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ASYMPTOTIC CONSISTENT EXPONENTIAL-TYPE INTEGRATORS FOR KLEIN-GORDON-SCHRÖDINGER SYSTEMS FROM RELATIVISTIC TO NON-RELATIVISTIC REGIMES*

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Abstract. In this paper we propose asymptotic consistent exponential-type integrators for the Klein-Gordon-Schrödinger system. This novel class of integrators allows us to solve the system from slowly varying relativistic up to challenging highly oscillatory non-relativistic regimes without any step size restriction. In particular, our first- and second-order exponential-type integrators are asymptotically consistent in the sense of asymptotically converging to the corresponding decoupled free Schrödinger limit system.

Key words. highly oscillatory, Klein-Gordon-Schrödinger, asymptotic consistency, exponential-type integrators

AMS subject classifications. 35C20, 65M12, 35L05

1. Introduction.

The Klein-Gordon-Schrödinger (KGS) system

$$
\begin{aligned}
&c^{-2}\partial_{tt}z(t,x) - \Delta z(t,x) + c^2 z(t,x) = |n(t,x)|^2,\\
&i\partial_t n(t,x) + \Delta n(t,x) + n(t,x)z(t,x) = 0
\end{aligned}
\tag{1.1}
$$

describes the dynamics of a complex-valued nucleon field n interacting with a neutral real-valued scalar meson field z. It arises from coupling a Klein-Gordon (KG) equation nonlinearly to a classical Schrödinger equation. For existence and uniqueness of global smooth solutions we refer to [12, 13, 14] and references therein. Numerically, the Klein-Gordon-Schrödinger system is extensively studied in the *relativistic regime* $c = 1$; see, for instance, [3, 22, 23]. In contrast, the *non-relativistic regime*, where the speed of light c formally tends to infinity, is, due to the highly oscillatory behavior of the solution, much more numerically demanding. Classical numerical methods break down as they fail to resolve the oscillations within the solution. In particular, severe step size restrictions need to be imposed which leads to huge computational effort and does not permit reasonably accurate simulations. Even more suitable so-called Gautschi-type methods, which are especially designed for the numerical solution of oscillatory second-order differential equations (see, e.g., [2, 17, 19]), do not allow a reasonable approximation as they fail to capture the highly oscillatory parts. This phenomenon is illustrated in Figure 1.1, in the slowly varying relativistic regime ($c = 1$) the Gautschi-type method allows a precise approximation of the solution, whereas it fails in the highly oscillatory non-relativistic regime ($c \gg 1$). For classical splitting-type methods we observe a similar error behavior as for the Gautschi-type methods and refer to [10, 26] for their analysis in the context of Schrödinger equations.

Based on a multiscale expansion technique an unconditionally stable accurate method for the Klein-Gordon-Schrödinger system with (or without) damping was recently presented in [4] (see also [1, 8] for results on classical Klein-Gordon equations). The derived method converges, for sufficiently smooth solutions, uniformly in time with linear convergence rate $\mathcal{O}(\tau)$ for $c \in [1,\infty)$. However, optimal quadratic convergence rate $\mathcal{O}(\tau^2)$ is only reached in the regime when either $c = \mathcal{O}(1)$ or $c\tau \geq 1$.

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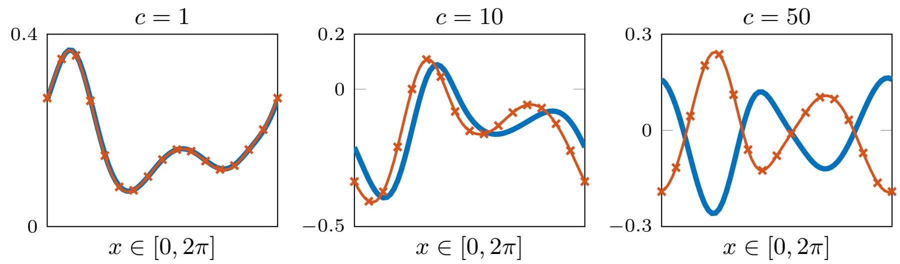

FIG. 1.1. *Numerical simulation (red, cross) simulated with time step size $\tau \approx 10^{-2}$ of the Klein-Gordon-Schrödinger system with a Gautschi-type method (see, e.g., [2]) for increasing values of c. Reference solution (blue, continuous). In the non-relativistic regime, i.e., for large values of c, the approximation fails.*

In comparison we establish a novel class of exponential-type integrators which allow convergence with second-order accuracy in time uniformly for all $c > 0$. The key idea thereby lies in exploiting the so-called *twisted variables* which are well known in the analysis of partial differential equations at low regularity (see, e.g., [6, 7, 15, 29]) and also well known in physics as the so-called "interaction picture". In addition, they appear in numerical analysis, for instance in the context of the modulated Fourier expansion [9, 17], adiabatic integrators [17, 25] as well as Lawson-type Runge–Kutta methods [24]. Recently, this technique was also established in the numerical analysis of low-regularity problems [21, 28] and introduced for the highly oscillatory Klein-Gordon equation in [5]. In the latter we could develop uniformly accurate exponential-type integrators for the classical Klein-Gordon equation up to order two for the first time. Due to the coupled structure the analysis in the Klein-Gordon-Schrödinger setting is, however, much more involved. In particular, their nonlinear resonance interaction strongly differs. Therefore, we need to develop new, adapted techniques.

Let us explain the underlying strategy in a nutshell.

Strategy. In a first step we reformulate the Klein-Gordon part (in z) as a *first-order system in time* via the transformation

$$u = z - ic^{-1}\langle\nabla\rangle_c^{-1}\partial_t z$$

which transforms the KGS system (1.1) into a coupled first-order system in the new variables (u, n) (see Section 2 for details). This allows us to filter-out the highly oscillatory phases

$$\mathrm{e}^{\pm i\ell c^2 t} \quad \text{with} \quad \ell \in \mathbb{Z}$$

explicitly by introducing the key idea of *twisted variables* (u_*, n_*) (see Section 2). The major numerical advantage of looking at the system in (u_*, n_*) instead of (u, n) lies in the fact that $(\partial_t u_*, \partial_t n_*)$ is *bounded uniformly in* c, whereas $(\partial_t u, \partial_t n)$ is of order c^2. This allows us to develop a novel class of *uniformly accurate* exponential-type integrators by iterating Duhamel's formula in (u_*, n_*). The essential point thereby lies in integrating the interactions of the highly oscillatory phases exactly and only approximating the slowly varying parts; see Sections 3 and 4.

This strategy allows us to develop high-order asymptotic consistent numerical methods which approximate Klein-Gordon-Schrödinger solutions from relativistic $c = 1$ up to non-relativistic $c \gg 1$ regimes. Despite of this uniform approximation property, another advantage of the novel class of integrators compared to classical methods is the following: the method converges asymptotically (i.e., $c \to \infty$) to the numerical method of the corresponding decoupled free Schrödinger limit system ($c \to \infty$ in (1.1)); for details see Section 5.

Our theoretical convergence results are underlined with numerical experiments in Section 6.

For practical implementation we impose periodic boundary conditions, i.e., $x \in \mathbb{T}^d$, where $\mathbb{T}^d := [0, 2\pi]^d$. In the following let $r > d/2$. We denote by $\|\cdot\|_r$ the standard $H^r = H^r(\mathbb{T}^d)$ Sobolev norm, where we in particular exploit the well-known bilinear estimate

$$\|fg\|_r \leq c_{r,d}\|f\|_r\|g\|_r \tag{1.2}$$

which holds for some constant $c_{r,d} > 0$.

2. Twisting the variables. In a first step, we rewrite the Klein-Gordon part (in z) of the Klein-Gordon-Schrödinger system (1.1) as a first-order system in time. This will allow us to resolve the limit-behavior $c \to \infty$ of the solution. Therefore, we define for a given $c > 0$ the following operator (*Japanese bracket*)

$$\langle\nabla\rangle_c = \sqrt{-\Delta + c^2}.$$

Next we write (1.1) as a first-order system in time via the transformation (see, e.g., [27])

$$u = z - ic^{-1}\langle\nabla\rangle_c^{-1}\partial_t z, \tag{2.1}$$

such that as $z(t, x) \in \mathbb{R}$ we have

$$z = \frac{1}{2}(u + \overline{u}). \tag{2.2}$$

The corresponding KGS system in (u, n) reads

$$\begin{aligned} i\partial_t u &= -c\langle\nabla\rangle_c u + c\langle\nabla\rangle_c^{-1}|n|^2, \quad && u(0) = z(0) - ic^{-1}\langle\nabla\rangle_c^{-1}\partial_t z(0),\\ i\partial_t n &= -\Delta n - n\frac{1}{2}(u + \overline{u}), && n(0) = n_0. \end{aligned} \tag{2.3}$$

Note that the definition of the operator $\langle\nabla\rangle_c$ formally implies that for $c \to \infty$

$$c\langle\nabla\rangle_c = c^2 + \text{“lower order terms in c”}. \tag{2.4}$$

Next, following the approach in [5], we consider the corresponding *twisted variables* by multiplying u with the phases e^{-ic^2t} which creates the high oscillations in our problem. More precisely, we set

$$u_*(t) = \mathrm{e}^{-ic^2t}u(t).$$

Note that for the Schrödinger part n of the KGS system (2.3) we do not need to apply this twisting since no highly oscillatory action is linked to this variable. However, for notational reasons we write n_* instead of n.

A simple calculation shows that

$$i\partial_t u_* = -\mathcal{A}_c u_* + c\langle\nabla\rangle_c^{-1}\mathrm{e}^{-ic^2t}|n|^2 \quad \text{with} \quad \mathcal{A}_c = c\langle\nabla\rangle_c - c^2. \tag{2.5}$$

The advantage of looking at the twisted system in u_* (instead of u) lies in the fact that the leading operator formally satisfies $\mathcal{A}_c = \mathcal{O}(1)$ in c, whereas $c\langle\nabla\rangle_c = \mathcal{O}(c^2)$; see (2.4). This can be shown easily with the Taylor series expansion of the function $x \to \sqrt{1 + x^2}$ which formally implies that

$$\mathcal{A}_c = -\tfrac{1}{2}\Delta + \mathcal{O}\left(\frac{\Delta^2}{c^2}\right). \tag{2.6}$$

Replacing the first line in (2.3) by (2.5) yields the twisted KGS system

$$
\begin{aligned}
&i\partial_t u_* = -\mathcal{A}_c u_* + c\langle\nabla\rangle_c^{-1}\mathrm{e}^{-ic^2t}|n_*|^2, && u_*(0) = z(0) - ic^{-1}\langle\nabla\rangle_c^{-1}\partial_t z(0),\\
&i\partial_t n_* = -\Delta n_* - \tfrac{1}{2}\left(\mathrm{e}^{ic^2t}u_* + \mathrm{e}^{-ic^2t}\overline{u_*}\right)n_*, && n_*(0) = n(0),
\end{aligned}
\tag{2.7}
$$

with mild solutions

$$
\begin{aligned}
u_*(t_n+\tau) &= \mathrm{e}^{i\tau\mathcal{A}_c}u_*(t_n) - ic\langle\nabla\rangle_c^{-1}\int_0^\tau \mathrm{e}^{i(\tau-s)\mathcal{A}_c}\mathrm{e}^{-ic^2(t_n+s)}|n_*(t_n+s)|^2\mathrm{d}s,\\
n_*(t_n+\tau) &= \mathrm{e}^{i\tau\Delta}n_*(t_n) + \frac{i}{2}\int_0^\tau \mathrm{e}^{i(\tau-s)\Delta}\big[\mathrm{e}^{ic^2(t_n+s)}u_*(t_n+s)\\
&\qquad\qquad + \mathrm{e}^{-ic^2(t_n+s)}\overline{u_*}(t_n+s)\big]n_*(t_n+s)\mathrm{d}s;
\end{aligned}
\tag{2.8}
$$

see, e.g., [27, Section 2.1].

The crucial benefit in the above formulation is the uniform bound on the leading operator $\mathcal{A}_c$

$$
\|\mathcal{A}_c u\|_r \le \frac{1}{2}\|u\|_{r+2}\,,
\tag{2.9}
$$

as well as on the operator in front of the nonlinear coupling which satisfies

$$
\left\|c\langle\nabla\rangle_c^{-1}u\right\|_r \le \|u\|_r\,;
\tag{2.10}
$$

see [5, Lemma 3]. This in particular implies for all $t\in\mathbb{R}$ that (see [5, Lemma 4])

$$
\left\|\mathrm{e}^{it\mathcal{A}_c}\right\|_r = 1 \quad\text{and}\quad \left\|(\mathrm{e}^{-it\mathcal{A}_c}-1)u\right\|_r \le \frac{1}{2}|t|\,\|u\|_{r+2}\,.
\tag{2.11}
$$

Thanks to the essential bound (2.9) uniform bounds also hold on the derivatives $(u_*'(t), n_*'(t))$. More precisely, the solutions of (2.7) satisfy

$$
\begin{aligned}
&\|u_*(t_n+s)-u_*(t_n)\|_r \le \frac{1}{2}|s|\,\|u_*(t_n)\|_{r+2} + |s|\sup_{0\le\xi\le s}\|n_*(t_n+\xi)\|_r^2\,,\\
&\|n_*(t_n+s)-n_*(t_n)\|_r \le |s|\,\|n_*(t_n)\|_{r+2} + |s|\sup_{0\le\xi\le s}\left(\|u_*(t_n+\xi)\|_r\,\|n_*(t_n+\xi)\|_r\right).
\end{aligned}
\tag{2.12}
$$

The above estimates on the derivatives can be proven using Duhamel's formula for u_* and n_*, respectively, and employing the estimates (2.10) and (2.11); see [5, Lemma 5].

Next we state the necessary local well-posedness assumptions.

ASSUMPTION 2.1. *Fix $r > d/2$ and assume that there exists a $T_r > 0$ such that the solution $u_*(t)$, $n_*(t)$ of (2.7) satisfies*

$$
\sup_{0\le t\le T_r}\left(\|u_*(t)\|_r + \|n_*(t)\|_r\right) \le M,
\tag{2.13}
$$

uniformly in c.

REMARK 2.2. Note that Assumption 2.1 holds under the following conditions on the initial data

$$
\|n(0)\|_r \le M_1, \qquad \|z(0)\|_r + \left\|c^{-1}\langle\nabla\rangle_c^{-1}\partial_t z(0)\right\|_r \le M_2,
$$

where M_1, M_2 do not depend on c. This can be easily seen by using a classical fixed point argument in Duhamel's formula (2.8) together with the essential uniform bound (2.10) and (2.11).

For further details on the local well-posedness of highly oscillatory Klein-Gordon equations we refer to [27] and references therein.

In our analysis we will employ the concept of the so-called φ-functions [20] which are defined as follows.

DEFINITION 2.3 (The φ-functions [20]). *For $\xi \in \mathbb{C}$ set*

$$\varphi_0(\xi) := \mathrm{e}^{\xi} \qquad \textit{and} \qquad \varphi_k(\xi) := \int_0^1 \mathrm{e}^{(1-\theta)\xi} \frac{\theta^{k-1}}{(k-1)!} \mathrm{d}\theta \quad \textit{for} \quad k \geq 1,$$

such that in particular we have that

$$\varphi_0(\xi) = \mathrm{e}^{\xi}, \qquad \varphi_1(\xi) = \frac{\mathrm{e}^{\xi} - 1}{\xi}, \qquad \varphi_2(\xi) = \frac{\varphi_1(\xi) - 1}{\xi}.$$

In addition, we define

$$\Psi_k(\xi) := \int_0^1 \mathrm{e}^{\theta\xi} \frac{\theta^{k-1}}{(k-1)!} \mathrm{d}\theta \quad \textit{for} \quad k \geq 1,$$

such that, in particular, we have that

$$\Psi_2(\xi) = \frac{\varphi_0(\xi) - \varphi_1(\xi)}{\xi}.$$

3. Construction of a first-order asymptotic consistent integrator. In this section, we derive a first-order exponential-type integrator for the solution (u_*, n_*) based on Duhamel's formula (2.8). We also refer to [5] for the analysis in the classical Klein-Gordon setting. In order to construct a scheme of first order, we need to impose some additional regularity assumptions on the exact solutions.

ASSUMPTION 3.1. *Fix $r > d/2$ and assume that $u_*, n_* \in \mathcal{C}([0,T]; H^{r+2}(\mathbb{T}^d))$ with, in particular,*

$$\sup_{0 \leq t \leq T} \left(\|u_*(t)\|_{r+2} + \|n_*(t)\|_{r+2} \right) \leq M_3,$$

where M_3 can be bounded uniformly in c.

Note that the above assumption can be easily played back to the initial values thanks to Remark 2.2.

Below we give a detailed derivation of the numerical scheme for u_*^{n+1} approximating $u_*(t_{n+1})$ (with $t_{n+1} = t_n + \tau$) followed by a more compact derivation of the schemes for n_*^{n+1}. Recall Duhamel's formula for u_* (see (2.8))

$$u_*(t_n + \tau) = \mathrm{e}^{i\tau\mathcal{A}_c} u_*(t_n) - ic\langle\nabla\rangle_c^{-1} \int_0^\tau \mathrm{e}^{i(\tau-s)\mathcal{A}_c} \mathrm{e}^{-ic^2(t_n+s)} |n_*(t_n + s)|^2 \mathrm{d}s.$$

The exponential term $\mathrm{e}^{i\tau\mathcal{A}_c}$ is uniformly bounded in c thanks to (2.11). Therefore, the remaining task lies in resolving the highly oscillatory phases in the integral. Using the formal Taylor series expansions

$$n_*(t_n + s) = n_*(t_n) + \mathcal{O}(s n_*') \quad \text{and} \quad \mathrm{e}^{-is\mathcal{A}_c} = 1 + \mathcal{O}(s\mathcal{A}_c) \tag{3.1}$$

in the above integral allows us to integrate the highly oscillatory phases

$$\int_0^\tau \mathrm{e}^{-ic^2 s}\mathrm{d}s = \tau\varphi_1\left(-ic^2\tau\right)$$

exactly. The formal expansion of $\mathrm{e}^{is\mathcal{A}_c}$ given in (3.1) is thereby understood as the application of the operator $\mathrm{e}^{is\mathcal{A}_c}$ to some sufficiently smooth function f in the sense that

$$\mathrm{e}^{-is\mathcal{A}_c} f = f + s\, R(\mathcal{A}_c f), \tag{3.2}$$

where the remainder $R(\mathcal{A}_c f)$ satisfies the bound

$$\|R(\mathcal{A}_c f)\|_r \leq \frac{1}{2}\|f\|_{r+2}.$$

The above bound on the remainder is a direct consequence of (2.11). It is important to note that additional smoothness on f is needed in the expansion (3.2)

Together with the definition of φ_1 (Definition 2.3) we thus obtain that

$$\begin{aligned} u_*(t_n+\tau) =& \mathrm{e}^{i\tau\mathcal{A}_c}u_*(t_n) - ic\langle\nabla\rangle_c^{-1}\mathrm{e}^{i\tau\mathcal{A}_c}\mathrm{e}^{-ic^2 t_n}\tau\varphi_1(-ic^2\tau)|n_*(t_n)|^2 \\ &+ R_1(\tau, t_n, u_*, n_*), \end{aligned} \tag{3.3}$$

where the remainder $R_1(\tau, t_n, u_*, n_*)$ satisfies, thanks to the bounds (2.9), (2.10) and (2.12) (which hold uniformly in c),

$$\|R_1(\tau, t_n, u_*, n_*)\|_r \leq \tau^2 k_r(M_3) \tag{3.4}$$

for a constant k_r which can be chosen independently of c.

This motivates us to define the following numerical scheme in u_*

$$u_*^{n+1} = \mathrm{e}^{i\tau\mathcal{A}_c}u_*^n - i\tau c\langle\nabla\rangle_c^{-1}\mathrm{e}^{i\tau\mathcal{A}_c}\mathrm{e}^{-ic^2 t_n}\varphi_1(-i\tau c^2)|n_*^n|^2.$$

Given the numerical scheme in u_*^{n+1} we can easily compute z^{n+1} as follows (see (2.2))

$$z^{n+1} = \frac{1}{2}\left(u_*^{n+1} + \overline{u_*^{n+1}}\right).$$

For n_* we proceed as follows. Recall Duhamel's formula (see (2.8))

$$\begin{aligned} n_*(t_n+\tau) =& \mathrm{e}^{i\tau\Delta}n_*(t_n) \\ &+ \frac{i}{2}\int_0^\tau \mathrm{e}^{i(\tau-s)\Delta}\left[\mathrm{e}^{ic^2(t_n+s)}u_*(t_n+s)\right. \\ &\left.+\mathrm{e}^{-ic^2(t_n+s)}\overline{u_*}(t_n+s)\right] n_*(t_n+s)\mathrm{d}s. \end{aligned}$$

Carrying out the formal Taylor series expansions

$$u_*(t_n+s) = u_*(t_n)+\mathcal{O}(su_*'), \quad n_*(t_n+s) = n_*(t_n)+\mathcal{O}(sn_*'), \quad \text{and} \quad \mathrm{e}^{-is\Delta} = 1+\mathcal{O}(s\Delta) \tag{3.5}$$

in the above integral allows us to integrate the highly oscillatory phases $\mathrm{e}^{\pm ic^2 s}$ exactly. Together with the definition of φ_1 (Definition 2.3) we therefore obtain that

$$\begin{aligned} n_*(t_n+\tau) =& \mathrm{e}^{i\tau\Delta}n_*(t_n) \\ &+ \frac{i}{2}\mathrm{e}^{i\tau\Delta}\tau\left[\mathrm{e}^{ic^2 t_n}\varphi_1(ic^2\tau)u_*(t_n)n_*(t_n)\right. \\ &\left.+\mathrm{e}^{-ic^2 t_n}\varphi_1(-ic^2\tau)\overline{u_*}(t_n)n_*(t_n)\right] \\ &+ R_1(\tau, t, u_*, n_*), \end{aligned} \tag{3.6}$$

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where the remainder $R_1(\tau, t, u_*, n_*)$ satisfies a similar (in particular uniform) bound to (3.4) thanks to (2.12).

This motivates us to define the following numerical scheme in n_*

$$n_*^{n+1} = \mathrm{e}^{i\tau\Delta} n_*^n + \frac{i}{2}\tau \mathrm{e}^{i\tau\Delta}\left[\mathrm{e}^{ic^2 t_n}\varphi_1(ic^2\tau) u_*^n n_*^n + \mathrm{e}^{-ic^2 t_n}\varphi_1(-ic^2\tau)\overline{u_*^n} n_*^n\right].$$

Collecting the results yields the following full numerical scheme in u_* and n_*

$$\begin{aligned} u_*^{n+1} &= \mathrm{e}^{i\tau\mathcal{A}_c} u_*^n - i\tau \mathrm{e}^{-ic^2 t_n}\varphi_1(-i\tau c^2) c\langle\nabla\rangle_c^{-1}\mathrm{e}^{i\tau\mathcal{A}_c}|n_*^n|^2,\\ u_*^0 &= z(0) - ic^{-1}\langle\nabla\rangle_c^{-1}\partial_t z(0)\\ n_*^{n+1} &= \mathrm{e}^{i\tau\Delta} n_*^n + \frac{i}{2}\tau \mathrm{e}^{i\tau\Delta}\left[\mathrm{e}^{ic^2 t_n}\varphi_1(ic^2\tau) u_*^n n_*^n + \mathrm{e}^{-ic^2 t_n}\varphi_1(-ic^2\tau)\overline{u_*^n} n_*^n\right],\\ n_*^0 &= n_0, \end{aligned} \tag{3.7}$$

where we used the transformation (2.1) for the initial value.

3.1. Convergence analysis of the first-order asymptotic consistent scheme. The exponential-type integration scheme (3.7) converges (by construction) with first order in time uniformly with respect to c; see Theorem 3.2 below.

THEOREM 3.2 (Convergence bound for the first-order scheme). *Fix $r > d/2$ and assume that Assumption 3.1 holds. For u_* defined in (3.7) we set*

$$z^n := \frac{1}{2}\left(\mathrm{e}^{ic^2 t_n} u_*^n + \mathrm{e}^{-ic^2 t_n}\overline{u_*^n}\right).$$

Then, there exists a $T > 0$ and $\tau_0 > 0$ such that for $\tau \le \tau_0$ and $t_n \le T$ we have for all $c > 0$ that

$$\|z(t_n) - z^n\|_r + \|n(t_n) - n^n\|_r \le \tau K_{r,T,M,M_3},$$

where the constant K_{r,T,M,M_3} can be chosen independently of c.

Proof. Fix $r > d/2$.

Stability. In the following we set for $f, g \in H^r$

$$\begin{aligned} \Phi_\tau(f,g) &:= \mathrm{e}^{i\tau\mathcal{A}_c} f - i\tau \mathrm{e}^{-ic^2 t_n}\varphi_1(-i\tau c^2) c\langle\nabla\rangle_c^{-1}\mathrm{e}^{i\tau\mathcal{A}_c}|g|^2\\ \Psi_\tau(f,g) &:= \mathrm{e}^{i\tau\Delta} g + \frac{i}{2}\tau \mathrm{e}^{i\tau\Delta}\left[\mathrm{e}^{ic^2 t_n}\varphi_1(ic^2\tau) f g + \mathrm{e}^{-ic^2 t_n}\varphi_1(-ic^2\tau)\overline{f} g\right] \end{aligned}$$

such that, in particular, $u_*^{n+1} = \Phi_\tau(u_*^n, n_*^n)$ and $n_*^{n+1} = \Psi_\tau(u_*^n, n_*^n)$.

Note that for all $t \in \mathbb{R}$ we have that $\|\mathrm{e}^{it\mathcal{A}_c}\|_r = 1$ and $\|c\langle\nabla\rangle_c^{-1}\|_r \le 1$ (see (2.10) and (2.11), respectively). Furthermore, the following stability bound holds on the φ_1 function

$$\left\|\varphi_1(i\tau c^2\xi)\right\|_r \le 1 \quad \text{for all} \quad \xi \in \mathbb{R}; \tag{3.8}$$

see also [20]. This implies (together with the bilinear estimate (1.2)) that

$$\|\Phi_\tau(f_1, g_1) - \Phi_\tau(f_2, g_2)\|_r \le \|f_1 - f_2\|_r + \tau K\left(\|g_1\|_r, \|g_2\|_r\right)\|g_1 - g_2\|_r,$$

where the constant K depends on $\|g_1\|_r$ and $\|g_2\|_r$, but can be chosen independently of c. A similar bound holds for Ψ.

Global error. Thanks to the local error bound given in (3.4) the assertion then follows by induction, respectively, a *Lady Windermere's fan* argument; see, for example [18, 26]. ∎

In the next section we derive the second-order asymptotic consistent method for the KGS system and state the corresponding convergence result.

4. Construction of a second-order asymptotic consistent integrator. In this section we derive a second-order integrator for the KGS system (1.1) based on Duhamel's formula (2.8) in the twisted variables (u_*, n_*).

Naïvely, one would think that the second-order integrator can be easily derived by simply including the next terms (of order s) in the Taylor series expansions (3.1) and (3.5). This would, however, *not allow a uniform approximation* in c due to the observation that formally

$$\partial_t u_* = \mathcal{O}(1) \quad \text{in } c\text{, however,} \qquad \partial_{tt} u_*(t) = \mathcal{O}(c^2)$$

(similarly for n_*). The construction of a numerical scheme based on a second-order Taylor series expansion of $u_*(t)$ would thus introduce an error of order $\mathcal{O}(\tau^2 c^2)$, but would not yield the desired uniform second-order error bound $\mathcal{O}(\tau^2)$.

Therefore, we need to carry out a much more careful analysis by iterating Duhamel's formula twice which allows us to integrate the highly oscillatory terms $\mathrm{e}^{\pm ic^2 \ell t}$ (with $\ell \in \mathbb{Z}$) exactly.

To obtain second-order approximations we need to impose additional regularity on the exact solutions $u_*(t)$ and $n_*(t)$.

ASSUMPTION 4.1. *Fix $r > d/2$ and assume that $u_*, n_* \in \mathcal{C}([0,T]; H^{r+4}(\mathbb{T}^d))$ with in particular*

$$\sup_{0\le t\le T} \Big(\|u_*(t)\|_{r+4} + \|n_*(t)\|_{r+4} \Big) \le M_4,$$

where M_4 can be bounded uniformly in c.

4.1. Second-order approximation of u_*. In a first step we iterate Duhamel's formula (2.8) in $u_*(t_n+\tau)$ by plugging Duhamel's formula for $n_*(t_n+s)$ into the corresponding integral in $u_*(t_n+\tau)$. This yields

$$\begin{aligned}
u_*(t_n+\tau) = & \\
& \mathrm{e}^{i\tau\mathcal{A}_c} u_*(t_n) - ic\langle\nabla\rangle_c^{-1} \int_0^\tau \mathrm{e}^{i(\tau-s)\mathcal{A}_c} \mathrm{e}^{-ic^2(t_n+s)} \bigg| \mathrm{e}^{is\Delta} n_*(t_n) \\
& + \frac{i}{2}\int_0^s \mathrm{e}^{i(s-\theta)\Delta} n_*(t_n+\theta)\big(\mathrm{e}^{ic^2(t_n+\theta)} u_*(t_n+\theta) \\
& + \mathrm{e}^{-ic^2(t_n+\theta)}\overline{u_*}(t_n+\theta)\big)\mathrm{d}\theta \bigg|^2 \mathrm{d}s \\
=: & \mathrm{e}^{i\tau\mathcal{A}_c} u_*(t_n) \\
& - ic\langle\nabla\rangle_c^{-1} \int_0^\tau \mathrm{e}^{i(\tau-s)\mathcal{A}_c} \mathrm{e}^{-ic^2(t_n+s)} U_1\left(n_*(t_n+s), u_*(t_n+s)\right) \mathrm{d}s\,.
\end{aligned} \tag{4.1}$$

The Taylor series expansions (3.1) and (3.5) imply that

$$\begin{aligned}
& U_1\left(n_*(t_n+s), u_*(t_n+s)\right) = \\
& \quad \left| \mathrm{e}^{is\Delta} n_*(t_n) + \frac{i}{2} s n_*(t_n) \left(\mathrm{e}^{ic^2 t_n}\varphi_1(ic^2 s) u_*(t_n) + \mathrm{e}^{-ic^2 t_n}\varphi_1(-ic^2 s)\overline{u_*}(t_n)\right)\right|^2 \\
& \qquad + R_3(s, t_n, u_*, n_*),
\end{aligned}$$

where the remainder satisfies the estimate

$$\|R_3(s,t_n,u_*,n_*)\|_r \le s^2 k_r(M_3)$$

uniformly in c. Simplifying the absolute value square and employing the Taylor series expansion $\mathrm{e}^{is\Delta} = 1 + is\Delta + \mathcal{O}(s^2\Delta^2)$ in the terms of order s furthermore implies that

$$\begin{aligned} U_1\left(n_*(t_n+s), u_*(t_n+s)\right) = |n_*(t_n)|^2 - is\left(\Delta\overline{n_*}(t_n)\right)n_*(t_n) + is\left(\Delta n_*(t_n)\right)\overline{n_*}(t_n) \\ + R_4(s, t_n, u_*, n_*). \end{aligned}$$

Plugging U_1 into (4.1) we thus obtain, together with the observation that $\mathcal{A}_c + c^2 = c\langle\nabla\rangle_c$, the following second-order expansion in u_*

$$\begin{aligned} u_*(t_n+\tau) =& \mathrm{e}^{i\tau\mathcal{A}_c}u_*(t_n) - ic\langle\nabla\rangle_c^{-1}\mathrm{e}^{i\tau\mathcal{A}_c}\mathrm{e}^{-ic^2t_n} \\ & \int_0^\tau \mathrm{e}^{-isc\langle\nabla\rangle_c}\Big(|n_*(t_n)|^2 - is\left(\Delta\overline{n_*}(t_n)\right)n_*(t_n) + is\left(\Delta n_*(t_n)\right)\overline{n_*}(t_n)\Big)\mathrm{d}s \\ & + R_4(\tau, t_n, u_*, n_*), \end{aligned}$$

where the remainder satisfies

$$\|R_4(\tau, t_n, u_*, n_*)\|_r \le \tau^3 k_r(M_4) \tag{4.2}$$

uniformly in c.

In order to derive a *stable numerical scheme* we carry out the following manipulation in the exponential based on the observation (2.6) which implies that

$$s\mathrm{e}^{-isc\langle\nabla\rangle_c} = s\mathrm{e}^{-is\left(c\langle\nabla\rangle_c - \frac{1}{2}\Delta\right)} + \mathcal{O}(s^2\Delta).$$

The above relation allows the following expansion of $u_*(t_n+\tau)$:

$$\begin{aligned} u_*(t_n+\tau) = & \mathrm{e}^{i\tau\mathcal{A}_c}u_*(t_n) - ic\langle\nabla\rangle_c^{-1}\mathrm{e}^{i\tau\mathcal{A}_c}\mathrm{e}^{-ic^2t_n} \\ & \int_0^\tau \mathrm{e}^{-isc\langle\nabla\rangle_c}|n_*(t_n)|^2 \\ & \quad + is\mathrm{e}^{-is\left(c\langle\nabla\rangle_c - \frac{1}{2}\Delta\right)}\Big(- \left(\Delta\overline{n_*}(t_n)\right)n_*(t_n) + \left(\Delta n_*(t_n)\right)\overline{n_*}(t_n)\Big)\mathrm{d}s \\ & + R_4(\tau, t_n, u_*, n_*), \end{aligned}$$

where the remainder R_4 satisfies the bound (4.2). Integration by parts together with Definition 2.3 yields

$$\begin{aligned} \int_0^\tau \mathrm{e}^{-isc\langle\nabla\rangle_c}\mathrm{d}s &= \tau\varphi_1\big(-i\tau c\langle\nabla\rangle_c\big), \\ \int_0^\tau s\mathrm{e}^{-is\left(c\langle\nabla\rangle_c - \frac{1}{2}\Delta\right)}\mathrm{d}s &= \tau^2\Psi_2\left(-i\tau\big(c\langle\nabla\rangle_c - \tfrac{1}{2}\Delta\big)\right), \end{aligned}$$

which yields

$$\begin{aligned} u_*(t_n+\tau) = & \mathrm{e}^{i\tau\mathcal{A}_c}u_*(t_n) - ic\langle\nabla\rangle_c^{-1}\mathrm{e}^{i\tau\mathcal{A}_c}\mathrm{e}^{-ic^2t_n}\Big(\tau\varphi_1\big(-i\tau c\langle\nabla\rangle_c\big)|n_*(t_n)|^2 \\ & + i\tau^2\Psi_2\left(-i\tau\big(c\langle\nabla\rangle_c - \tfrac{1}{2}\Delta\big)\right)\Big(\overline{n_*}(t_n)\left(\Delta n_*(t_n)\right) - n_*(t_n)\left(\Delta\overline{n_*}(t_n)\right)\Big)\Big) \\ & + R_4(\tau, t_n, u_*, n_*). \end{aligned}$$

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This motivates us to define the following scheme in u_*:

$$u_*^{n+1} = \mathrm{e}^{i\tau\mathcal{A}_c} u_*^n - ic\langle\nabla\rangle_c^{-1} \mathrm{e}^{i\tau\mathcal{A}_c} \mathrm{e}^{-ic^2 t_n} I_{u_*}^n\left(n_*^n\right) \tag{4.3}$$

with

$$\begin{aligned} I_{u_*}^n\left(n_*^n\right) := {}& \tau\varphi_1\big(-i\tau c\langle\nabla\rangle_c\big)|n_*^n|^2 \\ & + i\tau^2\Psi_2\left(-i\tau\big(c\langle\nabla\rangle_c - \tfrac{1}{2}\Delta\big)\right)\Big(\overline{n_*^n}\left(\Delta n_*^n\right) - n_*^n\left(\Delta\overline{n_*^n}\right)\Big). \end{aligned}$$

4.2. Second-order approximation of n_*. To approximate n_* up to second order uniformly in c we proceed as above. Recall Duhamel's formula (2.8) in the twisted variable n_*

$$\begin{aligned} n_*(t_n+\tau) = {}& \mathrm{e}^{i\tau\Delta} n_*(t_n) + \frac{i}{2}\int_0^\tau \mathrm{e}^{i(\tau-s)\Delta}\Big[\mathrm{e}^{ic^2(t_n+s)} u_*(t_n+s) \\ & + \mathrm{e}^{-ic^2(t_n+s)}\overline{u_*}(t_n+s)\Big] n_*(t_n+s)\mathrm{d}s. \end{aligned} \tag{4.4}$$

In a first step we derive uniform approximations in $n_*(t_n+s)$ and $u_*(t_n+s)$ up to order s^2 .

1) Approximation of $n_*(t_n+s)$*:* Thanks to the first-order approximation in n_* given in (3.6) we know that

$$\begin{aligned} n_*(t_n+s) = {}& \mathrm{e}^{is\Delta} n_*(t_n) + \frac{i}{2}\mathrm{e}^{ic^2 t_n} s\varphi_1\big(ic^2 s\big) n_*(t_n) u_*(t_n) \\ & + \frac{i}{2}\mathrm{e}^{-ic^2 t_n} s\varphi_1\big(-ic^2 s\big) n_*(t_n)\overline{u_*}(t_n) + R_3(s,t_n,u_*,n_*), \end{aligned} \tag{4.5}$$

where the remainder satisfies

$$\|R_3(s,t_n,u_*,n_*)\|_r \le s^2 k_r(M_3) \tag{4.6}$$

uniformly in c.

2) Approximation of $u_*(t_n+s)$*:* Thanks to the first-order approximation (3.3) we obtain together with (3.1) that

$$u_*(t_n+s) = \mathrm{e}^{is\mathcal{A}_c} u_*(t_n) - i\mathrm{e}^{-ic^2 t_n} c\langle\nabla\rangle_c^{-1} s\varphi_1\left(-ic^2 s\right)|n_*(t_n)|^2 + R_3(s,t_n,u_*,n_*), \tag{4.7}$$

where the remainder satisfies (4.6) for some constant $k_r(M_3)$ independent of c.

Plugging the first-order approximations (4.5) and (4.7) into (4.4) yields

$$\begin{aligned} n_*(t_n+\tau) = {}& \mathrm{e}^{i\tau\Delta} n_*(t_n) + \frac{i}{2}\mathrm{e}^{i\tau\Delta}\int_0^\tau \mathrm{e}^{-is\Delta} \\ & \cdot\Big[\mathrm{e}^{is\Delta} n_*(t_n) + \frac{i}{2}\mathrm{e}^{ic^2 t_n} s\varphi_1\big(ic^2 s\big) n_*(t_n) u_*(t_n) \\ & + \frac{i}{2}\mathrm{e}^{-ic^2 t_n} s\varphi_1\big(-ic^2 s\big) n_*(t_n)\overline{u_*}(t_n)\Big] \\ & \cdot\Big[\mathrm{e}^{ic^2(t_n+s)}\mathrm{e}^{is\mathcal{A}_c} u_*(t_n) - i\mathrm{e}^{ic^2 s} c\langle\nabla\rangle_c^{-1} s\varphi_1\left(-ic^2 s\right)|n_*(t_n)|^2 \\ & + \mathrm{e}^{-ic^2(t_n+s)}\mathrm{e}^{-is\mathcal{A}_c}\overline{u_*}(t_n) + i\mathrm{e}^{-ic^2 s} c\langle\nabla\rangle_c^{-1} s\varphi_1\left(ic^2 s\right)|n_*(t_n)|^2\Big]\,\mathrm{d}s \\ & + R_3(\tau,t_n,u_*,n_*), \end{aligned} \tag{4.8}$$

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where the remainder satisfies (4.6) for some constant $k_r(M_3)$ independent of c.

3) Approximation of the integral $I_{n_*}(u_*(t_n), n_*(t_n))$: The remaining task lies in the approximation of the integral in (4.8), called I_{n_*} henceforth. Using the approximation $s\mathrm{e}^{-is\Delta} = s + \mathcal{O}(s^2\Delta)$ and $s\mathrm{e}^{-is\mathcal{A}_c} = s + \mathcal{O}(s^2\mathcal{A}_c)$ we obtain that

$$
\begin{aligned}
I_{n_*} = &\int_0^\tau \mathrm{e}^{-is\Delta}\left[\left(\mathrm{e}^{is\Delta}n_*(t_n)\right)\left(\mathrm{e}^{ic^2(t_n+s)}\mathrm{e}^{is\mathcal{A}_c}u_*(t_n)\right)\right]\mathrm{d}s\\
&+\int_0^\tau \mathrm{e}^{-is\Delta}\left[\left(\mathrm{e}^{is\Delta}n_*(t_n)\right)\left(\mathrm{e}^{-ic^2(t_n+s)}\mathrm{e}^{-is\mathcal{A}_c}\overline{u_*}(t_n)\right)\right]\mathrm{d}s\\
&+i\int_0^\tau sn_*(t_n)\left[c\langle\nabla\rangle_c^{-1}|n_*(t_n)|^2\right]\\
&\cdot\left(-\mathrm{e}^{ic^2s}\varphi_1\left(-ic^2s\right)+\mathrm{e}^{-ic^2s}\varphi_1\left(ic^2s\right)\right)\mathrm{d}s\\
&+\frac{i}{2}\int_0^\tau s\left[\mathrm{e}^{ic^2t_n}\varphi_1\left(ic^2s\right)n_*(t_n)u_*(t_n)\right.\\
&\left.+\mathrm{e}^{-ic^2t_n}\varphi_1\left(-ic^2s\right)n_*(t_n)\overline{u_*}(t_n)\right]\\
&\cdot\left[\mathrm{e}^{ic^2(t_n+s)}u_*(t_n)+\mathrm{e}^{-ic^2(t_n+s)}\overline{u_*}(t_n)\right]\mathrm{d}s\\
&+R_4(\tau,t_n,u_*,n_*),
\end{aligned}
\tag{4.9}
$$

where the remainder R_4 satisfies

$$
\|R_4(\tau,t_n,u_*,n_*)\|_r \le \tau^3 k_r(M_4)
\tag{4.10}
$$

uniformly in c.

The latter two integrals can be easily solved by exploiting the relations for $\sigma\in\mathbb{R}$,

$$
\begin{aligned}
\int_0^\tau s\,\mathrm{e}^{-\sigma ic^2s}\varphi_1(\sigma ic^2s)\mathrm{d}s &= \int_0^\tau s\,\varphi_1(-\sigma ic^2s)\mathrm{d}s = \tau^2\varphi_2\left(-\sigma ic^2\tau\right)\\
\int_0^\tau s\,\mathrm{e}^{\sigma ic^2s}\varphi_1(\sigma ic^2s)\mathrm{d}s &= \sigma\frac{1}{ic^2}\int_0^\tau\left(\varphi_0(\sigma 2ic^2s)-\varphi_0(\sigma ic^2s)\right)\mathrm{d}s\\
&= \sigma\frac{\tau}{ic^2}\left(\varphi_1(\sigma 2ic^2\tau)-\varphi_1(\sigma ic^2\tau)\right),
\end{aligned}
$$

which follow from the observation

$$
\mathrm{e}^{\sigma ic^2\tau}\varphi_1\left(-\sigma ic^2\tau\right)=\varphi_1\left(\sigma ic^2\tau\right)
$$

together with integration by parts and Definition 2.3.

The first two integrals need to be analysed with care. For the first integral $I_{n_*,1}$ we obtain by Taylor series expansion together with the relation (see also Definition 2.3)

$$
\int_0^\tau s\mathrm{e}^{\sigma is(c^2-\Delta)}\mathrm{d}s = \tau^2\Psi_2\left(\sigma i\tau(c^2-\Delta)\right),\quad \sigma=\pm1
\tag{4.11}
$$

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that

$$
\begin{aligned}
I_{n_*,1} :=& \int_0^\tau \mathrm{e}^{-is\Delta}\Big[\left(\mathrm{e}^{is\Delta} n_*(t_n)\right)\left(\mathrm{e}^{ic^2(t_n+s)}\mathrm{e}^{is\mathcal{A}_c} u_*(t_n)\right)\Big]\mathrm{d}s\\
=&\mathrm{e}^{ic^2 t_n}\int_0^\tau \mathrm{e}^{is(c^2-\Delta)}\Big[n_*(t_n)u_*(t_n) + \left(is\Delta n_*(t_n)\right)u_*(t_n)\\
&+ n_*(t_n)\left(is\mathcal{A}_c u_*(t_n)\right)\Big]\mathrm{d}s + R_4(\tau, t_n, u_*, n_*)\\
=&\mathrm{e}^{ic^2 t_n}\tau\varphi_1\left(i\tau(c^2-\Delta)\right)n_*(t_n)u_*(t_n)\\
&+ \tau^2 \mathrm{e}^{ic^2 t_n}\Psi_2\left(i\tau(c^2-\Delta)\right)\\
&\cdot\Big[\left(i\Delta n_*(t_n)\right)u_*(t_n) + n_*(t_n)\left(i\mathcal{A}_c u_*(t_n)\right)\Big] + R_4(\tau, t_n, u_*, n_*).
\end{aligned}
\tag{4.12}
$$

For the second integral $I_{n_*,2}$ we similarly have

$$
\begin{aligned}
I_{n_*,2} :=& \int_0^\tau \mathrm{e}^{-is\Delta}\Big[\left(\mathrm{e}^{is\Delta} n_*(t_n)\right)\left(\mathrm{e}^{-ic^2(t_n+s)}\mathrm{e}^{-is\mathcal{A}_c}\overline{u_*}(t_n)\right)\Big]\mathrm{d}s\\
=&\mathrm{e}^{-ic^2 t_n}\int_0^\tau \mathrm{e}^{-is(c^2-\Delta)}\mathrm{e}^{-2is\Delta}\Big[\left(\mathrm{e}^{is\Delta} n_*(t_n)\right)\left(\mathrm{e}^{-is\mathcal{A}_c}\overline{u_*}(t_n)\right)\Big]\mathrm{d}s\\
=&\mathrm{e}^{-ic^2 t_n}\int_0^\tau \mathrm{e}^{-is(c^2-\Delta)}\Big[n_*(t_n)\overline{u_*}(t_n)\Big]\mathrm{d}s\\
&+ \mathrm{e}^{-ic^2 t_n}\int_0^\tau \mathrm{e}^{-is(c^2-\Delta)}\left(-2is\Delta\right)\Big[n_*(t_n)\overline{u_*}(t_n)\Big]\mathrm{d}s\\
&+ \mathrm{e}^{-ic^2 t_n}\int_0^\tau \mathrm{e}^{-is(c^2-\Delta)}\Big[\left(is\Delta n_*(t_n)\right)\overline{u_*}(t_n) + n_*(t_n)\left(-is\mathcal{A}_c\overline{u_*}(t_n)\right)\Big]\mathrm{d}s\\
&+ R_4(\tau, t_n, u_*, n_*).
\end{aligned}
$$

Together with the definition of the φ_1 function (Definition 2.3) and relation (4.11) we thus obtain that

$$
\begin{aligned}
I_{n_*,2} =& \mathrm{e}^{-ic^2 t_n}\tau\varphi_1\left(-i\tau(c^2-\Delta)\right)\Big[n_*(t_n)\overline{u_*}(t_n)\Big]\\
&+ \mathrm{e}^{-ic^2 t_n}\tau^2\Psi_2\left(-i\tau(c^2-\Delta)\right)(-2i\Delta)\Big[n_*(t_n)\overline{u_*}(t_n)\Big]\\
&+ \mathrm{e}^{-ic^2 t_n}\tau^2\Psi_2\left(-i\tau(c^2-\Delta)\right)\Big[\left(i\Delta n_*(t_n)\right)\overline{u_*}(t_n) + n_*(t_n)\Big(-i\mathcal{A}_c\overline{u_*}(t_n)\Big)\Big]\\
&+ R_4(\tau, t_n, u_*, n_*).
\end{aligned}
\tag{4.13}
$$

Recall that by (4.8) and (4.9) we have that

$$
n_*(t_n+\tau) = \mathrm{e}^{i\tau\Delta} n_*(t_n) + \frac{i}{2}\mathrm{e}^{i\tau\Delta} I_{n_*}(u_*(t_n), n_*(t_n)).
$$

Thus, plugging (4.12) and (4.13) into (4.9) motivates us (together with (4.3)) to define the following numerical scheme

$$
\begin{aligned}
u_*^{n+1} &= \mathrm{e}^{i\tau\mathcal{A}_c}u_*^n - ic\langle\nabla\rangle_c^{-1}\mathrm{e}^{i\tau\mathcal{A}_c}\mathrm{e}^{-ic^2 t_n} I_{u_*}^n(n_*^n),\\
n_*^{n+1} &= \mathrm{e}^{i\tau\Delta}n_*^n + \frac{i}{2}\mathrm{e}^{i\tau\Delta} I_{n_*}^n(u_*^n, n_*^n)
\end{aligned}
\tag{4.14}
$$

with

$$
\begin{aligned}
I^n_{u_*}(n^n_*) := {}& \tau\varphi_1\big(-i\tau c\langle\nabla\rangle_c\big)|n^n_*|^2\\
&+ i\tau^2\Psi_2\left(-i\tau\big(c\langle\nabla\rangle_c - \tfrac{1}{2}\Delta\big)\right)\Big(\overline{n^n_*}\left(\Delta n^n_*\right) - n^n_*\left(\Delta\overline{n^n_*}\right)\Big)
\end{aligned}
\tag{4.15}
$$

and

$$
\begin{aligned}
I^n_{n_*} := {}& \mathrm{e}^{ic^2t_n}\tau\varphi_1\left(i\tau(c^2-\Delta)\right)n^n_*u^n_*\\
&+\tau^2\mathrm{e}^{ic^2t_n}\Psi_2\left(i\tau(c^2-\Delta)\right)\Big[\left(i\Delta n^n_*\right)u^n_* + n^n_*\left(i\mathcal{A}_cu^n_*\right)\Big]\\
&+\mathrm{e}^{-ic^2t_n}\tau\varphi_1\left(-i\tau(c^2-\Delta)\right)\Big[n^n_*\overline{u^n_*}\Big]\\
&+\mathrm{e}^{-ic^2t_n}\tau^2\Psi_2\left(-i\tau(c^2-\Delta)\right)\Big[\left(-2i\Delta\right)\left(n^n_*\overline{u^n_*}\right)\\
&+\left(i\Delta n^n_*\right)\overline{u^n_*} + n^n_*\Big(-i\mathcal{A}_c\overline{u^n_*}\Big)\Big]\\
&+\frac{\tau}{2c^2}\mathrm{e}^{2ic^2t_n}\Big(\varphi_1\left(2ic^2\tau\right)-\varphi_1\left(ic^2\tau\right)\Big)n^n_*(u^n_*)^2\\
&-\frac{\tau}{2c^2}\mathrm{e}^{-2ic^2t_n}\Big(\varphi_1\left(-2ic^2\tau\right)-\varphi_1\left(-ic^2\tau\right)\Big)n^n_*(\overline{u^n_*})^2\\
&+i\tau^2\Big(-\varphi_2\left(ic^2\tau\right)+\varphi_2\left(-ic^2\tau\right)\Big)n^n_*\left(c\langle\nabla\rangle_c^{-1}|n^n_*|^2\right)\\
&+\frac{i\tau^2}{2}\Big(\varphi_2\left(ic^2\tau\right)+\varphi_2\left(-ic^2\tau\right)\Big)n^n_*|u^n_*|^2
\end{aligned}
\tag{4.16}
$$

with φ_1, φ_2 and Ψ_2 given in Definition 2.3.

4.3. Convergence analysis of the second-order scheme. The exponential-type integration scheme (4.14) converges (by construction) with second order in time uniformly with respect to c, see Theorem 4.2 below.

THEOREM 4.2 (Convergence bound for the second-order scheme). *Fix $r > d/2$ and assume that Assumption 4.1 holds. For u_* defined in (4.14) we set*

$$
z^n := \frac{1}{2}\left(\mathrm{e}^{ic^2t_n}u^n_* + \mathrm{e}^{-ic^2t_n}\overline{u^n_*}\right).
$$

Then, there exists a $T > 0$ and $\tau_0 > 0$ such that for $\tau \le \tau_0$ and $t_n \le T$ we have for all $c > 0$ that

$$
\|z(t_n) - z^n\|_r + \|n(t_n) - n^n\|_r \le \tau^2 K_{r,T,M,M_4},
$$

where the constant K_{r,T,M_4} can be chosen independently of c.

Proof. Fix $r > d/2$.

Stability. In the following we set for $f, g \in H^r$ and

$$
\begin{aligned}
\Phi_\tau(f,g) &:= \mathrm{e}^{i\tau\mathcal{A}_c}f - ic\langle\nabla\rangle_c^{-1}\mathrm{e}^{i\tau\mathcal{A}_c}\mathrm{e}^{-ic^2t_n}I^n_{u_*}(g),\\
\Psi_\tau(f,g) &:= \mathrm{e}^{i\tau\Delta}g + \frac{i}{2}\mathrm{e}^{i\tau\Delta}I^n_{n_*}(f,g)
\end{aligned}
$$

such that, in particular, $u^{n+1}_* = \Phi_\tau(u^n_*, n^n_*)$ and $n^{n+1}_* = \Psi_\tau(u^n_*, n^n_*)$.

Note that for all $t \in \mathbb{R}$ we have that $\|\mathrm{e}^{it\mathcal{A}_c}\|_r = 1$ and $\|c\langle\nabla\rangle_c^{-1}\|_r \le 1$; see (2.10) and (2.11), respectively. Recall that by Definition 2.3 we have that

$$
\Psi_2(\xi) = \frac{\varphi_0(\xi) - \varphi_1(\xi)}{\xi}.
$$

This implies (by looking at the corresponding operators in Fourier space) that the kth Fourier coefficient satisfies

$$\tau\Psi_2\Big(i\tau\big(c\langle\nabla\rangle_c - \frac{1}{2}\Delta\big)\Big)_k = \frac{\varphi_0\left(i\tau\big(c\sqrt{c^2+|k|^2}+\frac{1}{2}|k|^2\big)\right) - \varphi_1\left(i\tau\big(c\sqrt{c^2+|k|^2}+\frac{1}{2}|k|^2\big)\right)}{i\big(c\sqrt{c^2+|k|^2}+\frac{1}{2}|k|^2\big)}.$$

Note that for all $k \in \mathbb{Z}^d$ we have

$$\frac{|k|^2}{c\sqrt{c^2+|k|^2}+\frac{1}{2}|k|^2} \le 2.$$

As $|\varphi_0(i\xi)| \le 1$ for all $\xi \in \mathbb{R}$ and φ_1 satisfies (3.8) this allows us to derive the essential stability bound

$$\tau^2 \left\|\Psi_2\Big(i\tau\big(c\langle\nabla\rangle_c - \frac{1}{2}\Delta\big)\Big)\Delta f\right\|_r \le 4\tau\|f\|_r.$$

Similarly, we obtain due to the observations for the kth Fourier coefficients

$$\left(\frac{-\Delta}{c^2-\Delta}\right)_k = \frac{|k|^2}{c^2+|k|^2} \le 1 \quad \text{and} \quad \left(\frac{\mathcal{A}_c}{c^2-\Delta}\right)_k = \frac{c\sqrt{c^2+|k|^2}-c^2}{c^2+|k|^2} \le 1$$

that

$$\tau^2\left\|\Psi_2\big(\pm i\tau(c^2-\Delta)\big)Op\, f\right\|_r \le K\tau\|f\|_r \quad \text{for} \quad Op = \Delta \quad \text{or} \quad Op = \mathcal{A}_c$$

for some constant $K > 0$ independent of c.

Furthermore, by the definition of φ_2 together with the relation $\varphi_2(\xi) = \frac{\varphi_1(\xi)-1}{\xi}$ (see Definition 2.3) we readily obtain that

$$\tau^2\left|\varphi_2(i\ell c^2\tau)\right| \le \tau \min\left\{\frac{2}{|\ell|c^2}, \tau\right\} \quad \text{for all } \ell \in \mathbb{Z}, \ell \neq 0$$

such that

$$\tau^2\left\|\varphi_2(i\ell c^2\tau)f\right\|_r \le \tau\min\left\{\frac{2}{|\ell|c^2},\tau\right\}\|f\|_r \quad \text{for all } \ell \in \mathbb{Z}, \ell \neq 0.$$

Together with the bilinear estimate (1.2) we thus obtain that

$$\|\Phi_\tau(f_1,g_1) - \Phi_\tau(f_2,g_2)\|_r \le \|f_1-f_2\|_r + \tau K\left(\|g_1\|_r, \|g_2\|_r\right)\|g_1-g_2\|_r,$$

where the constant K depends on $\|g_1\|_r$ and $\|g_2\|_r$, but can be chosen independently of c. A similar bound holds for Ψ.

Global error. Thanks to the local error bound given in (4.2) and (4.10), respectively, the assertion then follows by induction, respectively, a *Lady Windermere's fan* argument; see, for example [18, 26]. ∎

5. Asymptotic consistency. In this section we show that our novel class of exponential-type integrators of first and second order is indeed asymptotically consistent: in the non-relativistic limit ($c \to \infty$) the schemes converge to the numerical solution of the corresponding non-relativistic limit system (i.e., $c \to \infty$ in (1.1)). The latter can be derived with, for instance, Modulated Fourier Expansion techniques; see [9, 11, 16, 17] and references therein. In particular, the leading order term z_∞ in the asymptotic expansion of z reads

$$z_\infty(t,x) = \frac{1}{2}\left(\mathrm{e}^{ic^2 t} u_\infty(t,x) + \mathrm{e}^{-ic^2 t}\overline{u_\infty}(t,x)\right), \tag{5.1}$$

where (u_∞, n_∞) solve the decoupled free Schrödinger limit system

$$\begin{aligned} \partial_t u_\infty(t,x) &= -\tfrac{i}{2}\Delta u_\infty(t,x), \qquad & u_\infty(0) &= z(0) - ic^{-2}\partial_t z(0),\\ \partial_t n_\infty(t,x) &= i\Delta n_\infty(t,x), & n_\infty(0) &= n_0. \end{aligned} \tag{5.2}$$

For sufficiently smooth solutions (and well prepared initial data) asymptotic convergence of order two holds, i.e.,

$$z(t,x) - z_\infty(t,x) = \mathcal{O}(c^{-2}) \quad \text{and} \quad n(t,x) - n_\infty(t,x) = \mathcal{O}(c^{-2}).$$

The crucial difference between the limit Schrödinger system (5.2) and the full nonlinear Klein-Gordon-Schrödinger system (1.1) lies in the fact that the limit system is linear. Therefore, it can be solved exactly in time. Nevertheless, in order to compare its solution with our asymptotic consistent schemes, we formulate it as a numerical integration scheme as follows

$$\begin{aligned} u_\infty^{n+1} &= \mathrm{e}^{-\frac{i}{2}\tau\Delta} u_\infty^n, \quad & u_\infty^0 &= z(0) - ic^{-2}\partial_t z(0),\\ n_\infty^{n+1} &= \mathrm{e}^{i\tau\Delta} n_\infty^n, & n_\infty^0 &= n_0 \end{aligned} \tag{5.3}$$

with solutions

$$z_\infty^{n+1} = \frac{1}{2}\left(\mathrm{e}^{ic^2 t_{n+1}} u_\infty^{n+1} + \mathrm{e}^{-ic^2 t_{n+1}}\overline{u_\infty^{n+1}}\right) \quad \text{and} \quad n_\infty^{n+1}. \tag{5.4}$$

Asymptotic convergence of the first-order method. We now motivate the asymptotic convergence of our first-order asymptotic consistent exponential-type integrator (3.7) towards the limit solution (5.3). Thereby we use (2.6) and (2.10) which yields

$$\begin{aligned} \left\| \left(\mathcal{A}_c - \tfrac{1}{2}\Delta\right) u_*(t)\right\|_r + \left\| \left(c\langle\nabla\rangle_c^{-1} - 1\right) u_*(t)\right\|_r &\le c^{-2} k \,\|u_*(t)\|_{r+4},\\ \left\|\tau\varphi_1(\pm i\tau c^2)\right\|_r &\le \frac{2}{c^2} \end{aligned} \tag{5.5}$$

for some constant $k > 0$ independent of c. Applying (5.5) to (3.7) formally yields

$$u_*^{n+1} = \mathrm{e}^{-\frac{i}{2}\tau\Delta} u_*^n + \mathcal{O}(c^{-2}), \quad n_*^{n+1} = \mathrm{e}^{i\tau\Delta} n_*^n + \mathcal{O}(c^{-2}).$$

Hence, for sufficiently smooth solutions the exponential-type integration scheme (3.7) converges asymptotically to the solution of the corresponding free Schrödinger limit system (5.3).

Asymptotic convergence of the second-order method. Techniques similar to (5.5) allow us to show that formally

$$I_{u_*}^n = \mathcal{O}(c^{-2}) \quad \text{and} \quad I_{n_*}^n = \mathcal{O}(c^{-2}).$$

Applying the observation (5.5) in (4.14) implies that also our second-order exponential-type integration scheme (4.14) formally converges asymptotically with order c^{-2} to the solution of the corresponding free Schrödinger limit system (5.3).

The asymptotic consistent behaviour of our novel class of integrators is illustrated with numerical experiments in the following section.

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6. Numerical experiments. In this section we numerically illustrate the convergence properties of our first- and second-order integrators. For the space-discretization we use a standard Fourier pseudospectral method. In our numerical experiments we choose the highest Fourier mode $M = 256$ in our discretization (which corresponds to $\Delta x \approx 0.0245$) and integrate the initial values

$$z(0,x) = \frac{1}{2}\frac{\cos(x)^2}{2-\cos(x)}, \quad \partial_t z(0,x) = \frac{1}{2}c^2\frac{\sin(x)\cos(x)}{2-\cos(x)}, \quad n(0,x) = 1 + i\frac{\sin(x)}{2-\cos(x)}$$

up to $T = 1$.

Time convergence plots: In Figure 6.1 and Figure 6.2 we plot the time-step size versus the discrete H^1-error of the first-order (3.7), respectively, second-order scheme (4.14), in double logarithmic scale.

Asymptotic consistency plots: Figure 6.3 shows the asymptotic convergence of the first- and second-order integrators towards their limit approximation (5.3) with rate c^{-2} (measured in H^1). In the simulation we use a time step size $\tau \approx 10^{-7}$.

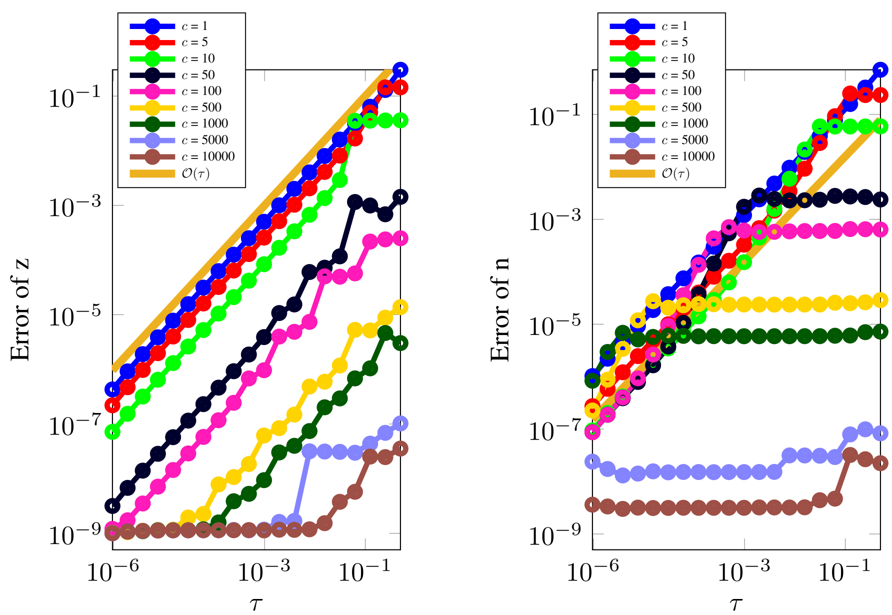

FIG. 6.1. *Order plots of the first-order asymptotic consistent method* (3.7) *for different values of* $c = 1, 5, 10, 50, 100, 500, 1000, 5000, 10000$.

In the numerical experiments we observe that the error does not increase for increasing values of c which is the aim of our novel developed methods. In particular, it is indicated that the error introduced by our schemes reduces with increasing c. This might be due to the fact that our numerical schemes asymptotically converge with order $\mathcal{O}(c^{-2})$ (see also Figure 6.3) to the decoupled free Schrödinger limit system (5.2) which is indeed solved exactly in time. Our numerical observations, in particular, suggest a global error behavior of type $\min\{\tau, c^{-2}\}$ and $\min\{\tau^2, c^{-2}\}$ for the first-order (3.7) and second-order (4.14) exponential-type integrator, respectively.

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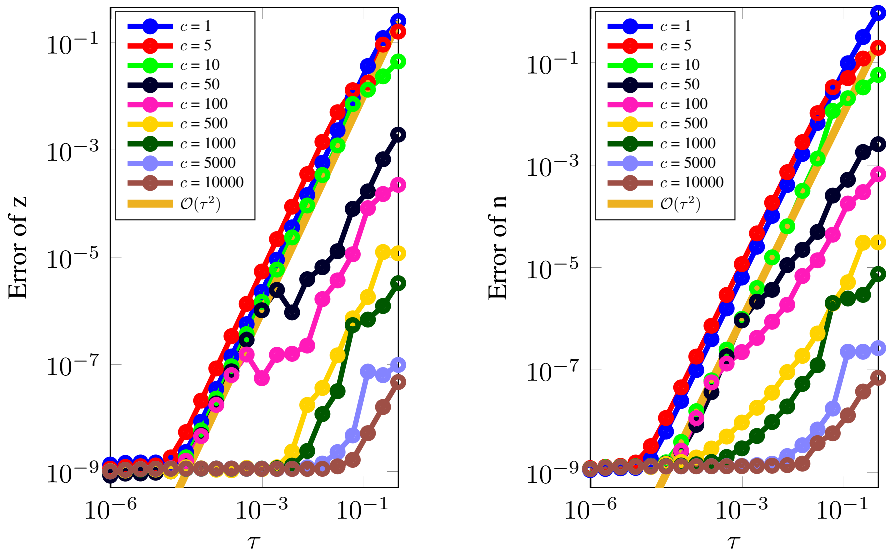

FIG. 6.2. *Order plots of the second-order asymptotic consistent method* (4.14) *for different values of* $c = 1, 5, 10, 50, 100, 500, 1000, 5000, 10000$*.*

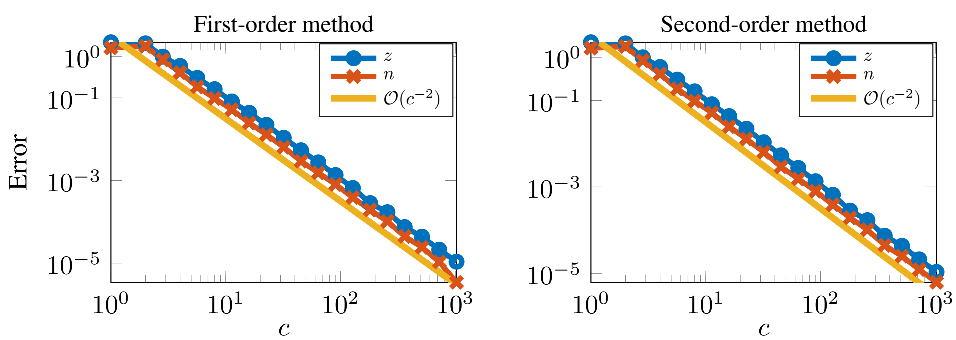

FIG. 6.3. *Asymptotic consistency plot. The derived integrators converge asymptotically with rate* c^{-2} *to the limit solutions* (5.3)*.*

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