})\big) - \mathrm{e}^{\mathrm{i}\tau\zeta/\varepsilon^2} \varphi_1\big(\mathrm{i}\tau(\sigma\mathcal{D}_\varepsilon - \frac{\delta+\zeta}{\varepsilon^2}\mathrm{Id})\big)\right), & \zeta \neq 0, \\ \tau^2 \mathrm{e}^{\mathrm{i}\tau\delta/\varepsilon^2} \varphi_2\big(\mathrm{i}\tau(\sigma\mathcal{D}_\varepsilon - \delta/\varepsilon^2\mathrm{Id})\big), & \zeta = 0, \end{cases}
\end{aligned}
$$

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

$$
\begin{aligned}
I_\sigma^1(t,u) = &\sum_{j\in\{-1,1\}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2} \mathcal{A}_\sigma(j-\sigma) \Pi_\sigma^\varepsilon \left[W u_j\right] \\
&+ \sum_{j\in\{-1,1\}} \sum_{\substack{p=-4\\ p \text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj)t/\varepsilon^2} \mathcal{B}_\sigma(j-\sigma, pj) \Pi_\sigma^\varepsilon \left[W \widehat{G}_j^{(p)}(u)[u]\right] \qquad (3.15)
\end{aligned}
$$

and

$$
\begin{aligned}
I^2_\sigma(t,u) &= \sum_{\substack{j=-3\\ j\text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2} \mathcal{A}_\sigma(j-\sigma)\Pi^\varepsilon_\sigma\left[(u_{-j_1})^* u_{j_2} u_{j_3}\right] \\
&+ \sum_{\substack{j=-3\\ j\text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \sum_{\substack{p=-4\\ p\text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj_1)t/\varepsilon^2} \mathcal{B}_\sigma(j-\sigma,pj_1)\Pi^\varepsilon_\sigma\left[\left(\widehat{G}^{(p)}_{-j_1}(u)[u]\right)^* u_{j_2} u_{j_3}\right] \\
&+ \sum_{\substack{j=-3\\ j\text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \sum_{\substack{p=-4\\ p\text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj_2)t/\varepsilon^2} \mathcal{B}_\sigma(j-\sigma,pj_2)\Pi^\varepsilon_\sigma\left[(u_{-j_1})^* \widehat{G}^{(p)}_{j_2}(u)[u] u_{j_3}\right] \\
&+ \sum_{\substack{j=-3\\ j\text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \sum_{\substack{p=-4\\ p\text{ even}}}^{2} \mathrm{e}^{\mathrm{i}(j-\sigma+pj_3)t/\varepsilon^2} \mathcal{B}_\sigma(j-\sigma,pj_3)\Pi^\varepsilon_\sigma\left[(u_{-j_1})^* u_{j_2} \widehat{G}^{(p)}_{j_3}(u)[u]\right]. \qquad (3.16)
\end{aligned}
$$

3.1.4 Specification of the time integrator and local error bound

Eq. (3.13) immediately suggests a time integrator: Replacing $\phi(t_n)$ by numerical approximations $\phi^n = \left(\phi^n_{-1}, \phi^n_{+1}\right)$ (thus also replacing $\widehat{G}^{(p)}_\sigma(t_n) = \widehat{G}^{(p)}_\sigma(\phi(t_n))[\phi(t_n)]$ by $\widehat{G}^{(p)}_\sigma(\phi^n)[\phi^n]$) and omitting the $\mathcal{O}\left(\tau^3\right)$ terms yields the recursion

$$
\phi^{n+1} = \mathbf{\Phi}_{\mathrm{NPI}}(t_n, \phi^n), \qquad n = 0, 1, 2, \ldots \qquad (3.17)
$$

with the numerical flow[1]

$$
\mathbf{\Phi}_{\mathrm{NPI}}(t,u) = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\tau\mathcal{D}_\varepsilon} u_{-1} - \mathrm{i} I^1_{-1}(t,u) - \mathrm{i} I^2_{-1}(t,u) \\ \mathrm{e}^{+\mathrm{i}\tau\mathcal{D}_\varepsilon} u_{+1} - \mathrm{i} I^1_{+1}(t,u) - \mathrm{i} I^2_{+1}(t,u) \end{pmatrix}. \qquad (3.18)
$$

The operator $\mathbf{\Phi}_{\mathrm{NPI}}$ 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 clear. The method (3.17) is fully explicit. If the exact solution $\phi = (\phi_{-1}, \phi_{+1})$ of (2.13) is in $\mathbf{H^4}$ for all times, then by construction its local error

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

is bounded by

$$
\left|\!\left|\!\left| \ell^{n+1}_{\mathrm{NPI}} \right|\!\right|\!\right|_{\mathbf{L^2}} \leq C\tau^3 \qquad (3.19)
$$

for some constant C that is independent of τ and ε. This is one of the ingredients that 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.

[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.

Remark 3.2. *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.* (3.4) *in step 1, the potential W (appearing in $G_\sigma^{(-2)}$ and $G_\sigma^{(0)}$) 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* (3.3)*, 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 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 3.3. *In [10], the authors presented the NPI-2, which is based on the same ideas. There are however some differences. Firstly, they work in the context of the* original Dirac equation (2.1)*. This means that they cannot use an approximation of the type $\psi(t_n + r) \approx \psi(t_n)$ (as we did for the transformed variables, cf.* (3.5)*), since this would induce large errors when ε is small due to the oscillatory dynamics of ψ. That is why in [10] the approximation*

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

was used instead, which is again motivated by Duhamel's formula together with the decomposition (2.8)*. Secondly, they used 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* (3.17)*, which is why we will also refer to our version as NPI-2. However, having formulated the method in the transformed variables $\phi = (\phi_{-1}, \phi_{+1})$ 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.*

3.2 Nonresonant nested Picard iterative integrator (NRNPI)

For the NPI-2 (3.17), one can derive a second-order global error bound with a constant that does not depend on ε, as mentioned in [10, Sec. 4]. To do so, one has to combine the local error bound (3.19) 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 (3.18) contains evaluations of $I_\pm^1$ and $I_\pm^2$, 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 (3.13) of an exact solution $\phi = (\phi_{-1}, \phi_{+1})$ of (2.13) 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. (3.16). If I^2_σ is evaluated with arguments t_n and $\phi(t_n)$ as in (3.13), then each of the addends is of the type

$$\mathrm{e}^{\mathrm{i}qt_n/\varepsilon^2}\mathcal{B}_\sigma(\delta,\zeta)\Pi^\varepsilon_\sigma\left[z(t_n)\right] \tag{3.20}$$

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

$$z(t) = u(t)^* v(t) w(t) \tag{3.21}$$

where u, v and w each are either ϕ_σ for some $\sigma \in \{-1,+1\}$ or $\widehat{G}^{(p)}_\sigma(\phi(\cdot))[\phi(\cdot)]$ for some $\sigma \in \{-1,+1\}$, $p \in \{-4,-2,0,2\}$. We suggest a method where all terms of the type (3.20) 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 (3.20) contain the prefactor $\mathrm{e}^{\mathrm{i}qt_n/\varepsilon^2}$. This is a complex number oscillating on the unit circle throughout the time steps. For $q \neq 0$, two consecutive numbers $\mathrm{e}^{\mathrm{i}qt_n/\varepsilon^2}$ and $\mathrm{e}^{\mathrm{i}qt_{n+1}/\varepsilon^2} = \mathrm{e}^{\mathrm{i}q\tau/\varepsilon^2}\mathrm{e}^{\mathrm{i}qt_n/\varepsilon^2}$ 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 $\phi = (\phi_{-1}, \phi_{+1})$ of (2.13) 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 $\mathcal{B}_\sigma(\delta,\zeta)\Pi^\varepsilon_\sigma\left[z(t_n)\right]$ 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. 4.5) to show that neglecting terms of the form (3.20) 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 $I^1_\sigma(t_n, \phi(t_n))$.

Let us now establish our new method in detail. In each of the last three lines of I^2_σ, defined in (3.16), 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 of four terms here. Overall, we replace $I_\sigma^1(t,u)$ and $I_\sigma^2(t,u)$ in the numerical flow (3.18) of the full method by $J_\sigma^1(t,u)[u]$ and $J_\sigma^2(t,u)[u]$ where for $u=(u_{-1},u_{+1})\in\mathbf{H^2}$ the operators $J_\sigma^1(t,u)$ and $J_\sigma^2(t,u)$ are given by

$$\begin{aligned} J_\sigma^1(t,u)[v] &= \sum_{j\in\{-1,1\}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2}\mathcal{A}_\sigma(j-\sigma)\Pi_\sigma^\varepsilon\left[Wv_j\right] \\ &\quad + \sum_{j\in\{-1,1\}} \mathcal{B}_\sigma(j-\sigma,\sigma-j)\Pi_\sigma^\varepsilon\left[W\widehat{G}_j^{(\sigma j-1)}(u)[v]\right], \end{aligned} \tag{3.22}$$

$$\begin{aligned} J_\sigma^2(t,u)[v] &= \sum_{\substack{j=-3\\ j\text{ odd}}}^{3}\sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2}\mathcal{A}_\sigma(j-\sigma)\Pi_\sigma^\varepsilon\left[u_{-j_1}^* u_{j_2}v_{j_3}\right] \\ &\quad + \sum_{\substack{j=-3\\ j\text{ odd}}}^{3}\sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathcal{B}_\sigma(j-\sigma,\sigma-j)\Pi_\sigma^\varepsilon\left[\left(\widehat{G}_{-j_1}^{(j_1(\sigma-j))}(u)[u]\right)^* u_{j_2}v_{j_3}\right] \\ &\quad + \sum_{\substack{j=-3\\ j\text{ odd}}}^{3}\sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathcal{B}_\sigma(j-\sigma,\sigma-j)\Pi_\sigma^\varepsilon\left[u_{-j_1}^*\widehat{G}_{j_2}^{(j_2(\sigma-j))}(u)[u]v_{j_3}\right] \\ &\quad + \sum_{\substack{j=-3\\ j\text{ odd}}}^{3}\sum_{\substack{J\in\mathcal{J}\\ \#J=j}} \mathcal{B}_\sigma(j-\sigma,\sigma-j)\Pi_\sigma^\varepsilon\left[u_{-j_1}^* u_{j_2}\widehat{G}_{j_3}^{(j_3(\sigma-j))}(u)[v]\right], \end{aligned} \tag{3.23}$$

$v=(v_{-1},v_{+1})\in\mathbf{L^2}$. The reason why we distinguished between the arguments u and v is that now, for every $u\in\mathbf{H^2}$, $J_\sigma^1(t,u)$ and $J_\sigma^2(t,u)$ 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

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

with the numerical flow

$$\mathbf{\Phi}_{\mathrm{NRNPI}}(t,u)[v]=\begin{pmatrix}\mathrm{e}^{-\mathrm{i}\tau\mathcal{D}_\varepsilon}v_{-1}-\mathrm{i}J_{-1}^1(t,u)[v]-\mathrm{i}J_{-1}^2(t,u)[v]\\ \mathrm{e}^{+\mathrm{i}\tau\mathcal{D}_\varepsilon}v_{+1}-\mathrm{i}J_{+1}^1(t,u)[v]-\mathrm{i}J_{+1}^2(t,u)[v]\end{pmatrix} \tag{3.24}$$

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

Remark 3.4. *The terms J_σ^1 and J_σ^2 have to be computed in every time step. They include products of the numerical approximations ϕ_σ^n 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 afterwards 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_σ^1 and the last three lines of J_σ^2, 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_σ^1 and J_σ^2.

Remark 3.5. *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 3.2 and omit terms according to the strategies from above. Consequently, the same additional assumptions on the potential W as in Remark 3.2 are required.*

Remark 3.6. *The techniques from this section can be used to construct similar time integrators for other equations, such as the Klein-Gordon-Dirac system.*

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 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

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

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 (3.17), which we collect in $\ell_{\mathrm{diff}}^{n+1}$,

$$\ell^{n+1} = \underbrace{\phi(t_{n+1}) - \mathbf{\Phi}_{\mathrm{NPI}}(t_n, \phi(t_n))}_{=\ell_{\mathrm{NPI}}^{n+1}} + \underbrace{\mathbf{\Phi}_{\mathrm{NPI}}(t_n, \phi(t_n)) - \mathbf{\Phi}_{\mathrm{NRNPI}}(t_n, \phi(t_n))[\phi(t_n)]}_{=:\ell_{\mathrm{diff}}^{n+1}}. \tag{4.1}$$

From (3.19), we have $\left|\!\left|\!\left|\ell_{\mathrm{NPI}}^{n+1}\right|\!\right|\!\right|_{\mathbf{L^2}} \leq C\tau^3$. Comparing (3.18) and (3.24), we further find

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

This representation will allow to derive the following lemma concerning the structure and properties of $\ell_{\mathrm{diff}}^{n+1}$, whose proof can be found in Section 6.

Lemma 4.1. *Let Assumptions 2.1 hold. Further, Let ϕ be the exact solution of* (2.13) *and $\ell_{\mathrm{diff}}^{n+1}$ as above. Set $\mathcal{Q} = \{-6, -4, -2, 2, 4, 6\}$. Then, we can write*

$$\ell_{\mathrm{diff}}^{n+1} = \sum_{q \in \mathcal{Q}} \tau^2 \mathrm{e}^{\mathrm{i}qt_n/\varepsilon^2} E_q^n \tag{4.2}$$

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

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

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

The next lemma addresses the stability of the numerical flow $\mathbf{\Phi}_{\mathrm{NRNPI}}$.

Lemma 4.2. *Let Assumption 2.1* (A) *hold. Then, for $R > 0$, we have*

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

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

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

$$\begin{aligned}
&\mathbf{\Phi}_{\mathrm{NRNPI}}^{n,k}[u] = \mathbf{\Phi}_{\mathrm{NRNPI}}(t_{n-1}, \phi^{n-1})\Big[\mathbf{\Phi}_{\mathrm{NRNPI}}(t_{n-2}, \phi^{n-2})\Big[\ \ldots\ \mathbf{\Phi}_{\mathrm{NRNPI}}(t_k, \phi^k)\big[u\big]\Big]\Big], && k < n\\
&\mathbf{\Phi}_{\mathrm{NRNPI}}^{n,k}[u] = u, && k \geq n
\end{aligned}$$

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

Assumption 4.3. *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. [16, 20]. This step size restriction is not critical, since it is independent of ε.

Lemma 4.4. *Under Assumptions 2.1* (A) *and 4.3, we have for all $k, n \in \mathbb{N}$ with $k, n \leq \lfloor T/\tau \rfloor$ that*

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

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

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 4.5. *Let Assumptions 2.1 and 4.3 hold and let τ_0 be the constant from the latter. Further, for $\varepsilon \in (0,1)$ arbitrary, let ϕ be the exact solution of* (2.13) *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, we have*

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

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

$$K(\tau,\varepsilon) := \min_{q \in \{2,4,6\}} \left| \mathrm{e}^{\mathrm{i}q\tau/\varepsilon^2} - 1 \right|. \tag{4.3}$$

According to (3.2), the theorem directly yields an error bound for the approximations $\psi^n \approx \psi(t_n)$ defined in (3.1):

Corollary 4.6. *Under the assumptions of and with the constant $C_\star$ from Theorem 4.5, we have*

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

Before we continue with the proof of Theorem 4.5, 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

$$\tau = \frac{(2k-1)}{4}\pi\varepsilon^2, \qquad k \in \mathbb{N}. \tag{4.4}$$

It follows from (4.3) 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 (4.4) *optimal*. On the other hand, one should avoid the *resonant step sizes*

$$\tau = \frac{k}{2}\pi\varepsilon^2 \qquad \text{or} \qquad \tau = \frac{k}{3}\pi\varepsilon^2, \qquad k \in \mathbb{N}, \tag{4.5}$$

for which $K(\tau,\varepsilon) = 0$. This is the reason why these step sizes were excluded in Theorem 4.5. 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 1 (a) in Section 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 $\sin(x) > \frac{2\sqrt{2}}{\pi}x$ 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 4.7. *In the setting of Corollary 4.6, we have*

$$\begin{aligned}
&\|\psi^n - \psi(t_n)\|_{L^2} \le C_\star\left(1 + \frac{1}{\sqrt{2}}\right)\tau^2 && \text{for optimal } \tau \ge \frac{\pi}{4}\varepsilon^2,\\
&\|\psi^n - \psi(t_n)\|_{L^2} \le C_\star\left(1 + \frac{1}{\sqrt{2}}\right)\frac{\pi}{4}\varepsilon^2\tau && \text{for } \tau < \frac{\pi}{4}\varepsilon^2.
\end{aligned}$$

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 4.5. Let $e^n = \phi(t_n) - \phi^n$ be the global error at time t_n. The linearity of $\mathbf{\Phi}_{\mathrm{NRNPI}}(t,u)$ for fixed u allows to decompose e^n as

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

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

$$d^n := \mathbf{\Phi}_{\mathrm{NRNPI}}(t_{n-1},\phi(t_{n-1}))[\phi(t_{n-1})] - \mathbf{\Phi}_{\mathrm{NRNPI}}(t_{n-1},\phi^{n-1})[\phi(t_{n-1})] \tag{4.6}$$

accounting for perturbations in the linear flow operator $\mathbf{\Phi}_{\mathrm{NRNPI}}$. Dissolving the recursion formula yields

$$\begin{aligned}
e^n &= \ell^n + d^n + \mathbf{\Phi}_{\mathrm{NRNPI}}(t_{n-1},\phi^{n-1})\left[\ell^{n-1} + d^{n-1} + \mathbf{\Phi}_{\mathrm{NRNPI}}(t_{n-2},\phi^{n-2})[e^{n-2}]\right]\\
&= \ldots = \sum_{k=1}^{n} \mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}\big[\ell^k\big] + \sum_{k=1}^{n} \mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}\big[d^k\big].
\end{aligned} \tag{4.7}$$

Here, we used the definition and linearity of $\mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}$ and that $e^0 = \phi(t_0) - \phi^0 = 0$. Again using the linearity of $\mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}$ and the decomposition of the local error ℓ^k from (4.1), the first sum can be decomposed to

$$\sum_{k=1}^{n} \mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}\big[\ell^k\big] = \sum_{k=1}^{n} \mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}\big[\ell^k_{\mathrm{NPI}}\big] + \sum_{k=1}^{n} \mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}\big[\ell^k_{\mathrm{diff}}\big]. \tag{4.8}$$

Now, the several lemmas established before allow to derive suitable bounds for the norm of each of the sums appearing in (4.7) or (4.8). In the first sum of (4.8), we can "afford" to loose one τ since ℓ^k_{NPI} is in $\mathcal{O}\big(\tau^3\big)$. Thus, we can use triangle inequality together with Lemma 4.4 to obtain

$$\begin{aligned}\left|\!\left|\!\left|\sum_{k=1}^{n} \mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}\left[\ell^k_{\mathrm{NPI}}\right]\right|\!\right|\!\right|_{\mathbf{L^2}} &\leq \sum_{k=1}^{n} \left|\!\left|\!\left|\mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}\left[\ell^k_{\mathrm{NPI}}\right]\right|\!\right|\!\right|_{\mathbf{L^2}} \leq \sum_{k=1}^{n} \mathrm{e}^{Ct_n} \left|\!\left|\!\left|\ell^k_{\mathrm{NPI}}\right|\!\right|\!\right|_{\mathbf{L^2}} \\ &\leq \sum_{k=1}^{n} C\mathrm{e}^{Ct_n}\tau^3 \leq CT\mathrm{e}^{CT}\tau^2. \end{aligned} \tag{4.9}$$

To control the second sum in (4.8), 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^k_{diff} from Lemma 4.1 and using summation by parts, we have

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

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

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

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

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

for all $q \in \mathcal{Q}$. Together with the uniform bound for the norm of E_q^{n-1} from Lemma 4.1, we infer that the first term is in $\mathcal{O}\Big(\frac{\tau^2}{K(\tau,\varepsilon)}\Big)$. Further, using the properties of $\mathbf{\Phi}_{\mathrm{NRNPI}}$ and $\mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}$ from Lemmas 4.2 and 4.4, respectively, and the properties for the error components E_q from Lemma 4.1, we obtain for $k \leq n-1$ that

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

Overall, we have

$$\left|\!\left|\!\left| \sum_{k=1}^{n} \mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}} \left[\ell^k_{\mathrm{diff}}\right] \right|\!\right|\!\right|_{\mathbf{L^2}} \leq \tau^2 \sum_{q\in\mathcal{Q}} C\frac{2}{K(\tau,\varepsilon)} + \tau^2 \sum_{q\in\mathcal{Q}} \sum_{k=1}^{n-1} C\tau \mathrm{e}^{CT} \frac{2}{K(\tau,\varepsilon)} \leq \tau^2 \frac{CT\mathrm{e}^{CT}}{K(\tau,\varepsilon)}. \tag{4.10}$$

Now, it remains to control the second sum in (4.7). Recall the definition of d^k from (4.6). Since $\phi(t_{k-1}) \in \mathbf{B^2}(M_{\mathrm{ex}})$ and $\phi^{k-1} \in \mathbf{B^2}(M_{\mathrm{num}})$ by assumptions 2.1 and 4.3, respectively, we can use Lemma 4.2 (iii) with $R = \max\{M_{\mathrm{ex}}, M_{\mathrm{num}}\}$ to obtain

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

Triangle inequality together with Lemma 4.4 then yields

$$\left|\!\left|\!\left| \sum_{k=1}^{n} \mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}[d^k] \right|\!\right|\!\right|_{\mathbf{L^2}} \leq \mathrm{e}^{Ct_n} \sum_{k=1}^{n} \left|\!\left|\!\left| d^k \right|\!\right|\!\right|_{\mathbf{L^2}} \leq C\mathrm{e}^{CT}\tau \sum_{k=1}^{n} \left|\!\left|\!\left| e^{k-1} \right|\!\right|\!\right|_{\mathbf{L^2}}. \tag{4.11}$$

Finally, combining (4.7) - (4.11), we have

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

The discrete Gronwall Lemma inequality implies

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

□

Remark 4.8. *Since the local errors of the NRNPI contain those of the NPI-2 (ℓ^k_{NPI}) and additionally the terms that have been omitted from it (ℓ^k_{diff}), 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 [10], 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* (3.15)-(3.18) *and* (3.22)-(3.24)*, respectively, that made the error analysis in this section manageable. In fact, Lemmas 4.2, 4.4 and 6.1 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.*

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.

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

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

with a two-component solution $\psi(t,x)\in\mathbb{C}^2$ 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. [1]. 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.

For 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 [1, 2, 10]. 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 [1, 10], i.e.

$$\psi_1^0(x) = e^{-x^2/2}, \quad \psi_2^0(x) = e^{-(x-1)^2/2}, \quad V(x) = \frac{1-x}{1+x^2}, \quad A_1(x) = \frac{(x+1)^2}{1+x^2}$$

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 step sizes $\tau = T/N$, where $N\in\mathbb{N}$ is the number of time steps. This means, in particular, that not all 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 (3.1). For all error plots, we then compare the approximations ψ^N at the final time $t_N=T$ with

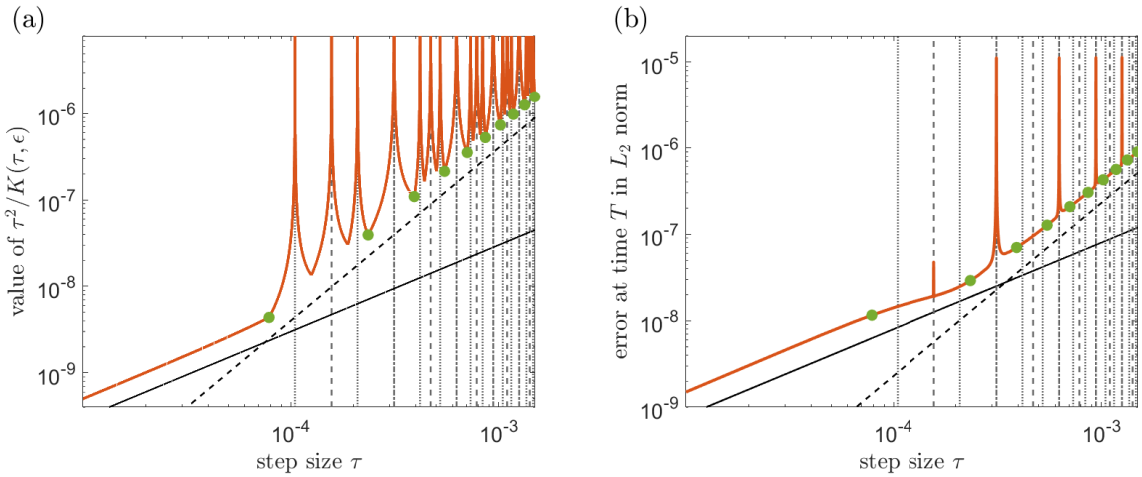

Figure 1: The behaviour of the function $\tau \mapsto \frac{\tau^2}{K(\tau,\varepsilon)}$ (left) compared to the error at time $T = 0.3360\pi$ of the NRNPI (right) for $\varepsilon = 0.01$. In both plots, the axis limits for the step size τ are the same. The green dots depict the function values for the optimal step sizes (4.4). Further, the vertical gray lines mark the resonant step sizes (4.5), 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.

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 $\widehat{u}_k \in \mathbb{C}^2, k \in \mathbb{Z}$.

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 (4.4) and for resonant step sizes (4.5). 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

$$N = \frac{2T}{k\pi}\varepsilon^{-2} = \frac{T}{2k\pi}10^4 = \frac{3360}{2k} \tag{5.1}$$

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 (5.1) 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 (4.4).

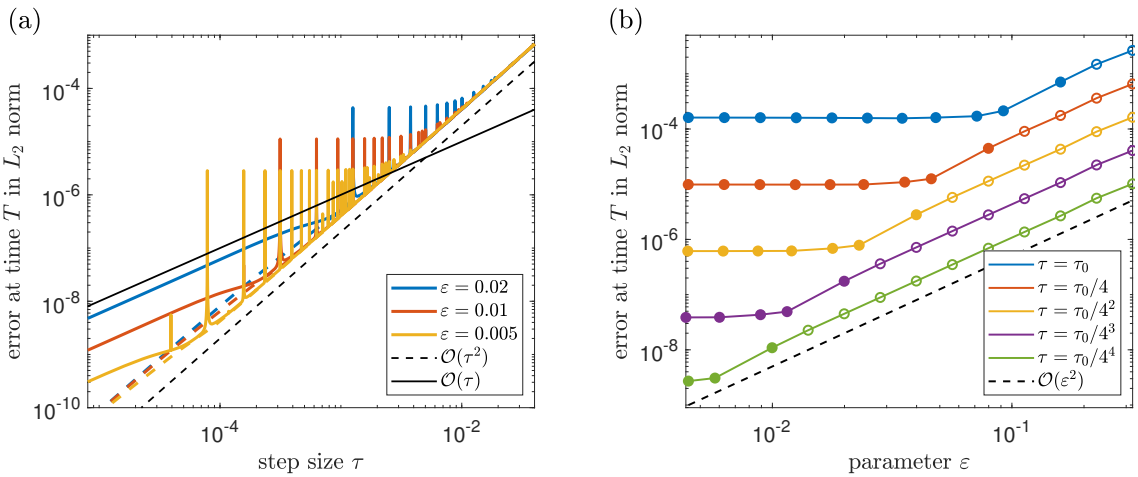

Figure 2: Left: L_2-error of the NRNPI (solid) and the NPI-2 (dashed) at time $T = 0.3360\pi$ in dependency of the step size τ for three different values of ε. Right: L_2-error of the NRNPI at time $T = 1$ in dependency of ε for five different step sizes τ, namely $\tau_0 = 0.02$ and fractions thereof. The filled markers correspond to ε-values for which the respective step size is optimal.

Figure 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 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 4.6 and 4.7. 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 2 (a). The red line is the same as in Figure 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 4.6 and 4.7. 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 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. (4.4), 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 4.7. 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 4.7.

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 1, it seems that not all resonant step sizes (4.5) 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 (3.20) 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 (3.16). 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 $u = \phi(t_n) = \big(\phi_{-1}(t_n), \phi_{+1}(t_n)\big)$ of the transformed Dirac equation, is

$$\mathrm{e}^{6\mathrm{i}t/\varepsilon^2}\mathcal{B}_{-1}(4,2)\Pi^{\varepsilon}_{-1}\left[\left(\widehat{G}^{(2)}_{-1}(\phi(t_n))[\phi(t_n)]\right)^{*}\phi_{+1}(t_n)\phi_{+1}(t_n)\right] \tag{5.2}$$

with

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

Noting that ϕ_{-1} and ϕ_{+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 [8, Eq. (3.25) and (3.26)], however, that

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

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

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

Thus, the terms in (5.2) 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 (5.2). 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 1 (b) and 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.

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 (4.5), which is illustrated in Figure 1 (a). Hence, Corollary 4.6 suggests that the error of the NRNPI would be unbounded if a resonant step size was used. In contrast, Figure 1 (b) reveals that even at those resonant step sizes where spikes indeed appear, the error grows only to a finite level. The reason is that two additional error bounds for the NRNPI could be derived that also hold for the resonant step sizes. First, Lemma 4.1 implies that the local error of the NRNPI is at least in $\mathcal{O}(\tau^2)$ for *all* step sizes τ. Without even considering the special structure of the local error, a Lady Windermere's fan argument yields a uniform (w.r.t. ε) first-order global error bound. Indeed, the furthermost left large spikes for the different values of ε in Figure 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 (3.20) that have been omitted from the numerical flow of the full NPI-2. By the definition of $\mathcal{B}_\sigma(\delta, \zeta)$, cf. (3.14), 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 $\mathcal{O}(\tau\varepsilon^2)$ norm bound 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 (4.4) provide a suitable choice for τ, many other nonresonant step sizes yield equally good results.

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

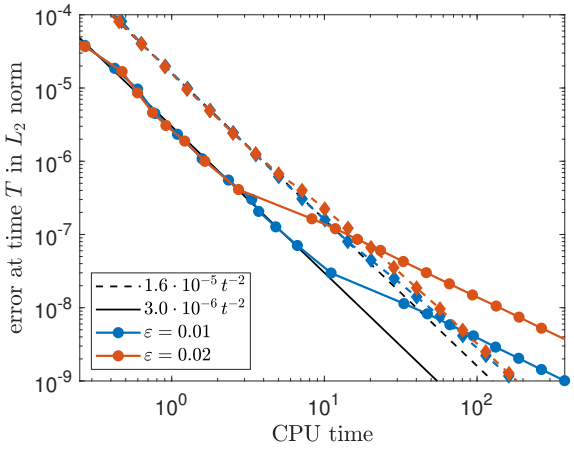

Figure 3: L_2-error of the NRNPI (solid, circles) and the NPI-2 (dashed, diamonds) at time $T = 1$ in dependency of the computing time for two different values of ε.

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. 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.

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.

6 Proof of auxiliary lemmas

In this chapter, we present the proofs of the Lemmas 4.1, 4.2 and 4.4. In preparation thereto, we prove an additional lemma concerning properties of the operators $\widehat{G}_\sigma^{(p)}$ in Section 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

$$u^*v - \widetilde{u}^*\widetilde{v} = u^*\,(v-\widetilde{v}) + (u-\widetilde{u})^*\,\widetilde{v}, \tag{6.1}$$

$$u^*vw - \widetilde{u}^*\widetilde{v}\widetilde{w} = u^*v\,(w-\widetilde{w}) + u^*\,(v-\widetilde{v})\,\widetilde{w} + (u-\widetilde{u})^*\,\widetilde{v}\widetilde{w} \tag{6.2}$$

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

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

Lemma 6.1. *Let Assumption 2.1 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) $\left\|\widehat{G}_\sigma^{(p)}(u)[v]\right\|_{L^2} \le \dfrac{C}{\tau}\,|||v|||_{\mathbf{L^2}}$ *for all $v \in \mathbf{L^2}$,*

(ii) $\left\|\widehat{G}_\sigma^{(p)}(u)[v]\right\|_{H^2} \le \dfrac{C}{\tau}\,|||v|||_{\mathbf{H^2}}$ *for all $v \in \mathbf{H^2}$,*

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

Moreover, the inequalities

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

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

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

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 (2.4) and (2.6) yield

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

Together with the bound (2.7) for products with the potential W, the fact that $\left\|\Pi_{\mp1}^\varepsilon\right\| = 1$, and the estimate (3.7) for the norm of $\widehat{\mathcal{D}_\varepsilon}(\tau)$, the assertion follows from the definition of $\widehat{G}_\sigma^{(p)}$.

(ii) As (i), but using that H^2 is an algebra instead of inequalities (2.4) and (2.6).

(iii) As (ii), but using the estimate (3.8) instead of (3.7) for $\widehat{\mathcal{D}_\varepsilon}(\tau)$.

(iv) Let $u, \widetilde{u} \in \mathbf{B^2}(R)$. First, note that with (3.7), we have

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

For three indices $j_1, j_2, j_3 \in \{-1, +1\}$, a decomposition of the form 6.2 together with the inequalities (2.4) and (2.6) imply that

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

On top of that, (2.7) yields

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

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

(v) Instead of (3.7), we use the estimate (3.8) to obtain

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

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).

□

6.2 Lemma 4.1: structure of the local error of the NRNPI

Proof of Lemma 4.1. Let $\sigma \in \{-1, +1\}$. The terms that have been omitted in $J_\sigma^2(t_n, \phi(t_n))[\phi(t_n)]$ compared to $I_\sigma^2(t_n, \phi(t_n))$ are exactly those of the form (3.20) with $q \neq 0$, i.e. $q \in \mathcal{Q}$, and with z given by (3.21). Those terms omitted in $J_\sigma^1(t_n, \phi(t_n))[\phi(t_n)]$ compared to $I_\sigma^1(t_n, \phi(t_n))$ are also of the form (3.20) with $q \in \mathcal{Q}$, but with

$$z(t) = W\widehat{G}_j^{(p)}(\phi(t))[\phi(t)] \tag{6.3}$$

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 $\phi_{\pm 1}$ is uniformly bounded w.r.t. ε in H^2, Taylor's theorem yields $\|\phi_j(t_{n+1}) - \phi_j(t_n)\|_{H^2} \leq C\tau$ and thus also

$$\|\phi_j(t_{n+1}) - \phi_j(t_n)\|_{L^2} \leq C\tau \tag{6.4}$$

with the constant $C = C_D$ from (2.15). Further, since for all $t \in [0,T]$, $\|\phi_j(t)\|_{H^4} \leq M_{\mathrm{ex}}$ by (2.10), we have $\phi(t) = (\phi_{-1}(t), \phi_{+1}(t)) \in \mathbf{B^4}(2M_{\mathrm{ex}}) \subset \mathbf{B^2}(2M_{\mathrm{ex}})$. Now it follows from Lemma 6.1 (v) that for $j \in \{-1,+1\}$,

$$\left\| \widehat{G}_j^{(p)}(\phi(t_{n+1}))[\phi(t_{n+1})] - \widehat{G}_j^{(p)}(\phi(t_n))[\phi(t_n)] \right\|_{L^2} \leq C \left\| \phi(t_{n+1}) - \phi(t_n) \right\|_{\mathbf{H^2}} \leq C\tau \quad (6.5)$$

for 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 (3.21). Regardless of whether $u = \phi_\sigma$ or $u = \widehat{G}_\sigma^{(p)}(\phi(\cdot))[\phi(\cdot)]$, from (2.10) and Lemma 6.1 (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 (6.4) and (6.5) 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 (6.2) together with the Sobolev inequalities (2.4) and (2.6) yields

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

When z is of the form (6.3), the same estimate follows from (6.5) together with the bounds for products with the potential (2.7). Since $\left\|\Pi_{\mp 1}^\varepsilon\right\| = 1$ 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. □

6.3 Lemma 4.2: stability of the numerical flow of the NRNPI

Proof of Lemma 4.2. (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

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

Each addend of $J_\sigma^1(t,u)[v]$ and $J_\sigma^2(t,u)[v]$ 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 6.1 (i), we have $\left\| \widehat{G}_\sigma^{(p)}(u)[v] \right\|_{L^2} \leq C \|v\|_{\mathbf{L^2}}$ for some constant C that depends on R, but not on τ. Using that $u \in \mathbf{B^2}(R)$ together with the estimates (2.4), (2.6) and (2.7) yields

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

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

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

Since $v_\sigma \in \left(H^2(\mathbb{R}^3)\right)^4$ for $\sigma \in \{-1,+1\}$, Lemma 3.1 yields

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

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

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

because $\left|\!\left|\!\left| v \right|\!\right|\!\right|_{\mathbf{L^2}} \leq \left|\!\left|\!\left| v \right|\!\right|\!\right|_{\mathbf{H^2}}$. 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* $\mathbf{\Phi}_{\mathrm{NRNPI}}(t,u)[v]$ and $\mathbf{\Phi}_{\mathrm{NRNPI}}(t,\widetilde{u})[v]$, 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

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

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 (3.23), 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

$$\sum_{\substack{j=-3 \\ j \text{ odd}}}^{3} \sum_{\substack{J\in\mathcal{J} \\ \#J=j}} \mathrm{e}^{\mathrm{i}(j-\sigma)t/\varepsilon^2} \mathcal{A}_\sigma(j-\sigma) \Pi^\varepsilon_\sigma \left(u^*_{-j_1} u_{j_2} - \widetilde{u}^*_{-j_1} \widetilde{u}_{j_2} \right) v_{j_3}. \tag{6.6}$$

With (2.4) and the fact that $\left\| v_{j_3} \right\|_{H^2} \leq \left|\!\left|\!\left| v \right|\!\right|\!\right|_{\mathbf{H^2}} \leq R$, 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 (6.1) together with (2.6) and $\left\| u_j \right\|_{H^2} \leq \left|\!\left|\!\left| u \right|\!\right|\!\right|_{\mathbf{H^2}} \leq R$ for $j \in \{-1,+1\}$ leads to

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

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 $C\tau \left|\!\left|\!\left| u - \widetilde{u} \right|\!\right|\!\right|_{\mathbf{L^2}}$ for the L_2-norm of the first double sum (6.6).

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 (6.1) together with estimate (2.6) and then applying Lemma 6.1 (ii) and (iv), we find

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

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 (6.2) instead of (6.1) is required here. Apart from that, the same arguments as for the previous sums lead to a bound of the form $C\tau \left|\!\left|\!\left| u - \widetilde{u} \right|\!\right|\!\right|_{\mathbf{L^2}}$ 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. (3.22). 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. □

6.4 Lemma 4.4: Stability of $\mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}$

Proof of Lemma 4.4. Let $u \in \mathbf{L^2}$. For $k \ge n$ the assertion is trivial because $\mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}} = \mathrm{Id}$. For $k < n$, $\mathbf{\Phi}^{n,k}_{\mathrm{NRNPI}}$ is given by

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

Now, we can apply Lemma 4.2 (i) for $\mathbf{\Phi}_{\mathrm{NRNPI}}(t_k,\phi^k)$, then for $\mathbf{\Phi}_{\mathrm{NRNPI}}(t_{k+1},\phi^{k+1})$ and so forth. The constant of the Lemma can be chosen identically each time by Assumption 4.3.

Thus, we obtain

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

□

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