Numerical Integrators for Maxwell–Klein–Gordon and Maxwell–Dirac Systems in Highly to Slowly Oscillatory Regimes

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Referent: JProf. Dr. Katharina Schratz
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ABSTRACT

Maxwell–Klein–Gordon (MKG) and Maxwell–Dirac (MD) systems physically describe the mutual interaction of moving relativistic particles with their self-generated electromagnetic field. Solving these systems in the nonrelativistic limit regime, i.e. when the speed of light c formally tends to infinity, is numerically very delicate as the solution becomes highly oscillatory in time. In order to resolve the oscillations, standard time integrations schemes require severe restrictions on the time step $\tau \sim c^{-2}$ depending on the small parameter c^{-2} which leads to high computational costs. Within this thesis we propose and analyse two types of numerical integrators to efficiently integrate the MKG and MD systems in highly oscillatory nonrelativistic limit regimes to slowly oscillatory relativistic regimes.

The idea for the first type relies on asymptotically expanding the exact solution in the small parameter c^{-1}. This results in non-oscillatory Schrödinger–Poisson (SP) limit systems which can be solved efficiently by using classical splitting schemes. We will see that standard Strang splitting schemes, applied to the latter SP systems with step size τ, allow error bounds of order $\mathcal{O}\left(\tau^2 + c^{-N}\right)$ for $N \in \mathbb{N}$ without any time step restriction. Thus, in the nonrelativistic limit regime $c \to \infty$ these methods are very efficient and allow an accurate approximation to the exact solution.

The second type of numerical integrator is based on "twisted variables" which have been originally introduced for the Klein–Gordon equation in [18]. In the case of MKG and MD systems however, due to the strong nonlinear coupling between the components of the solution, the construction and analysis is much more involved. We thereby exploit the main advantage of the "twisted variables" that they have bounded derivatives with respect to $c \to \infty$. Together with a splitting approach, this allows us to construct an exponential-type splitting method which is first order accurate in time uniformly in c. Due to error bounds of order $\mathcal{O}(\tau)$ independent of c without any restriction on the time step τ, these schemes are efficient in highly to slowly oscillatory regimes.

Keywords:

Klein–Gordon, Dirac, Maxwell, Wave Equations, Schrödinger, Highly Oscillatory, Nonrelativistic Limit, Numerical Time Integration, Uniformly Accurate, Splitting

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CHAPTER ONE

MOTIVATION AND INTRODUCTION

In the last decades, scientists paid a lot of attention to (highly oscillatory) Klein–Gordon and Dirac equations. The latter type of wave equations arose when physicists researched on a relativistic description of high-energy particles. "High-energy" thereby means that the particles move at high velocity v_p close to the speed of light c_0. This effort resulted in the Klein–Gordon equation which was set up by *Schrödinger* (1926), *Gordon* (1926) and *Klein* (1927) ([78, Chapter 5.1]). However, the observation of negative probability densities in the Klein–Gordon equation, led to its rejection at first. Later, a reinterpretation of the Klein–Gordon equation by *Pauli* and *Weisskopf* in (1939) served as a basis for the description of spin-0 particles such as π-mesons ([78, Chapter 5.1]). To also incorporate the spin-1/2 of electrons into a relativistic equation, *Paul Dirac* invented his famous equation in 1929 ([87, Chapter 1.1]).

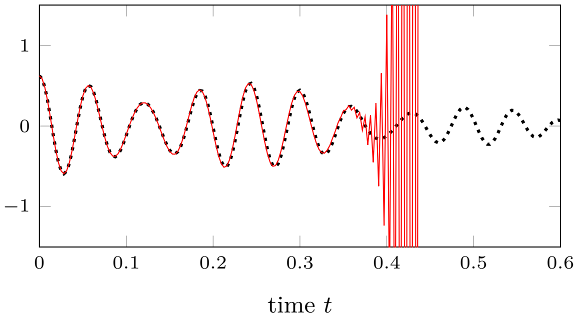
It is well known that moving charged particles create their own time dependent electromagnetic field ([74, Chapter 4.5.5]). The Maxwell–Klein–Gordon (MKG) and Maxwell–Dirac (MD) systems incorporate the interaction of the particle with this self-generated electromagnetic field by coupling the Klein–Gordon and Dirac equation to Maxwell's potentials ([42, 59]).

For the time evolution of solutions to Klein–Gordon and Dirac type equations, the ratio of the constant speed of light c_0 and the velocity v_p of the moving particle, i.e. $c := c_0/v_p$, plays an important role. Scientists distinguish between

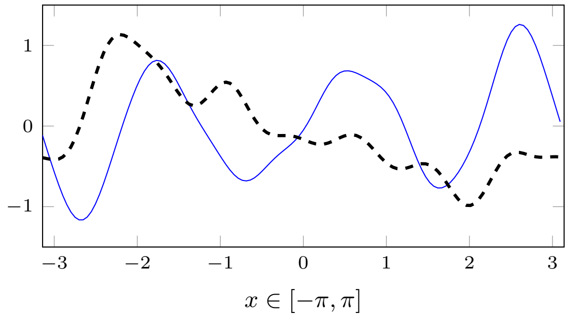
- the relativistic regime $v_p \approx c_0$, where the ratio $c = c_0/v_p$ is small and
- the nonrelativistic limit regime $v_p \to 0$, where the ratio $c = c_0/v_p \to \infty$ is large.

A large ratio $c = c_0/v_p \gg 1$ thereby leads to high oscillations in the solution. In this highly oscillatory regime, the numerical time integration of Klein–Gordon and Dirac type equation becomes very challenging since the high oscillations in the solution impose severe time step restrictions to standard integration schemes. On the one hand, applying classical explicit schemes such as adapted Störmer-Verlet schemes (Expt-FD,[9]) to a spatial discretization of the Klein–Gordon equation leads to strong CFL[①] conditions

[①] **C**ourant–**F**riedrichs–**L**ewy, see for instance [32, 39]



(a) (Classical explit schemes, $c = 10$, step size $\tau \approx 3.1 \cdot 10^{-3}$): Classical explicit schemes (red solid line) suffer from severe stability issues, even for small step sizes. The black dotted line represents the exact solution in the space point $x = 0$.



(b) (Exponential Gautschi-type schemes, $c = 17.8$, step size $\tau = 10^{-2}$): Exponential Gautschi-type schemes (blue solid line) suffer from severe time step restrictions due to numerical errors depending on the large parameter c. The black dashed line represents the exact solution at time $t = 1$.

Figure 1.1: Numerical solution to nonlinear Klein–Gordon equations. Classical explicit schemes (left) require strong CFL conditions $\tau \lesssim c^{-2}$ to ensure stability. Standard exponential integration schemes (right) suffer from large error bounds of order $\mathcal{O}\left(\tau^2 c^4\right)$.

on the maximal time step size in order to guarantee numerical stability. In [9, Theorem 1], the authors proved that for numerical stability issues the allowed time step size τ must be smaller than $1/c^2$ (cf. Fig. 1.1a). Additionally, due to numerical error bounds depending on $\tau^2 c^6$ ([9, Theorem 2]), we retain numerical convergence only for very small time step sizes. On the other hand, choosing (semi-)implicit integration schemes ((S)Impt(-EC)-FD, [9]) helps to overcome a CFL condition but still leaves large numerical errors depending on $\tau^2 c^6$ ([9, Theorem 4,5]).

Another class of numerical integration schemes for wave-type problems are exponential Gautschi-type methods ([9, 50–52, 54]). Despite being unconditionally stable ([9, 50, 51]) and thus not suffering from a CFL condition, their application to nonlinear Klein–Gordon equations also leads to large numerical errors depending on $\tau^2 c^4$ (cf. [9, 50–52, 54]). In order to retain a good accuracy of the corresponding numerical approximation for large values of $c \gg 1$, we therefore need to choose very small time steps τ, which causes high computational costs (cf. Fig. 1.1b).

But not only the numerical time integration of Klein–Gordon equations is challenging. We encounter similar difficulties for the (Maxwell–)Dirac equations in the highly oscillatory regime $c \gg 1$. The analysis of several explicit Leapfrog-type (LFFD,[16]) and (semi-)implicit (SIFD1,SIFD2,CNFD,[16]) time integration schemes for the Dirac equation led to strong CFL conditions for the explicit LFFD scheme and to large numerical error bounds for all mentioned schemes. Again, due to these bounds, only very small time step sizes smaller than $1/c^3$ allow numerical convergence of these schemes. The authors proved that also a symmetric exponential wave integrator (sEWI-FP,[16]) suffers from a c-dependent CFL condition. Among the methods proposed and analysed in the latter paper the unconditionally stable time-splitting Fourier pseudo-spectral method (TSFP,[16]) performed best, but still requires severe time step restrictions due to error bounds depending on $\tau^2 c^4$ ([16, Lemma 4.1 and subsequent paragraph],[15, Theorem 4.3]). A similar numerical result is given in the paper [10], in which the authors construct a numerical scheme for solving the Maxwell–Dirac system in Lorenz gauge[②] , combining the TSFP method with an exponential Gautschi-type integration scheme.

An idea to overcome these severe time step restrictions relies on the asymptotic behaviour of (Maxwell–) Klein–Gordon and (Maxwell–)Dirac systems in the nonrelativistic limit regime. Exploiting analytical convergence results of the latter highly oscillatory systems towards non-oscillatory nonlinear Schrödinger and Schrödinger–Poisson equations in the limiting case $c \to \infty$ ([19, 21, 22, 69, 70]), the authors Faou and Schratz [45] and the authors Krämer and Schratz of [63] recently constructed and analysed efficient numerical time integration schemes for highly oscillatory Klein–Gordon and Maxwell–Klein–Gordon system in the regime $c \gg 1$. A similar scheme has been proposed in [57] for the Maxwell–Dirac system, where a rigorous numerical convergence analysis of this scheme is missing. Given a time step size τ, the latter schemes allow numerical error bounds of order $\mathcal{O}\left(\tau^2 + c^{-2}\right)$. This means they are efficient only in the regime, where $c \gg 1$ is very large and where $c^{-2} \lesssim \tau^2$.

In the recent years, mathematicians also paid a lot of attention to the construction of uniformly accurate time integration schemes for nonlinear Klein–Gordon ([13, 18, 28]), Klein–Gordon–Zakharov ([11]), Klein–Gordon–Schrödinger ([12]) and Dirac ([14]) equations. These schemes are based on a multiscale expansion of the solution and are efficient also in the intermediate slowly oscillatory regimes where c is too small for the application of schemes which exploit the solution's asymptotic limit behaviour. It turns out that these multiscale time integrator Fourier/sine psudeo-spectral schemes (MTI-FP/MTI-SP,[12–14]) allow two error bounds of order τ^2+c^{-2} and τ^2c^2 which are independent of each other and imply a (non-optimal) uniform in c first order in time convergence. The non-optimality of these MTI-FP/SP schemes gave rise to the construction of uniformly accurate time integration schemes for the Klein–Gordon equation in [18] based on "twisted variables" which allow an arbitrary high convergence order in time uniformly in c. The authors Baumstark et al. of [18] have been the first to use the "twisted variables" for the construction of uniformly accurate schemes.

The literature mentioned above mainly uses Fourier techniques (cf. [44, 66]) or finite difference methods ([39]) for the discretization in space of the (Maxwell–)Klein–Gordon and (Maxwell–)Dirac systems. A finite element discretization in space of the Maxwell–Klein–Gordon system in temporal gauge is discussed in [29].

Aims and Results

In this thesis we construct efficient numerical time integration schemes for Maxwell–Klein–Gordon and Maxwell–Dirac systems in highly to slowly oscillatory regimes using Fourier techniques for the spatial discretization ([44, 66]).

Thereby, in the highly oscillatory nonrelativistic limit regime $c \gg 1$, we extend the ideas of the authors Krämer and Schratz in [63] to construct efficient limit time integration schemes of arbitrary high order in c^{-1} for Maxwell–Klein–Gordon and Maxwell–Dirac systems. The analysis of these schemes then provides rigorous numerical convergence bounds of order $\mathcal{O}\left(\tau^2 + c^{-N}\right)$. In particular, it also provides a rigorous proof of the heuristically investigated error bounds $\mathcal{O}\left(\tau^2 + c^{-1}\right)$ given in [57], which correspond to the numerical asymptotic limit approximation to the solution of the MD system.

[②]Named after Ludvig Lorenz (1829 – 1891).

We furthermore construct and analyse numerical time integration schemes for the Maxwell–Klein–Gordon and Maxwell–Dirac system which are uniformly accurate in $c \geq 1$ and which allow an efficient integration of the latter systems in the slowly oscillatory as well as in the highly oscillatory regimes. These schemes are based on the "twisted variables" which recently have been successfully used in [18] to construct uniformly accurate schemes for Klein–Gordon systems.

Our numerical experiments finally provide an overview of the efficiency in the different regimes of our asymptotic and uniformly accurate schemes in comparison to standard exponential Gautschi-type and time-splitting integrators from [9, 10, 15, 16, 51]. It turns out that already for small values of c our schemes outperform the standard schemes.

Outline of the Thesis

The following provides a rough overview of the outline of this thesis.

In the current Chapter 1, we motivate this thesis and collect our aims and results. We introduce some notation and provide a short introduction to Klein–Gordon and Dirac equations from the mathematical point of view.

In Chapter 2, we introduce the Maxwell–Klein–Gordon and Maxwell–Dirac systems and shed a light on the connection between the underlying Klein–Gordon/Dirac and Maxwell's equations. A reformulation of the latter systems as first order systems in time provides the basis for the construction of our time integration schemes.

In Chapter 3, we shall derive and analyse the asymptotic Schrödinger–Poisson limit systems for both model problems for $c \gg 1$ using the technique of a modulated Fourier expansion in the solution. Based on the asymptotic behaviour of the solution, we furthermore construct efficient Strang splitting time integration schemes.

In Chapter 4, we exploit the technique of "twisted variables" to construct uniformly accurate time integration schemes for the Maxwell–Klein–Gordon and Maxwell–Dirac systems and give rigorous numerical error bounds. Thereby, we rewrite the highly oscillatory first order systems from Chapter 2 as first order systems in time which admit bounded derivatives in the solution with respect to $c \to \infty$. In the application of this scheme to the Maxwell–Dirac system, we discuss a special choice of initial data for this system.

In Chapter 5, numerical experiments shall underline the theoretical convergence bounds of our schemes. Besides the efficiency of our schemes in different regimes we also discuss numerical energy and norm conservation properties.

Chapter 6 provides an overview of open questions which might be topic of interesting future research.

In Appendix A, we collect auxiliary tools which shall help the reader understanding selected topics of this thesis.

1.1 Notational Remarks

Based on [6, 45, 70, 85], the following notation shall be used throughout the thesis. For more details and further references, see also Appendix A. The sets $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{R}$, $\mathbb{C}$ denote the usual set of natural numbers, integers, real and complex numbers, respectively. Moreover, let $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. Let $i = \sqrt{-1}$ denote the imaginary unit. We denote the complex conjugate of $z = a + ib \in \mathbb{C}$ with $a, b \in \mathbb{R}$ by $\overline{z} := a - ib$. The real and imaginary parts of z are denoted by $a = \mathrm{Re}\,(z)$ and $b = \mathrm{Im}\,(z)$ respectively.

For $m \in \mathbb{N}$ and $Z, W \in \mathbb{C}^m$ we define the dot product by

$$Z \cdot W := Z^\top W = (Z_1, \dots, Z_m) \cdot \begin{pmatrix} W_1 \\ \vdots \\ W_m \end{pmatrix} = Z_1 W_1 + \dots + Z_m W_m.$$

In particular, $|Z|^2 := Z \cdot \overline{Z}$ denotes the square of the Eucledian norm of $Z \in \mathbb{C}^m$, where $\overline{Z} = (\overline{Z_1}, \dots, \overline{Z_m})^\top$.

Let $d \in \mathbb{N}$ denote the spatial dimension and let $\mathbb{T}^d := (\mathbb{R}/2\pi\mathbb{Z})^d$ be the d-dimensional torus. We may refer to $\mathbb{T}$ as the 2π-periodically continued set $[-\pi, \pi]$ and simply write $\mathbb{T} = [-\pi, \pi]$. Furthermore let $T > 0$. Within this thesis, $t \in [0, T]$ denotes the time variable and $x = (x^1, \dots, x^d)^\top \in \mathbb{T}^d$ denotes the spatial variable. Considering a function $u : [0, T] \times \mathbb{T}^d \to \mathbb{C}^m$, with $m \in \mathbb{N}$, depending on time and space, we may leave out the spatial argument for sake of simplicity. More precisely, we may sometimes write $u(t) : \mathbb{T}^d \to \mathbb{C}^m$ for $t \in [0, T]$.

Let $k = (k^1, \dots, k^d)^\top \in \mathbb{Z}^d$ and let $\widehat{u}_k$ denote the k-th Fourier coefficient corresponding to the Fourier series expansion of u

$$u(t, x) = \sum_{k \in \mathbb{Z}^d} \widehat{u}_k(t) e^{ik \cdot x}, \qquad \text{where for } k \in \mathbb{Z}^d \qquad \widehat{u}_k = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} u(x) e^{-ik \cdot x} dx.$$

For a sufficiently smooth function $f : [0, T] \times \mathbb{T}^d \to \mathbb{C}$ and vector field $G : [0, T] \times \mathbb{T}^d \to \mathbb{C}^d$, we denote by

$$\partial_t f(t, x) = \frac{\partial}{\partial t} f(t, x) \qquad \text{the derivative of } f \text{ with respect to } t, \text{ and by}$$

$$\partial_j f(t, x) = \partial_{x^j} f(t, x) = \frac{\partial}{\partial x^j} f(t, x) \qquad \text{the derivative of } f \text{ with respect to } x^j,$$

for $j = 1, \dots, d$, where the spatial derivatives ∂_j have to be understood in the weak Sobolev sense.

We furthermore use the notation for $m \in \mathbb{N}$ and $j = 1, \dots, d$

$$\partial_t^2 f(t, x) = \partial_{tt} f(t, x) = \frac{\partial^2}{\partial t^2} f(t, x) \qquad \text{and} \qquad \partial_j^m f(t, x) = \frac{\partial^m}{\partial x_j^m} f(t, x).$$

We may leave out the arguments (t, x) and denote by

$$\nabla f = \mathrm{grad}\, f := (\partial_1 f, \dots, \partial_d f)^\top \qquad \text{the spatial gradient of } f,$$

$$\nabla \cdot G = \mathrm{div}\, G := \sum_{j=1}^d \partial_j G_j \qquad \text{the spatial divergence of } G,$$

$$\Delta f = \nabla^2 f = \mathrm{div}\,\mathrm{grad}\, f := \sum_{j=1}^d \partial_j^2 f \qquad \text{the spatial Laplacian of } f,$$

where $G_j(t,x)$ denote the components of G for $j=1,\dots,d$. In particular, we define the spatial Laplacian of a vector field G via

$$\Delta G = (\Delta G_1, \dots, \Delta G_d)^\top.$$

In the special case of $d=3$, we furthermore denote the curl of G by

$$\nabla \times G = \operatorname{curl} G \coloneqq (\partial_2 G_3 - \partial_3 G_2,\ \partial_3 G_1 - \partial_1 G_3,\ \partial_1 G_2 - \partial_2 G_1)^\top. \tag{1.1}$$

By a simple calculation we can verify the following zero-identities for the differential operators above, i.e.

$$\operatorname{div}\operatorname{curl} G = \nabla \cdot (\nabla \times G) = 0 \qquad \text{and} \qquad \operatorname{curl}\operatorname{grad} f = \nabla \times (\nabla f) = 0. \tag{1.2}$$

In particular, if $G(t,x) = G(t,\tilde{x})$ with $x = (x^1, x^2, x^3)^\top \in \mathbb{T}^3$ only depends on the 2D spatial variable $\tilde{x} = (x^1, x^2)^\top$ and if we have a smooth vector field H of type

$$H(t,x) = H(t,\tilde{x}) = (H_1(t,\tilde{x}),\ H_2(t,\tilde{x}),\ H_3(t,\tilde{x}))^\top \coloneqq (G_1(t,\tilde{x}),\ G_2(t,\tilde{x}),\ 0)^\top,$$

then (1.1) admits

$$\nabla \times H = \operatorname{curl} H = (0, 0, \partial_1 G_2 - \partial_2 G_1)^\top. \tag{1.3}$$

Thus, identifying the vector field $H : \mathbb{T}^3 \to \mathbb{T}^3$ as a vector field $\tilde{H} : \mathbb{T}^2 \to \mathbb{T}^2$ with $\tilde{H} = (H_1, H_2)$ allows us to define also a curl operator for $d=2$, i.e.

$$\operatorname{curl} \tilde{H} = \partial_1 H_2 - \partial_2 H_1 \quad \text{defines a curl on } \mathbb{T}^2.$$

For $r \in \mathbb{N}_0$, we denote by $H^r(\mathbb{T}^d)$ the usual Sobolev spaces on the torus $\mathbb{T}^d$ with the norm

$$\|u\|_r^2 \coloneqq \sum_{k \in \mathbb{Z}^d} \langle k \rangle_1^{2r} |\widehat{u}_k|^2, \quad \text{where} \quad \langle k \rangle_1 \coloneqq \sqrt{|k|^2 + 1}.$$

We may sometimes also write $\langle k \rangle$ instead of $\langle k \rangle_1$. In particular, $H^0(\mathbb{T}^d)$ coincides with the usual $L^2(\mathbb{T}^d)$ space. We furthermore use the notation

$$\dot{H}^r(\mathbb{T}^d) = \left\{ u \in H^r(\mathbb{T}^d) \,|\, \int_{\mathbb{T}^d} u(x) dx = 0 \right\}$$

for the homogeneous Sobolev spaces of vanishing mean, equipped with the norm

$$\begin{cases} \|u\|_{r,0} \coloneqq \|\langle \nabla \rangle_0 u\|_{r-1} & \text{for } 1 \le r \in \mathbb{N} \\ \|u\|_{0,0} \coloneqq \sum_{k \in \mathbb{Z}^d \setminus \{0\}} |\widehat{u}_k|^2 & \text{for } r = 0 \end{cases}$$

In the following, we may use the notation $H^r = H^r(\mathbb{T}^d)$ and $\dot{H}^r = \dot{H}^r(\mathbb{T}^d)$ instead. Throughout this thesis, the operator $\langle \nabla \rangle_c \coloneqq \sqrt{-\Delta + c^2}$ for $c \in \mathbb{R}$ plays a major role. We define it via its Fourier representation

$$\langle \nabla \rangle_c u(t,x) \coloneqq \sum_{k \in \mathbb{Z}^d} \langle k \rangle_c\ \widehat{u}_k e^{ik \cdot x}, \quad \text{where} \quad \langle k \rangle_c \coloneqq \sqrt{|k|^2 + c^2}.$$

In the literature, the symbol $\langle k \rangle_c$ is often called *Japanese bracket*, see for instance [85, Preface].

For fixed $c \in \mathbb{R}$, the operator $\langle \nabla \rangle_c$ maps the Sobolev space H^{r+1} into H^r (see Lemma A.5). Within this thesis, we in particular focus on the limit case $c \to \infty$ for which $\|\langle \nabla \rangle_c u\|_r$ is unbounded for all $r \geq 0$. However, Lemma A.11 shows that for all $w \in H^{r+2}$

$$\left\|(c\langle \nabla \rangle_c - c^2)w\right\|_r \leq K \|w\|_{r+2} \quad \text{uniformly for all } c \in \mathbb{R}$$

with a constant K independent of $c \in \mathbb{R}$. For the interested reader, we collect additional details and properties of Sobolev spaces in Appendix A.1.

In our analysis, we often use the Landau notation $\mathcal{O}(\cdot)$ to express the dependence of an upper bound on a specific parameter. Let X, Y be vector spaces equipped with norms $\|\cdot\|_X : X \to [0,\infty)$ and $\|\cdot\|_Y : Y \to [0,\infty)$. Furthermore, let $f : \mathbb{R} \to X$ and $g : \mathbb{R} \to Y$. For $\omega \in \mathbb{R}$, we say that $f(\omega) = \mathcal{O}(g(\omega))$ (is large $\mathcal{O}$ of $g(\omega)$) in the sense of the X norm if

$$\|f(\omega)\|_X \leq K \|g(\omega)\|_Y$$

with a constant K independent of ω. Note that within this thesis the constants K are generic constants. A dependence on specific properties will be given explicitly.

Next, we give a short introduction to basic aspects of Klein–Gordon and Dirac equations.

1.2 Some Aspects of Klein–Gordon Equations

Based on [69, 75, 78, 80, 87], we provide a brief introduction to Klein–Gordon equations in this section and point out the ideas for the construction of efficient integration schemes given in [18, 45, 63] for (Maxwell–)Klein–Gordon equations.

Brief Physical Background of Klein–Gordon Equations

This section is based on [40, 75, 78, 87]. The interested reader finds further details in the latter books and refrences therein. For physicists, the *correspondence principle* is an important concept in order to set up relativistic wave equations for moving particles of velocity v_p and rest mass m_0. The idea behind this concept relies on replacing classical physical quantities like the energy $\mathcal{E}$ and the momentum $\boldsymbol{p}$ with operators, i.e.

- the energy $\mathcal{E}$ is identified with $i\hbar\partial_t$ and
- the momentum $\boldsymbol{p}$ is identified with $-i\hbar\nabla$,

where $\hbar$ is *Planck's* constant.

The classical energy-momentum relation $\mathcal{E} = \boldsymbol{p}^2/(2m_0)$ in non-relativistic regimes of small velocity v_p results in the time-dependent Schrödinger equation

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m_0}\nabla^2\psi.$$

Since the *principles of special relativity* require that the order of time and space derivatives must be equal in a relativistic equation ([75]), the latter Schrödinger equation is not suitable for a relativistic description of particles. Due to the asymmetry of time and space derivatives, it is not invariant under Lorentz transforms[③] — and thus the principles of special relativity are violated — which means that it changes its structure in the transition from one inertial system into another one. This invariance gains more and more importance the closer the velocity v_p approaches the speed of light c_0. In the relativistic regime where $v_p \approx c_0$, we thus need to consider a different relation in order to describe the motion of our particle which reads

$$c_0^{-2}\mathcal{E}^2 - \boldsymbol{p}^2 = m_0^2 c_0^2. \tag{1.4}$$

Replacing $\mathcal{E}$ and $\boldsymbol{p}$ by their respective operators we thus obtain the Klein–Gordon equation for a scalar field ψ

$$-\hbar^2 \partial_t^2 \psi = \left(-\hbar^2 c_0^2 \nabla^2 + m_0^2 c_0^4\right)\psi \tag{1.5}$$

which has been proposed by *Schrödinger* (1926), *Gordon* (1926) and *Klein* (1927) for the relativistic description of charged particles, see for instance [78, Chapter 5.1]. Later in 1939, *Pauli* and *Weisskopf* reinterpreted it as an equation for the relativistic description of spin-less particles such as for instance π-mesons, after it had been rejected as an equation for the description of electrons which have spin-1/2.

Next, we transform (1.5) into a dimensionless equation by applying a simple variable transform. Based on [77], we assign our particle moving at given velocity v_p the following

$$\textit{de Broglie} \text{ wave length} \qquad \lambda_s = \frac{\hbar}{m_0 v_p} \tag{1.6a}$$

and follow the idea from [12] to plug the transform $(t,x) \mapsto (t/t_s, x/\lambda_s)$ into (1.5) which determines the reference time t_s. A short calculation shows that the transform

$$(t,x) \mapsto (\tilde{t},\tilde{x}) = \left(\frac{t}{t_s}, \frac{x}{\lambda_s}\right) \quad \text{with} \quad t_s = \frac{m_0 \lambda_s^2}{\hbar} \qquad \text{and} \qquad c := \frac{c_0}{v_p} = c_0 \frac{\lambda_s m_0}{\hbar} \tag{1.6b}$$

provides the following Klein–Gordon equation in dimensionless units $\tilde{t}$ and $\tilde{x}$

$$-c^{-2}\partial_{\tilde{t}}^2 \psi(\tilde{t},\tilde{x}) = (-\nabla_{\tilde{x}}^2 + c^2)\psi(\tilde{t},\tilde{x}), \tag{1.7}$$

where $\nabla_{\tilde{x}}$ denotes the gradient with respect to the variable $\tilde{x}$. In the following, we omit the $\tilde{}$ in the dimensionless Klein–Gordon equation and proceed in the next subsection.

The Dimensionless Nonlinear Klein–Gordon Equation

This section is based on [10, 45, 69, 80, 87]. Adding a nonlinear self-interaction of the particle to (1.7) we obtain the following dimensionless nonlinear Klein–Gordon equation

$$\partial_t^2 \psi = -c^2(-\Delta + c^2)\psi + c^2 f[\psi], \quad \psi(0,x) = \psi_I(x), \quad \partial_t \psi(0,x) = c\,\langle\nabla\rangle_c\,\psi_I'(x) \tag{1.8}$$

for given initial data ψ_I, ψ_I' with a sufficiently smooth nonlinearity $f : \mathbb{C} \to \mathbb{C}$ satisfying

$$f[e^{i\omega}\psi] = e^{i\omega} f[\psi] \qquad \text{for} \qquad \omega \in \mathbb{R} \qquad \text{and} \qquad \overline{f[\psi]} = f[\overline{\psi}]. \tag{1.9}$$

Within this thesis, we consider (1.8) equipped with periodic boundary conditions on the torus $\mathbb{T}^d$ and on a finite time interval $[0,T]$.

Note that in the nonrelativistic limit regime $v_p \to 0$ we have $c = c_0/v_p \to \infty$. This means that the velocity of the particle is very large compared to the constant speed of light. A transition from the relativistic to the nonrelativistic regime can thus be seen as letting the speed of light formally tend to infinity.

[③] Named after Hendrik Antoon Lorentz (1853 – 1928).

Diagonalisation of the Klein–Gordon Equation

Based on [10, 45, 56, 69, 80, 87], our aim is now to transform the latter Klein–Gordon equation into an equivalent first order system in time which has a diagonal structure in its linear part. Later in this thesis, we may apply a similar transformation to the Maxwell–Klein–Gordon system. Based on the resulting first order system, we then construct efficient time integration schemes for the MKG system.

In the following, we replace $c^2 \langle\nabla\rangle_c^2 := c^2(-\Delta + c^2)$ in (1.8) and carry out a classical reformulation of the latter second order in time differential equation as first order system in time first. We collect the solution ψ and its first time derivative $\partial_t\psi$ in a vector $(\psi, \partial_t\psi)^\top$. The application of another time derivate then leads to

$$\partial_t \begin{pmatrix} \psi \\ \partial_t\psi \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & \mathcal{I} \\ -c^2 \langle\nabla\rangle_c^2 & 0 \end{pmatrix}}_{=:\mathfrak{A}} \begin{pmatrix} \psi \\ \partial_t\psi \end{pmatrix} + \begin{pmatrix} 0 \\ c^2 f[\psi] \end{pmatrix}.$$

Note that in Fourier space, the operator $\mathfrak{A}$ has the symbol

$$\widehat{\mathfrak{A}}(k) = \begin{pmatrix} 0 & 1 \\ -c^2 \langle k\rangle_c^2 & 0 \end{pmatrix} \qquad \text{for } k \in \mathbb{Z}^d$$

where $\langle k\rangle_c = \sqrt{|k|^2 + c^2}$ is the Fourier symbol of $\langle\nabla\rangle_c = \sqrt{-\Delta + c^2}$. A short calculation shows that we diagonalise $\widehat{\mathfrak{A}}(k)$ as (see for instance [80, Section 3.1] and [56, Section 7.2])

$$\widehat{\mathfrak{A}}(k) = \widehat{S}(k) \cdot \widehat{D}(k) \cdot \widehat{S}(k)^{-1} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ +ic\langle k\rangle_c & -ic\langle k\rangle_c \end{pmatrix} \begin{pmatrix} +ic\langle k\rangle_c & 0 \\ 0 & -ic\langle k\rangle_c \end{pmatrix} \begin{pmatrix} 1 & -ic^{-1}\langle k\rangle_c^{-1} \\ 1 & +ic^{-1}\langle k\rangle_c^{-1} \end{pmatrix}.$$

Identifying $\langle k\rangle_c$ with $\langle\nabla\rangle_c$, this diagonalisation finally motivates the transformation $(\psi, \partial_t\psi)^\top \to (u, v)^\top$, given by

$$\begin{aligned} u &= \psi - i\langle\nabla\rangle_c^{-1} \frac{\partial_t}{c}\psi, \\ \overline{v} &= \psi + i\langle\nabla\rangle_c^{-1} \frac{\partial_t}{c}\psi, \end{aligned} \tag{1.10}$$

which implies the identities

$$\psi = \frac{1}{2}(u + \overline{v}), \qquad \partial_t\psi = ic\langle\nabla\rangle_c \frac{1}{2}(u - \overline{v}).$$

Differentiating u and v with respect to time immediately yields the relations

$$\begin{cases} i\partial_t u = -c\langle\nabla\rangle_c u + c^{-1}\langle\nabla\rangle_c^{-1}\left(c^2 f[\frac{1}{2}(u+\overline{v})]\right) \\ i\partial_t v = -c\langle\nabla\rangle_c v + c^{-1}\langle\nabla\rangle_c^{-1}\left(c^2 \overline{f[\frac{1}{2}(u+\overline{v})]}\right). \end{cases}$$

Applying the transform (1.10) to our initial data and gathering the nonlinear terms in the system above in

$$F[w] = \left(f[\tfrac{1}{2}(u+\overline{v})] \,,\, \overline{f[\tfrac{1}{2}(u+\overline{v})]} \right)^\top$$

we obtain the following first order system in time for variables $w = (u, v)^\top$

$$i\partial_t w = -c\langle\nabla\rangle_c w + c\langle\nabla\rangle_c^{-1} F[w], \quad w(0) = \begin{pmatrix} \psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'} \end{pmatrix}.$$

The reader may compare the latter with the Maxwell–Klein–Gordon first order system (2.33).

Efficient Time Integration of Klein–Gordon Equations

Note that for $c \to \infty$, the latter system is highly oscillatory in time. In [45] the authors exploit that in this regime, the ansatz of writing

$$w(t) = e^{ic^2 t} w_0(t) + \mathcal{O}\left(c^{-1}\right) \tag{1.11}$$

together with the observation (see Lemma A.11)

$$\left\| (c \langle \nabla \rangle_c - (c^2 - \frac{1}{2}\Delta) w_0 \right\|_r \leq K \|w_0\|_{r+4} \qquad \text{for } w_0 \in H^{r+4}$$

leads to a first order system for slowly varying variables $w_0 = (u_0, v_0)^\top$ of type (cf. the limit system (3.108) for MKG)

$$i\partial_t w_0 = \frac{1}{2}\Delta w_0 + F_0[w_0], \quad w_0(0) = \begin{pmatrix} \psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'} \end{pmatrix}.$$

Thereby, the nonlinearity F_0 satisfies $F[w(t)] - e^{ic^2 t} F_0[w_0(t)] = \mathcal{O}\left(c^{-1}\right)$ in the sense of the H^r norm. The latter non-oscillatory Schrödinger system is then solved by an exponential Strang splitting scheme which yields error bounds of order $\mathcal{O}\left(\tau^2 + c^{-1}\right)$. In Chapter 3 we follow the same strategy and construct similar time integration schemes in the nonrelativistic limit regime for the Maxwell–Klein–Gordon and Maxwell–Dirac systems.

From the error bound $\mathcal{O}\left(\tau^2 + c^{-1}\right)$, it becomes clear that this scheme is only efficient in the regime, where $c \gg 1$ is very large. In order to construct an efficient scheme also in the slowly oscillatory regimes where c is of moderate size, the authors of [18] follow the idea of "twisted variables" making the ansatz (cf. (1.11))

$$w(t) = e^{ic^2 t} w_*(t).$$

Using that $(c \langle \nabla \rangle_c - c^2) w_0 = \mathcal{O}\left(\Delta w_0\right)$ (see Lemma A.11), this again leads to a first order system in time for slowly varying variables $w_* = (u_*, v_*)^\top$ (cf. the corresponding system (4.15) for MKG)

$$i\partial_t w_*(t) = (c \langle \nabla \rangle_c - c^2) w_*(t) + e^{-ic^2 t} c \langle \nabla \rangle_c^{-1} F_*[e^{ic^2 t} w_*(t)], \qquad w_*(0) = w(0).$$

The authors applied a special kind of exponential integrators ([55]) to the latter system which resulted in unifromly accurate time integration schemes satisfying uniform error bounds of order $\mathcal{O}\left(\tau^p\right)$ for p arbitrary large independent of c.

Later, in Chapter 4 we adapt this idea of twisted variables in order to construct efficient uniformly accurate schemes for our Maxwell–Klein–Gordon and Maxwell–Dirac systems.

1.3 Some Aspects of Dirac Equations

In this section, we discuss some aspects of Dirac equations based on [70, 75, 77, 78, 80, 87] and on Dirac's paper [40] from 1928. We start off with a short introduction to the physical background of this famous equation.

Brief Physical Background of Dirac Equations

This section is based on [40, 40, 75, 77, 78, 87]. In particular, the author Thaller provides a well structured derivation of Dirac's equation in [87, Chapter 1.1].

By virtue of the emerging quantum theory and special relativity ([40]), an equation to correctly describe the behaviour of electrons should satisfy the *principles of special relativity*, which requires symmetry of time and space derivatives, as well as the *principles of quantum mechanics*, which requires that it is a first order in time (linear) differential equation with a self-adjoint right hand side (see [75, 87]). Because the Klein–Gordon equation (1.5) is a second order differential equation, it had to be abandoned for this purpose.

After its rejection, *Paul Dirac* worked on an equation which conforms with both principles. So he started off with the square-root of the Klein–Gordon energy-momentum relation from (1.4)

$$\mathcal{E} = \sqrt{c_0^2 \boldsymbol{p}^2 + m_0^2 c_0^4} \tag{1.12}$$

and linearized it, such that for the momentum $\boldsymbol{p} = (p_1, p_2, p_3)^\top$ and yet unknown $m \times m$ matrices $\boldsymbol{\alpha}_1, \boldsymbol{\alpha}_2, \boldsymbol{\alpha}_3$ and $\boldsymbol{\beta}$ with yet unknown dimension $m \in \mathbb{N}$

$$\mathcal{E} = c_0 \boldsymbol{\alpha} \cdot \boldsymbol{p} + \boldsymbol{\beta} m_0 c_0^2, \qquad \text{with} \qquad \boldsymbol{\alpha} \cdot \boldsymbol{p} := \sum_{j=1}^{3} \boldsymbol{\alpha}_j p_j \tag{1.13}$$

is satisfied. But before he could apply the latter equation to the corresponding physical problem, he still had to determine the matrices in it. Closely following his arguments, we derive the latter matrices in the next section.

He demanded that the squares of the energy terms (1.4) and (1.13) are equal, which means that

$$\mathcal{E}^2 = \left(c_0 \boldsymbol{\alpha} \cdot \boldsymbol{p} + \boldsymbol{\beta} m_0 c_0^2\right)^2 \overset{!}{=} c_0^2 \boldsymbol{p}^2 + m_0^2 c_0^4, \qquad \text{where} \qquad \boldsymbol{\alpha} \cdot \boldsymbol{p} := \sum_{j=1}^{3} \boldsymbol{\alpha}_j p_j. \tag{1.14}$$

From this relation, we will in particular see, that his calculations provided $m = 4$ and the matrices given explicitly in (1.21)More details will be given later on.

Similar to the previous section, he replaced in the energy-momentum relation (1.13) the energy $\mathcal{E}$ with the operator $i\hbar\partial_t$ and the components of the momentum with the operators $-i\hbar\partial_j$ with $\hbar$ being *Planck's* constant. This led to his famous *Dirac* equation (1929)

$$i\hbar\partial_t \psi = -i\hbar c_0 \sum_{j=1}^{3} \boldsymbol{\alpha}_j \partial_j \psi + m_0 c_0^2 \boldsymbol{\beta} \psi \qquad \text{with solution } \psi(t,x) \in \mathbb{C}^4 \tag{1.15}$$

in its standard representation was born.

Because the presence of the matrices $\boldsymbol{\alpha}_j, \boldsymbol{\beta}$ for $j = 1, 2, 3$ incorporates the spin-1/2 of electrons into the Dirac equation (see [77, 78]), the four-component solution ψ is often called a *four-spinor*.

From (1.14), we see that *Dirac's* approach followed the idea of basically taking the square-root of the Klein–Gordon energy in order to set up his equation. Therefore, the Dirac equation is sometimes also called the "square-root of the Klein–Gordon equation" (see for instance [75]).

In the literature, one finds Dirac's equation very often also in its covariant form (1.16) which implies its invariance under Lorentz transforms (see [78] and [40]). To obtain this form, we multiply the latter equation by $\boldsymbol{\beta}/c_0$ and exploit the relations (1.18). This leads to ([22, 40, 70, 78, 87])

$$i\hbar\gamma_0\frac{\partial_t}{c_0}\psi = -i\hbar\sum_{j=1}^{3}\gamma_j\partial_j\psi + m_0c_0\psi \qquad \text{with solution } \psi(t,x)\in\mathbb{C}^4, \tag{1.16}$$

where the new set of matrices is given by (see [78, Chapter 5.3.4])

$$\boldsymbol{\gamma}_0 = \boldsymbol{\beta} \qquad \text{and} \qquad \boldsymbol{\gamma}_j = \boldsymbol{\beta}\boldsymbol{\alpha}_j \qquad \text{for } j=1,\dots,3.$$

In commemoration of *Paul Dirac's* important contributions to modern physics his equation has been inscribed to a plate in *Westminster Abbey* in the famous elegant and compact form ([75])

$$i\boldsymbol{\gamma}\cdot\boldsymbol{\partial}\psi = m\psi,$$

where $\boldsymbol{\gamma}\cdot\boldsymbol{\partial}\psi := (\boldsymbol{\gamma}_0 c_0^{-1}\partial_{\tilde{t}} + \boldsymbol{\gamma}_1\partial_1 + \boldsymbol{\gamma}_2\partial_2 + \boldsymbol{\gamma}_3\partial_3)\psi$ in normalized units $(\tilde{t},\tilde{x}) = c_0/\hbar\,(t,x)$. Next, we derive Dirac's matrices $\boldsymbol{\alpha}_1$, $\boldsymbol{\alpha}_2$, $\boldsymbol{\alpha}_3$ and $\boldsymbol{\beta}$.

A Derivation of Dirac's Matrices

Based on [75, 78, 87], and on *Dirac's* paper [40] from 1928, we now determine Dirac's matrices $\boldsymbol{\alpha}_1$, $\boldsymbol{\alpha}_2$, $\boldsymbol{\alpha}_3$ and $\boldsymbol{\beta}$ of dimension $m\times m$, and follow the line of argumentation in [87, Chapter 1.1] which is very close to the one of *Dirac* himself (see [40]).

In order to determine the latter matrices, *Dirac* demanded equality of the square of (1.12) and the square of (1.13) in the sense that

$$\mathcal{E}^2 = \left(c_0\boldsymbol{\alpha}\cdot\boldsymbol{p} + \boldsymbol{\beta}m_0c_0^2\right)^2 \overset{!}{=} c_0^2\boldsymbol{p}^2 + m_0^2c_0^4, \qquad \text{where} \qquad \boldsymbol{\alpha}\cdot\boldsymbol{p} := \sum_{j=1}^{3}\boldsymbol{\alpha}_j p_j \tag{1.17}$$

It turns out that the latter holds for matrices satisfying the following anticommuting relations (see [87, Chapter 1.1])

$$\boldsymbol{\alpha}_j\boldsymbol{\alpha}_k + \boldsymbol{\alpha}_k\boldsymbol{\alpha}_j = 2\delta_{j,k}\mathcal{I}_m, \qquad \boldsymbol{\alpha}_j\boldsymbol{\beta} + \boldsymbol{\beta}\boldsymbol{\alpha}_j = 0_m \qquad \text{and} \qquad \boldsymbol{\beta}^2 = \mathcal{I}_4 \tag{1.18}$$

for $j,k=1,2,3$ where $\mathcal{I}_m$ and 0_m denote the $m\times m$ identity matrix and zero matrix, respectively, and where $\delta_{j,k}$ denotes the Kronecker[④] symbol. Furthermore, because a quantum mechanical interpretation of (1.13) requires that its right hand side leads to a self-adjoint expression (see [87, Chapter 1.1 and 1.2]), we need $\boldsymbol{\alpha}_j$ and β to be Hermitian, i.e. we need that (cf. (1.21) below for $\boldsymbol{\sigma}_j$)

$$\boldsymbol{\alpha}_j = \overline{\boldsymbol{\alpha}_j}^\top \qquad (\text{and also} \quad \boldsymbol{\sigma}_j = \overline{\boldsymbol{\sigma}_j}^\top) \qquad \text{and} \qquad \boldsymbol{\beta} = \overline{\boldsymbol{\beta}}^\top, \qquad \text{for } j=1,2,3. \tag{1.19}$$

It remains to determine the dimension $m\in\mathbb{N}$ of the latter matrices. Therefore, we proceed as follows. Let $\operatorname{tr} A := \sum_{\ell=1}^{m} A_{\ell\ell}$ be the trace of an $m\times m$ matrix A (see for instance [6]). Combining the relations (1.18) with Proposition A.28 on the trace of products of matrices, we find for $j=1,2,3$

$$\operatorname{tr}\boldsymbol{\alpha}_j = \operatorname{tr}\boldsymbol{\beta}(\boldsymbol{\beta}\boldsymbol{\alpha}_j) = -\operatorname{tr}\boldsymbol{\beta}(\boldsymbol{\alpha}_j\boldsymbol{\beta}) \overset{\text{Prop. A.28}}{=} -\operatorname{tr}\boldsymbol{\alpha}_j\boldsymbol{\beta}^2 = -\operatorname{tr}\boldsymbol{\alpha}_j \quad \text{and thus} \quad \operatorname{tr}\boldsymbol{\alpha}_j = 0. \tag{1.20}$$

[④] $\delta_{j,k}=1$ for $j=k$ and $\delta_{j,k}=0$ for $j\neq k$

Furthermore, the relations (1.18) and (1.19) imply $\mathcal{I}_m = \boldsymbol{\alpha}_j^2 = \boldsymbol{\alpha}_j \overline{\boldsymbol{\alpha}_j}^\top$, which means that $\boldsymbol{\alpha}_j$ are unitary matrices. By virtue of the latter identity, the matrices $\boldsymbol{\alpha}_j$ can only have the real eigenvalues ± 1, which we denote by $\lambda_{j,1}, \dots, \lambda_{j,m}$ for $j = 1, \dots, m$. From (1.20) and Proposition A.28 we thus deduce that m must be an even number.

In the case $m = 2$ we find at most three linearly independent anticommuting matrices satisfying the first condition in (1.18). A possible choice are the Pauli matrices

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.21a}$$

which together with the identity matrix $\mathcal{I}_2$ form a basis of Hermitian 2×2 matrices. Thus, we cannot find an additional linearly independent Hermitian 2×2 matrix $\boldsymbol{\beta}$ satisfying the second relation in (1.18). However, in the case $m = 4$ choosing

$$\boldsymbol{\alpha}_j = \begin{pmatrix} 0_2 & \boldsymbol{\sigma}_j \\ \boldsymbol{\sigma}_j & 0_2 \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} \mathcal{I}_2 & 0_2 \\ 0_2 & -\mathcal{I}_2 \end{pmatrix}, \qquad \text{for } j = 1, \dots, 3 \tag{1.21b}$$

we obtain a set of matrices which satisfy the relation (1.18). Furthermore, we observe that

$$\mathcal{I}_4 - \boldsymbol{\beta} = \begin{pmatrix} 0_2 & 0_2 \\ 0_2 & 2\,\mathcal{I}_2 \end{pmatrix} \qquad \text{and} \qquad \mathcal{I}_4 + \boldsymbol{\beta} = \begin{pmatrix} 2\,\mathcal{I}_2 & 0_2 \\ 0_2 & 0_2 \end{pmatrix} \tag{1.22a}$$

and similarly

$$\mathcal{I}_2 - \boldsymbol{\sigma}_3 = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix} \qquad \text{and} \qquad \mathcal{I}_2 + \boldsymbol{\sigma}_3 = \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}. \tag{1.22b}$$

In the next subsection we discuss properties of a dimensionless version of Dirac's equation (1.15).

The Dimensionless Dirac Equation

This section is based on [10, 15, 16, 70, 77, 87]. Applying the variable transform (1.6) of the previous section to Dirac's equation (1.15) allows us to rewrite it as the following dimensionless system, depending on the dimensionless parameter $c = c_0/v_p$, (see also [10, Section 2.1])

$$i\frac{\partial_t}{c}\psi = -i\sum_{j=1}^{d} \boldsymbol{\alpha}_j \partial_j \psi + c\boldsymbol{\beta}\psi, \quad \psi(0,x) = \psi_I(x) \tag{1.23}$$

with given initial data ψ_I and with the four-spinor solution $\psi(t,x) \in \mathbb{C}^4$. Note that we consider the latter system on the torus $\mathbb{T}^d$ and on a finite time interval $[0,T]$. The Pauli matrices $\boldsymbol{\sigma}_j$ and the Dirac matrices $\boldsymbol{\alpha}_j, \boldsymbol{\beta}$ for $j = 1, 2, 3$ are given explicitly in (1.21).

Recall, that in the previous subsection we have seen the following relations of the latter matrices ([78, 87])

$$\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k + \boldsymbol{\sigma}_k\boldsymbol{\sigma}_j = 2\delta_{j,k}\mathcal{I}_2, \quad \boldsymbol{\alpha}_j\boldsymbol{\alpha}_k + \boldsymbol{\alpha}_k\boldsymbol{\alpha}_j = 2\delta_{j,k}\mathcal{I}_4, \quad \boldsymbol{\alpha}_j\boldsymbol{\beta} + \boldsymbol{\beta}\boldsymbol{\alpha}_j = 0, \quad \boldsymbol{\beta}^2 = \mathcal{I}_4. \tag{1.24a}$$

For $d = 1, 2, 3$ and $\xi \in \mathbb{C}^d$, this immediately provides the following identities

$$\sum_{j=1}^{d}\sum_{k=1}^{d} \boldsymbol{\sigma}_j\boldsymbol{\sigma}_k \xi_j\xi_k = \frac{1}{2}\sum_{j=1}^{d}\sum_{k=1}^{d} (\boldsymbol{\sigma}_j\boldsymbol{\sigma}_k + \boldsymbol{\sigma}_k\boldsymbol{\sigma}_j)\xi_j\xi_k = \sum_{j=1}^{d} \boldsymbol{\sigma}_j^2 \xi_j^2 = |\xi|^2\,\mathcal{I}_2 \tag{1.24b}$$

and analogously

$$\sum_{j=1}^{d}\sum_{k=1}^{d} \boldsymbol{\alpha}_j \boldsymbol{\alpha}_k \xi_j \xi_k = |\xi|^2 \mathcal{I}_4. \tag{1.24c}$$

In particular, applying the operator $-i\partial_t/c$ to the Dirac equation (1.23) we see that the latter identities allow a reformulation of (1.23) as a Klein–Gordon equation (cf. (1.8))

$$\partial_t^2 \psi_\ell = -c^2(-\Delta + c^2)\psi_\ell, \quad \ell = 1,2,3,4,$$

where

$$\psi(0) = \psi_I \qquad \text{and} \qquad \partial_t \psi(0) = c \langle \nabla \rangle_c \psi_I' \quad \text{with} \quad \psi_I' := -i\boldsymbol{\beta} c \langle \nabla \rangle_c^{-1} \psi_I - \langle \nabla \rangle_c^{-1} \sum_{j=1}^{d} \boldsymbol{\alpha}_j \partial_j \psi_I.$$

This means that each component of the four-spinor solution

$$\psi(t,x) = (\psi_1(t,x), \psi_2(t,x), \psi_3(t,x), \psi_4(t,x))^\top \in \mathbb{C}^4$$

satisfies a Klein-Gordon equation. Note that this procedure can be seen as taking the square of the Dirac equation which correlates to the energy equality (1.17).

The main difference between the original KG equation and this reformulation of Dirac's equation is the incorporation of the coupling between the components $\psi_\ell, \ell = 1,2,3,4$ through the initial data ψ_I'.

Next, we discuss the ideas for the construction of efficient integration schemes.

Efficient Time Integration of Dirac Equations

We have seen that we can reformulate the Dirac equation (1.23) as a Klein–Gordon equation (1.25), where the coupling between the components of the solution is incorporated via the corresponding initial data.

By virtue of this reformulation, we now apply similar techniques as described in Section 1.2, in order to efficiently compute numerical solutions to the Dirac equation in the different regimes. Note that later in this thesis, we are interested in numerically solving a Maxwell–Dirac system (2.36), which involves also nonlinear terms coupling the Dirac four-spinor solution to Maxwell's potentials .

More precisely in the following we assume the presence of nonlinear terms $f : \mathbb{C}^4 \to \mathbb{C}^4$ and $g^{\boldsymbol{\alpha}} : \mathbb{C}^4 \to \mathbb{C}^4$ in (1.25) such that (cf. the MKG reformulation (2.38) of the MD system)

$$\begin{cases} \partial_t^2 \psi_\ell = -c^2(-\Delta + c^2)\psi_\ell + c^2 \Big(f_\ell[\psi_\ell] + g^{\boldsymbol{\alpha}}[\psi] \Big), \quad \ell = 1,2,3,4 \\ \psi(0) = \psi_I, \qquad \partial_t \psi(0) = c \langle \nabla \rangle_c \psi_I', \end{cases} \tag{1.26}$$

where f and $g^{\boldsymbol{\alpha}}$ satisfy assumptions of type (1.9). The particular choice of $g^{\boldsymbol{\alpha}}$ to involve terms $\boldsymbol{\alpha}_j \psi$ for $j = 1,2,3$ realizes an additional coupling of the components of the four-spinor ψ to each other.

More precisely, a diagonalisation of the Klein–Gordon reformulation (1.26) as in the previous section yields a diagonal first order system in time of type (cf. the corresponding system (2.41) for MD)

$$\begin{cases} i\partial_t w = -c \langle \nabla \rangle_c w + c \langle \nabla \rangle_c^{-1} \Big(F[w] + G^{\boldsymbol{\alpha}}[w] \Big), \\ w(0) = w_I := \begin{pmatrix} (\mathcal{I}_4 - c \langle \nabla \rangle_c^{-1} \boldsymbol{\beta})\psi_I + i \langle \nabla \rangle_c^{-1} \sum_{j=1}^{d} \boldsymbol{\alpha}_j \partial_j \psi_I \\ (\mathcal{I}_4 + c \langle \nabla \rangle_c^{-1} \boldsymbol{\beta})\overline{\psi_I} + i \langle \nabla \rangle_c^{-1} \sum_{j=1}^{d} \overline{\boldsymbol{\alpha}_j} \partial_j \overline{\psi_I} \end{pmatrix} \end{cases} \tag{1.27}$$

with solution $w = (u, v)^\top$. Note that later in Chapter 3, we see that in the Maxwell–Dirac first order system in time (2.41) the influence of the respective nonlinearity of type $G^{\boldsymbol{\alpha}}$ vanishes as $c \to \infty$. Therefore we assume in the following that $G^{\boldsymbol{\alpha}} = \mathcal{O}\left(c^{-1}\right)$ in the sense of the H^r norm. The particular structure of the initial data is induced by the choice of ψ_I' in (1.25). Note that we recover the solution ψ through the identity

$$\psi = \frac{1}{2}(u + \overline{v}).$$

We now follow the ideas from [45, 63] as in Section 1.2 for an asymptotic limit approximation of type

$$w(t) = e^{ic^2 t} w_0(t) + \mathcal{O}\left(c^{-1}\right)$$

in the nonrelativistic limit regime $c \to \infty$. Note that because of the assumption that $G^{\boldsymbol{\alpha}}$ vanishes as $c \to \infty$, also the coupling between the components of ψ vanishes. Thus, we obtain the following Schrödinger system for the non-oscillatory function $w_0 = (u_0, v_0)^\top$ with the same arguments as before (cf. the limit system (3.108) for the MD system)

$$i\partial_t w_0 = \frac{1}{2}\Delta w_0 + F_0[w_0], \qquad w_0(0) = w_{I,0} = (u_{I,0}, v_{I,0})^\top, \tag{1.28}$$

where w_I is given in (1.29) below and where F_0 satisfies

$$F[w] - e^{ic^2 t} F_0[w_0] = \mathcal{O}\left(c^{-1}\right) \qquad \text{in the sense of the } H^r \text{ norm.}$$

Due to Lemma A.11 we furthermore observe that $\langle\nabla\rangle_c^{-1} \psi = c^{-1}\psi + \mathcal{O}\left(c^{-1}\right)$ and consequently find

$$(\mathcal{I}_4 \mp c \langle\nabla\rangle_c^{-1} \boldsymbol{\beta})\psi = (\mathcal{I}_4 \mp \boldsymbol{\beta})\psi + \mathcal{O}\left(c^{-1}\right).$$

Employing the latter into the initial data w_I in (1.27) and combining it with the identities for $(\mathcal{I}_4 \mp \boldsymbol{\beta})$ in (1.22), we obtain initial data $w_{I,0}$ of a very particular structure

$$w_{I,0} = (u_{I,0}, v_{I,0})^\top \qquad \text{where} \qquad u_I = \begin{pmatrix} 0 \\ 2\psi_I^- \end{pmatrix} \quad \text{and} \quad v_{I,0} = \begin{pmatrix} 2\overline{\psi_I^+} \\ 0 \end{pmatrix}. \tag{1.29}$$

Note that here we decomposed the initial data

$$\psi_I = (\psi_I^+, \psi_I^-)^\top \qquad \text{such that} \qquad \psi_I^\pm(x) \in \mathbb{C}^2.$$

Furthermore, exploiting the ideas from [18] and using the "twisted variables"

$$w(t) = e^{ic^2 t} w_*(t)$$

in highly to slowly oscillatory regimes, then yields the following system with slowly varying solution $w_* = (u_*, v_*)^\top$ (cf. (4.15))

$$\begin{cases} i\partial_t w_*(t) = (c\langle\nabla\rangle_c - c^2) w_*(t) + e^{-ic^2 t} c \langle\nabla\rangle_c^{-1} \left(F[e^{ic^2 t} w_*(t)] + G^{\boldsymbol{\alpha}}[e^{ic^2 t} w_*(t)] \right), \\ w_*(0) = w(0). \end{cases} \tag{1.30}$$

Based on the equations (1.28) and (1.30) with slowly varying solution, we proceed as described in Section 1.2, in order to construct efficient approximation schemes in the different regimes.

In Sections 3.5 and 3.6 we carry out the construction and analysis of limit approximation schemes in the regime $c \gg 1$ for Maxwell–Klein–Gordon and Maxwell–Dirac systems. Afterwards, in Sections 4.2 and 4.3 we propose and analyse uniformly accurate time integration schemes for the latter systems based on the “twisted variables” from [18].

In the next chapter we proceed with the derivation of the Maxwell–Klein–Gordon and Maxwell–Dirac systems in the Coulomb gauge.

CHAPTER

TWO

MAXWELL–KLEIN–GORDON AND MAXWELL–DIRAC SYSTEMS

In this chapter we provide an insight into the model problems which shall be considered within this thesis and highlight some of their properties. It is based on [20–22, 70, 71, 79, 80] and also on the paper [63] by Krämer and Schratz. For details on physical topics, we refer to [42, 59, 78].

Firstly, in Section 2.1, we derive the Maxwell–Klein–Gordon (MKG) system (2.20) and reformulate it as a first order system in time (2.33). Afterwards, in Section 2.2, we transfer this reformulation to the Maxwell–Dirac (MD) system (2.36) by bypassing an equivalent MKG reformulation (2.38) and applying the same ansatz as before. This yields again a first order system in time (2.41) similar to the MKG case, but with additional terms.

Both systems physically describe the interaction of charged particles with their self-generated electromagnetic fields via a coupling of the Klein–Gordon equation in the MKG case, and of the Dirac equation in the MD case, to Maxwell's potentials ([70, 78, 87]).

2.1 The Maxwell–Klein–Gordon System

In this section, based on [21, 60, 62, 70, 71, 76, 79] and references therein, we derive the Maxwell–Klein–Gordon (MKG) system in Coulomb gauge. For details on physical topics we refer to [42, 58, 59, 78]. The MKG system in Coulomb gauge is a system consisting of a Klein–Gordon equation for a complex function $\psi(t,x) \in \mathbb{C}$ coupled to an electromagnetic field expressed by real electromagnetic potentials $(\phi(t,x), \boldsymbol{\mathcal{A}}(t,x))^\top \in \mathbb{R}^{1+d}$ satisfying the

$$\text{Coulomb gauge condition} \qquad \operatorname{div} \boldsymbol{\mathcal{A}} = 0.$$

From the physical point of view, the MKG system incorporates the influence of a self-generated electromagnetic field described by potentials $(\phi, \boldsymbol{\mathcal{A}})^\top$ corresponding to a moving charged particle into the

Klein–Gordon equation. In Coulomb gauge, it reads

$$\begin{cases} \frac{1}{c^2}\partial_{tt}\psi + \big(-\Delta + c^2\big)\psi = \frac{1}{c^2}\Big(\phi^2\psi - 2i\phi\partial_t\psi - i(\partial_t\phi)\psi\Big) - \frac{|\boldsymbol{\mathcal{A}}|^2}{c^2}\psi - 2i\frac{\boldsymbol{\mathcal{A}}}{c}\cdot\nabla\psi, \\ \partial_{tt}\boldsymbol{\mathcal{A}} - c^2\Delta\boldsymbol{\mathcal{A}} = c\mathcal{P}_{\mathrm{df}}\left[\boldsymbol{J}[\psi,\boldsymbol{\mathcal{A}}]\right], \qquad \boldsymbol{J}[\psi,\boldsymbol{\mathcal{A}}] := \operatorname{Re}\big(i\psi\overline{\nabla\psi}\big) - \frac{\boldsymbol{\mathcal{A}}}{c}|\psi|^2 \\ -\Delta\phi = \rho[\psi,\phi], \qquad \rho[\psi,\phi] := -\frac{1}{c^2}\Big(\operatorname{Re}\big(i\psi\overline{\partial_t\psi}\big) + \phi|\psi|^2\Big) \\ \big(\psi(0,x), \partial_t^{[\phi(0,x)]}\psi(0,x)\big) = \big(\psi_I(x), \langle\nabla\rangle_c\,\psi_I'(x)\big) \\ \big(\boldsymbol{\mathcal{A}}(0), \partial_t\boldsymbol{\mathcal{A}}(0)\big) = \big(A_I(x), cA_I'(x)\big), \quad \operatorname{div} A_I = 0 = \operatorname{div} A_I', \\ \int_{\mathbb{T}^d}\phi(t,x)dx = 0, \qquad \operatorname{div}\boldsymbol{\mathcal{A}} = 0. \end{cases} \tag{2.1}$$

For practical implementation issues, we in particular focus on periodic boundary conditions on the torus $\mathbb{T}^d$ and consider a finite time interval $t \in [0,T]$. In the above system, we define the minimal coupling operator $\partial_t^{[\phi]} := c^{-1}(\partial_t + i\phi)$ (see also Definition A.23) and the orthogonal projection operator onto divergence-free vector fields $\mathcal{P}_{\mathrm{df}}[\boldsymbol{J}] = \boldsymbol{J}^{\mathrm{df}}$ with $\operatorname{div}\boldsymbol{J}^{\mathrm{df}} = 0$ (see Appendix A.4). Moreover, the assumption

$$\int_{\mathbb{T}^d}\phi(t,x)dx = 0$$

is a consequence of Remark 2.3. Because we can assume the latter without loss of generality (see Remark 2.3), we may omit this detail in the following for sake of simplicity.

Assuming that the initial data satisfy

$$\psi_I, \psi_I' \in H^r(\mathbb{T}^d) \qquad \text{and} \qquad A_I \in \mathcal{P}_{\mathrm{df}}H^r(\mathbb{T}^d), \quad A_I' \in \mathcal{P}_{\mathrm{df}}H^{r-1}(\mathbb{T}^d)$$

for $r > d/2$, we then look for solutions (see [21, 62, 70, 71, 79] and also the local well-posedness result in Proposition 2.4)

$$\psi(t) \in H^r(\mathbb{T}^d), \quad \phi(t) \in \dot{H}^{r+1}(\mathbb{T}^d) \quad \text{and} \quad \boldsymbol{\mathcal{A}}(t) \in \dot{H}^r(\mathbb{T}^d) \qquad \text{for all times } t \in [0,T].$$

The spaces $H^r(\mathbb{T}^d)$ and $\dot{H}^r(\mathbb{T}^d)$ are given in Definitions A.1 and A.3. Moreover, due to the definition of $\mathcal{P}_{\mathrm{df}} : H^r \to \dot{H}^r$ in Definition A.13, we naturally define

$$\mathcal{P}_{\mathrm{df}}H^r(\mathbb{T}^d) = \{A \in \dot{H}^r(\mathbb{T}^d) \quad \text{with} \quad \operatorname{div} A = 0\}, \quad \text{see Definition A.13.}$$

In Section 2.1.4, we apply to (2.1) a diagonalisation similar as in Section 1.2 and obtain the first order system in time

$$\begin{cases} i\partial_t w = -c\langle\nabla\rangle_c w + F[w,\phi,\mathfrak{a}], & w(0) = w_I = \begin{pmatrix}\psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'}\end{pmatrix}, \\ -\Delta\phi = \rho[w], \qquad \int_{\mathbb{T}^d}\phi(t,x)dx = 0 & \\ i\partial_t\mathfrak{a} = -c\langle\nabla\rangle_0\,\mathfrak{a} + \langle\nabla\rangle_0^{-1}\boldsymbol{J}^P[w,\mathfrak{a}], & \mathfrak{a}(0) = \mathfrak{a}_I = A_I - i\langle\nabla\rangle_0^{-1}A_I'. \end{cases}$$

with solutions $w = (u,v)^\top$ and $\mathfrak{a}$ satisfying

$$\psi = \frac{1}{2}(u + \overline{v}), \qquad \boldsymbol{\mathcal{A}} = \frac{1}{2}(\mathfrak{a} + \overline{\mathfrak{a}}).$$

The operator $\langle\nabla\rangle_c := \sqrt{-\Delta + c^2}$ is defined via its Fourier representation in Definition A.2.

Due to the following Remark 2.1, the operator $\langle\nabla\rangle_0^{-1}$ is well-defined on the spaces $\dot{H}^r(\mathbb{T}^d)$.

Remark 2.1. *Because for all $A \in \dot{H}^r(\mathbb{T}^d)$ we have that $\widehat{A}_0 = 0$ (see Definition A.3), we retain that the operator $\langle \nabla \rangle_0^{-1} : \dot{H}^r \to \dot{H}^r$ is well-defined on the spaces $\dot{H}^r(\mathbb{T}^d)$ spaces. In particular, due to the definition of $\mathcal{P}_{\mathrm{df}}$ in Appendix A.4, we have that $\mathcal{P}_{\mathrm{df}}[J] \in \dot{H}^r(\mathbb{T}^d)$ for all $J \in H^r(\mathbb{T}^d)$.*

We start off with some introductory information on Maxwell's potentials and gauge formalism. The reader who is already familiar with this topic may continue reading in Section 2.1.2 below.

2.1.1 Short Excursion on Maxwell's Potentials and Gauge Formalism

Before deriving the MKG system in details we discuss the electromagnetic potentials ϕ and $\boldsymbol{\mathcal{A}}$. We thereby mainly follow [42, 58, 59]. We consider the electromagnetic field $(\boldsymbol{E}, \boldsymbol{B})^\top$, where we denote by $\boldsymbol{E}(t,x) \in \mathbb{R}^3$ the electric and by $\boldsymbol{B}(t,x) \in \mathbb{R}^3$ the magnetic field. It is well-known that electromagnetic fields obey Maxwell's equations (here in dimensionless units, see [59, Appendix 2] for Maxwell's equations in different units)

$$\begin{aligned} \operatorname{div} \boldsymbol{B} &= 0, \qquad \operatorname{curl} \boldsymbol{E} + \frac{1}{c}\partial_t \boldsymbol{B} = 0, \\ \operatorname{div} \boldsymbol{E} &= \rho, \qquad \operatorname{curl} \boldsymbol{B} - \frac{1}{c}\partial_t \boldsymbol{E} = \frac{\boldsymbol{J}}{c}, \end{aligned} \tag{2.2}$$

where $\rho : [0,T] \times \mathbb{T}^d \to \mathbb{R}$ and $\boldsymbol{J} : [0,T] \times \mathbb{T}^d \to \mathbb{R}^d$ denote the dimensionless charge and current density depending on time $t \in [0,T]$ and space $x \in \mathbb{T}^d$. They fulfil the continuity equation

$$\partial_t \rho + \operatorname{div} \boldsymbol{J} = 0. \tag{2.3}$$

Maxwell's equations (2.2) now are the basis for the derivation of the electromagnetic potentials ϕ and $\boldsymbol{\mathcal{A}}$ corresponding to the electromagnetic field $(\boldsymbol{E}, \boldsymbol{B})^\top$.

Derivation of Maxwell's Potentials

Based on [58, 59] we now derive Maxwell's potentials from the equations (2.2). The first of Maxwell's equations, i.e. $\operatorname{div} \boldsymbol{B} = 0$, allows us to write $\boldsymbol{B}$ as the curl of a sufficiently smooth vector potential $\boldsymbol{\mathcal{A}}(t,x) \in \mathbb{R}^3$ such that (cf. (1.2))

$$\boldsymbol{B} = \nabla \times \boldsymbol{\mathcal{A}}. \tag{2.4}$$

Inserting $\boldsymbol{B} = \nabla \times \boldsymbol{\mathcal{A}}$ into the second equation, we find

$$\operatorname{curl} \boldsymbol{E} + \frac{1}{c}\partial_t \boldsymbol{B} = \operatorname{curl}(\boldsymbol{E} + \frac{1}{c}\partial_t \boldsymbol{\mathcal{A}}) = 0.$$

Because $\operatorname{curl}(\nabla f) = 0$ for every sufficiently smooth function $f(x) \in \mathbb{R}$ (see (1.2)), we thus make the ansatz

$$\boldsymbol{E} + \frac{1}{c}\partial_t \boldsymbol{\mathcal{A}} = -\nabla \phi \tag{2.5}$$

for a yet arbitrary scalar potential $\phi(t,x) \in \mathbb{R}$. The third and fourth of Maxwell's equations (2.2), i.e.

$$\operatorname{div} \boldsymbol{E} = \rho \quad \text{and} \quad \operatorname{curl} \boldsymbol{B} - \frac{1}{c}\partial_t \boldsymbol{E} = \frac{\boldsymbol{J}}{c} \quad \text{respectively,}$$

provide the following relation between $\boldsymbol{\mathcal{A}}$ and ϕ. Plugging (2.4) and (2.5) into the latter equations yields

$$\begin{cases} -\Delta \phi = \rho + \frac{1}{c}\partial_t(\operatorname{div} \boldsymbol{\mathcal{A}}), \\ \frac{1}{c^2}\partial_{tt} \boldsymbol{\mathcal{A}} - \Delta \boldsymbol{\mathcal{A}} = \frac{\boldsymbol{J}}{c} - \nabla(\operatorname{div} \boldsymbol{\mathcal{A}} + \frac{1}{c}\partial_t \phi). \end{cases} \tag{2.6}$$

Whenever the potentials ϕ and $\boldsymbol{\mathcal{A}}$ satisfy this set of equations, we refer to them as *Maxwell's potentials.*

The construction of ϕ and $\boldsymbol{\mathcal{A}}$ via (2.4) and (2.5) leaves some gauge freedom, i.e. if ϕ and $\boldsymbol{\mathcal{A}}$ satisfy (2.4) and (2.5) or (2.6) respectively, then also do (see [42, Chapter 3.3], [59, Chapter 6.3])

$$\boldsymbol{\mathcal{A}}' := \boldsymbol{\mathcal{A}} + c\nabla\chi \quad \text{and} \quad \phi' := \phi - \partial_t\chi \quad \text{with a smooth gauge function} \quad \chi(t,x) \in \mathbb{R}.$$

In particular, note that this gauge transform leaves the electric and magnetic field invariant, since by $\mathrm{curl}(\nabla f) = 0$ for any smooth function $f(x) \in \mathbb{R}$ we have (see Proposition A.25)

$$\begin{aligned} \boldsymbol{B} &= \nabla \times \boldsymbol{\mathcal{A}} = \nabla \times \boldsymbol{\mathcal{A}}'. \\ \boldsymbol{E} &= -\nabla\phi - \frac{1}{c}\partial_t\boldsymbol{\mathcal{A}} = -\nabla\phi' - \frac{1}{c}\partial_t\boldsymbol{\mathcal{A}}'. \end{aligned}$$

Usually the gauge function χ is chosen such that the coupled system (2.6) for ϕ and $\boldsymbol{\mathcal{A}}$ decouples. At this point, we name two popular gauges based on [58, 59] amongst which is the *Lorenz gauge*[①] with gauge condition $\frac{\partial_t}{c}\phi + \mathrm{div}\,\boldsymbol{\mathcal{A}} = 0$. Plugging the transformed potentials ϕ' and $\boldsymbol{\mathcal{A}}'$ into this condition leads to a gauge function χ satisfying $\partial_{tt}\chi - c^2\Delta\chi = 0$ and to a system of two wave equations for ϕ and $\boldsymbol{\mathcal{A}}$ which read

$$\begin{cases} \frac{1}{c^2}\partial_{tt}\phi - \Delta\phi = \rho, \\ \frac{1}{c^2}\partial_{tt}\boldsymbol{\mathcal{A}} - \Delta\boldsymbol{\mathcal{A}} = \frac{\boldsymbol{J}}{c}. \end{cases}$$

The second gauge is the *Coulomb gauge*[②] for which we have the condition $\mathrm{div}\,\boldsymbol{\mathcal{A}} = 0$. We give here only a short summary on the properties of the potentials ϕ and $\boldsymbol{\mathcal{A}}$ in this gauge. For the interested reader, more details are given later on and can be found in [58, 59] and references therein. The Coulomb gauge leads to a decoupled system of a Poisson equation for ϕ and a wave equation for $\boldsymbol{\mathcal{A}}$

$$\begin{cases} -\Delta\phi = \rho, \\ \frac{1}{c^2}\partial_{tt}\boldsymbol{\mathcal{A}} - \Delta\boldsymbol{\mathcal{A}} = \frac{1}{c}\mathcal{P}_{\mathrm{df}}[\boldsymbol{J}], \end{cases}$$

where $\mathcal{P}_{\mathrm{df}}[\boldsymbol{J}] = \boldsymbol{J}^{\mathrm{df}}$ with $\mathrm{div}\,\boldsymbol{J}^{\mathrm{df}} = 0$ denotes the orthogonal projection of $\boldsymbol{J}$ onto its divergence-free part $\boldsymbol{J}^{\mathrm{df}}$. The latter can be seen by incorporating the continuity equation (2.3) $\partial_t\rho + \mathrm{div}\,\boldsymbol{J} = 0$ for ρ and $\boldsymbol{J}$. In the following, we focus on the Coulomb gauge $\mathrm{div}\,\boldsymbol{\mathcal{A}} = 0$ and give some more details in the subsequent subsection.

Coulomb Gauge in more Detail

In the Coulomb gauge, i.e. for $\mathrm{div}\,\boldsymbol{\mathcal{A}} \equiv 0$, the coupled set of equations (2.6) for ϕ and $\boldsymbol{\mathcal{A}}$ reduces to

$$\begin{cases} -\Delta\phi = \rho, \\ \frac{1}{c^2}\partial_{tt}\boldsymbol{\mathcal{A}} - \Delta\boldsymbol{\mathcal{A}} = \frac{\boldsymbol{J}}{c} - \nabla\left(\frac{\partial_t}{c}\phi\right). \end{cases} \tag{2.7}$$

Note that the solution ϕ to Poisson's equation $-\Delta\phi = \rho$ describes the Coulomb potential due to the charge density ρ which gives this gauge the name "Coulomb gauge", see also [59, Chapter 6.3].

Our aim is now to show that in the latter system (2.7) the right hand side of the second equation can be identified with an orthogonal projection of $\boldsymbol{J}/c$ onto its divergence-free part and proceed as follows.

[①] Named after Ludvig Lorenz (1829 – 1891).
[②] Named after Charles Augustin de Coulomb (1736 – 1806).

By Helmholtz's theorem in [7, Chapter 1.16] and due to [37, Chapter 0], there exists an orthogonal decomposition of a given vector field $\tilde{\boldsymbol{J}}$ into a divergence-free part $\tilde{\boldsymbol{J}}^{\mathrm{df}}$ and a curl-free part $\tilde{\boldsymbol{J}}^{\mathrm{cf}}$ such that

$$\tilde{\boldsymbol{J}} = \tilde{\boldsymbol{J}}^{\mathrm{df}} + \tilde{\boldsymbol{J}}^{\mathrm{cf}}, \quad \text{where} \quad \operatorname{div} \tilde{\boldsymbol{J}}^{\mathrm{df}} = 0 \quad \text{and} \quad \operatorname{curl} \tilde{\boldsymbol{J}}^{\mathrm{cf}} = 0. \tag{2.8}$$

From the continuity equation (2.3) we deduce

$$\operatorname{div}(\boldsymbol{J} - \nabla \partial_t \phi) = \operatorname{div}(\boldsymbol{J}) - \Delta(\partial_t \phi) = \operatorname{div}(\boldsymbol{J}) + \partial_t \rho \overset{(2.3)}{=} 0. \tag{2.9}$$

On the other hand, the decomposition $\boldsymbol{J} = \boldsymbol{J}^{\mathrm{df}} + \boldsymbol{J}^{\mathrm{cf}}$ allows us to write

$$\operatorname{div}(\boldsymbol{J} - \nabla \partial_t \phi) \overset{(2.8)}{=} \operatorname{div}(\boldsymbol{J}^{\mathrm{cf}} - \nabla \partial_t \phi) \overset{(2.9)}{=} 0.$$

In particular, this means that $(\boldsymbol{J}^{\mathrm{cf}} - \nabla \partial_t \phi)$ is divergence-free. But due to the fact that for $\nabla \partial_t \phi$ being a gradient field also $\operatorname{curl}(\nabla \partial_t \phi) = 0$ holds (see (1.2)), we obtain

$$\operatorname{curl}(\boldsymbol{J}^{\mathrm{cf}} - \nabla \partial_t \phi) = 0.$$

Therefore the term $(\boldsymbol{J}^{\mathrm{cf}} - \nabla \partial_t \phi)$ is also curl-free. By virtue of (2.8), we thus conclude that

$$\boldsymbol{J}^{\mathrm{cf}}(t,x) - \nabla \partial_t \phi(t,x) = \big(\boldsymbol{J}(t,x) - \nabla \partial_t \phi(t,x)\big)^{\mathrm{cf}} = -M(t) \quad \text{for some } M(t) \in \mathbb{R}$$

can not depend on x and thus must be a constant function in space. This implies that

$$\boldsymbol{J} - \nabla \partial_t \phi = \boldsymbol{J}^{\mathrm{df}} - M(t) =: \mathcal{P}_{\mathrm{df}}[\boldsymbol{J}] \tag{2.10a}$$

is the orthogonal projection of $\boldsymbol{J}$ onto its divergence-free part $\boldsymbol{J}^{\mathrm{df}}$ up to a constant function $M(t)$ in space. Let us now give a rough definition of the projection $\mathcal{P}_{\mathrm{df}}[\boldsymbol{J}]$. For more details on the operator $\mathcal{P}_{\mathrm{df}}$ we refer to Appendix A.4 and references therein. Denoting the solution operator to Poisson's equation

$$-\Delta \phi = \rho$$

formally by $\dot{\Delta}^{-1}$ such that $\phi(t,x) = -\dot{\Delta}^{-1}\rho(t,x)$ — a precise definition of $\dot{\Delta}^{-1}$ on the torus $x \in \mathbb{T}^d$ is given in Appendix A.3 — we have that from the continuity equation (2.3) above

$$\mathcal{P}_{\mathrm{df}}[\boldsymbol{J}] = \boldsymbol{J} - \nabla \partial_t \phi = \boldsymbol{J} - \nabla \dot{\Delta}^{-1} \operatorname{div} \boldsymbol{J}, \tag{2.10b}$$

see also [41, Section 2.1] and [85, Exercise A.23].

In particular, if $\boldsymbol{\mathcal{A}}$ does not satisfy the Coulomb gauge condition, i.e. if $\operatorname{div} \boldsymbol{\mathcal{A}}(t,x) \neq 0$ for at least one $(t,x) \in [0,T] \times \mathbb{T}^d$, we choose the gauge function χ such that the gauge transform $\boldsymbol{\mathcal{A}}' = \boldsymbol{\mathcal{A}} + c\nabla\chi$ of $\boldsymbol{\mathcal{A}}$ satisfies $\operatorname{div} \boldsymbol{\mathcal{A}}' = 0$, i.e.

$$0 = \operatorname{div} \boldsymbol{\mathcal{A}}' = \operatorname{div} \boldsymbol{\mathcal{A}} + c\Delta\chi.$$

In this case, the function χ satisfies the Poisson equation

$$-\Delta\chi = \frac{1}{c} \operatorname{div} \boldsymbol{\mathcal{A}}.$$

Then, similar to (2.10b), we formally denote by $\chi = -\frac{1}{c}\Delta^{-1} \operatorname{div} \boldsymbol{\mathcal{A}}$ the solution to this equation and obtain that the transformation

$$\boldsymbol{\mathcal{A}}' = \boldsymbol{\mathcal{A}} + c\nabla\chi = \boldsymbol{\mathcal{A}} - \nabla\dot{\Delta}^{-1} \operatorname{div} \boldsymbol{\mathcal{A}} = \mathcal{P}_{\mathrm{df}}[\boldsymbol{\mathcal{A}}']$$

can be identified with the projection onto the divergence-free part of $\boldsymbol{\mathcal{A}}$ (cf. (2.10b)).

Finally collecting (2.7) together with (2.10b), in the Coulomb gauge, Maxwell's equations (2.2) reduce to the decoupled set of equations for the potentials ϕ and $\boldsymbol{\mathcal{A}}$

$$\begin{cases} -\Delta\phi = \rho, \\ \frac{1}{c^2}\partial_{tt}\boldsymbol{\mathcal{A}} - \Delta\boldsymbol{\mathcal{A}} = = \frac{1}{c}\mathcal{P}_{\mathrm{df}}[\boldsymbol{J}]. \end{cases} \tag{2.11}$$

The electric field $\boldsymbol{E}$ and the magnetic field $\boldsymbol{B}$ are then given through (2.4) and (2.5)

$$\begin{aligned} \boldsymbol{E}(t,x) &= -\nabla\phi(t,x) - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t,x), \\ \boldsymbol{B}(t,x) &= \nabla\times\boldsymbol{\mathcal{A}}(t,x). \end{aligned} \tag{2.12}$$

In case of spatial dimension $d = 2$, within this thesis we consider vector potentials $\boldsymbol{\mathcal{A}} = (A_1, A_2, 0)^\top$ and refer to electromagnetic fields of type

$$\boldsymbol{E}(t,x) = -\begin{pmatrix} \partial_1\phi(t,x) \\ \partial_2\phi(t,x) \\ 0 \end{pmatrix} - \frac{\partial_t}{c}\begin{pmatrix} A_1(t,x) \\ A_2(t,x) \\ 0 \end{pmatrix} = \begin{pmatrix} E_1(t,x) \\ E_2(t,x) \\ 0 \end{pmatrix} \quad \text{and}$$

$$\boldsymbol{B}(t,x) = \nabla\times\begin{pmatrix} A_1(t,x) \\ A_2(t,x) \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \partial_1 A_2(t,x) - \partial_2 A_1(t,x) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ B_3(t,x) \end{pmatrix}$$

for $x \in \mathbb{T}^2$. For sake of simplicity, in the following we write $\boldsymbol{\mathcal{A}} = (A_1, \ldots, A_d)^\top$ for $d = 1, 2, 3$.

2.1.2 Coupling the Klein–Gordon Equation to an Electromagnetic Field

The content of this section is based on [78, Chapter 5.3.5.4 and Appendix F] and [69–71, 80]. Note that we use the *Japanese bracket* notation $\langle\nabla\rangle_c := \sqrt{-\Delta + c^2}$ as in the given literature. Our goal in this section is to couple the Klein–Gordon (KG) equation

$$c^{-2}\partial_{tt}\psi + (-\Delta + c^2)\psi = f[\psi], \quad \psi(0) = \psi_I, \quad \partial_t\psi(0) = c\,\langle\nabla\rangle_c\,\psi_I', \tag{2.13}$$

to the electromagnetic field $(\boldsymbol{E}, \boldsymbol{B})^\top$. This coupling shall preserve the gauge invariance of the corresponding potentials $(\phi, \boldsymbol{\mathcal{A}})^\top$ in the Coulomb gauge, i.e. with $\operatorname{div}\boldsymbol{\mathcal{A}} = 0$, as well as of the Klein–Gordon solution ψ. We focus on KG equations with a sufficiently smooth nonlinearity $f : \mathbb{C} \to \mathbb{C}$ such that

$$f[e^{i\omega}\psi] = e^{i\omega} f[\psi] \quad \text{for all } \omega \in \mathbb{R}. \tag{2.14}$$

Furthermore, we assume that the charge density ρ and the current density $\boldsymbol{J}$ in (2.11) satisfy the continuity equation (2.3) $\partial_t\rho + \operatorname{div}\boldsymbol{J} = 0$.

We carry out the coupling of the KG solution ψ to the influence of an electromagnetic field via a suitable transform of the differentiation operators $\frac{\partial_t}{c}$ and ∇ which leaves the resulting system invariant under gauge transformations. This motivates the Definition A.23 of the "minimal coupling operators" $\partial_t^{[\phi]}$ and $\nabla^{[\boldsymbol{\mathcal{A}}]}$

$$\partial_t^{[\phi]}\psi := \big(\frac{\partial_t}{c} + i\frac{\phi}{c}\big)\psi \qquad \text{and} \qquad \nabla^{[\boldsymbol{\mathcal{A}}]}\psi := \big(\nabla - i\frac{\boldsymbol{\mathcal{A}}}{c}\big)\psi. \tag{2.15}$$

More details on these operators can be found in [78, Chapter 5.3.5.4] and [70, 71, 78, 80, 87]. In a next step, we replace the differential operators ∂_t/c and ∇ in the Klein–Gordon equation (2.13) with $\partial_t^{[\phi]}$ and $\nabla^{[\boldsymbol{\mathcal{A}}]}$ and obtain the coupled system

$$\begin{cases} (\partial_t^{[\phi]})^2\psi - (\nabla^{[\boldsymbol{\mathcal{A}}]})^2\psi + c^2\psi = f[\psi], \\ \qquad\qquad\qquad\qquad -\Delta\phi = \rho, \\ \qquad \frac{1}{c^2}\partial_{tt}\boldsymbol{\mathcal{A}} - \Delta\boldsymbol{\mathcal{A}} = \frac{1}{c}\mathcal{P}_{\mathrm{df}}\left[\boldsymbol{J}\right]. \end{cases} \tag{2.16}$$

We emphasize here, that the operators $\partial_t^{[\phi]}$ and $\nabla^{[\boldsymbol{\mathcal{A}}]}$ are now depending also on time and space, since they involve the potentials $(\phi, \boldsymbol{\mathcal{A}}) : [0, T] \times \mathbb{T}^d \to \mathbb{R}^{1+3}$. In particular, $(\partial_t^{[\phi]})^2\psi$ and $(\nabla^{[\boldsymbol{\mathcal{A}}]})^2\psi$ are given explicitly in Corollary A.24. With the aid of Proposition A.25, we see that the latter system is gauge invariant under the gauge transform (see [70, 71])

$$\boldsymbol{\mathcal{A}}' = \boldsymbol{\mathcal{A}} + c\nabla\chi, \qquad \phi' = \phi - \partial_t\chi \qquad \text{and} \qquad \psi' := e^{i\chi}\psi.$$

In other words, if $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ solves (2.16), then also $(\psi', \phi', \boldsymbol{\mathcal{A}}')^\top$ does.

The system (2.16) looks very similar to the desired MKG system (2.1). In fact, only a back coupling of Maxwell's potentials to the KG solution ψ is still missing. Note that so far, the charge and current density ρ and $\boldsymbol{J}$ did not satisfy any particular condition besides the continuity equation (2.3). In order to couple back the electromagnetic potentials $\phi, \boldsymbol{\mathcal{A}}$ to the KG solution ψ, we need suitably chosen densities ρ and $\boldsymbol{J}$. We proceed with the derivation of the full Maxwell–Klein–Gordon system in the subsequent section. For the interested reader we provide the above-mentioned Definition A.23, Corollary A.24, and Proposition A.25 in Appendix A.6.

2.1.3 The Maxwell–Klein–Gordon System

In this section we collect the findings of the previous sections and derive the full Maxwell–Klein–Gordon system (2.1) as it is given in [20, 21, 70, 71] and also in the paper [63] by Krämer and Schratz.

So far we considered *external* electromagnetic fields represented by potentials $\phi, \boldsymbol{\mathcal{A}}$, which influence the motion of a charged spinless particle ([78, 87]) described by the coupled Klein–Gordon equation (2.16). In particular, because moving charges create their own time variant electromagnetic field (see [74, Chapter 4.5.5]), we are especially interested in the interaction of the particle with its *self-generated* field. Within this work we shall only focus on this self-interaction. The results can be adapted in order to incorporate the influence of *external* fields into the system.

In order to describe the mutual interaction between the charged particle and its electromagnetic field, we modify (2.16) such that not only the KG solution ψ depends on the potentials ϕ and $\boldsymbol{\mathcal{A}}$ but also vice versa. We carry out the back coupling via a suitable ψ-dependent choice for the density ρ and current density $\boldsymbol{J}$ satisfying the continuity equation (2.3). In the following we consider the system (2.16) for vanishing nonlinearity $f[\psi] \equiv 0$.

Derivation of the Charge and Current Density

According to [78, Chapter 5.2.2] we derive ρ and $\boldsymbol{J}$ corresponding to the linear Klein–Gordon problem (2.13) for $f \equiv 0$ as follows: Assume that ψ solves the KG equation. Then

$$0 = \overline{\psi} \cdot \left(c^{-2}\partial_{tt}\psi - \Delta\psi + c^2\psi\right) - \psi \cdot \overline{\left(c^{-2}\partial_{tt}\psi - \Delta\psi + c^2\psi\right)}.$$

Using that

$$(\overline{\psi}\partial_{tt}\psi - \psi\overline{\partial_{tt}\psi}) = \partial_t\left(\overline{\psi}\partial_t\psi - \psi\overline{\partial_t\psi}\right) \qquad \text{and} \qquad (\overline{\psi}\Delta\psi - \psi\overline{\Delta\psi}) = \operatorname{div}\left(\overline{\psi}\nabla\psi - \psi\overline{\nabla\psi}\right)$$

we thus obtain that the latter equation takes the form of a continuity equation, i.e.

$$0 = 2i\partial_t \operatorname{Im}\left(-c^{-2}\psi\overline{\partial_t\psi}\right) + 2i\operatorname{div}(\operatorname{Im}\left(\psi\overline{\nabla\psi}\right)),$$

if we divide by $-2i$ and set

$$\tilde{\rho} = \operatorname{Im}\left(c^{-2}\psi\overline{\partial_t\psi}\right) = -\operatorname{Re}\left(i\frac{\psi}{c}\overline{(\frac{\partial_t}{c}\psi)}\right) \quad \text{and} \quad \tilde{\boldsymbol{J}} = \operatorname{Im}\left(-\psi\overline{\nabla\psi}\right) = \operatorname{Re}\left(i\psi\overline{\nabla\psi}\right).$$

Replacing the operators $\frac{\partial_t}{c}$ and ∇ in $\tilde{\rho}$ and $\tilde{\boldsymbol{J}}$ with the minimal coupling operators $\partial_t^{[\phi]}$ and $\nabla^{[\boldsymbol{\mathcal{A}}]}$, respectively, (see (2.15)), this ansatz transfers directly to the coupled system (2.16). More precisely, according to [70, Section 1] and [71] we define

$$\begin{aligned} \rho = \quad & \rho[\psi,\phi] & := -\operatorname{Re}\left(i\frac{\psi}{c}\cdot\overline{\partial_t^{[\phi]}\psi}\right) = -\frac{1}{c^2}\left(\operatorname{Re}\left(i\psi\overline{\partial_t\psi}\right) + \phi\,|\psi|^2\right), \\ \boldsymbol{J} = \quad & \boldsymbol{J}[\psi,\boldsymbol{\mathcal{A}}] & := \operatorname{Re}\left(i\psi\cdot\overline{\nabla^{[\boldsymbol{\mathcal{A}}]}\psi}\right) = \qquad \operatorname{Re}\left(i\psi\overline{\nabla\psi}\right) - \frac{\boldsymbol{\mathcal{A}}}{c}\,|\psi|^2. \end{aligned} \tag{2.18}$$

In the following we may also write $\rho(t), \boldsymbol{J}(t)$ instead of $\rho[\psi(t),\phi(t)], \boldsymbol{J}[\psi(t),\boldsymbol{\mathcal{A}}(t)]$, if the context is clear. Plugging this choice of ρ and $\boldsymbol{J}$ into (2.16) we obtain a system which describes the mutual interaction of the moving charged particle with its self-generated electromagnetic field in the Coulomb gauge. We call the resulting system (2.20) the *Maxwell–Klein–Gordon* (MKG) system. In Proposition 2.2 below, we prove that ρ and $\boldsymbol{J}$ as in (2.18) satisfy indeed a continuity equation.

Proposition 2.2 ([70, 78], Continuity equation for MKG)**.** *Let* $(\psi,\phi,\boldsymbol{\mathcal{A}})^\top$ *satisfy the MKG system* (2.20) *below. Then the charge density* ρ *and the current density* $\boldsymbol{J}$ *defined in* (2.18) *satisfy the continuity equation*

$$\partial_t\rho + \operatorname{div}\boldsymbol{J} = 0. \tag{2.19}$$

Proof (see also [70, 78])*:* The proof of this lemma is a straight forward calculation, exploiting equation (2.20a). We compute

$$\begin{aligned} -\partial_t\rho &= \operatorname{Re}\left(i(\left|\frac{\partial_t}{c}\psi\right|^2 + \psi\frac{\overline{\partial_t^2\psi}}{c^2}\right) + \frac{1}{c^2}\partial_t\phi\,|\psi|^2 + 2\phi\operatorname{Re}\left(\psi\overline{\partial_t\psi}\right) \\ &= \operatorname{Re}\left(i\left(\psi\overline{\Delta\psi} - c^2\,|\psi|^2 + \frac{1}{c^2}\left(\phi^2\,|\psi|^2 + 2i\phi\psi\overline{\partial_t\psi} + i(\partial_t\phi)\,|\psi|^2\right)\right.\right. \\ &\qquad \left.\left. - \frac{|\boldsymbol{\mathcal{A}}|^2}{c^2}\,|\psi|^2 + 2i\psi\cdot\frac{\boldsymbol{\mathcal{A}}}{c}\cdot\overline{\nabla\psi}\right)\right) \\ &\quad + \frac{1}{c^2}\partial_t\phi\,|\psi|^2 + \frac{2}{c^2}\phi\operatorname{Re}\left(\psi\overline{\partial_t\psi}\right) \\ &= \operatorname{Re}\left(i\psi\overline{\Delta\psi} - 2\frac{\boldsymbol{\mathcal{A}}}{c}\psi\overline{\nabla\psi}\right)\right). \end{aligned}$$

On the other hand, we have

$$\begin{aligned}\operatorname{div} \boldsymbol{J} &= \operatorname{Re}\Big(i\big(\,|\nabla\psi|^2 + \psi\overline{\Delta\psi}\Big) - \big(\frac{\operatorname{div}\boldsymbol{\mathcal{A}}}{c}\,|\psi|^2 + 2\frac{\boldsymbol{\mathcal{A}}}{c}\operatorname{Re}\big(\psi\overline{\nabla\psi}\big)\\ &= \operatorname{Re}\Big(i\psi\overline{\Delta\psi} - 2\frac{\boldsymbol{\mathcal{A}}}{c}\psi\overline{\nabla\psi}\Big)\\ &= -\,\partial_t\rho.\end{aligned}$$

This finishes the proof. □

The Maxwell–Klein–Gordon System

Plugging the choice for ρ and $\boldsymbol{J}$ from (2.18) into the system (2.16), we obtain the Maxwell–Klein–Gordon system with solution $(\psi,\phi,\boldsymbol{\mathcal{A}})^\top$ under the Coulomb gauge constraint $\operatorname{div}\boldsymbol{\mathcal{A}} = 0$

$$\begin{cases} \frac{1}{c^2}\partial_{tt}\psi + \big(-\Delta + c^2\big)\psi = \frac{1}{c^2}\Big(\phi^2\psi - 2i\phi\partial_t\psi - i(\partial_t\phi)\psi\Big) - \frac{|\boldsymbol{\mathcal{A}}|^2}{c^2}\psi - 2i\frac{\boldsymbol{\mathcal{A}}}{c}\cdot\nabla\psi, & (2.20a)\\ \partial_{tt}\boldsymbol{\mathcal{A}} - c^2\Delta\boldsymbol{\mathcal{A}} = c\mathcal{P}_{\mathrm{df}}\left[\boldsymbol{J}[\psi,\boldsymbol{\mathcal{A}}]\right], \qquad \operatorname{div}\boldsymbol{\mathcal{A}} = 0 & (2.20b)\\ -\Delta\phi = \rho[\psi,\phi], \qquad \int_{\mathbb{T}^d}\phi(t,x)dx = 0, & (2.20c)\\ \big(\psi(0,x), \partial_t^{[\phi(0,x)]}\psi(0,x)\big) = \big(\psi_I(x), \langle\nabla\rangle_c\,\psi_I'(x)\big) & (2.20d)\\ \big(\boldsymbol{\mathcal{A}}(0), \partial_t\boldsymbol{\mathcal{A}}(0)\big) = \big(A_I(x), cA_I'(x)\big), & (2.20e)\\ \rho\,\text{and}\,\boldsymbol{J} \quad \text{as in (2.18)}, \end{cases}$$

where the projection $\mathcal{P}_{\mathrm{df}}$ onto divergence-free fields is given explicitly in Appendix A.4. Note that due to Proposition 2.2, the densities ρ and $\boldsymbol{J}$ indeed satisfy a continuity equation.

For simplicity, we assume that the total charge ([42, 59, 78]) in the above system

$$\mathcal{Q}(t) := \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d}\rho(t,x)dx = 0 \qquad \text{at time } t = 0$$

is zero (see also [63, Remark 1]). Note that due to Remark 2.3, we can assume without loss of generality

$$\widehat{\phi}_0(t) \overset{\text{Prop. A.4}}{=} \int_{\mathbb{T}^d}\phi(t,x)dx = 0 \qquad \text{for all } t$$

and thus may omit this detail in the following. In particular, this means that we look for $\phi(t) \in \dot{H}^{\tilde{r}}(\mathbb{T}^d)$ for all $t \in [0,T]$. Poisson's equation (2.20c) is well-posed in $\dot{H}^{\tilde{r}}(\mathbb{T}^d)$ for $\tilde{r} \geq 0$.

Remark 2.3 ([63, Remark 1 and 3])**.** *The continuity equation (2.19) together with $\mathcal{Q}(0) = 0$ implies that*

$$\int_{\mathbb{T}^d}\rho(t,x)dx = \int_{\mathbb{T}^d}\rho(0,x)dx = 0 \qquad \textit{for all } t. \tag{2.21}$$

Note that this implies that the Fourier mode corresponding to $k = 0$ (see [63, Remark 1] and also Proposition A.4)

$$\widehat{\rho}_0(t) = \widehat{\rho}_0(0) = 0 \qquad \textit{is zero for all } t$$

and thus the Poisson equation (2.20c) is solvable. If initially $\widehat{\rho}_0(0) \neq 0$, we consider instead

$$\tilde{\rho} = \rho - \widehat{\rho}_0(0), \quad \textit{such that (2.21) is satisfied for all } t.$$

Moreover, the gauge freedom in the MKG system (see Proposition A.25) allows us to add to ϕ a spatial constant function depending on t. More precisely, if (see [63, Remark 3])

$$0 \neq \widehat{\phi}_0(t) = \int_{\mathbb{T}^d} \phi(t,x)dx =: M(t) \in \mathbb{R},$$

we may choose

$$\phi' = \phi - \partial_t \chi, \qquad \text{with} \qquad \chi(t) = M(0) + \int_0^t M(s)ds$$

instead. Proposition A.25 then implies that if $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ solves (2.20), then also does the triplet $(e^{i\chi}\psi, \phi', \boldsymbol{\mathcal{A}})^\top$.

The basis for our numerical methods, which shall be presented within this thesis relies on reformulating the latter MKG system as a first order system in time. We proceed in the subsequent subsection.

2.1.4 Reformulation of MKG as a First Order System in Time

In this section, based on [45, 69–71, 80] and also on the paper [63] of Krämer and Schratz, we reformulate the MKG system (2.20) with solution $(\psi, \boldsymbol{\mathcal{A}}, \phi)^\top$ as a first order system in time for variables $(u, v, \phi, \mathfrak{a})^\top$ satisfying

$$\psi = \frac{1}{2}(u + \overline{v}), \qquad \boldsymbol{\mathcal{A}} = \frac{1}{2}(\mathfrak{a} + \overline{\mathfrak{a}}). \tag{2.22}$$

We thereby exploit the diagonalisation of wave-type equations as described in Section 1.2 and use, as before, the *Japanese bracket* notation $\langle \nabla \rangle_c := \sqrt{-\Delta + c^2}$.

We start off by reformulating the Klein–Gordon part (2.20a) for ψ and the Poisson part (2.20c) for the scalar potential ϕ. Then, we also transform the wave equation (2.20b) for the vector potential $\boldsymbol{\mathcal{A}}$ into a first order system in time of similar type using the same techniques.

(i) Reformulation of the Klein–Gordon part:

Following the ideas from Section 1.2 we transform $(\psi, \partial_t^{[\phi]}\psi)^\top$ into variables $w = (u, v)^\top$ by making the ansatz

$$\begin{aligned} u =& \psi - i \langle \nabla \rangle_c^{-1} \partial_t^{[\phi]} \psi, \\ v =& \overline{\psi} - i \langle \nabla \rangle_c^{-1} \overline{\partial_t^{[\phi]} \psi}, \end{aligned} \tag{2.23}$$

where we replaced ∂_t / c in (1.10) by its minimal coupling operator $\partial_t^{[\phi]} = c^{-1}(\partial_t + i\phi)$ given in Definition A.23. Because $\phi(t,x) \in \mathbb{R}$ is a real potential, we observe that $\psi = \frac{1}{2}(u + \overline{v})$ and that

$$\begin{aligned} \partial_t^{[\phi]} \psi =& i \langle \nabla \rangle_c (u - \psi) \quad \Rightarrow \quad \partial_t \psi = ic \langle \nabla \rangle_c (u - \psi) - i\phi\psi \\ \overline{\partial_t^{[\phi]} \psi} =& i \langle \nabla \rangle_c (v - \overline{\psi}) \quad \Rightarrow \quad \partial_t \overline{\psi} = ic \langle \nabla \rangle_c (v - \overline{\psi}) + i\phi\overline{\psi}. \end{aligned} \tag{2.24}$$

Applying the first time derivative to u and v in (2.23), we obtain

$$\begin{aligned} \partial_t u =& \partial_t \psi - ic^{-1} \langle \nabla \rangle_c^{-1} \big(\partial_{tt} \psi + i\partial_t(\phi\psi)\big), \\ \partial_t v =& \partial_t \overline{\psi} - ic^{-1} \langle \nabla \rangle_c^{-1} \big(\overline{\partial_{tt} \psi} - i\partial_t(\phi\overline{\psi})\big). \end{aligned}$$

In a next step, replacing in the latter equation the terms $\partial_{tt}\psi$ and $\partial_t\psi$ with their equivalents from (2.20a) and (2.24), this yields the following first order system in time for $w = (u, v)^\top$

$$i\partial_t w = -c \langle\nabla\rangle_c w + F[w, \phi, \mathfrak{a}], \quad w(0) = w_I = \begin{pmatrix} \psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'} \end{pmatrix}, \tag{2.25}$$

where due to (2.23) the initial data w_I are given by

$$w_I = \begin{pmatrix} \psi(0) - i \langle\nabla\rangle_c^{-1} \partial_t^{[\phi(0)]}\psi(0) \\ \overline{\psi(0) - i \langle\nabla\rangle_c^{-1} \partial_t^{[\phi(0)]}\psi(0)} \end{pmatrix} = \begin{pmatrix} \psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'} \end{pmatrix}.$$

Thanks to the identity $\boldsymbol{\mathcal{A}} = \frac{1}{2}(\mathfrak{a} + \overline{\mathfrak{a}})$ (cf. (2.29) below), the nonlinearity F reads

$$\begin{aligned} F[w, \phi, \mathfrak{a}] = &\frac{1}{2}\big(\phi + \langle\nabla\rangle_c^{-1} \phi \langle\nabla\rangle_c\big)\begin{pmatrix} u \\ -v \end{pmatrix} + \frac{1}{2}\big(\phi - \langle\nabla\rangle_c^{-1} \phi \langle\nabla\rangle_c\big)\begin{pmatrix} \overline{v} \\ -\overline{u} \end{pmatrix} \\ &- \frac{1}{8}c^{-1} \langle\nabla\rangle_c^{-1} \begin{pmatrix} |\mathfrak{a} + \overline{\mathfrak{a}}|^2 (u + \overline{v}) \\ |\mathfrak{a} + \overline{\mathfrak{a}}|^2 (\overline{u} + v) \end{pmatrix} + i\frac{1}{2} \langle\nabla\rangle_c^{-1} \begin{pmatrix} -(\mathfrak{a} + \overline{\mathfrak{a}}) \cdot \nabla(u + \overline{v}) \\ (\mathfrak{a} + \overline{\mathfrak{a}}) \cdot \nabla(\overline{u} + v) \end{pmatrix}. \end{aligned} \tag{2.26}$$

(ii) Reformulation of Poisson's equation:

If we insert $\psi = \frac{1}{2}(u + \overline{v})$ into the definition of the charge density ρ in (2.18), we have by (2.24) that

$$\rho[\psi, \phi] = -\frac{1}{c^2} \operatorname{Re}\big(i\psi \cdot \big(ic \langle\nabla\rangle_c (v - \overline{\psi})\big)\big) = -\frac{1}{4} \operatorname{Re}\big((u + \overline{v})c^{-1} \langle\nabla\rangle_c (\overline{u} - v)\big) =: \rho[w]. \tag{2.27}$$

Thus, the Poisson equation (2.20c) corresponding to the first order in time setting reads

$$-\Delta\phi = \rho[w]. \tag{2.28}$$

(iii) Reformulation of the Maxwell Wave Equation:

Next, we also rewrite the wave equation (2.20b) for the vector potential $\boldsymbol{\mathcal{A}}$ as a first order system in time, applying the same ideas as in (2.23) and replacing $\langle\nabla\rangle_c$ with $\langle\nabla\rangle_0$. Because $\boldsymbol{\mathcal{A}}(t, x) \in \mathbb{R}^d$ is real vector valued, we obtain one single equation for the variable

$$\mathfrak{a} = \boldsymbol{\mathcal{A}} - i \langle\nabla\rangle_0^{-1} \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}, \tag{2.29}$$

which implies $\boldsymbol{\mathcal{A}} = \frac{1}{2}(\mathfrak{a} + \overline{\mathfrak{a}})$ and

$$\partial_t\boldsymbol{\mathcal{A}} = ic \langle\nabla\rangle_0 (\mathfrak{a} - \boldsymbol{\mathcal{A}}). \tag{2.30}$$

Note that later on, we look for solutions $\boldsymbol{\mathcal{A}} \in \dot{H}^r$ (see Definition A.3) for which the operator $\langle\nabla\rangle_0^{-1}$ is well-defined. Taking the first time derivative of $\mathfrak{a}$ in (2.29) and using the identities (2.20b) and (2.30) for $\partial_{tt}\boldsymbol{\mathcal{A}}$ and $\partial_t\boldsymbol{\mathcal{A}}$, respectively, gives

$$i\partial_t\mathfrak{a} = -c \langle\nabla\rangle_0 \mathfrak{a} + \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P[w, \mathfrak{a}], \quad \mathfrak{a}(0) = \mathfrak{a}_I = A_I - i \langle\nabla\rangle_0^{-1} A_I', \tag{2.31}$$

where for $w = (u, v)^\top$ the nonlinearity $\boldsymbol{J}^P$ is given by

$$\begin{aligned} \boldsymbol{J}^P[w, \mathfrak{a}] =& \mathcal{P}_{\mathrm{df}}\Big[\boldsymbol{J}\big[\tfrac{1}{2}(u + \overline{v}), \tfrac{1}{2}(\mathfrak{a} + \overline{\mathfrak{a}})\big]\Big] \\ =& \mathcal{P}_{\mathrm{df}}\Big[\operatorname{Re}\Big(i\frac{1}{4}(u + \overline{v})\nabla(\overline{u} + v)\Big) - \frac{1}{c}\frac{1}{8}(\mathfrak{a} + \overline{\mathfrak{a}})\, |u + \overline{v}|^2\Big]. \end{aligned} \tag{2.32}$$

Altogether, the steps (i), (ii), (iii) yield the following first order system in time

for the variables $(w, \phi, \mathfrak{a})^\top$ for $x \in \mathbb{T}^d$ and $t \in [0, T]$,

composed of (2.25),(2.28) and (2.31), i.e.

$$\begin{cases} i\partial_t w = -c\langle\nabla\rangle_c w + F[w,\phi,\mathfrak{a}], & w(0) = w_I = \begin{pmatrix}\psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'}\end{pmatrix}, \quad (2.33a) \\ -\Delta\phi = \rho[w], \qquad \int_{\mathbb{T}^d}\phi(t,x)dx = 0, & (2.33b) \\ i\partial_t\mathfrak{a} = -c\langle\nabla\rangle_0\mathfrak{a} + \langle\nabla\rangle_0^{-1}\boldsymbol{J}^P[w,\mathfrak{a}], & \mathfrak{a}(0) = \mathfrak{a}_I = A_I - i\langle\nabla\rangle_0^{-1}A_I'. \quad (2.33c)\end{cases}$$

equipped with periodic boundary conditions. By (2.26),(2.27) and (2.32) the nonlinear terms read

$$\begin{aligned} F[w,\phi,\mathfrak{a}] = {} & \phi\begin{pmatrix}u \\ -v\end{pmatrix} - \frac{1}{2}\left(\phi - \langle\nabla\rangle_c^{-1}\phi\langle\nabla\rangle_c\right)\begin{pmatrix}u-\overline{v} \\ \overline{u}-v\end{pmatrix} & (2.33d) \\ & - \frac{1}{8}c^{-1}\langle\nabla\rangle_c^{-1}\begin{pmatrix}|\mathfrak{a}+\overline{\mathfrak{a}}|^2(u+\overline{v}) \\ |\mathfrak{a}+\overline{\mathfrak{a}}|^2(\overline{u}+v)\end{pmatrix} + i\frac{1}{2}\langle\nabla\rangle_c^{-1}\begin{pmatrix}-(\mathfrak{a}+\overline{\mathfrak{a}})\cdot\nabla(u+\overline{v}) \\ (\mathfrak{a}+\overline{\mathfrak{a}})\cdot\nabla(\overline{u}+v)\end{pmatrix} \\ \rho[w] = {} & -\frac{1}{4}\operatorname{Re}\left((u+\overline{v})c^{-1}\langle\nabla\rangle_c(\overline{u}-v)\right) & (2.33e) \\ \boldsymbol{J}^P[w,\mathfrak{a}] = {} & \mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i\frac{1}{4}(u+\overline{v})\nabla(\overline{u}+v)\right) - \frac{1}{c}\frac{1}{8}(\mathfrak{a}+\overline{\mathfrak{a}})\,|u+\overline{v}|^2\right]. & (2.33f)\end{aligned}$$

Recall that for the system (2.33) the following identities hold

$$\psi = \frac{1}{2}(u+\overline{v}), \quad \boldsymbol{\mathcal{A}} = \frac{1}{2}(\mathfrak{a}+\overline{\mathfrak{a}}), \quad \partial_t\boldsymbol{\mathcal{A}} = \frac{1}{2}ic\langle\nabla\rangle_0(\mathfrak{a}-\overline{\mathfrak{a}}). \tag{2.34}$$

Concerning the usage of $\langle\nabla\rangle_0^{-1}$ in the above system, note Remark 2.1 above. Furthermore note that $\mathcal{P}_{\mathrm{df}}H^r(\mathbb{T}^d) \subset \dot{H}^r(\mathbb{T}^d)$ (see Definition A.13) for all $r \geq 1$. Thus, combining the local well-posedness result in Proposition 2.4 for $r > d/2$ with Corollary A.15 on the zero mode of the solution $\mathfrak{a}(t)$ of (2.33c) for all times $t \in [0, T]$, we deduce that

$$\text{if} \quad A_I \in \mathcal{P}_{\mathrm{df}}H^r(\mathbb{T}^d) \quad \text{and} \quad A_I' \in \mathcal{P}_{\mathrm{df}}H^{r-1}(\mathbb{T}^d), \quad \text{then} \quad \mathfrak{a}_I \in \mathcal{P}_{\mathrm{df}}H^r(\mathbb{T}^d)$$

and then in particular the zero Fourier mode of the solution $\mathfrak{a}(t)$ of (2.33c) satisfies by Corollary A.15

$$\left(\widehat{\mathfrak{a}(t)}\right)_0 = 0 \qquad \text{for all } t \in [0, T].$$

We thus look for solutions of the MKG first order system (2.33) which satisfy (see [21, 62, 70, 79] and also the local well-posedness result in Proposition 2.4 below)

$$(w(t), \phi(t), \mathfrak{a}(t))^\top \in H^r(\mathbb{T}^d) \times \dot{H}^{r+1}(\mathbb{T}^d) \times \dot{H}^r(\mathbb{T}^d) \qquad \text{for all times } t \in [0, T].$$

2.1.5 Local Well-Posedness of the MKG First Order System

Based on [21, 60, 62, 70, 76, 79] and references therein, we now formulate the following local well-posedness result on the MKG first order system in time (2.33). The interested reader may find more details in the latter papers.

Proposition 2.4 ([21, 60, 62, 70, 76, 79] and references therein). *Let $c > 0$ and let $r > d/2$. Let the initial data of the MKG system (2.20) satisfy $(\psi_I, \psi'_I, A_I, A'_I) \in H^r(\mathbb{T}^d) \times H^r(\mathbb{T}^d) \times \mathcal{P}_{df}H^r(\mathbb{T}^d) \times \mathcal{P}_{df}H^{r-1}(\mathbb{T}^d)$ (see Definitions A.1 and A.13 for the Definition of Sobolev spaces). Then there exist constants $T_r, B_r > 0$ independent of c such that the solution $(w, \phi, \mathfrak{a})^\top$ of the MKG first order system in time (2.33) satisfies*

$$\|w(t)\|_r + \|\phi(t)\|_{r+1,0} + \|\mathfrak{a}(t)\|_{r,0} \leq B_r$$

and thus

$$(w(t), \phi(t), \mathfrak{a}(t))^\top \in H^r(\mathbb{T}^d) \times \dot{H}^{r+1}(\mathbb{T}^d) \times \dot{H}^r(\mathbb{T}^d)$$

for all $t \in [0, T_r]$.

Proof (see also [21, 62, 70, 79] and references therein)*:* For the proof of the bounds on $w(t) = (u(t), v(t))^\top$ and $\mathfrak{a}(t)$ see the local well-posedness results in [21, 62, 70, 79] and references therein. Additionally, note that by (2.33), we have

$$-\Delta\phi = -\frac{1}{4}\,\mathrm{Re}\left((u + \overline{v})c^{-1}\langle\nabla\rangle_c(\overline{u} - v)\right).$$

Applying the solution operator

$$\dot{\Delta}^{-1} : H^{\tilde{r}}(\mathbb{T}^d) \to \dot{H}^{\tilde{r}+2}(\mathbb{T}^d) \quad \text{for} \quad \tilde{r} \geq 1 \text{ given in (A.4)}$$

to the latter Poisson equation we thus find

$$\|\phi\|_{r+1,0} = \left\|\dot{\Delta}^{-1}\left(\frac{1}{4}\,\mathrm{Re}\left((u + \overline{v})c^{-1}\langle\nabla\rangle_c(\overline{u} - v)\right)\right)\right\|_{r+1,0}$$
$$\overset{\text{Lemma A.8}}{\leq} K\,\|w\|_r\,\left\|c^{-1}\langle\nabla\rangle_c w\right\|_{r-1} \overset{\text{Lemma A.11}}{\leq} K\,\|w\|_r^2,$$

with a constant K independent of c exploiting bilinear Sobolev product estimates from Lemma A.8 and properties of the operator $c^{-1}\langle\nabla\rangle_c$ from Lemma A.11. □

In the subsequent section we derive the Maxwell–Dirac system.

2.2 The Maxwell–Dirac System

In this section, based on [10, 14, 22, 34, 35, 78, 87], we derive the Maxwell–Dirac (MD) system in Coulomb gauge. Recall, that in Section 2.1 we derived the MKG system (2.20) by coupling the Klein–Gordon (KG) equation (2.13) with solution $\psi(t, x) \in \mathbb{C}$ to a Poisson and a wave equation (2.11) for Maxwell's potentials $(\phi(t, x), \boldsymbol{\mathcal{A}}(t, x))^\top \in \mathbb{R}^{1+d}$. We carried out this coupling by replacing the operators $\frac{\partial_t}{c}$ and ∇ in the KG equation (2.13) with the corresponding minimal coupling operators (see Definition A.23)

$$\partial_t^{[\phi]} = \frac{\partial_t}{c} + i\frac{\phi}{c} \quad \text{and} \quad \nabla^{[\boldsymbol{\mathcal{A}}]} = \nabla - i\frac{\boldsymbol{\mathcal{A}}}{c}.$$

Furthermore, we have chosen the charge and current densities $\rho, \boldsymbol{J}$ suitably for the Maxwell–Klein–Gordon setting (see (2.18) in Section 2.1.3).

Following the same strategy as in Section 2.1 for the MKG case, we derive the Maxwell–Dirac system (2.36) by replacing $\frac{\partial_t}{c}$ and ∇ with $\partial_t^{[\phi]}$ and $\nabla^{[\boldsymbol{\mathcal{A}}]}$, respectively, in the Dirac equation (1.23)

$$i\left(\frac{\partial_t}{c}\psi+\sum_{j=1}^{d}\boldsymbol{\alpha}_j\partial_j\psi\right)-c\boldsymbol{\beta}\psi=0,\quad \psi(0,x)=\psi_I(x), \tag{2.35}$$

with solution $\psi(t,x)=(\psi_1(t,x),\dots,\psi_4(t,x))^\top\in\mathbb{C}^4$. In the literature, the solution of the Dirac equation is often called four-spinor (see for instance [87]). The matrices $\boldsymbol{\alpha}_j,\boldsymbol{\beta}, j=1,2,3$ were given in (1.21). Combining the latter Dirac equation with Maxwell's potentials $(\phi(t,x),\boldsymbol{\mathcal{A}}(t,x))^\top\in\mathbb{R}^{1+d}$ satisfying the Poisson and wave equations (2.11), we thus obtain the Maxwell–Dirac system ([70]) in the Coulomb gauge $\operatorname{div}\boldsymbol{\mathcal{A}}=0$

$$\begin{cases} i\left(\frac{\partial_t}{c}\psi+\sum_{j=1}^{d}\boldsymbol{\alpha}_j\partial_j\psi\right)=c\boldsymbol{\beta}\psi+\frac{1}{c}\left(\phi-\sum_{j=1}^{d}\boldsymbol{\alpha}_jA_j\right)\psi & (2.36a)\\ \partial_{tt}\boldsymbol{\mathcal{A}}-c^2\Delta\boldsymbol{\mathcal{A}}=c\mathcal{P}_{\text{df}}\left[\boldsymbol{J}[\psi]\right], \qquad \operatorname{div}\boldsymbol{\mathcal{A}}=0 & (2.36b)\\ -\Delta\phi=\rho[\psi], \qquad \int_{\mathbb{T}^d}\phi(t,x)dx=0 & (2.36c)\\ \psi(0,x)=\psi_I(x) & (2.36d)\\ \big(\boldsymbol{\mathcal{A}}(0,x),\partial_t\boldsymbol{\mathcal{A}}(0,x)\big)=\big(A_I(x),cA_I'(x)\big). & (2.36e)\end{cases}$$

In Section 2.2.4 below, we show that the choice of ρ and $\boldsymbol{J}$ as

$$\rho=\rho[\psi]=|\psi|^2, \qquad \boldsymbol{J}=\boldsymbol{J}[\psi]=c\psi\cdot\overline{\boldsymbol{\alpha}\psi}=(J_j)_{j=1}^d, \quad J_j=c\psi\cdot\overline{\boldsymbol{\alpha}_j\psi}. \tag{2.36f}$$

satisfies the continuity equation (see also [70])

$$\partial_t\rho+\operatorname{div}\boldsymbol{J}=0.$$

Assuming initial data satisfying

$$\psi_I\in H^r(\mathbb{T}^d) \qquad \text{and} \qquad A_I\in\dot{H}^r(\mathbb{T}^d),\quad A_I'\in\dot{H}^{r-1}(\mathbb{T}^d)$$

for $r>d/2$, we then look for solutions (see [22, 34, 35, 70, 71] and also the local well-posedness result in Proposition 2.7)

$$\psi(t)\in H^r(\mathbb{T}^d),\quad \phi(t)\in\dot{H}^{r+2}(\mathbb{T}^d)\quad\text{and}\quad \boldsymbol{\mathcal{A}}(t)\in\dot{H}^r(\mathbb{T}^d) \qquad \text{for all times } t\in[0,T].$$

The spaces $H^r(\mathbb{T}^d)$ and $\dot{H}^r(\mathbb{T}^d)$ are given in Definitions A.1 and A.3. Exploiting Proposition A.25, we observe that the MD system (2.36) is invariant under the gauge transform (see [70] and Section 2.1.1)

$$\boldsymbol{\mathcal{A}}'=\boldsymbol{\mathcal{A}}+c\nabla\chi, \qquad \phi'=\phi-\partial_t\chi \qquad \text{and} \qquad \psi':=e^{i\chi}\psi,$$

i.e. if $(\psi,\phi,\boldsymbol{\mathcal{A}})^\top$ solves (2.16), then also $(\psi',\phi',\boldsymbol{\mathcal{A}}')^\top$ does (cf. Section 2.1.2).

For simplicity, we assume that the total charge ([42, 59, 78]) in the above MD system (2.36) and in the MD first order in time reformulation (2.41) satisfies

$$\mathcal{Q}(t):=\frac{1}{(2\pi)^d}\int_{\mathbb{T}^d}\rho(t,x)dx=0 \qquad \text{at time } t=0.$$

As before, due to Remark 2.3, we can assume without loss of generality

$$\widehat{\phi}_0(t) \overset{\text{Prop. A.4}}{=} \int_{\mathbb{T}^d} \phi(t,x)dx = 0 \qquad \text{for all } t.$$

This allows us to omit the corresponding condition in (2.36) for further reading. Note that the Poisson equation (2.20c) is well-posed in the spaces $\dot{H}^{\tilde{r}}(\mathbb{T}^d)$ for $\tilde{r} \geq 0$.

Reduction of the MD System in Lower Dimensions

Note that based on [10, 14–16, 87], in lower spatial dimension $d = d_{\text{low}} \in \{1,2\}$ the Dirac equation (2.36a) with *four-spinor* solution $\psi(t,x) \in \mathbb{C}^4$ reduces to a Dirac equation with *two-spinor* solution $\Psi(t,x) = (\psi_1(t,x), \psi_4(t,x))^\top \in \mathbb{C}^2$ via a simple variable transform, see Remark 2.5. In particular, in our numerical experiments in Chapter 5, we exploit this peculiarity and consider the reduced MD system (2.37) instead of the full Maxwell–Dirac system. However, the theoretical results of this thesis remain valid for both the reduced and the full system.

Afterwards, the subsequent sections are dedicated to derive a first order system in time of type (2.33) by bypassing a second order in time MKG reformulation of the MD system.

Remark 2.5 ([10, 14–16, 87], Reduced MD System in Lower Dimension)**.** *In lower spatial dimensions, i.e. $d = 1,2$ we can reduce the Dirac system for the four-spinor ψ to two Dirac systems for two-spinors ([87]) $\Psi, \tilde{\Psi}$ by setting $\Psi = (\psi_1, \psi_4)^\top$ and $\tilde{\Psi} = (\psi_2, \psi_3)^\top$. In particular the system for the two-spinor $\tilde{\Psi}$ is equivalent to the system for Ψ if we apply a transformation $y \mapsto \tilde{y} = -y$, $A_2 \mapsto \tilde{A}_2 = -A_2$.*
Hence in dimensions $d = 1,2$ it is enough to consider the system for the two-spinor Ψ:

$$\begin{cases} i\partial_t \Psi = -ic\sum_{j=1}^{d} \sigma_j \partial_{x_j} \Psi + c^2 \boldsymbol{\sigma}_3 \Psi + \left(\phi - \sum_{j=1}^{d} \boldsymbol{\sigma}_j A_j\right) \Psi \\ \partial_{tt} \boldsymbol{\mathcal{A}} = c^2 \Delta \boldsymbol{\mathcal{A}} + c\mathcal{P}_{\text{df}}[\boldsymbol{J}], \quad \boldsymbol{J} = c\Psi \cdot \overline{\boldsymbol{\sigma}\Psi} \\ -\Delta\phi = \rho, \qquad \int_{\mathbb{T}^d} \phi(t,x)dx = 0, \qquad \rho = |\Psi|^2 \\ \Psi(0) = \Psi_I := (\psi_1(0), \psi_4(0))^\top, \quad \boldsymbol{\mathcal{A}}(0) = A_I, \quad \partial_t \boldsymbol{\mathcal{A}}(0) = cA'_I, \end{cases} \tag{2.37}$$

This means in particular that all the results on the solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MD system (2.36) within this work remain valid for the solution $(\Psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the reduced system (2.37) if we replace $\boldsymbol{\alpha}_j$ by $\boldsymbol{\sigma}_j$, $j = 1,2$ and $\boldsymbol{\beta}$ by $\boldsymbol{\sigma}_3$ (see (1.21) and [87] for definition of the Dirac matrices).

Therefore, we exploit that according to [22, Lemma 2.1] and [70], we can reformulate the MD system (2.36) as an equivalent MKG system of type (2.20), but with additional nonlinear terms. Then the ideas of the previous Section 2.1.4 immediately provide the desired MD first order system in time (see (2.41) below). We proceed in the subsequent subsections.

2.2.1 Maxwell–Dirac in Form of a MKG System

This section is based on [22, 70].

Before we reformulate the MD system (2.36) as a diagonal first order system in time of type (2.33) in the subsequent Section 2.2.2, we rewrite it as an equivalent Maxwell–Klein–Gordon type system at first. In contrast to the standard MKG system (2.20), the latter involves additional terms due to the presence of the Dirac matrices $\boldsymbol{\alpha}_j$ and $\boldsymbol{\beta}$ for $j = 1, \dots, d$.

Recall that the minimal coupling operators read (cf. Definition A.23)

$$\partial_t^{[\phi]} = \frac{\partial_t}{c} + i\frac{\phi}{c} \quad \text{and} \quad \nabla^{[\boldsymbol{\mathcal{A}}]} = \nabla - i\frac{\boldsymbol{\mathcal{A}}}{c}.$$

We apply the operator $(-i\partial_t^{[\phi]})$ to the Dirac equation (2.36a) and obtain (see [70, Section 5])

$$\begin{cases} (-i\partial_t^{[\phi]})(i\partial_t^{[\phi]}\psi) = (-i\partial_t^{[\phi]})\Big(-i\sum_{j=1}^{d}\boldsymbol{\alpha}_j\nabla^{[\boldsymbol{\mathcal{A}}]}\psi + c\boldsymbol{\beta}\psi\Big), \\ \psi(0) = \psi_I, \quad -i\partial_t^{[\phi(0)]}\psi(0) = i\sum_{j=1}^{d}\boldsymbol{\alpha}_j\big(\nabla^{[\boldsymbol{\mathcal{A}}(0)]}\big)_j\psi - c\boldsymbol{\beta}\psi =: -i\left\langle\nabla\right\rangle_c\psi_I'. \end{cases}$$

Due to Proposition A.26, this yields the following Maxwell–Klein–Gordon type system for the four-spinor $\psi(t,x) \in \mathbb{C}^4$ and the potentials $(\phi(t,x), \boldsymbol{\mathcal{A}}(t,x))^\top \in \mathbb{R}^{1+d}$

$$\begin{cases} c^{-2}(\partial_t + i\phi)^2\psi = \Big(\nabla - i\frac{\boldsymbol{\mathcal{A}}}{c}\Big)^2\psi - c^2\psi + \frac{i}{c}\mathfrak{D}^{\boldsymbol{\alpha}}[\phi, \boldsymbol{\mathcal{A}}]\psi & (2.38a) \\ \partial_{tt}\boldsymbol{\mathcal{A}} = c^2\Delta\boldsymbol{\mathcal{A}} + c\mathcal{P}_{\text{df}}[\boldsymbol{J}], \quad \boldsymbol{J} = c\psi\cdot\overline{\boldsymbol{\alpha}\psi} & (2.38b) \\ -\Delta\phi = \rho, \qquad \rho = |\psi|^2, & (2.38c) \\ \psi(0) = \psi_I, \quad \partial_t^{[\phi(0))]}\psi(0) = \left\langle\nabla\right\rangle_c\psi_I' := -\sum_{j=1}^{d}\boldsymbol{\alpha}_j(\nabla^{[\boldsymbol{\mathcal{A}}(0)]})_j\psi_I - ic\boldsymbol{\beta}\psi_I, & (2.38d) \\ \boldsymbol{\mathcal{A}}(0) = A_I, \quad \partial_t\boldsymbol{\mathcal{A}}(0) = cA_I'. & (2.38e) \end{cases}$$

The additional nonlinearity $\mathfrak{D}^{\boldsymbol{\alpha}}[\phi, \boldsymbol{\mathcal{A}}]\psi$ is given through (cf. [70, Section 5])

$$\begin{aligned} \mathfrak{D}^{\boldsymbol{\alpha}}[\phi, \boldsymbol{\mathcal{A}}] &:= \mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\phi] + \mathfrak{D}^{\boldsymbol{\alpha}}_0[\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}] + \mathfrak{D}^{\boldsymbol{\alpha}}_{\text{curl}}[\boldsymbol{\mathcal{A}}] \qquad \text{with} \\ \mathfrak{D}^{\boldsymbol{\alpha}}_{\text{curl}}[\boldsymbol{\mathcal{A}}] &:= -\frac{1}{2}\sum_{\substack{j,k=1 \\ j\neq k}}^{d}\boldsymbol{\alpha}_j\boldsymbol{\alpha}_k[(\partial_j(A_k)) - (\partial_k(A_j))], \quad \mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\phi] := \sum_{j=1}^{d}\boldsymbol{\alpha}_j(\partial_j\phi), \\ \mathfrak{D}^{\boldsymbol{\alpha}}_0[\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}] &:= \sum_{j=1}^{d}\boldsymbol{\alpha}_j(\frac{\partial_t}{c}A_j). \end{aligned} \tag{2.38f}$$

Note that in the MKG type system (2.38), the choice of the charge and current density ρ and $\boldsymbol{J}$, respectively, is the same as in the Maxwell–Dirac system (2.36). Furthermore, note that the additional nonlinearity $\mathfrak{D}^{\boldsymbol{\alpha}}[\phi, \boldsymbol{\mathcal{A}}]$ in (2.38) above is due to the particular coupling between the components of the solution ψ of the Dirac equation (2.36a) via the Dirac matrices $\boldsymbol{\alpha}_j$ for $j = 1, \dots, d$ given in (1.21).

For later use, we collect the operators $\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{curl}}$, $\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}$ and $\mathfrak{D}^{\boldsymbol{\alpha}}_0$ in the following Definition 2.6. We proceed in the subsequent subsection with the reformulation of the MKG type system (2.38) as a diagonal first order system in time using the techniques of the previous Section 2.1.4.

Definition 2.6 ([70]). *For a smooth vector field $\boldsymbol{\mathcal{B}}(t,x) = (B_1(t,x),\dots,B_d(t,x)) \in \mathbb{C}^d$ and a smooth function $\mathcal{W}(t,x) \in \mathbb{C}$ we define the operators*

$$\begin{aligned}\mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{curl}}[\boldsymbol{\mathcal{B}}] &\coloneqq -\frac{1}{2}\sum_{\substack{j,k=1\\ j\neq k}}^{d} \boldsymbol{\alpha}_j\boldsymbol{\alpha}_k[(\partial_j(B_k)) - (\partial_k(B_j))], \quad \mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{div}}[\mathcal{W}] \coloneqq \sum_{j=1}^{d}\boldsymbol{\alpha}_j(\partial_j W),\\ \mathfrak{D}^{\boldsymbol{\alpha}}_{0}[\boldsymbol{\mathcal{B}}] &\coloneqq \sum_{j=1}^{d}\boldsymbol{\alpha}_j(B_j),\end{aligned}$$

where the Dirac matrices $\alpha_j, j = 1,\dots,d$ are given in (1.21).

2.2.2 Reformulation of the MKG Representation as a First Order System in Time

Based on [22, 70, 71] and also based on the paper [63] by Krämer and Schratz, we now reformulate the MD system (2.36) as a first order system in time similar to (2.33) with solutions $w = (u,v)^\top$, ϕ and $\boldsymbol{\mathfrak{a}}$ satisfying the identities (cf. (2.34))

$$\psi = \frac{1}{2}(u+\overline{v}), \quad \boldsymbol{\mathcal{A}} = \frac{1}{2}(\boldsymbol{\mathfrak{a}}+\overline{\boldsymbol{\mathfrak{a}}}), \quad \partial_t\boldsymbol{\mathcal{A}} = i\frac{1}{2}c\,\langle\nabla\rangle_0\,(\boldsymbol{\mathfrak{a}}-\overline{\boldsymbol{\mathfrak{a}}}). \tag{2.39}$$

Bypassing the MKG type system (2.38) corresponding to the MD system (2.36), allows us to use the same techniques for this purpose as before in the previous Section 2.1.4. Note that according to [22, Lemma 2.1] the MD system (2.36), its MKG reformulation (2.38) and finally the corresponding first order system (2.41) below are equivalent.

Therefore, we proceed as in Section 2.1.4 and make the ansatz

$$\begin{aligned} u &= \psi - i\,\langle\nabla\rangle_c^{-1}\,\partial_t^{[\phi]}\psi,\\ v &= \overline{\psi} - i\,\langle\nabla\rangle_c^{-1}\,\overline{\partial_t^{[\phi]}\psi}, \qquad \text{where} \quad \partial_t^{[\phi]} = \frac{\partial_t}{c} + \frac{\phi}{c} \quad \text{(see Definition A.23)}.\\ \boldsymbol{\mathfrak{a}} &= \boldsymbol{\mathcal{A}} - i\,\langle\nabla\rangle_0^{-1}\,\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}, \end{aligned} \tag{2.40}$$

We observe that the variables $w = (u,v)^\top$ and $\boldsymbol{\mathfrak{a}}$ satisfy the identities in (2.39) for ψ and $\boldsymbol{\mathcal{A}}$. Differentiating $w, \boldsymbol{\mathfrak{a}}$ with respect to time t analogously to Section 2.1.4, we obtain a diagonal first order system in time system with a structure similar to (2.33). Plugging the relations (2.39) for $\boldsymbol{\mathcal{A}}$, $\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}$ into the additional nonlinear term $\mathfrak{D}^{\boldsymbol{\alpha}}[\phi,\boldsymbol{\mathcal{A}}] = \mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{div}}[\phi] + \mathfrak{D}^{\boldsymbol{\alpha}}_0[\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}] + \mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{curl}}[\boldsymbol{\mathcal{A}}]$ in (2.38), we find that (see Definition 2.6)

$$\begin{aligned}\mathfrak{D}^{\boldsymbol{\alpha}}_0[\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}] &= i\frac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_0[\langle\nabla\rangle_0\,(\boldsymbol{\mathfrak{a}}-\overline{\boldsymbol{\mathfrak{a}}})]\\ \mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{curl}}[\boldsymbol{\mathcal{A}}] &= \frac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{curl}}[\boldsymbol{\mathfrak{a}}+\overline{\boldsymbol{\mathfrak{a}}}].\end{aligned}$$

The term $\frac{i}{c}\mathfrak{D}^{\boldsymbol{\alpha}}[\phi,\boldsymbol{\mathcal{A}}]\psi$ then manifests in an additional nonlinearity $G[w,\phi,\boldsymbol{\mathfrak{a}}]$ in the resulting first order system in time

with solution $(w,\phi,\boldsymbol{\mathfrak{a}})^\top$ for $x \in \mathbb{T}^d$ and $t \in [0,T]$, which reads (cf. [70])

$$
\begin{cases}
i\partial_t w = - c\langle\nabla\rangle_c w + F[w,\phi,\mathfrak{a}] + G[w,\phi,\mathfrak{a}], & (2.41a)\\
w(0) = w_I = \begin{pmatrix} \psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'} \end{pmatrix}, & \\
-\Delta\phi = \rho[w], \qquad \int_{\mathbb{T}^d} \phi(t,x)dx = 0, & \\
i\partial_t \mathfrak{a} = - c\langle\nabla\rangle_0 \mathfrak{a} + \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P[w], & (2.41b)\\
\mathfrak{a}(0) = \mathfrak{a}_I = A_I - i\langle\nabla\rangle_0^{-1} A_I', &
\end{cases}
$$

equipped with periodic boundary conditions. The terms ρ and $\boldsymbol{J}^P := \mathcal{P}_{\mathrm{df}}[\boldsymbol{J}]$ are obtained by plugging $\psi = \frac{1}{2}(u+\overline{v})$ into (2.36f). We thus find

$$
\begin{aligned}
F[w,\phi,\mathfrak{a}] = \phi\begin{pmatrix} u \\ -v \end{pmatrix} &- \frac{1}{2}\left(\phi - \langle\nabla\rangle_c^{-1}\phi\langle\nabla\rangle_c\right)\begin{pmatrix} u-\overline{v} \\ \overline{u}-v \end{pmatrix} \qquad (2.41c)\\
&- \frac{1}{8}c^{-1}\langle\nabla\rangle_c^{-1}\begin{pmatrix} |\mathfrak{a}+\overline{\mathfrak{a}}|^2(u+\overline{v}) \\ |\mathfrak{a}+\overline{\mathfrak{a}}|^2(\overline{u}+v) \end{pmatrix} + i\frac{1}{2}\langle\nabla\rangle_c^{-1}\begin{pmatrix} -(\mathfrak{a}+\overline{\mathfrak{a}})\cdot\nabla(u+\overline{v}) \\ (\mathfrak{a}+\overline{\mathfrak{a}})\cdot\nabla(\overline{u}+v) \end{pmatrix},
\end{aligned}
$$

$$
G[w,\phi,\mathfrak{a}] = i\frac{1}{2}\langle\nabla\rangle_c^{-1}\begin{pmatrix} \left(\frac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{curl}}[\mathfrak{a}+\overline{\mathfrak{a}}] + \mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{div}}[\phi] + \frac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_0[i\langle\nabla\rangle_0(\mathfrak{a}-\overline{\mathfrak{a}})]\right)(u+\overline{v}) \\ -\left(\frac{1}{2}\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\mathrm{curl}}[\mathfrak{a}+\overline{\mathfrak{a}}] + \mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\mathrm{div}}[\phi] + \frac{1}{2}\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_0[i\langle\nabla\rangle_0(\mathfrak{a}-\overline{\mathfrak{a}})]\right)(\overline{u}+v) \end{pmatrix}, \qquad (2.41d)
$$

$$
\rho[w] = \frac{1}{4}(|u|^2 + |v|^2 + 2\,\mathrm{Re}\,(u\cdot v)), \qquad (2.41e)
$$

$$
\boldsymbol{J}^P[w] = c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[(u+\overline{v})\overline{\boldsymbol{\alpha}}(\overline{u}+v)\right]. \qquad (2.41f)
$$

In particular, using (2.38) we can write the initial data as

$$
w(0) = w_I = \begin{pmatrix} \left(\mathcal{I}_4 - \boldsymbol{\beta}c\langle\nabla\rangle_c^{-1}\right)\psi_I \\ \left(\mathcal{I}_4 + \boldsymbol{\beta}c\langle\nabla\rangle_c^{-1}\right)\overline{\psi_I} \end{pmatrix} + i\langle\nabla\rangle_c^{-1}\sum_{j=1}^d \begin{pmatrix} \boldsymbol{\alpha}_j(\nabla^{[A_I]})_j\psi_I \\ \overline{\boldsymbol{\alpha}_j(\nabla^{[A_I]})_j\psi_I} \end{pmatrix}.
$$

Recall that by Remark 2.1 above, the operator $\langle\nabla\rangle_0^{-1}$ is well-defined on the spaces $\dot{H}^r(\mathbb{T}^d)$. Furthermore, note that $\mathcal{P}_{\mathrm{df}}H^r(\mathbb{T}^d) \subset \dot{H}^r(\mathbb{T}^d)$ (see Definition A.13) for all $r \geq 1$. Thus, combining the local well-posedness result in Proposition 2.7 for $r > d/2$, with Corollary A.15 on the zero mode of the solution $\mathfrak{a}(t)$ of (2.41b) for all times $t \in [0,T]$, we deduce that

$$
\text{if} \quad A_I \in \mathcal{P}_{\mathrm{df}}H^r(\mathbb{T}^d) \quad \text{and} \quad A_I' \in \mathcal{P}_{\mathrm{df}}H^{r-1}(\mathbb{T}^d), \quad \text{then} \quad \mathfrak{a}_I \in \mathcal{P}_{\mathrm{df}}H^r(\mathbb{T}^d)
$$

and then in particular the zero Fourier mode of the solution $\mathfrak{a}(t)$ of (2.41b) satisfies by Corollary A.15

$$
\left(\widehat{\mathfrak{a}(t)}\right)_0 = 0 \qquad \text{for all } t \in [0,T].
$$

We thus look for solutions of the MD first order system (2.41) which satisfy (see [22, 34, 35] and also the local well-posedness result in Proposition 2.7 below)

$$
(w(t),\phi(t),\mathfrak{a}(t))^\top \in H^r(\mathbb{T}^d) \times \dot{H}^{r+2}(\mathbb{T}^d) \times \dot{H}^r(\mathbb{T}^d) \qquad \text{for all times } t \in [0,T].
$$

The system (2.41) is very similar to system (2.33). In fact, the nonlinearity $F[w,\phi,\mathfrak{a}]$ has the same structure as in Section 2.1.4. However, because $\psi(t,x) \in \mathbb{C}^4$ also the variables $u, v \in \mathbb{C}^4$ take values in $\mathbb{C}^4$ and thus $F[w,\phi,\mathfrak{a}]$ takes values in $\mathbb{C}^4 \times \mathbb{C}^4$. Another difference to (2.33) is found in $\rho[w], \boldsymbol{J}^P[w]$ which we obtain simply by replacing ψ in their definitions in (2.38) by $\psi = \frac{1}{2}(u+\overline{v})$.

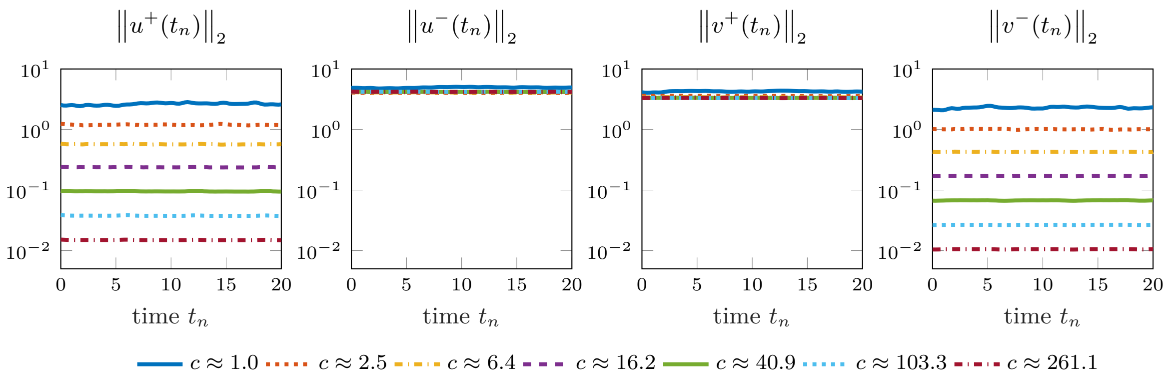


Figure 2.1: (MD, Simulation of the H^2 norm of $w(t_n) = (u^+(t_n), u^-(t_n), v^+(t_n), v^-(t_n))^\top$). For the case of $d = 2$ we observe that $\|u^\pm(t_n)\|_2$ and $\|v^\pm(t_n)\|_2$ behave as in (2.42) for $t_n \in [0, 20]$. Note that in the outer left and outer right semi-logarithmic (in the y-axis) plot the lines corresponding to the norms of u^+ and v^+ for the values $c = 1.59^{2\ell}, \ell = 0, 1, \ldots, 6$ are equidistant which underlines the $\mathcal{O}\left(c^{-1}\right)$ behaviour of u^+ and v^+ (cf. (2.42)). The numerical approximation to the solution w of the MD first order system (2.41) at time $t_n = n\tau, n = 1, \ldots, 20/\tau$ for the time step $\tau \approx 0.004$ is obtained via the "twisted" time integration scheme Ψ_*^τ (with $\gamma = 1$) given in (4.39) (see Chapter 4) with initial data corresponding to Experiment 5.4 (see Section 5.4).

In view of the block structure of $\mathcal{I}_4 \mp \boldsymbol{\beta}$ from (1.22), we decompose the solution $w = (u, v)^\top$ into upper and lower components ([19, 22, 87]), i.e. in the notation $u^+(t,x), u^-(t,x), v^+(t,x), v^-(t,x) \in \mathbb{C}^2$ we have

$$u = \begin{pmatrix} u^+ \\ u^- \end{pmatrix} \quad \text{and} \quad v = \begin{pmatrix} v^+ \\ v^- \end{pmatrix}. \tag{2.42a}$$

Then, equation (1.22) together with the inequality $\left\|(1 - c\langle\nabla\rangle_c^{-1})w\right\|_r \leq c^{-2}\|w\|_{r+2}$ from Lemma A.11, yields that the initial data $w_I = (u_I^+, u_I^-, v_I^+, v_I^-)^\top$ satisfy (see also (3.37))

$$\begin{aligned}
\|u_I^+\|_r \leq & & c^{-1}K(\|\psi_I\|_{r+2}, \|A_I\|_r),\\
\|u_I^-\|_r \leq 2\|\psi^-\|_r + & & c^{-1}K(\|\psi_I\|_{r+1}, \|A_I\|_r),\\
\|v_I^+\|_r \leq 2\|\psi^+\|_r + & & c^{-1}K(\|\psi_I\|_{r+1}, \|A_I\|_r),\\
\|v_I^-\|_r \leq & & c^{-1}K(\|\psi_I\|_{r+2}, \|A_I\|_r).
\end{aligned} \tag{2.42b}$$

The local well-posedness result ([22, 34, 35, 70]) on MD from Proposition 2.7 in Section 2.2.3 below, then shows that this structure is also transported in the solution $w(t)$ of (2.41a) for all times t, i.e. we find that for all $t \in [0, T]$ in the sense of the H^r norm for $r > d/2$

$$\begin{aligned}
u^+(t) =& \mathcal{O}\left(c^{-1}\right), & v^+(t) =& \mathcal{O}\left(1\right),\\
u^-(t) =& \mathcal{O}\left(1\right), & v^-(t) =& \mathcal{O}\left(c^{-1}\right).
\end{aligned} \tag{2.42c}$$

The latter is underlined by Fig. 2.1. We obtain a proof of this structure as a subsidiary result of the rigorous convergence analysis of the nonrelativistic limit approximation to the MD system in Section 3.4.3.

Next, we state a local well-posedness result on the MD first order system in time (2.41) in the subsequent subsection. Afterwards in Section 2.2.4, we provide a derivation of the MD charge and current density ρ and $\boldsymbol{J}$ (see (2.36f) above), respectively. In the subsequent chapter, we then continue with the construction of efficient numerical time integration schemes in the nonrelativistic limit regime $c \gg 1$.

2.2.3 Local Well-Posedness of the MD First Order System

Based on [22, 34, 35, 70, 71] and references therein, we formulate the following local well-posedness result on the MD first order system in time (2.41). The interested reader may find more details in the latter papers.

Proposition 2.7 ([22, 34, 35, 70, 71]). *Let $c > 0$ and let $r > d/2$. Let the initial data of the MD system (2.36) satisfy $(\psi_I, A_I, A'_I) \in H^r(\mathbb{T}^d) \times \mathcal{P}_{df} H^r(\mathbb{T}^d) \times \mathcal{P}_{df} H^{r-1}(\mathbb{T}^d)$ (see Definitions A.1 and A.13 for the Definition of Sobolev spaces). Then there exist constants $T_r, B_r > 0$ independent of c, such that the solution $(w, \phi, \mathfrak{a})^\top$ of the MD first order system in time (2.41) satisfies*

$$\|w(t)\|_r + \|\phi(t)\|_{r+2,0} + \|\mathfrak{a}(t)\|_{r,0} \leq B_r$$

and thus

$$(w(t), \phi(t), \mathfrak{a}(t))^\top \in H^r(\mathbb{T}^d) \times \dot{H}^{r+2}(\mathbb{T}^d) \times \dot{H}^r(\mathbb{T}^d) \quad \text{for all } t \in [0, T_r].$$

Proof (see [22, 34, 35] and references therein)*:* For the proof of the bounds on $w(t) = (u(t), v(t))^\top$ and $\mathfrak{a}(t)$ see the local well-posedness results in [22, 34, 35] and references therein. Additionally, note that by (2.41), we have

$$-\Delta\phi = \frac{1}{4}(|u|^2 + |v|^2 + 2\,\mathrm{Re}\,(u \cdot v)).$$

Applying the solution operator

$$\dot{\Delta}^{-1} : H^{\tilde{r}}(\mathbb{T}^d) \to \dot{H}^{\tilde{r}+2}(\mathbb{T}^d) \quad \text{for} \quad \tilde{r} \geq 0 \text{ given in (A.4)}$$

to the latter Poisson equation we thus find for a constant K independent of c

$$\begin{aligned} \|\phi\|_{r+2,0} &= \left\| \dot{\Delta}^{-1} \left(\frac{1}{4}(|u|^2 + |v|^2 + 2\,\mathrm{Re}\,(u \cdot v)\right) \right\|_{r+2,0} \\ &\overset{\text{Lemma A.8}}{\leq} K \|w\|_r^2, \end{aligned}$$

exploiting bilinear Sobolev product estimates from Lemma A.8. □

2.2.4 Derivation of the MD Charge and Current Density

This section is dedicated to derive the MD charge and current density ρ and $\boldsymbol{J}$ (see (2.36f) above) and is based on [70] and [78, Chapter 5.3.2]. In order to derive these quantities suitably for the (Maxwell–)Dirac equation (2.36) we consider its Dirac part (2.36a)

$$i \left(\frac{\partial_t}{c}\psi + \sum_{j=1}^{d} \boldsymbol{\alpha}_j \partial_j \psi \right) = c\boldsymbol{\beta}\psi + \frac{1}{c}\left(\phi - \sum_{j=1}^{d} \boldsymbol{\alpha}_j A_j \right) \psi, \tag{2.43}$$

We proceed as in [78, Chapter 5.3.2] and multiply equation (2.43) from left with the complex conjugate transpose of its solution ψ and subtract the complex conjugate of the resulting product.

More precisely, exploiting that by (1.19)

$$\boldsymbol{\alpha}_j^\top = \overline{\boldsymbol{\alpha}_j}, \; j = 1, \ldots, d \quad \text{and that the potentials} \quad (\phi(t,x), \boldsymbol{\mathcal{A}}(t,x))^\top \in \mathbb{R}^{1+d}$$

are real vector valued, we find that

$$\begin{aligned}
0 =& \overline{\psi}^\top \left(i\frac{\partial_t}{c}\psi + i\sum_{j=1}^{d} \boldsymbol{\alpha}_j \partial_j \psi - c\boldsymbol{\beta}\psi \right) - \psi^\top \left(-i\overline{\frac{\partial_t}{c}\psi} - i\sum_{j=1}^{d} \overline{\boldsymbol{\alpha}_j}\,\overline{\partial_j \psi} - c\boldsymbol{\beta}\overline{\psi} \right) \\
=& \frac{i}{c}\left(\overline{\psi}^\top \partial_t \psi + \psi^\top \overline{\partial_t \psi} \right) + \frac{i}{c}\left(c\sum_{j=1}^{d} \overline{\psi}^\top \boldsymbol{\alpha}_j \partial_j \psi + \psi^\top \overline{\boldsymbol{\alpha}_j}\,\overline{\partial_j \psi} \right) \\
=& \frac{i}{c}\left(\partial_t \big(\psi^\top \overline{\psi}\big) + \operatorname{div}\big(c(\psi^\top \overline{\boldsymbol{\alpha}_j}\,\overline{\psi})_{j=1}^d \big) \right).
\end{aligned}$$

If we define the charge and current density by

$$\rho = |\psi|^2 \quad \text{and} \quad \boldsymbol{J} = c(\psi \cdot \overline{\boldsymbol{\alpha}_j}\,\overline{\psi})_{j=1}^d, \quad \text{respectively.}$$

the latter takes the form of a continuity equation

$$\partial_t \rho + \operatorname{div} \boldsymbol{J} = 0$$

Note that due to the relation $\boldsymbol{\alpha}_j^\top = \overline{\boldsymbol{\alpha}_j}, j = 1, \dots, d$ from (1.19) the current $\boldsymbol{J}(t,x) \in \mathbb{R}^d$ is real vector valued.

In the next chapter, we shall continue with the construction of efficient numerical time integration schemes in the nonrelativistic limit regime $c \gg 1$ by exploiting the asymptotic behaviour of the highly oscillatory solution of the MKG/MD first order systems in time (2.33)/(2.41).

CHAPTER

THREE

NUMERICAL INTEGRATORS FOR MKG AND MD IN THE NONRELATIVISTIC LIMIT REGIME

Based on [19–22, 45, 68–71, 81] and on the paper [63] by Krämer and Schratz in this chapter, we construct and analyse efficient numerical integrators for the Maxwell–Klein–Gordon and Maxwell–Dirac systems

$$\text{in the nonrelativistic limit regime where } c \gg 1,$$

and where the solution becomes highly oscillatory in time, exploiting

$$\text{the asymptotic behaviour of the highly oscillatory solution} \quad (\psi, \phi, \boldsymbol{\mathcal{A}})^\top \quad \text{as } c \to \infty$$

which was analytically investigated in [19–22, 63, 69, 70] in low regularity Sobolev spaces. More precisely, in the latter papers, the authors proved the convergence of the highly oscillatory MKG/MD systems (2.20)/(2.36) towards non-oscillatory Schrödinger–Poisson (SP) systems of type

$$\begin{cases} i\partial_t w_0 = \frac{1}{2}\Delta w_0 + \phi_0 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix} \\ -\Delta\phi_0 = \rho_0 = \begin{cases} -\frac{1}{4}\left(|u_0|^2 - |v_0|^2\right) & \text{in case of MKG,} \\ \frac{1}{4}\left(|u_0|^2 + |v_0|^2\right) & \text{in case of MD,} \end{cases} \\ i\partial_t \boldsymbol{a}_0 = -c\left\langle \nabla \right\rangle_0 \boldsymbol{a}_0 \end{cases} \tag{3.1}$$

with solution $(w_0, \phi_0, \boldsymbol{a}_0)^\top$, where $w_0 = (u_0, v_0)^\top$, in the sense that

$$\begin{pmatrix} w(t) \\ \phi(t) \\ \mathfrak{a}(t) \end{pmatrix} \longrightarrow \begin{pmatrix} e^{ic^2 t} w_0(t) \\ \phi_0(t) \\ \boldsymbol{a}_0(t) \end{pmatrix} \quad \text{as } c \to \infty, \text{ (see Theorems 3.3 and 3.4 below).} \tag{3.2}$$

For the convergence of the MD system in Lorenz gauge in semiclassical and nonrelativistic limit regimes, see [68, 81, 82].

Recall that $(w, \phi, \mathfrak{a})^\top$ denotes the solution to the MKG (2.33) and MD (2.41) first order system in time (here $\delta_{\mathrm{MD}} = 0$ in case of MKG and $\delta_{\mathrm{MD}} = 1$ in case of MD)

$$\begin{cases} i\partial_t w = -c\left\langle \nabla \right\rangle_c w + F[w,\phi,\mathfrak{a}] + \delta_{\mathrm{MD}} G[w,\phi,\mathfrak{a}], & w(0) = w_I = \begin{pmatrix} \psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'} \end{pmatrix} \\ -\Delta\phi = \rho[w] & \\ i\partial_t \mathfrak{a} = -c\left\langle \nabla \right\rangle_0 \mathfrak{a} + \left\langle \nabla \right\rangle_0^{-1} \boldsymbol{J}^P[w,\mathfrak{a}], & \mathfrak{a}(0) = \mathfrak{a}_I = A_I - i\left\langle \nabla \right\rangle_0^{-1} A_I', \end{cases} \tag{3.3}$$

with solutions $w = (u,v)^\top$, ϕ and $\mathfrak{a}$ satisfying the identities

$$\psi = \frac{1}{2}(u + \overline{v}), \quad \boldsymbol{\mathcal{A}} = \frac{1}{2}(\mathfrak{a} + \overline{\mathfrak{a}}), \quad \partial_t \boldsymbol{\mathcal{A}} = i\frac{1}{2}c\left\langle \nabla \right\rangle_0 (\mathfrak{a} - \overline{\mathfrak{a}}).$$

Recall that Remark 2.1 provides well-posedness of the operator $\left\langle \nabla \right\rangle_0^{-1}$ on the spaces $\dot{H}^r(\mathbb{T}^d)$ given in Definition A.3. Despite small differences in the dimension m of $w(t,x) = (u(t,x), v(t,x))^\top \in \mathbb{C}^m \times \mathbb{C}^m$ (i.e. $m = 1$ for MKG, $m = 4$ for MD), in the initial data $w(0)$ and in the charge and current densities ρ and $\boldsymbol{J}^P$ in case of MKG and MD, the first order systems (3.3) have a very similar structure in both cases. Thus, within this chapter, many aspects in the construction and analysis of our schemes will be very similar. We may point out important differences explicitly.

In this chapter we now follow [45, 69, 70] and the paper [63] by Krämer and Schratz in order to derive the SP system (3.1) as the nonrelativistic of the MKG and MD system (2.20) and (2.36), respectively, in a constructive way. We therefore exploit the technique of a Modulated Fourier Expansion (MFE) in Sections 3.1, 3.2.2 and 3.3 below (see [52, Chapter XIII.5] and [30, 31, 49]). This technique allows us to (formally) derive analytic asymptotic approximations which are (at first formally) converging towards the exact solution with a convergence rate of order $\mathcal{O}\left(c^{-N}\right)$ for $N \in \mathbb{N}$ (see (3.33),(3.61)). We carry out a rigorous analysis of this convergence in Section 3.4.

In Section 3.4, based on [19–22, 70], we prove the asymptotic behaviour (3.2) rigorously and give rigorous analytical convergence bounds depending on the small parameter c^{-N}, see Theorems 3.3 and 3.4 below. More precisely, we show rigorous bounds for the approximations

$$\psi_0(t) = \frac{1}{2}(e^{ic^2t}u_0(t) + e^{-ic^2t}\overline{v_0}(t)), \quad \phi_0(t) \quad \text{and} \quad \boldsymbol{\mathcal{A}}_0 = \frac{1}{2}(\boldsymbol{a}_0(t) + \overline{\boldsymbol{a}_0}(t))$$

to the solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MKG and MD systems (2.20) and (2.36), respectively. Thereby, the functions $w_0 = (u_0, v_0)^\top$, ϕ_0 and $\boldsymbol{a}_0$ solve (3.1). Because of the identities $\psi = \frac{1}{2}(u+\overline{v})$ and $\boldsymbol{\mathcal{A}} = \frac{1}{2}(\mathfrak{a}+\overline{\mathfrak{a}})$, the convergence bounds can be played back to bounds of the form (see [19–22, 69, 70] and the paper [63] by Krämer and Schratz)

$$\left\| w(t) - e^{ic^2t}w_0(t) \right\|_r + \|\phi(t) - \phi_0(t)\|_{r+2,0} + \|\mathfrak{a}(t) - \boldsymbol{a}_0(t)\|_{r,0} = \mathcal{O}\left(c^{-1}\right), \tag{3.4}$$

where $w = (u,v)^\top$, ϕ and $\mathfrak{a}$ solve (3.3). For more details see Section 3.4 below.

Later in Section 3.5, we carry out the construction of efficient numerical time integration schemes for solving the highly oscillatory first order system in time (3.3) in the nonrelativistic limit regime $c \gg 1$. We therefore exploit the analytic asymptotic convergence (3.4). The construction of efficient schemes thus relies on numerically solving the non-oscillatory Schrödinger–Poisson system (3.1) with classical splitting schemes of order p. The resulting scheme then admits

$$\text{error bounds of order} \quad \mathcal{O}\left(c^{-1} + \tau^p\right).$$

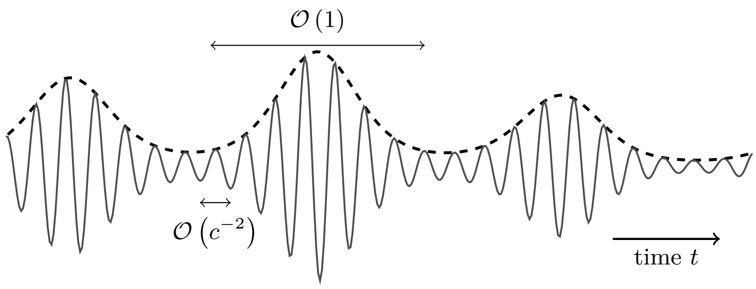


Figure 3.1: (Multiple Time Scales in a System). A highly oscillatory function of the form $\tilde{w}(t) = e^{ic^2 t}\tilde{w}_0(t)$ (solid line) involves the oscillatory phases $e^{ic^2 t}$. The amplitude of $\tilde{w}$ is governed by the non-oscillatory modulation function $\tilde{w}_0$ (dashed line). The fast oscillations happen at the time scale $c^2 t$ whereas the modulation happens at time scale t.

Note that for the case of MKG, these schemes have been already constructed and analysed in the paper [63] by Krämer and Schratz. Furthermore, note that in [57] for the case of MD a similar scheme, based on numerically solving the SP system (3.1) with an exponential Strang splitting method ([44, 65]) has been proposed. The authors Huang et al. of [57] only numerically investigated numerical experiments that their scheme is convergent of order $\mathcal{O}\left(c^{-1} + \tau^2\right)$, but they did not rigorously prove these numerical error bounds. Our analysis provides a rigorous proof for the latter and furthermore provides a constructive way to improve the

$$\text{numerical error bounds up to order} \quad \mathcal{O}\left(c^{-N} + \tau^p\right) \quad \text{for } N \in \mathbb{N}$$

for a given time step τ by exploiting higher order analytical asymptotic approximations.

In Section 3.6 we finally prove rigorous numerical convergence results given in Theorem 3.15.

As a first step in the derivation of the SP limit system (3.1) we reformulate the first order system (3.3) as a multiscale system depending on various time scales of the solution. We continue in the subsequent section.

3.1 A Multiscale System in Time for MKG and MD

For the content of this section see also [45, 69, 70] and also the paper [63] by Krämer and Schratz. In this section, we rewrite the first order system (3.3), which is given in the time variable t and space variable x, as a multiscale system depending on multiple time scales t, $\theta := c^2 t$ and $\varphi := c\langle\nabla\rangle_0 t$, which are present in the time evolution of the solution, and on space x. Let us shortly discuss the meaning of these time scales. This formal ansatz allows us to formally analyse the internal oscillatory structure of the solution and to separate highly oscillatory from slowly varying parts of the solution. A rigorous analysis of this oscillatory behaviour shall be subject of later sections.

We observe that for $c \gg 1$ the dominant terms in (3.3) are of order c^2 and $c\langle\nabla\rangle_0$ due to Lemma A.11. These terms impose fast oscillations to the solutions w and $\mathfrak{a}$ happening at the fast time scales $\theta := c^2 t$ and $\varphi := c\langle\nabla\rangle_0 t$. According to results from perturbation theory ([52, 61, 72, 73]) the amplitude of these fast oscillations, due to the corresponding highly oscillatory phases $e^{ia\theta}$ and $e^{ib\varphi}$ for $a, b \in \mathbb{Z}$, is governed by slowly varying modulation functions $w_n^{(a,b_j)}$ and $\mathfrak{a}_n^{(a,b_j)}$ depending on the slow time t (see Fig. 3.1

and cf. (3.6)). To incorporate these different time scales into the solution, we proceed as in [45, 63] and make the formal ansatz of expanding the solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MKG/MD equation and the solution $(w, \phi, \mathfrak{a})^\top$ of the corresponding first order system into a *Modulated Fourier Expansion* (MFE) (see [52, Chapter XIII.5] and [30, 31, 49] for more details on MFE) in variables

$$t, \quad \varphi(t) := ct\,\langle\nabla\rangle_0 \quad \text{and} \quad \theta(t) := c^2 t. \tag{3.5}$$

In the following, we omit the explicit dependence of φ and θ on the slow time t. More precisely, similar to [45, 63], we make the ansatz

$$\begin{aligned}
\begin{pmatrix}\psi(t)\\ \phi(t)\\ \boldsymbol{\mathcal{A}}(t)\end{pmatrix} &\simeq \begin{pmatrix}\Psi(t,\varphi,\theta)\\ \Phi(t,\varphi,\theta)\\ \mathbb{A}(t,\varphi,\theta)\end{pmatrix} = \sum_{n=0}^{\infty} c^{-n}\begin{pmatrix}\Psi_n(t,\varphi,\theta)\\ \Phi_n(t,\varphi,\theta)\\ \mathbb{A}_n(t,\varphi,\theta)\end{pmatrix}, \\
\begin{pmatrix}w(t)\\ \phi(t)\\ \mathfrak{a}(t)\end{pmatrix} &\simeq \begin{pmatrix}\mathbb{W}(t,\varphi,\theta)\\ \Phi(t,\varphi,\theta)\\ \mathbb{a}(t,\varphi,\theta)\end{pmatrix} = \sum_{n=0}^{\infty} c^{-n}\begin{pmatrix}\mathbb{W}_n(t,\varphi,\theta)\\ \Phi_n(t,\varphi,\theta)\\ \mathbb{a}_n(t,\varphi,\theta)\end{pmatrix},
\end{aligned} \tag{3.6a}$$

where the coefficients $(\mathbb{W}_n, \Phi_n, \mathbb{a}_n)^\top$ are given by products of plane wave solutions, see [30, Section 4]. More precisely, we look for solutions of the form

$$\begin{pmatrix}\mathbb{W}_n(t,\varphi,\theta,x)\\ \Phi_n(t,\varphi,\theta,x)\\ \mathbb{a}_n(t,\varphi,\theta,x)\end{pmatrix} = \sum_{a\in\mathbb{Z}} e^{ia\theta}\begin{pmatrix}\widetilde{\mathbb{W}}_n^{(a)}(t,\varphi,x)\\ \widetilde{\Phi}_n^{(a)}(t,\varphi,x)\\ \widetilde{\mathbb{a}}_n^{(a)}(t,\varphi,x)\end{pmatrix} = \sum_{a\in\mathbb{Z}} e^{ia\theta}\sum_{\substack{\boldsymbol{b}\in\mathbb{Z}^M\\ M\in\mathbb{N}_0}}\prod_{j=1}^{M} e^{ib_j\varphi}\begin{pmatrix}w_n^{(a,b_j)}(t,x)\\ \phi_n^{(a,b_j)}(t,x)\\ \mathfrak{a}_n^{(a,b_j)}(t,x)\end{pmatrix} \tag{3.6b}$$

in the time variables t, φ and θ and in the space variable x. Note that our ansatz involves φ and θ only in the phases $e^{ia\theta}$ and $e^{ib\varphi}$ for $a, b \in \mathbb{Z}$. This admits the additional assumption that $\theta \in \mathbb{T}$ and $\widehat{\varphi}_k \in \mathbb{T}$ for $k \in \mathbb{Z}^d$, where the latter describes the Fourier representation of the operator time scale $\varphi = ct\,\langle\nabla\rangle_0$.

Introducing variables $\mathbb{U}, \mathbb{V}, \mathbb{U}_n, \mathbb{V}_n$ such that

$$\mathbb{W}(t,\varphi,\theta) = (\mathbb{U}(t,\varphi,\theta), \mathbb{V}(t,\varphi,\theta))^\top \quad \text{and} \quad \mathbb{W}_n(t,\varphi,\theta) = (\mathbb{U}_n(t,\varphi,\theta), \mathbb{V}_n(t,\varphi,\theta))^\top$$

and respecting the relations $\psi = \frac{1}{2}(u + \overline{v})$ and $\boldsymbol{\mathcal{A}} = \frac{1}{2}(\mathfrak{a} + \overline{\mathfrak{a}})$ in (2.22), we remark that for all $n \in \mathbb{N}_0$ we have

$$\Psi_n = \frac{1}{2}(\mathbb{U}_n + \overline{\mathbb{V}_n}), \qquad \mathbb{A}_n = \frac{1}{2}(\mathbb{a}_n + \overline{\mathbb{a}_n}). \tag{3.7}$$

By (2.33) and (2.41) the nonlinearity $F[w, \phi, \mathfrak{a}]$ has the same structure in both the MKG as the MD first order system. Plugging in the expansions $\mathbb{W}, \Phi, \mathbb{a}$ into F we find $\mathbb{F} := F[\mathbb{W}, \Phi, \mathbb{a}]$ with expansion

$$F[w(t), \phi(t), \mathfrak{a}(t)] \simeq \mathbb{F}(t,\varphi,\theta) = \sum_{n=0}^{\infty} c^{-n}\mathbb{F}_n(t,\varphi,\theta). \tag{3.8a}$$

In a similar way we expand $\mathbb{G} := G[\mathbb{W}, \Phi, \mathbb{a}]$, $\mathbb{p} := \rho[\mathbb{W}]$ and $\mathbb{J}^P := \boldsymbol{J}^P[\mathbb{W}, \mathbb{a}]$ such that

$$\begin{aligned}
G[w(t), \phi(t), \mathfrak{a}(t)] &\simeq \mathbb{G}(t,\varphi,\theta) = \sum_{n=0}^{\infty} c^{-n}\mathbb{G}_n(t,\varphi,\theta),\\
\rho[w(t)] &\simeq \mathbb{p}(t,\varphi,\theta) = \sum_{n=0}^{\infty} c^{-n}\mathbb{p}_n(t,\varphi,\theta),\\
\boldsymbol{J}^P[w(t), \mathfrak{a}(t)] &\simeq \mathbb{J}^P(t,\varphi,\theta) = \sum_{n=0}^{\infty} c^{-n}\mathbb{J}^P_n(t,\varphi,\theta) + c\mathbb{J}^P_{-1}(t,\varphi,\theta).
\end{aligned} \tag{3.8b}$$

Note the presence of a term $\mathbb{J}^P_{-1}$ corresponding to the order c^1 in the expansion $\mathbb{J}^P$ which vanishes in case of MKG but is necessary for the analysis in case of MD due to the definition of $\boldsymbol{J}^P$ in (2.41).

Due to the explicit dependence of the multiscale ansatz functions $\mathbb{W}, \Phi, \mathbb{a}$ on the time scales t, $\varphi = ct\langle\nabla\rangle_0$ and $\theta = c^2 t$ from (3.5), we introduce the multiscale time derivative motivated by the chain rule of differentiation

$$\partial_{[\theta,\varphi,t]} := (c^2\partial_\theta + c\langle\nabla\rangle_0\partial_\varphi + \partial_t)$$

such that $\partial_t w(t) \simeq \partial_{[\theta,\varphi,t]}\mathbb{W}(t,\varphi,\theta)$.

Plugging the MFE ansatz (3.6) into the first order system (3.3), yields for both the MKG first order (MKGfo) system (2.33) and the MD first order (MDfo) system (2.41) the following multiscale system. For the expansion of $c\langle\nabla\rangle_c w$ we refer to Proposition A.12 and for the usage of $\langle\nabla\rangle_0^{-1}$ see Remark 2.1. Then

$$\begin{cases} c^2(i\partial_\theta + 1)\mathbb{W}_0(t,\varphi,\theta) + c\Big((i\partial_\theta + 1)\mathbb{W}_1(t,\varphi,\theta) + i\langle\nabla\rangle_0\partial_\varphi\mathbb{W}_0(t,\varphi,\theta)\Big) \\ \qquad = \sum_{n=0}^{\infty} c^{-n}\Big(- (i\partial_\theta + 1)\mathbb{W}_{n+2}(t,\varphi,\theta) - i\langle\nabla\rangle_0\partial_\varphi\mathbb{W}_{n+1}(t,\varphi,\theta) \\ \qquad\qquad - i\partial_t\mathbb{W}_n(t,\varphi,\theta) + \frac{1}{2}\Delta\mathbb{W}_n(t,\varphi,\theta) + \mathbb{F}_n(t,\varphi,\theta) + \mathbb{G}_n(t,\varphi,\theta) \\ \qquad\qquad - \sum_{\substack{m,\ell\in\mathbb{N}_0 \\ 2m+\ell=n+2 \\ m\geq 2}} \tilde{\alpha}_m(-\Delta)^m\mathbb{W}_\ell(t,\varphi,\theta)\Big), \\ c^2 i\partial_\theta\mathbb{a}_0(t,\varphi,\theta) + c\Big(i\partial_\theta\mathbb{a}_1(t,\varphi,\theta) + \langle\nabla\rangle_0(i\partial_\varphi + 1)\mathbb{a}_0(t,\varphi,\theta) - \langle\nabla\rangle_0^{-1}\mathbb{J}^P_{-1}(t,\varphi,\theta)\Big) \\ \qquad = \sum_{n=0}^{\infty} c^{-n}\Big(- i\partial_\theta\mathbb{a}_{n+2}(t,\varphi,\theta) - i\partial_t\mathbb{a}_n(t,\varphi,\theta) \\ \qquad\qquad - \langle\nabla\rangle_0(i\partial_\varphi + 1)\mathbb{a}_{n+1}(t,\varphi,\theta) + \langle\nabla\rangle_0^{-1}\mathbb{J}^P_n(t,\varphi,\theta)\Big) \\ \qquad 0 = \sum_{n=0}^{\infty} c^{-n}(-\Delta\Phi_n(t,\varphi,\theta) - \mathbb{p}_n(t,\varphi,\theta) \\ \mathbb{W}(0,0,0) = \sum_{n=0}^{\infty} c^{-n}\mathbb{W}_n(0,0,0) = \sum_{n=0}^{\infty} c^{-n} w_{I,n}, \qquad w_{I,n} = \begin{pmatrix} \psi_{I,n} - i\psi'_{I,n} \\ \overline{\psi_{I,n} - i\psi'_{I,n}} \end{pmatrix}, \\ \mathbb{a}(0,0,0) = \sum_{n=0}^{\infty} c^{-n}\mathbb{a}_n(0,0,0) = \sum_{n=0}^{\infty} c^{-n}\mathfrak{a}_{I,n}, \qquad \mathfrak{a}_{I,n} = A_{I,n} - i\langle\nabla\rangle_0^{-1}A'_{I,n}, \end{cases} \tag{3.9a}$$

where we assume that we can asymptotically expand the initial data $\psi_I, \psi'_I, A_I, A'_I$ such that

$$\begin{aligned} \psi_I &= \sum_{n=0}^{\infty} c^{-n}\psi_{I,n}, \quad \psi'_I = \sum_{n=0}^{\infty} c^{-n}\psi'_{I,n}, \\ A_I &= \sum_{n=0}^{\infty} c^{-n}A_{I,n}, \quad A'_I = \sum_{n=0}^{\infty} c^{-n}A'_{I,n}. \end{aligned} \tag{3.9b}$$

Note once more, that the structure of the nonlinearity F and thus the structure of its multiscale expansion $\mathbb{F}$ is the same in both the MKG and the MD case. Then, by definition of F in (2.33) and (2.41), respectively,

$$F[w,\phi,\mathfrak{a}] = \phi\begin{pmatrix} u \\ -v \end{pmatrix} - \frac{1}{2}\left(\phi - \langle\nabla\rangle_c^{-1}\phi\langle\nabla\rangle_c\right)\begin{pmatrix} u-\overline{v} \\ \overline{u}-v \end{pmatrix}$$
$$- \frac{1}{8}c^{-1}\langle\nabla\rangle_c^{-1}\begin{pmatrix} |\mathfrak{a}+\overline{\mathfrak{a}}|^2(u+\overline{v}) \\ |\mathfrak{a}+\overline{\mathfrak{a}}|^2(\overline{u}+v) \end{pmatrix} + i\frac{1}{2}\langle\nabla\rangle_c^{-1}\begin{pmatrix} -(\mathfrak{a}+\overline{\mathfrak{a}})\cdot\nabla(u+\overline{v}) \\ (\mathfrak{a}+\overline{\mathfrak{a}})\cdot\nabla(\overline{u}+v) \end{pmatrix}$$

together with Proposition A.12 and Proposition A.29 we obtain the coefficients $\mathbb{F}_n, n \geq 0$

$$\begin{aligned}\mathbb{F}_n =& \sum_{j=0}^{n}\Phi_j\begin{pmatrix} \mathbb{U}_{n-j} \\ -\mathbb{V}_{n-j} \end{pmatrix} + \frac{1}{2}\sum_{\substack{k,\ell,m\in\mathbb{N}_0 \\ 2(m+k)+\ell=n \\ m+k\neq 0}}\sum_{j=0}^{\ell}\tilde{\beta}_k(-\Delta)^k\left(\Phi_j\cdot\tilde{\alpha}_m(-\Delta)^m\begin{pmatrix} \mathbb{U}_{\ell-j}-\overline{\mathbb{V}_{\ell-j}} \\ \overline{\mathbb{U}_{\ell-j}}-\mathbb{V}_{\ell-j} \end{pmatrix}\right) \\ &- \frac{1}{8}\sum_{\substack{k,\ell\in\mathbb{N}_0 \\ 2k+\ell=n-2}}\sum_{j=0}^{\ell}\sum_{m=0}^{\ell-j}\tilde{\beta}_k(-\Delta)^k\begin{pmatrix} (\mathbb{a}_j+\overline{\mathbb{a}_j})\cdot(\mathbb{a}_m+\overline{\mathbb{a}_m})\cdot(\mathbb{U}_{\ell-j-m}+\overline{\mathbb{V}_{\ell-j-m}}) \\ (\mathbb{a}_j+\overline{\mathbb{a}_j})\cdot(\mathbb{a}_m+\overline{\mathbb{a}_m})\cdot(\overline{\mathbb{U}_{\ell-j-m}}+\mathbb{V}_{\ell-j-m}) \end{pmatrix} \\ &+ i\frac{1}{2}\sum_{\substack{k,\ell\in\mathbb{N}_0 \\ 2k+\ell=n-1}}\sum_{j=0}^{\ell}\tilde{\beta}_k(-\Delta)^k\begin{pmatrix} -(\mathbb{a}_j+\overline{\mathbb{a}_j})\cdot\nabla(\mathbb{U}_{\ell-j}+\overline{\mathbb{V}_{\ell-j}}) \\ (\mathbb{a}_j+\overline{\mathbb{a}_j})\cdot\nabla(\overline{\mathbb{U}_{\ell-j}}+\mathbb{V}_{\ell-j}) \end{pmatrix}.\end{aligned} \tag{3.10a}$$

In particular, the first terms $\mathbb{F}_0$ and $\mathbb{F}_1$ read

$$\mathbb{F}_0 = \Phi_0\begin{pmatrix} \mathbb{U}_0 \\ -\mathbb{V}_0 \end{pmatrix}, \quad \mathbb{F}_1 = \Phi_0\begin{pmatrix} \mathbb{U}_1 \\ -\mathbb{V}_1 \end{pmatrix} + \Phi_1\begin{pmatrix} \mathbb{U}_0 \\ -\mathbb{V}_0 \end{pmatrix} + i\frac{1}{2}\begin{pmatrix} -(\mathbb{a}_0+\overline{\mathbb{a}_0})\cdot\nabla(\mathbb{U}_0+\overline{\mathbb{V}_0}) \\ (\mathbb{a}_0+\overline{\mathbb{a}_0})\cdot\nabla(\overline{\mathbb{U}_0}+\mathbb{V}_0) \end{pmatrix}. \tag{3.10b}$$

Next, we collect the terms of same power of c in (3.9) which yields a sequence of partial differential equation for the coefficients $\mathbb{W}_n, \Phi_n, \mathbb{a}_n, n \geq 0$. Successively solving these equations, we illustrate the formal derivation of the first terms in the MFE expansion (3.6) in the subsequent Sections 3.2 and 3.3.

3.2 First Terms for the Maxwell–Klein–Gordon System

This section is based on [20–22, 45, 70] and on the paper [63] by Krämer and Schratz. Our aim is now to (formally) derive the first coefficients of the MFE expansion (3.6) for the Maxwell–Klein–Gordon system. Note that the calculations within this section are of a formal nature. A rigorous analysis for the formally derived approximations to the solution will be given later in Section 3.4. The analytic convergence results based on [20, 21, 70] are gathered in Theorem 3.3.

Recall that in case of the MKG first order system (2.33) the nonlinearity $G[w,\phi,\mathfrak{a}] \equiv 0$ vanishes. Thus, for all $n \in \mathbb{N}_0$ also the terms $\mathbb{G}_n, n \geq 0$ vanish in the multiscale system (3.9). The MFE coefficients corresponding to the nonlinear MKG charge and current density $\mathbb{p}$ and $\mathbb{J}^P$ (see (2.33) and cf. (3.8)) shall be given in the subsequent section.

3.2.1 MFE Coefficients of the Nonlinear Terms for MKG

In this section, we gather the coefficients $\mathbb{p}_n$ and $\mathbb{J}^P_{-1}, \mathbb{J}^P_n$ for $n \geq 0$ from the MFE expansion (3.8) for the Maxwell–Klein–Gordon charge and current densities

$$\rho[w] = -\frac{1}{4}\operatorname{Re}\left((u+\overline{v})c^{-1}\langle\nabla\rangle_c(\overline{u}-v)\right)$$
$$\boldsymbol{J}^P[w,\mathfrak{a}] = \mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i\frac{1}{4}(u+\overline{v})\nabla(\overline{u}+v)\right) - \frac{1}{c}\frac{1}{8}(\mathfrak{a}+\overline{\mathfrak{a}})|u+\overline{v}|^2\right],$$

given in (2.33). We carry out the derivation of the corresponding coefficients by plugging the expansion (3.6) into the latter. Propositions A.12 and A.29 then show that $\mathbb{J}^P_{-1} \equiv 0$ vanishes in the expansion (3.8), since $\boldsymbol{J}^P$ does not involve any term of order c^1. For $n \geq 0$ we thus obtain

$$\begin{aligned}
\mathbb{p}_n =& -\frac{1}{4}\sum_{j=0}^{n} \operatorname{Re}\Bigg((\mathbb{U}_j + \overline{\mathbb{V}_j}) \cdot \sum_{\substack{m,\ell\in\mathbb{N}_0 \\ 2m+\ell=n-j}} \tilde{\alpha}_m(-\Delta)^m(\overline{\mathbb{U}_\ell} - \mathbb{V}_\ell)\Bigg) \\
\mathbb{J}^P_n =& \sum_{m=0}^{n} \frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i(\mathbb{U}_m + \overline{\mathbb{V}_m})\nabla(\overline{\mathbb{U}_{n-m}} + \mathbb{V}_{n-m})\right)\right] \\
& - \sum_{j=0}^{n-1}\sum_{\ell=0}^{n-1-j} \frac{1}{8}\mathcal{P}_{\mathrm{df}}\left[(\mathbb{a}_j + \overline{\mathbb{a}_j}) \cdot (\mathbb{U}_\ell + \overline{\mathbb{V}_\ell}) \cdot (\overline{\mathbb{U}_{(n-1-j)-\ell}} + \mathbb{V}_{(n-1-j)-\ell})\right].
\end{aligned} \tag{3.11a}$$

In particular, the first coefficients for $n = 0, 1$ read

$$\begin{aligned}
\mathbb{p}_0 =& -\frac{1}{4}\operatorname{Re}\Bigg(|\mathbb{U}_0|^2 - |\mathbb{V}_0|^2 \underbrace{-\mathbb{U}_0 \cdot \mathbb{V}_0 + \overline{\mathbb{U}_0} \cdot \overline{\mathbb{V}_0}}_{\in i\mathbb{R}} \Bigg) = -\frac{1}{4}\left(|\mathbb{U}_0|^2 - |\mathbb{V}_0|^2 \right) \\
\mathbb{p}_1 =& -\frac{1}{2}\operatorname{Re}\left(\mathbb{U}_0\overline{\mathbb{U}_1} - \mathbb{V}_0\overline{\mathbb{V}_1}\right) \\
\mathbb{J}^P_0 =& \frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i(\mathbb{U}_0 + \overline{\mathbb{V}_0})\nabla(\overline{\mathbb{U}_0} + \mathbb{V}_0)\right)\right] \\
\mathbb{J}^P_1 =& \frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i(\mathbb{U}_0 + \overline{\mathbb{V}_0})\nabla(\overline{\mathbb{U}_1} + \mathbb{V}_1) + i(\mathbb{U}_1 + \overline{\mathbb{V}_1})\nabla(\overline{\mathbb{U}_0} + \mathbb{V}_0)\right)\right] \\
& - \frac{1}{8}\mathcal{P}_{\mathrm{df}}\left[(\mathbb{a}_0 + \overline{\mathbb{a}_0}) \cdot (\mathbb{U}_0 + \overline{\mathbb{V}_0}) \cdot (\overline{\mathbb{U}_0} + \mathbb{V}_0)\right].
\end{aligned} \tag{3.11b}$$

We make use of this expansion in the subsequent section.

3.2.2 First Terms for MKG

The next steps in the derivation of the nonrelativistic limit system (3.1) rely on the collection of the terms in (3.9), which correspond to the same power of c as in [45]. This procedure then leads to a sequence of partial differential equations. Successively solving the latter, then provides the MFE coefficients $(\mathbb{W}_n, \Phi_n, \mathbb{a}_n)^\top$ for all $n \geq 0$. Note that we assume boundedness with respect to c of the coefficients $\mathbb{W}_n, \Phi_n, \mathbb{a}_n$ for all $n \in \mathbb{N}_0$. We may repeatedly make use of Corollary A.27, which states a result from [45] on the solvability of differential equations for solutions of the form (3.6). More precisely, a differential equation with given inhomogeneity $g^{(a)}$ for all $a \in \mathbb{Z}$

$$(i\partial_\theta + m)W(t,\theta) = e^{im\theta}g^{(m)}(t) + \sum_{a\in\mathbb{Z}\setminus\{m\}} e^{ia\theta}g^{(a)}(t), \qquad W(0,0) \quad \text{given}, \quad m \in \mathbb{Z},$$

allows solutions W of the form $W(t,\theta) = \sum_{a\in\mathbb{Z}} e^{ia\theta}w^{(a)}(t)$, if $g^{(m)} \equiv 0$ vanishes, since $e^{im\theta}g^{(m)}(t)$ is a solution to the homogeneous equation and thus lies in the kernel of $(i\partial_\theta + m)$. See Corollary A.27 for more details.

Let us conduct this procedure for the first terms. We start off at the highest order c^2.

Order c^2: The terms of order c^2 in (3.9) admit the relation

$$\begin{aligned}
(i\partial_\theta + 1)\mathbb{W}_0(t,\varphi,\theta) =& 0, \\
i\partial_\theta\mathbb{a}_0(t,\varphi,\theta) =& 0
\end{aligned}$$

which according to Corollary A.27 allows solutions of the form

$$\begin{aligned} \mathbb{W}_0(t,\varphi,\theta) =& e^{i\theta}\widetilde{\mathbb{w}}_0^{(1)}(t,\varphi), \\ \mathbb{a}_0(t,\varphi,\theta) =& \widetilde{\mathbb{a}}_0^{(0)}(t,\varphi). \end{aligned} \tag{3.12}$$

In particular, $\mathbb{a}_0$ must be independent of θ. Note that the upper index $^{(a)}$ for $a \in \mathbb{Z}$ in the coefficients $\widetilde{\mathbb{w}}_0^{(a)}$ and $\widetilde{\mathbb{a}}_0^{(a)}$ denotes the correspondence to the phase $e^{ia\theta}$ in the fast variable $\theta = c^2 t$, see (3.6). Due to the relation $\mathbb{A}_n = \frac{1}{2}(\mathbb{a}_n + \overline{\mathbb{a}}_n)$ from (3.7), we thus have $\partial_\theta \mathbb{A}_0 = 0$. This implies that also $\mathbb{A}_0(t,\varphi,\theta) = \widetilde{\mathbb{A}}_0(t,\varphi)$ is independent of θ. In the following we may omit the superscript in $\widetilde{\mathbb{w}}_0^{(1)}$ and $\widetilde{\mathbb{a}}_0^{(0)}$ if the context is clear. The functions $\widetilde{\mathbb{w}}_0 = \widetilde{\mathbb{w}}_0^{(1)}$ and $\widetilde{\mathbb{a}}_0 = \widetilde{\mathbb{a}}_0^{(0)}$ will be determined in the successive steps.

Order c^1: At order c^1 we plug in (3.12) and obtain due to $\mathbb{J}_{-1}^P \equiv 0$ that

$$\begin{aligned} (i\partial_\theta + 1)\mathbb{W}_1(t,\varphi,\theta) =& -i\left\langle \nabla \right\rangle_0 \partial_\varphi\big(e^{i\theta}\widetilde{\mathbb{w}}_0(t,\varphi)\big), \\ i\partial_\theta \mathbb{a}_1(t,\varphi,\theta) =& -\left\langle \nabla \right\rangle_0 (i\partial_\varphi + 1)\widetilde{\mathbb{a}}_0(t,\varphi). \end{aligned} \tag{3.13}$$

We observe that the terms $\left\langle \nabla \right\rangle_0 \partial_\varphi\big(e^{i\theta}\widetilde{\mathbb{w}}_0(t,\varphi)\big)$ and $-\left\langle \nabla \right\rangle_0 (i\partial_\varphi + 1)\widetilde{\mathbb{a}}_0(t,\varphi)$ lie in the kernel of the operator $(i\partial_\theta + 1)$ and of $i\partial_\theta$, respectively. Thus, motivated by Corollary A.27, we demand that these terms vanish, i.e.

$$-i\left\langle \nabla \right\rangle_0 \partial_\varphi \widetilde{\mathbb{w}}_0(t,\varphi) \stackrel{!}{=} 0, \quad -\left\langle \nabla \right\rangle_0 (i\partial_\varphi + 1)\widetilde{\mathbb{a}}_0(t,\varphi) \stackrel{!}{=} 0.$$

This implies that $\widetilde{\mathbb{w}}_0(t,\varphi) = w_0^{(1,0)}(t)$ is independent of φ and we obtain

$$\mathbb{W}_0(t,\varphi,\theta) = e^{i\theta} w_0^{(1,0)}(t), \qquad \mathbb{a}_0(t,\varphi,\theta) = \widetilde{\mathbb{a}}_0(t,\varphi) = e^{i\varphi}\boldsymbol{a}_0^{(0,1)}(t) + C_{\mathbb{a}_0}. \tag{3.14}$$

Here, $w_0^{(1,0)}$ and $\boldsymbol{a}_0^{(0,1)}$ are the coefficients of $\mathbb{W}_0, \mathbb{a}_0$ corresponding to expansion (3.6) and $C_{\mathbb{a}_0} \in \mathbb{C}$ is a constant independent of t, φ, θ, x and in particular independent of c. We will see later that we can arbitrarily choose $C_{\mathbb{a}_0} \in \mathbb{C}$. In the following we omit the superscript and write $w_0 = w_0^{(1,0)}$ and $\boldsymbol{a}_0 = \boldsymbol{a}_0^{(0,1)}$ respectively.

The relation (3.13) for $\mathbb{W}_1, \mathbb{a}_1$ then becomes

$$\begin{aligned} (i\partial_\theta + 1)\mathbb{W}_1(t,\varphi,\theta) =& 0, \\ i\partial_\theta \mathbb{a}_1(t,\varphi,\theta) =& 0, \end{aligned}$$

which allows solutions of the form

$$\begin{aligned} \mathbb{W}_1(t,\varphi,\theta) =& e^{i\theta}\widetilde{\mathbb{w}}_1^{(1)}(t,\varphi), \\ \mathbb{a}_1(t,\varphi,\theta) =& \widetilde{\mathbb{a}}_1^{(0)}(t,\varphi), \end{aligned} \tag{3.15}$$

where $\widetilde{\mathbb{w}}_1 = \widetilde{\mathbb{w}}_1^{(1)}, \widetilde{\mathbb{a}}_1 = \widetilde{\mathbb{a}}_1^{(0)}$ are determined later on. Again, this implies that $\mathbb{A}_1 = \frac{1}{2}(\mathbb{a}_1 + \overline{\mathbb{a}_1})$ is independent of θ.

Plugging the representation (3.14) of $\mathbb{W}_0 = (\mathbb{U}_0, \mathbb{V}_0)^\top$ into (3.11), we deduce that

$$\Phi_0(t,\varphi,\theta) = \phi_0(t) \quad \text{independent of } \varphi, \theta \tag{3.16a}$$

solves

$$-\Delta\Phi_0(t,\varphi,\theta) = \mathbb{p}_0(t,\varphi,\theta) = -\frac{1}{4}\big(|u_0(t)|^2 - |v_0(t)|^2\big) =: \rho_0(t). \tag{3.16b}$$

Due to (3.11), the φ-independence of $\mathbb{W}_0$ furthermore yields the φ-independence of $\mathbb{J}_0^P$. In particular, we have

$$\begin{aligned}\mathbb{J}_0^P(t,\theta) =&\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\mathrm{Re}\left(i\big(u_0(t)\nabla\overline{u_0}(t)+\overline{v_0}(t)\nabla v_0(t)\big)\right)\right]\\ &+\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\mathrm{Re}\left(i\big(e^{2i\theta}u_0(t)\nabla v_0(t)+e^{-2i\theta}\overline{v_0}(t)\nabla\overline{u_0}(t)\big)\right)\right].\end{aligned}$$

Respecting ansatz (3.6), we thus expand $\mathbb{J}_0^P$ as follows

$$\begin{aligned}\mathbb{J}_0^P(t,\theta) =&\boldsymbol{J}_0^{(0,0)}(t)+e^{2i\theta}\boldsymbol{J}_0^{(2,0)}(t)+e^{-2i\theta}\boldsymbol{J}_0^{(-2,0)}(t),\\ \boldsymbol{J}_0^{(0,0)} =&\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\mathrm{Re}\left(i\big(u_0\nabla\overline{u_0}+\overline{v_0}\nabla v_0\big)\right)\right]\\ \boldsymbol{J}_0^{(2,0)} =&\frac{1}{8}i\mathcal{P}_{\mathrm{df}}\left[u_0\nabla v_0-v_0\nabla u_0\right]\\ \boldsymbol{J}_0^{(-2,0)} =&-\frac{1}{8}i\mathcal{P}_{\mathrm{df}}\left[\overline{u_0}\nabla\overline{v_0}-\overline{v_0}\nabla\overline{u_0}\right]=\overline{\boldsymbol{J}_0^{(2,0)}}.\end{aligned} \tag{3.17}$$

Order c^0: In view of the identities for $\mathbb{W}_j,\mathbb{a}_j, j=0,1$ in (3.14) and (3.15) and exploiting the representation of $\mathbb{F}_0$, Φ_0 and $\mathbb{J}_0^P$ in (3.10),(3.16) and (3.17) respectively and because $\mathbb{G}_n\equiv 0, n\geq 0$ in case of MKG, the terms of order c^0 in the multiscale system (3.9) admit the relation

$$\begin{aligned}&(i\partial_\theta+1)\mathbb{W}_2(t,\varphi,\theta)\\ &\quad=e^{i\theta}\left(-i\left\langle\nabla\right\rangle_0\partial_\varphi\widetilde{\mathbb{w}}_1(t,\varphi)-i\partial_t w_0(t)+\frac{1}{2}\Delta w_0(t)+\phi_0(t)\begin{pmatrix}u_0(t)\\-v_0(t)\end{pmatrix}\right),\\ &i\partial_\theta\mathbb{a}_2(t,\varphi,\theta)=-\left\langle\nabla\right\rangle_0\big(i\partial_\varphi+1\big)\widetilde{\mathbb{a}}_1(t,\varphi)-ie^{i\varphi}\partial_t\boldsymbol{a}_0(t)+\left\langle\nabla\right\rangle_0^{-1}\boldsymbol{J}_0^{(0,0)}(t)\\ &\qquad+e^{2i\theta}\left\langle\nabla\right\rangle_0^{-1}\boldsymbol{J}_0^{(2,0)}(t)+e^{-2i\theta}\left\langle\nabla\right\rangle_0^{-1}\boldsymbol{J}_0^{(-2,0)}(t).\end{aligned} \tag{3.18}$$

As before, we demand that in the latter system, the terms lying in the kernel of $(i\partial_\theta+1)$ and $i\partial_\theta$ respectively, must vanish. We obtain the relations

$$\begin{aligned}i\left\langle\nabla\right\rangle_0\partial_\varphi\widetilde{\mathbb{w}}_1(t,\varphi)&\stackrel{!}{=}\left(-i\partial_t w_0(t)+\frac{1}{2}\Delta w_0+\phi_0(t)\begin{pmatrix}u_0(t)\\-v_0(t)\end{pmatrix}\right),\\ \left\langle\nabla\right\rangle_0\big(i\partial_\varphi+1\big)\widetilde{\mathbb{a}}_1(t,\varphi)&\stackrel{!}{=}-ie^{i\varphi}\partial_t\boldsymbol{a}_0(t)+\left\langle\nabla\right\rangle_0^{-1}\boldsymbol{J}_0^{(0,0)}(t),\end{aligned} \tag{3.19}$$

which involve terms that lie in the kernel of the left hand side operators $i\left\langle\nabla\right\rangle_0\partial_\varphi$ and $\left\langle\nabla\right\rangle_0\big(i\partial_\varphi+1\big)$, respectively. Again due to Corollary A.27, we set these terms equal to zero such that for $w_0,\boldsymbol{a}_0$

$$i\partial_t w_0\stackrel{!}{=}\frac{1}{2}\Delta w_0+\phi_0\begin{pmatrix}u_0\\-v_0\end{pmatrix},\qquad i\partial_t\boldsymbol{a}_0\stackrel{!}{=}0,$$

In particular, thus $\boldsymbol{a}_0(t)=\boldsymbol{a}_0(0)$ is constant for all t. Moreover, the identity (3.14) for $\mathbb{W}_0$ and $\mathbb{a}_0$ implies the initial data (cf. (3.9))

$$w_0(0)=\mathbb{W}_0(0,0,0)=w_{I,0},\quad \boldsymbol{a}_0(0)=\mathbb{a}_0(0,0,0)-C_{\mathbb{a}_0}=\mathfrak{a}_{I,0}-C_{\mathbb{a}_0}.$$

Gathering the latter results, we obtain the following Schrödinger–Poisson system

$$\begin{cases} i\partial_t w_0=\dfrac{1}{2}\Delta w_0+\phi_0\begin{pmatrix}u_0\\-v_0\end{pmatrix}, & w_0(0)=w_{I,0}=\begin{pmatrix}\psi_{I,0}-i\psi'_{I,0}\\ \overline{\psi_{I,0}-i\psi'_{I,0}}\end{pmatrix},\\ -\Delta\phi_0=-\dfrac{1}{4}\big(|u_0|^2-|v_0|^2\big)=:\rho_0, & \end{cases} \tag{3.20}$$

with solution $(w_0,\phi_0)^\top$. Due to (3.14), the first coefficients in (3.6) then read with $C_{\mathbb{a}_0}=0$

$$\mathbb{W}_0(t,\theta)=e^{i\theta}w_0(t),\quad \mathbb{a}_0(t,\varphi,\theta)=e^{i\varphi}\mathfrak{a}_{I,0}=e^{i\varphi}(A_{I,0}-i\left\langle\nabla\right\rangle_0^{-1}A'_{I,0}). \tag{3.21}$$

Note that by virtue of Remark 2.1, the operator $\langle\nabla\rangle_0^{-1}$ is well-defined on the spaces $\dot{H}^r(\mathbb{T}^d)$ in which we are especially interested, see Definition A.3. The latter will become more clear later on, in the convergence analysis in Section 3.4 below. The identity $\mathbb{A}_0 = \frac{1}{2}(\mathfrak{a}_0 + \overline{\mathfrak{a}_0})$ and the fact that the coefficients $A_{I,n}, A'_{I,n}$ are real vector valued for all $n \in \mathbb{N}_0$ yields that

$$\mathbb{A}_0(t,\varphi,\theta) = \cos(\varphi)A_{I,0} + \frac{\sin(\varphi)}{\langle\nabla\rangle_0}A'_{I,0}. \tag{3.22}$$

Especially note that due to $\varphi = ct\langle\nabla\rangle_0$, the Fourier symbol of $\langle\nabla\rangle_0^{-1}\sin(\varphi)$ reads

$$\left(\widehat{\frac{\sin(\varphi)}{\langle\nabla\rangle_0}}\right)_k = ct\frac{\sin(ct\langle k\rangle_0)}{ct\langle k\rangle_0} = ct\,\mathrm{sinc}(ct\langle k\rangle_0) \qquad \text{for all } k\in\mathbb{Z}^d.$$

This implies, that for fixed $c \in \mathbb{R}$ and for all $t \in [0,T]$ the operator $\frac{\sin(\varphi)}{\langle\nabla\rangle_0} : H^r \to H^r$ is bounded.

Collecting (3.16), (3.20), (3.21) and (3.22) we have determined the first MFE coefficients of the expansion (3.6). They read $\mathfrak{a}_0(t,\varphi,\theta) = e^{i\varphi}\mathbf{a}_{I,0}$, $\Phi_0(t,\varphi,\theta) = \phi_0(t)$ and

$$\mathbb{W}_0(t,\varphi,\theta) = (\mathbb{U}_0(t,\varphi,\theta),\mathbb{V}_0(t,\varphi,\theta))^\top = e^{i\theta}(u_0(t),v_0(t))^\top.$$

Thus, we obtain from the identities in (3.7)

$$\Psi_0(t,\varphi,\theta) = \frac{1}{2}\left(e^{i\theta}u_0(t) + e^{-i\theta}\overline{v_0}(t)\right) \quad \text{and} \quad \mathbb{A}_0(t,\varphi,\theta) = \cos(\varphi)A_{I,0} + \frac{\sin(\varphi)}{\langle\nabla\rangle_0}A'_{I,0}.$$

Next, we continue with the derivation of higher order terms in the MFE expansion.

3.2.3 Higher Order Terms for MKG

The results of the previous section imply for the remaining terms in (3.19)

$$\begin{aligned} i\langle\nabla\rangle_0\partial_\varphi\widetilde{\mathbb{w}}_1(t,\varphi) &\overset{!}{=} 0,\\ \langle\nabla\rangle_0\left(i\partial_\varphi + 1\right)\widetilde{\mathfrak{a}}_1(t,\varphi) &\overset{!}{=} \langle\nabla\rangle_0^{-1}\boldsymbol{J}_0^{(0,0)}(t), \end{aligned}$$

which yields that $\widetilde{\mathbb{w}}_1(t,\varphi) = w_1^{(1,0)}(t)$ is independent of φ. Together with (3.15) we obtain solutions of the form

$$\begin{aligned} \mathbb{W}_1(t,\theta) &= e^{i\theta}w_1^{(1,0)}(t),\\ \widetilde{\mathfrak{a}}_1(t,\varphi) &= e^{i\varphi}\boldsymbol{a}_1^{(0,1)}(t) + \langle\nabla\rangle_0^{-2}\boldsymbol{J}_0^{(0,0)}(t) + C_{\mathfrak{a}_1} = \mathfrak{a}_1(t,\varphi,\theta), \end{aligned} \tag{3.23}$$

where $C_{\mathfrak{a}_1} \in \mathbb{C}$ is a constant independent of t, φ, θ, x and in particular independent of c. As before, the constant $C_{\mathfrak{a}_1} \in \mathbb{C}$ can be chosen arbitrarily and we set $C_{\mathfrak{a}_1} = 0$. In the following we may also write w_1 and $\boldsymbol{a}_1$ instead of $w_1^{(1,0)}$ and $\boldsymbol{a}_1^{(0,1)}$, respectively.

Moreover, the relations for $\mathbb{W}_2, \mathfrak{a}_2$ in (3.18) thus reduce to

$$\begin{aligned} (i\partial_\theta + 1)\mathbb{W}_2(t,\varphi,\theta) &= 0,\\ i\partial_\theta\mathfrak{a}_2(t,\varphi,\theta) &= e^{2i\theta}\langle\nabla\rangle_0^{-1}\boldsymbol{J}_0^{(2,0)}(t) + e^{-2i\theta}\langle\nabla\rangle_0^{-1}\boldsymbol{J}_0^{(-2,0)}(t). \end{aligned}$$

The latter allows bounded solutions of the form

$$\begin{aligned} \mathbb{W}_2(t,\varphi,\theta) &= e^{i\theta}\widetilde{\mathbb{w}}_2^{(1)}(t,\varphi)\\ \mathfrak{a}_2(t,\varphi,\theta) &= \widetilde{\mathfrak{a}}_2^{(0)}(t,\varphi) - \frac{1}{2}e^{2i\theta}\langle\nabla\rangle_0^{-1}\boldsymbol{J}_0^{(2,0)}(t) + \frac{1}{2}e^{-2i\theta}\langle\nabla\rangle_0^{-1}\boldsymbol{J}_0^{(-2,0)}(t). \end{aligned} \tag{3.24}$$

The coefficients $\widetilde{\mathbb{w}}_2^{(1)}$ and $\widetilde{\mathbb{a}}_2^{(0)}$ are determined later on. We plug the identities $\mathbb{W}_j(t,\theta) = e^{i\theta} w_j(t)$, $j = 0,1$ given in (3.21) and (3.23), respectively, into the densities $\mathbb{p}_1$ and $\mathbb{J}_1^P$ (see (3.11)) and obtain similar to (3.16) that

$$\Phi_1(t,\varphi,\theta) = \phi_1(t) \quad \text{solves} \quad -\Delta\phi_1(t) = -\frac{1}{2}\operatorname{Re}\left(u_0(t)\overline{u_1}(t) - v_0(t)\overline{v_1}(t)\right) =: \rho_1(t) \tag{3.25}$$

independent of φ and θ. Moreover, we obtain

$$\begin{aligned}\mathbb{J}_1^P(t,\varphi,\theta) =& \boldsymbol{J}_1^{(0,0)}(t) + \tilde{\mathbb{J}}_1^{(0)}(t,\varphi) \\ &+ e^{2i\theta}\Big(\boldsymbol{J}_1^{(2,0)}(t) + \tilde{\mathbb{J}}_1^{(2)}(t,\varphi)\Big) + e^{-2i\theta}\Big(\boldsymbol{J}_1^{(-2,0)}(t) + \tilde{\mathbb{J}}_1^{(-2)}(t,\varphi)\Big)\end{aligned} \tag{3.26a}$$

where the coefficients $\boldsymbol{J}_1^{(a,b)}$ are given by

$$\begin{aligned}\boldsymbol{J}_1^{(0,0)} &= \frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i\big(u_0\nabla\overline{u_1} + u_1\nabla\overline{u_0} + \overline{v_0}\nabla v_1 + \overline{v_1}\nabla v_0\big)\right)\right], \\ \boldsymbol{J}_1^{(2,0)} &= +\frac{1}{8}i\mathcal{P}_{\mathrm{df}}\left[u_0\nabla v_1 + u_1\nabla v_0 + v_0\nabla u_1 + v_1\nabla u_0\right], \\ \boldsymbol{J}_1^{(-2,0)} &= -\frac{1}{8}i\mathcal{P}_{\mathrm{df}}\left[\overline{u_0}\nabla\overline{v_1} + \overline{u_1}\nabla\overline{v_0} + \overline{v_0}\nabla\overline{u_1} + \overline{v_1}\nabla\overline{u_0}\right] = \overline{\boldsymbol{J}_1^{(2,0)}}, \\ \tilde{\mathbb{J}}_1^{(0)} &= -\frac{1}{8}\mathcal{P}_{\mathrm{df}}\left[\big(e^{i\varphi}\mathfrak{a}_{I,0} + e^{-i\varphi}\overline{\mathfrak{a}_{I,0}}\big)\cdot\big(|u_0|^2 + |v_0|^2\big)\right], \\ \tilde{\mathbb{J}}_1^{(2)} &= -\frac{1}{8}\mathcal{P}_{\mathrm{df}}\left[\big(e^{i\varphi}\mathfrak{a}_{I,0} + e^{-i\varphi}\overline{\mathfrak{a}_{I,0}}\big)\cdot u_0 v_0\right], \\ \tilde{\mathbb{J}}_1^{(-2)} &= -\frac{1}{8}\mathcal{P}_{\mathrm{df}}\left[\big(e^{i\varphi}\mathfrak{a}_{I,0} + e^{-i\varphi}\overline{\mathfrak{a}_{I,0}}\big)\cdot \overline{u_0 v_0}\right] = \overline{\tilde{\mathbb{J}}_1^{(2)}}.\end{aligned} \tag{3.26b}$$

Order c^{-1}: We exploit the relations (3.21), (3.23) and (3.24) for $\mathbb{W}_0, \mathbb{a}_0$, for $\mathbb{a}_1, \mathbb{W}_1$ and for $\mathbb{a}_2, \mathbb{W}_2$, respectively, and substitute them into $\mathbb{F}_1$ in (3.10) and into $\mathbb{J}_1^P$ in (3.26). The terms of order c^{-1} in (3.9) then read

$$\begin{aligned}&(i\partial_\theta + 1)\mathbb{W}_3(t,\varphi,\theta) \\ &\quad= e^{i\theta}\Bigg(-i\langle\nabla\rangle_0\,\partial_\varphi\widetilde{\mathbb{w}}_2^{(1)}(t,\varphi) \\ &\qquad + i\frac{1}{2}\begin{pmatrix}-(e^{i\varphi}\mathfrak{a}_{I,0})\cdot\nabla u_0(t) \\ (e^{i\varphi}\mathfrak{a}_{I,0})\cdot\nabla v_0(t)\end{pmatrix} + i\frac{1}{2}\begin{pmatrix}-(e^{-i\varphi}\overline{\mathfrak{a}_{I,0}})\cdot\nabla u_0(t) \\ (e^{-i\varphi}\overline{\mathfrak{a}_{I,0}})\cdot\nabla v_0(t)\end{pmatrix} \\ &\qquad - i\partial_t w_1(t) + \frac{1}{2}\Delta w_1(t) + \phi_0(t)\begin{pmatrix}u_1(t) \\ -v_1(t)\end{pmatrix} + \phi_1(t)\begin{pmatrix}u_0(t) \\ -v_0(t)\end{pmatrix}\Bigg) \\ &\quad + e^{-i\theta}\Bigg(i\frac{1}{2}\begin{pmatrix}-(e^{i\varphi}\mathfrak{a}_{I,0})\cdot\nabla\overline{v_0}(t) \\ (e^{i\varphi}\mathfrak{a}_{I,0})\cdot\nabla\overline{u_0}(t)\end{pmatrix} + i\frac{1}{2}\begin{pmatrix}-(e^{-i\varphi}\overline{\mathfrak{a}_{I,0}})\cdot\nabla\overline{v_0}(t) \\ (e^{-i\varphi}\overline{\mathfrak{a}_{I,0}})\cdot\nabla\overline{u_0}(t)\end{pmatrix}\Bigg) \\ &i\partial_\theta\mathbb{a}_3(t,\varphi,\theta) \\ &\quad= -\langle\nabla\rangle_0\,(i\partial_\varphi + 1)\widetilde{\mathbb{a}}_2^{(0)}(t,\varphi) + \langle\nabla\rangle_0^{-1}\boldsymbol{J}_1^{(0,0)}(t) - i\langle\nabla\rangle_0^{-2}\partial_t\boldsymbol{J}_0^{(0,0)}(t) \\ &\qquad - ie^{i\varphi}\partial_t\boldsymbol{a}_1^{(0,1)}(t) - \frac{1}{8}\langle\nabla\rangle_0^{-1}\mathcal{P}_{\mathrm{df}}\left[\big(e^{i\varphi}\mathfrak{a}_{I,0} + e^{-i\varphi}\overline{\mathfrak{a}_{I,0}}\big)\cdot\big(|u_0(t)|^2 + |v_0(t)|^2\big)\right], \\ &\qquad + e^{2i\theta}\Big(\frac{1}{2}\boldsymbol{J}_0^{(2,0)}(t) + \langle\nabla\rangle_0^{-1}\big(\boldsymbol{J}_1^{(2,0)}(t) + \tilde{\mathbb{J}}_1^{(2)}(t,\varphi)\big)\Big) \\ &\qquad + e^{-2i\theta}\Big(-\frac{1}{2}\boldsymbol{J}_0^{(-2,0)}(t) + \langle\nabla\rangle_0^{-1}\big(\boldsymbol{J}_1^{(-2,0)}(t) + \tilde{\mathbb{J}}_1^{(-2)}(t,\varphi)\big)\Big).\end{aligned} \tag{3.27}$$

The same arguments as before together with equation (3.25)

$$\phi_1(t) = \Phi_1(t,\varphi,\theta), \tag{3.28a}$$

provide the following Schrödinger–Poisson system (see [69, Theorem 1.4] for the second terms in case of nonlinear Klein–Gordon) for w_1, ϕ_1

$$\begin{cases} i\partial_t w_1 = \frac{1}{2}\Delta w_1 + \phi_0 \begin{pmatrix} u_1 \\ -v_1 \end{pmatrix} + \phi_1 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix}, \quad w_1(0) = w_{I,1} = \begin{pmatrix} \psi_{I,1} - i\psi'_{I,1} \\ \overline{\psi_{I,1} - i\psi'_{I,1}} \end{pmatrix}, \\ -\Delta\phi_1 = -\frac{1}{2}\operatorname{Re}\left(u_0\overline{u_1} - v_0\overline{v_1}\right) = \rho_1. \end{cases} \tag{3.28b}$$

The initial data $w_1(0)$ was chosen according to (3.9) and (3.23).

Furthermore, the remaining right hand side terms of (3.27) which lie in the kernel of $(i\partial_\theta + 1)$ provide a relation which determines $\widetilde{\mathbb{w}}_2^{(1)}$ (see Corollary A.27). The integration of the latter relation for $\widetilde{\mathbb{w}}_2^{(1)}$ with respect to φ, together with (3.24) then yields

$$\begin{aligned} \mathbb{W}_2(t,\varphi,\theta) =& e^{i\theta}\widetilde{\mathbb{w}}_2^{(1)}(t,\varphi) \\ =& e^{i\theta}\left(w_2^{(1,0)}(t) + i\frac{1}{2}\langle\nabla\rangle_0^{-1} \begin{pmatrix} (e^{i\varphi}\mathfrak{a}_{I,0} - e^{-i\varphi}\overline{\mathfrak{a}_{I,0}})\cdot\nabla u_0(t) \\ -(e^{i\varphi}\mathfrak{a}_{I,0} - e^{-i\varphi}\overline{\mathfrak{a}_{I,0}})\cdot\nabla v_0(t) \end{pmatrix} \right). \end{aligned}$$

Finally, the right hand side in the equation (3.27) for $\mathbb{W}_3$ reduces simplifies to terms with the phase $e^{-i\theta}$. Solving for $\mathbb{W}_3$ then yields

$$\mathbb{W}_3(t,\varphi,\theta) = e^{i\theta}\widetilde{\mathbb{w}}_3^{(1)}(t,\varphi) + i\frac{1}{4}e^{-i\theta}\begin{pmatrix} -(e^{i\varphi}\mathfrak{a}_{I,0} + e^{-i\varphi}\overline{\mathfrak{a}_{I,0}})\cdot\nabla\overline{v_0}(t) \\ (e^{i\varphi}\mathfrak{a}_{I,0} + e^{-i\varphi}\overline{\mathfrak{a}_{I,0}})\cdot\nabla\overline{u_0}(t) \end{pmatrix}.$$

Considering the equation for $\mathbb{a}_3$ in (3.27) we observe that the terms on the right hand side lying in the kernel of $i\partial_\theta$ — these are the terms not corresponding to $e^{\pm 2i\theta}$ — admit a relation for $\widetilde{\mathbb{a}}_2^{(0)}$ very similar to (3.19)

$$\begin{aligned} &\langle\nabla\rangle_0 \left(i\partial_\varphi + 1\right)\widetilde{\mathbb{a}}_2^{(0)}(t,\varphi) \\ &= \langle\nabla\rangle_0^{-1}\boldsymbol{J}_1^{(0,0)}(t) - i\langle\nabla\rangle_0^{-2}\partial_t\boldsymbol{J}_0^{(0,0)}(t) \\ &\quad - ie^{i\varphi}\partial_t\boldsymbol{a}_1^{(0,1)}(t) - \frac{1}{8}\langle\nabla\rangle_0^{-1}\mathcal{P}_{\mathrm{df}}\left[\left(e^{i\varphi}\mathfrak{a}_{I,0} + e^{-i\varphi}\overline{\mathfrak{a}_{I,0}}\right)\cdot\left(|u_0(t)|^2 + |v_0(t)|^2\right)\right]. \end{aligned}$$

Collecting the right hand side terms, corresponding to the kernel of $\langle\nabla\rangle_0\left(i\partial_\varphi + 1\right)$ then provide an equation which determines $\boldsymbol{a}_1^{(0,1)}(t)$. We proceed in the subsequent paragraph with the relations for the MFE coefficients arising from the terms of order $c^{-n}, n \geq 2$ in (3.9).

Order $c^{-n}, n \geq 2$: We have derived explicit formulas in this section for the first terms $\mathbb{W}_j, \Phi_j, \mathbb{a}_j$, $j = 0,1$ of the MKG first order system (3.9). To find higher order terms in the expansion (3.6) corresponding to c^{-n}, we iteratively solve the following system for each $n \geq 2$

$$\begin{cases} (i\partial_\theta + 1)\mathbb{W}_{n+2}(t,\varphi,\theta) + i\langle\nabla\rangle_0\partial_\varphi\mathbb{W}_{n+1}(t,\varphi,\theta) \\ \qquad = -i\partial_t\mathbb{W}_n(t,\varphi,\theta) + \frac{1}{2}\Delta\mathbb{W}_n(t,\varphi,\theta) + \mathbb{F}_n(t,\varphi,\theta) + \mathbb{G}_n(t,\varphi,\theta) \\ \qquad\quad - \sum_{\substack{m,\ell\in\mathbb{N}_0 \\ 2m+\ell=n+2 \\ m\geq 2}} \tilde{\alpha}_m(-\Delta)^m\mathbb{W}_\ell(t,\varphi,\theta) \\ i\partial_\theta\mathbb{a}_{n+2}(t,\varphi,\theta) = -\langle\nabla\rangle_0(i\partial_\varphi + 1)\mathbb{a}_{n+1}(t,\varphi,\theta) + \langle\nabla\rangle_0^{-1}\mathbb{J}_n^P(t,\varphi,\theta) \\ \qquad\quad - i\partial_t\mathbb{a}_n(t,\varphi,\theta) \\ -\Delta\Phi_n(t,\varphi,\theta) = \mathbb{p}_n(t,\varphi,\theta) \\ \mathbb{W}_n(0,0,0) = w_{I,n} = \begin{pmatrix} \psi_{I,n} - i\psi'_{I,n} \\ \overline{\psi_{I,n} - i\psi'_{I,n}} \end{pmatrix}, \\ \mathbb{a}_n(0,0,0) = \mathfrak{a}_{I,n} = A_{I,n} - i\langle\nabla\rangle_0^{-1}A'_{I,n}. \end{cases} \tag{3.29}$$

Similar to the case of nonlinear Klein–Gordon the structure of the MFE coefficients corresponding to $n \geq 2$ will be similar to those which we already derived. However, in the higher order terms the nonlinear coupling between the coefficients of $\mathbb{W}$, Φ and $\mathbb{A}$ in $\mathbb{F}_n, \mathbb{G}_n, \mathbb{p}_n, \mathbb{J}_n^P$ (cf. (3.10),(3.39),(3.11)) becomes stronger. This leads to more complicated equations for the coefficients.

3.2.4 Summary of the Asymptotic Approximation Results for MKG

In the end of this section, we collect the (formal) results on the first terms of the expansion (3.6) of the exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ to the MKG system (2.20) and $(w, \phi, \mathfrak{a})^\top$ to the MKG first order system (3.3), respectively. Moreover, we substitute the time scales $\varphi(t) = ct \langle\nabla\rangle_0$ and $\theta(t) = c^2 t$ by their definitions in (3.5) and write

$$\psi_0(t) = \Psi_0(t, \varphi(t), \theta(t)), \quad \boldsymbol{\mathcal{A}}_0(t) = \mathbb{A}(t, \varphi(t), \theta(t)), \quad \mathfrak{a}_0(t) = \mathbb{a}_0(t, \varphi(t), \theta(t)) = \widetilde{\mathbb{a}}_0(t, \varphi(t))$$

and analogously for the other MFE coefficients. Combining (3.7) and (3.14), we find

$$\psi_0(t) = \frac{1}{2}\big(e^{ic^2 t} u_0(t) + e^{-ic^2 t}\overline{v_0}(t)\big), \tag{3.30a}$$

where the non-oscillatory function $w_0 = (u_0, v_0)^\top$ together with the limit potential $\Phi_0 = \phi_0$ satisfy the Schrödinger–Poisson system (3.20). The terms $\boldsymbol{a}_0$ and $\boldsymbol{\mathcal{A}}_0$ are given by (3.21) and (3.22) respectively.

On a formal level, due to our ansatz (3.6), we thus have the (at first formal) approximation property $\psi = \psi_0 + \mathcal{O}\left(c^{-1}\right)$, and similar for the terms $\boldsymbol{\mathcal{A}}_0, \phi_0$. Solving the following Schrödinger–Poisson (3.30b) system in the nonrelativistic limit regime,

$$\begin{cases} i\partial_t w_0 = \frac{1}{2}\Delta w_0 + \phi_0 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix}, \qquad w_0(0) = w_{I,0} = \begin{pmatrix} \psi_{I,0} - i\psi'_{I,0} \\ \overline{\psi_{I,0} - i\psi'_{I,0}} \end{pmatrix}, \\ -\Delta\phi_0 = -\frac{1}{4}\left(|u_0|^2 - |v_0|^2 \right) = \rho_0, \\ \boldsymbol{a}_0(t) = e^{ic\langle\nabla\rangle_0 t}\mathfrak{a}_{I,0}, \quad \mathfrak{a}_{I,0} = A_{I,0} - i\langle\nabla\rangle_0^{-1} A'_{I,0} \\ \boldsymbol{\mathcal{A}}_0(t) = \cos(c\langle\nabla\rangle_0 t) A_{I,0} + \frac{\sin(c\langle\nabla\rangle_0 t)}{\langle\nabla\rangle_0} A'_{I,0}, \end{cases} \tag{3.30b}$$

where the initial data satisfies

$$\begin{aligned} \psi_I &= \psi_{I,0} + \mathcal{O}\left(c^{-1}\right), \qquad \psi'_I = \psi'_{I,0} + \mathcal{O}\left(c^{-1}\right), \\ A_I &= A_{I,0} + \mathcal{O}\left(c^{-1}\right), \qquad A'_I = A'_{I,0} + \mathcal{O}\left(c^{-1}\right), \end{aligned} \tag{3.31}$$

we thus obtain an approximation to the exact solution. More precisely, assuming boundedness of $\Psi_n, \mathbb{W}_n, \Phi_n, \mathbb{A}_n$ for all $n \in \mathbb{N}_0$ and for $t \in [0, T]$ in the sense of the H^r norm, we finally (formally) obtain the approximations

$$\begin{pmatrix} \psi(t) \\ \phi(t) \\ \boldsymbol{\mathcal{A}}(t) \end{pmatrix} = \begin{pmatrix} \psi_0(t) \\ \phi_0(t) \\ \boldsymbol{\mathcal{A}}_0(t) \end{pmatrix} + \mathcal{O}\left(c^{-1}\right). \tag{3.32}$$

For a rigorous convergence analysis of these approximations, we refer to [21, 22, 70] and also Theorem 4.7 below. Furthermore, we can improve this convergence to a $\mathcal{O}\left(c^{-N}\right)$ bound for $N \in \mathbb{N}$ in the sense of the H^r norm if we take into account additional higher order approximation terms in the expansion (3.6).

The truncated expansions

$$\begin{aligned}\psi_\infty^{(N_1-1)} =&\psi_0 + c^{-1}\psi_1 + \cdots + c^{-(N_1-1)}\psi_{N_1-1}\\ \phi_\infty^{(N_2-1)} =&\phi_0 + c^{-1}\phi_1 + \cdots + c^{-(N_2-1)}\phi_{N_2-1} \qquad \text{for } N_1, N_2, N_3 \in \mathbb{N}\\ \boldsymbol{\mathcal{A}}_\infty^{(N_3-1)} =&\boldsymbol{\mathcal{A}}_0 + c^{-1}\boldsymbol{\mathcal{A}}_1 + \cdots + c^{-(N_3-1)}\boldsymbol{\mathcal{A}}_{N_3-1}\end{aligned} \tag{3.33a}$$

satisfy (formally, see [45, 69] for convergence bounds of higher order approximations in the case of nonlinear Klein–Gordon equations)

$$\begin{pmatrix}\psi(t)\\ \phi(t)\\ \boldsymbol{\mathcal{A}}(t)\end{pmatrix} = \begin{pmatrix}\psi_\infty^{(N_1-1)}(t)\\ \phi_\infty^{(N_2-1)}(t)\\ \boldsymbol{\mathcal{A}}_\infty^{(N_3-1)}(t)\end{pmatrix} + \mathcal{O}\left(\begin{pmatrix}c^{-N_1}\\ c^{-N_2}\\ c^{-N_3}\end{pmatrix}\right). \tag{3.33b}$$

Thus, in order to obtain a $\mathcal{O}\left(c^{-2}\right)$ convergence bound for an approximation to the exact solution $(\psi, \phi)^\top$ of the MKG system (2.20) we proceed as follows. Additionally to solving (3.30), we also solve the system (3.28) for $w_1 = (u_1, v_1)^\top$ and ϕ_1. In order to keep notational consistency to Section 3.3 on the case of MD below, we use the notation $\tilde{\phi}_1 = \phi_1$. Afterwards, we compute

$$\psi_1(t) =\frac{1}{2}(e^{ic^2t}u_1(t) + e^{-ic^2t}\overline{v_1}(t)) \quad \text{and} \quad \tilde{\phi}_1(t) = \phi_1(t).$$

More precisely, we solve (see [69, Theorem 1.4] for the second terms in case of nonlinear Klein–Gordon equations)

$$\begin{cases} i\partial_t w_1 =\frac{1}{2}\Delta w_1 + \phi_0\begin{pmatrix}u_1\\ -v_1\end{pmatrix} + \tilde{\phi}_1\begin{pmatrix}u_0\\ -v_0\end{pmatrix},\\ -\Delta\tilde{\phi}_1 = -\frac{1}{2}\operatorname{Re}\left(u_0\cdot\overline{u_1} - v_0\cdot\overline{v_1}\right) =: \tilde{\rho}_1, w_1(0) = \quad w_{I,1}, \end{cases} \tag{3.34a}$$

where the initial data

$$w_{I,1} = w_{I,1} = \begin{pmatrix}\psi_{I,1} - i\psi'_{I,1}\\ \overline{\psi_{I,1} - i\psi'_{I,1}}\end{pmatrix} \quad \text{is given through (3.9).} \tag{3.34b}$$

Then the (formal) convergence bounds hold

$$\begin{pmatrix}\psi(t)\\ \phi(t)\\ \boldsymbol{\mathcal{A}}(t)\end{pmatrix} = \begin{pmatrix}\psi_0(t) + c^{-1}\psi_1(t)\\ \phi_0(t) + c^{-1}\phi_1(t)\\ \boldsymbol{\mathcal{A}}_0(t)\end{pmatrix} + \begin{pmatrix}\mathcal{O}\left(c^{-2}\right)\\ \mathcal{O}\left(c^{-2}\right)\\ \mathcal{O}\left(c^{-1}\right)\end{pmatrix}. \tag{3.35}$$

Despite that within this thesis, we only focus on the rigorous convergence analysis of the first order asymptotic approximation terms ([21, 22, 70]) $(\psi_0, \phi_0, \boldsymbol{\mathcal{A}}_0)^\top$ towards the exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MKG/MD system (2.20)/(2.36), we underline the latter convergence bounds (3.35) by numerical experiments in Chapter 5. A rigorous convergence analysis for higher order asymptotic approximations in case of nonlinear Klein–Gordon can be found in [45, 69].

Next, we derive the first MFE coefficients corresponding to the solution of the Maxwell–Dirac system.

3.3 First Terms for the Maxwell–Dirac System

This section is based on [20–22, 45, 70] and on the paper [63] by Krämer and Schratz. Our aim is now to (formally) derive the first terms in the MFE expansion (3.6) for the Maxwell–Dirac system. Note that the calculations within this section are of a formal nature. A rigorous analysis for the formally derived approximations to the exact solution will be given later in Section 3.4. The analytic convergence results based on [19, 22, 70] are gathered in Theorem 3.3.

The derivation of the first terms for the Maxwell–Dirac system is very similar to the previous section. Before we start off with their derivation we highlight the peculiarities of this system with respect to its first order formulation (2.41). First of all, expanding its initial value

$$w(0) = w_I = \begin{pmatrix} \left(\mathcal{I}_4 - \boldsymbol{\beta} c \left\langle \nabla \right\rangle_c^{-1}\right)\psi_I \\ \overline{\left(\mathcal{I}_4 + \boldsymbol{\beta} c \left\langle \nabla \right\rangle_c^{-1}\right)\psi_I} \end{pmatrix} + i \left\langle \nabla \right\rangle_c^{-1} \sum_{j=1}^{d} \begin{pmatrix} \boldsymbol{\alpha}_j (\nabla^{[A_I]})_j \psi_I \\ \overline{\boldsymbol{\alpha}_j (\nabla^{[A_I]})_j \psi_I} \end{pmatrix}$$

with respect to c^{-1} as $w_I = \sum_{n=0}^{\infty} c^{-n} w_{I,n}$, and recalling that $\nabla^{[A_I]} = \nabla - i\frac{A_I}{c}$, Lemma A.11 yields for $n \geq 0$

$$\begin{aligned} w_{I,n} =& \begin{pmatrix} (\mathcal{I}_4 - \boldsymbol{\beta})\psi_{I,n} \\ \overline{(\mathcal{I}_4 + \boldsymbol{\beta})\psi_{I,n}} \end{pmatrix} - \sum_{\substack{m,\ell \in \mathbb{N}_0 \\ 2m+\ell = n \\ m \geq 1}} \tilde{\beta}_m (-\Delta)^m \begin{pmatrix} \boldsymbol{\beta} \psi_{I,\ell} \\ \overline{\boldsymbol{\beta} \psi_{I,\ell}} \end{pmatrix} + \sum_{j=1}^{d} \sum_{\substack{m_1,\ell_1 \in \mathbb{N}_0 \\ 2m_1+\ell_1 = n-1}} \tilde{\beta}_{m_1} (-\Delta)^{m_1} \begin{pmatrix} i\boldsymbol{\alpha}_j \partial_j \psi_{I,\ell_1} \\ \overline{i\boldsymbol{\alpha}_j \partial_j \psi_{I,\ell_1}} \end{pmatrix} \\ &+ \sum_{j=1}^{d} \sum_{\substack{m_2,\ell_2 \in \mathbb{N}_0 \\ 2m_2+\ell_2 = n-2}} \tilde{\beta}_{m_2} (-\Delta)^{m_2} \begin{pmatrix} (A_I)_j \boldsymbol{\alpha}_j \psi_{I,\ell_2} \\ -(A_I)_j \overline{\boldsymbol{\alpha}_j \psi_{I,\ell_2}} \end{pmatrix}, \end{aligned} \tag{3.36a}$$

where the first terms in this expansion are given by

$$\begin{aligned} w_{I,0} &= \begin{pmatrix} (\mathcal{I}_4 - \boldsymbol{\beta})\psi_{I,0} \\ \overline{(\mathcal{I}_4 + \boldsymbol{\beta})\psi_{I,0}} \end{pmatrix}, \qquad w_{I,1} = \begin{pmatrix} (\mathcal{I}_4 - \boldsymbol{\beta})\psi_{I,1} \\ \overline{(\mathcal{I}_4 + \boldsymbol{\beta})\psi_{I,1}} \end{pmatrix} + \sum_{j=1}^{d} \begin{pmatrix} i\boldsymbol{\alpha}_j \partial_j \psi_{I,0} \\ \overline{i\boldsymbol{\alpha}_j \partial_j \psi_{I,0}} \end{pmatrix}, \\ w_{I,2} &= \begin{pmatrix} (\mathcal{I}_4 - \boldsymbol{\beta})\psi_{I,2} \\ \overline{(\mathcal{I}_4 + \boldsymbol{\beta})\psi_{I,2}} \end{pmatrix} + \sum_{j=1}^{d} \begin{pmatrix} \boldsymbol{\alpha}_j \left(i\partial_j \psi_{I,1} + (A_I)_j \psi_{I,0}\right) \\ \overline{\boldsymbol{\alpha}_j} \left(\overline{i\partial_j \psi_{I,1} - (A_I)_j \psi_{I,0}}\right) \end{pmatrix} - \begin{pmatrix} \frac{1}{2}\Delta \boldsymbol{\beta} \psi_{I,0} \\ \frac{1}{2}\Delta \overline{\boldsymbol{\beta} \psi_{I,0}} \end{pmatrix}. \end{aligned} \tag{3.36b}$$

In particular, this suggests the same structure for the initial data $w_{I,0} = (u_{I,0}, v_{I,0})^\top$ as in (1.29). More precisely, the decomposition

$$\psi = (\psi^+, \psi^-)^\top \quad \text{into upper and lower component functions} \quad \psi^+(t,x),\ \psi^-(t,x) \in \mathbb{C}^2,$$

together with the identity (1.22) for $\mathcal{I}_4 \pm \boldsymbol{\beta}$ yields

$$u_{I,0} = \begin{pmatrix} 0 \\ 2\psi_{I,0}^- \end{pmatrix}, \qquad v_{I,0} = \begin{pmatrix} 2\overline{\psi_{I,0}^+} \\ 0 \end{pmatrix}. \tag{3.37}$$

In the subsequent subsection, we discuss in more detail the nonlinear terms $\mathbb{G}$, $\mathbb{p}$, $\mathbb{J}^P$ which are present in the MD multiscale system (3.9).

3.3.1 MFE Coefficients of the Nonlinear Terms for MD

In this section, we collect the MFE coefficients $\mathbb{G}_n$ of the nonlinearity G and $\mathbb{p}_n$, $\mathbb{J}_n^P$ of the densities ρ and $\boldsymbol{J}^P$, corresponding to the MD system (2.41). Exploiting the relation $\frac{\partial_t}{c}\boldsymbol{\mathcal{A}} = \frac{i}{2}\left\langle \nabla \right\rangle_0 (\mathfrak{a} - \overline{\mathfrak{a}})$ from (2.39) allows us to write (cf. (2.41))

$$\mathfrak{D}^{\boldsymbol{\alpha}}[\phi, \tfrac{1}{2}(\mathfrak{a} + \overline{\mathfrak{a}})] = \tfrac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{curl}}[\mathfrak{a} + \overline{\mathfrak{a}}] + \mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{div}}[\phi] + \tfrac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_0[i\left\langle \nabla \right\rangle_0 (\mathfrak{a} - \overline{\mathfrak{a}})].$$

Substituting the latter into G in (2.41), we find

$$G[w,\phi,\mathfrak{a}] = i\frac{1}{2}\langle\nabla\rangle_c^{-1}\begin{pmatrix}\mathfrak{D}^{\boldsymbol{\alpha}}[\phi,\frac{1}{2}(\mathfrak{a}+\overline{\mathfrak{a}})]\cdot(u+\overline{v})\\ -\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}[\phi,\frac{1}{2}(\mathfrak{a}+\overline{\mathfrak{a}})]\cdot(\overline{u}+v)\end{pmatrix}.$$

Moreover, the MD first order system (2.41) involves the nonlinear densities

$$\begin{aligned}\rho[w] =& \frac{1}{4}(|u|^2+|v|^2+2\,\mathrm{Re}\,(u\cdot v)),\\ \boldsymbol{J}^P[w] =& c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[(u+\overline{v})\cdot\overline{\boldsymbol{\alpha}}(\overline{u}+v)\right].\end{aligned}$$

Plugging the multiscale variables $\mathbb{W}_n, \Phi_n, \mathbb{a}_n$ from (3.6) into G, ρ and $\boldsymbol{J}^P$, we thus find the corresponding MF coefficients in the expansion (3.8) as

$$\begin{aligned}
n\geq 0: &\qquad \mathbb{G}_n = i\frac{1}{2}\sum_{\substack{k,\ell\in\mathbb{N}_0\\ 2k+\ell=n-1}}\tilde{\beta}_k(-\Delta)^k\sum_{j=0}^{\ell}\begin{pmatrix}\mathfrak{D}^{\boldsymbol{\alpha}}[\Phi_j,\frac{1}{2}(\mathbb{a}_j+\overline{\mathbb{a}_j})]\cdot(\mathbb{U}_{\ell-j}+\overline{\mathbb{V}_{\ell-j}})\\ -\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}[\Phi_j,\frac{1}{2}(\mathbb{a}_j+\overline{\mathbb{a}_j})]\cdot(\overline{\mathbb{U}_{\ell-j}}+\mathbb{V}_{\ell-j})\end{pmatrix},\\
n\geq 0: &\qquad \mathbb{p}_n = \frac{1}{4}\sum_{j=0}^{n}\mathbb{U}_j\cdot\overline{\mathbb{U}_{n-j}}+\mathbb{V}_j\cdot\overline{\mathbb{V}_{n-j}}+2\,\mathrm{Re}\,(\mathbb{U}_j\cdot\mathbb{V}_{n-j}),\\
n\geq -1: &\qquad \mathbb{J}_n^P = \frac{1}{4}\sum_{j=0}^{n+1}\mathcal{P}_{\mathrm{df}}\left[(\mathbb{U}_j+\overline{\mathbb{V}_j})\cdot\overline{\boldsymbol{\alpha}}(\overline{\mathbb{U}_{n+1-j}}+\mathbb{V}_{n+1-j})\right].
\end{aligned}\tag{3.39a}$$

In particular, the first terms read $\mathbb{G}_0\equiv 0$ and

$$\begin{aligned}
\mathbb{G}_1 =& i\frac{1}{2}\begin{pmatrix}\mathfrak{D}^{\boldsymbol{\alpha}}[\Phi_0,\frac{1}{2}(\mathbb{a}_0+\overline{\mathbb{a}_0})]\cdot(\mathbb{U}_0+\overline{\mathbb{V}_0})\\ -\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}[\Phi_0,\frac{1}{2}(\mathbb{a}_0+\overline{\mathbb{a}_0})]\cdot(\overline{\mathbb{U}_0}+\mathbb{V}_0)\end{pmatrix},\\
\mathbb{p}_0 =& \frac{1}{4}\left(|\mathbb{U}_0|^2+|\mathbb{V}_0|^2+2\,\mathrm{Re}\,(\mathbb{U}_0\cdot\mathbb{V}_0)\right),\\
\mathbb{p}_1 =& \frac{1}{2}\,\mathrm{Re}\left(\mathbb{U}_0\cdot\overline{\mathbb{U}_1}+\mathbb{V}_0\cdot\overline{\mathbb{V}_1}+\mathbb{U}_0\cdot\mathbb{V}_1+\mathbb{U}_1\cdot\mathbb{V}_0\right),\\
\mathbb{J}_{-1}^P =& \frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\mathbb{U}_0\cdot\overline{\boldsymbol{\alpha}}\overline{\mathbb{U}_0}+\overline{\mathbb{V}_0}\cdot\overline{\boldsymbol{\alpha}}\mathbb{V}_0+\mathbb{U}_0\cdot\overline{\boldsymbol{\alpha}}\mathbb{V}_0+\overline{\mathbb{V}_0}\cdot\overline{\boldsymbol{\alpha}}\overline{\mathbb{U}_0}\right],\\
\mathbb{J}_0^P =& \frac{1}{2}\mathcal{P}_{\mathrm{df}}\left[\mathrm{Re}\left(\mathbb{U}_0\cdot\overline{\boldsymbol{\alpha}}\overline{\mathbb{U}_1}+\overline{\mathbb{V}_0}\cdot\overline{\boldsymbol{\alpha}}\mathbb{V}_1\right)\right]\\
&+\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\mathbb{U}_0\cdot\overline{\boldsymbol{\alpha}}\mathbb{V}_1+\mathbb{U}_1\cdot\overline{\boldsymbol{\alpha}}\mathbb{V}_0+\overline{\mathbb{V}_1}\cdot\overline{\boldsymbol{\alpha}}\overline{\mathbb{U}_0}+\overline{\mathbb{V}_0}\cdot\overline{\boldsymbol{\alpha}}\overline{\mathbb{U}_1}\right].
\end{aligned}\tag{3.39b}$$

Thereby, a short calculation provided that for $\xi,\eta\in\mathbb{C}^4$ we have $\overline{\xi\cdot\overline{\boldsymbol{\alpha}_j}\eta}=\eta\cdot\overline{\boldsymbol{\alpha}_j}\overline{\xi}$ exploiting the hermitian property $\boldsymbol{\alpha}_j=\overline{\boldsymbol{\alpha}_j}^\top$ for $j=1,2,3$ from (1.19). We make use of the latter MFE coefficients in the subsequent section.

3.3.2 First Terms for MD

In this section, we shall derive the first terms of the expansion (3.6) in case of the MD first order system (2.41) exploiting the multiscale system (3.9). Due to the many similarities of the systems in both cases, many steps in the derivation will be very similar in this section for the MD case as compared to Section 3.2.2 for the MKG case. We thus may omit some lengthy details and refer to Section 3.2.2 if necessary.

We now proceed as in Section 3.2.2 and collect in the multiscale system (3.9) the terms of same power of c. This provides a sequence of differential equations which shall be solved. we start off with the terms of highest order c^2.

Order c^2: The order c^2 admits as before solutions of the form (see (3.12))

$$\begin{aligned} \mathbb{W}_0(t,\varphi,\theta) =& e^{i\theta}\widetilde{\mathbb{w}}_0^{(1)}(t,\varphi), \\ \mathbb{a}_0(t,\varphi,\theta) =& \widetilde{\mathbb{a}}_0^{(0)}(t,\varphi), \end{aligned} \tag{3.40}$$

where in the following we write $\widetilde{\mathbb{w}}_0 = \widetilde{\mathbb{w}}_0^{(1)}$ and $\widetilde{\mathbb{a}}_0 = \widetilde{\mathbb{a}}_0^{(0)}$.

Order c^1: At order c^1 we find

$$\begin{aligned} (i\partial_\theta + 1)\mathbb{W}_1(t,\varphi,\theta) =& -i\langle\nabla\rangle_0\,\partial_\varphi\big(e^{i\theta}\widetilde{\mathbb{w}}_0(t,\varphi)\big), \\ i\partial_\theta\mathbb{a}_1(t,\varphi,\theta) =& -\langle\nabla\rangle_0\,(i\partial_\varphi+1)\widetilde{\mathbb{a}}_0(t,\varphi) + \langle\nabla\rangle_0^{-1}\,\mathbb{J}_{-1}^P(t,\varphi,\theta). \end{aligned} \tag{3.41}$$

Hence, we choose $\widetilde{\mathbb{w}}_0$ independent of φ such that $\mathbb{W}_0(t,\theta) = e^{i\theta}w_0^{(1,0)}(t)$, where in the following we abbreviate $w_0 = w_0^{(1,0)}$. In particular, this motivates the decomposition of $\mathbb{p}_0$ and $\mathbb{J}_{-1}^P$ from (3.39) as

$$\begin{aligned} \mathbb{J}_{-1}^P(t,\varphi,\theta) =& \boldsymbol{J}_{-1}^{(0,0)}(t) + e^{2i\theta}\boldsymbol{J}_{-1}^{(2,0)}(t) + e^{-2i\theta}\boldsymbol{J}_{-1}^{(-2,0)}(t), \\ \boldsymbol{J}_{-1}^{(0,0)} =& \frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_0\cdot\overline{\boldsymbol{\alpha}}\overline{u_0} + \overline{v_0}\cdot\overline{\boldsymbol{\alpha}}v_0\right] \\ \boldsymbol{J}_{-1}^{(2,0)} =& \frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_0\cdot\overline{\boldsymbol{\alpha}}v_0\right] \\ \boldsymbol{J}_{-1}^{(-2,0)} =& \frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\overline{v_0}\cdot\overline{\boldsymbol{\alpha}}\overline{u_0}\right], \end{aligned} \tag{3.42a}$$

and respectively

$$\begin{aligned} \mathbb{p}_0(t,\varphi,\theta) =& \rho_0^{(0,0)}(t) + e^{2i\theta}\rho_0^{(2,0)}(t) + e^{-2i\theta}\rho_0^{(-2,0)}(t), \\ \rho_0^{(0,0)}(t) =& \frac{1}{4}(|u_0|^2 + |v_0|^2), \quad \rho_0^{(2,0)}(t) = \frac{1}{4}(u_0\cdot v_0), \quad \rho_0^{(-2,0)}(t) = \frac{1}{4}(\overline{u_0}\cdot\overline{v_0}). \end{aligned} \tag{3.42b}$$

The solution to the Poisson equations $-\Delta\phi_0^{(m,0)}(t) = \rho_0^{(m,0)}(t), m = 0, \pm 2$ then define the corresponding potentials $\phi_0^{(m,0)}$ such that

$$\Phi_0(t,\varphi,\theta) = \phi_0^{(0,0)}(t) + e^{2i\theta}\phi_0^{(2,0)}(t) + e^{-2i\theta}\phi_0^{(-2,0)}(t), \tag{3.42c}$$

where we write $\phi_0 = \phi_0^{(0,0)}$ in the following. Moreover, we find that

$$\begin{aligned} \mathbb{W}_0(t,\theta) =& e^{i\theta}w_0(t), \\ \mathbb{a}_0(t,\varphi,\theta) = \widetilde{\mathbb{a}}_0(t,\varphi) =& e^{i\varphi}\boldsymbol{a}_0^{(0,1)}(t) + \langle\nabla\rangle_0^{-2}\,\boldsymbol{J}_{-1}^{(0,0)}(t). \end{aligned} \tag{3.43}$$

These findings then allow solutions to (3.41) of the form (cf. (3.24))

$$\begin{aligned} \mathbb{W}_1(t,\varphi,\theta) =& e^{i\theta}\widetilde{\mathbb{w}}_1^{(1)}(t,\varphi), \\ \mathbb{a}_1(t,\varphi,\theta) =& \widetilde{\mathbb{a}}_1^{(0)}(t,\varphi) - \frac{1}{2}e^{2i\theta}\langle\nabla\rangle_0^{-1}\boldsymbol{J}_{-1}^{(2,0)}(t) + \frac{1}{2}e^{-2i\theta}\langle\nabla\rangle_0^{-1}\boldsymbol{J}_{-1}^{(-2,0)}(t). \end{aligned}$$

The coefficients w_0, $\boldsymbol{a}_0 = \boldsymbol{a}_0^{(0,1)}$, $\widetilde{\mathbb{w}}_1 = \widetilde{\mathbb{w}}_1^{(1)}$ and $\widetilde{\mathbb{a}}_1 = \widetilde{\mathbb{a}}_1^{(0)}$ are determined in the successive steps.

Order c^0: Because $\mathbb{G}_0 = 0$ by (3.39) and from the definition of $\mathbb{F}_0$ in (3.10) together with the results on Φ_0 in (3.42), we obtain the terms of order c^0

$$
\begin{aligned}
(i\partial_\theta + 1)\mathbb{W}_2(t,\varphi,\theta) =& e^{i\theta}\Big(- i\langle\nabla\rangle_0 \partial_\varphi \widetilde{\mathbb{w}}_1(t,\varphi) \\
&- i\partial_t w_0(t) + \frac{1}{2}\Delta w_0(t) + \phi_0(t)\begin{pmatrix} u_0(t) \\ -v_0(t)\end{pmatrix} \Big) \\
&+ e^{3i\theta}\phi_0^{(2,0)}(t)\begin{pmatrix} u_0(t) \\ -v_0(t)\end{pmatrix} + e^{-i\theta}\phi_0^{(-2,0)}(t)\begin{pmatrix} u_0(t) \\ -v_0(t)\end{pmatrix} \\
i\partial_\theta \mathbb{a}_2(t,\varphi,\theta) =& - \langle\nabla\rangle_0 (i\partial_\varphi + 1)\mathbb{a}_1(t,\varphi,\theta) - i\partial_t \widetilde{\mathbb{a}}_0(t,\varphi) + \langle\nabla\rangle_0^{-1} \mathbb{J}_0^P(t,\varphi,\theta).
\end{aligned}
\tag{3.44}
$$

Because in the first equation for $\mathbb{W}_2$ the terms corresponding to $e^{i\theta}$ lie in the kernel of $(i\partial_\theta + 1)$, due to Corollary A.27, we thus demand

$$
i\langle\nabla\rangle_0 \partial_\varphi \widetilde{\mathbb{w}}_1(t,\varphi) \stackrel{!}{=} -i\partial_t w_0(t) + \frac{1}{2}\Delta w_0(t) + \phi_0(t)\begin{pmatrix} u_0(t) \\ -v_0(t)\end{pmatrix}.
$$

Since the right hand side of the latter equation does not depend on φ, it lies in the kernel of $(i\langle\nabla\rangle_0 \partial_\varphi)$. Therefore, again due to Corollary A.27 we demand

$$
i\partial_t w_0(t) = \frac{1}{2}\Delta w_0(t) + \phi_0(t)\begin{pmatrix} u_0(t) \\ -v_0(t)\end{pmatrix}. \tag{3.45}
$$

Thus, $\widetilde{\mathbb{w}}_1(t,\varphi) = w_1^{(1,0)}(t) = w_1(t)$ is independent of φ and we obtain

$$
\mathbb{W}_1(t,\varphi,\theta) = e^{i\theta} w_1(t). \tag{3.46}
$$

From $\mathbb{W}_0(t,\varphi,\theta) = e^{i\theta} w_0(t)$ given in (3.40) and due to (3.9), (3.36) and in particular due to (3.37), we obtain the initial data

$$
w_0(0) = w_{I,0} = (u_{I,0}, v_{I,0})^\top, \qquad u_{I,0} = \begin{pmatrix} 0 \\ 2\psi_{I,0}^- \end{pmatrix}, \quad v_{I,0} = \begin{pmatrix} 2\psi_{I,0}^+ \\ 0 \end{pmatrix}. \tag{3.47}
$$

Recall the decomposition of Φ_0 in (3.42c), i.e.

$$
\Phi_0(t,\varphi,\theta) = \phi_0(t) + e^{2i\theta}\phi_0^{(2,0)}(t) + e^{-2i\theta}\phi_0^{(-2,0)}(t), \tag{3.48a}
$$

where in particular ϕ_0 satisfies the Poisson equation

$$
-\Delta\phi_0(t) = \frac{1}{4}(|u_0(t)|^2 + |v_0(t)|^2) =: \rho_0(t). \tag{3.48b}
$$

In particular, by (3.51) below, the term $\phi_0^{(\pm 2,0)}(t) \equiv 0$ vanishes. Therefore, similar to (3.16) for the MKG system, we have

$$
\Phi_0(t,\varphi,\theta) = \phi_0(t) \quad \text{is independent of } \varphi, \theta. \tag{3.48c}
$$

Combining the latter relations (3.48) for ϕ_0 with Schrödinger's equation (3.45) for w_0 and plugging in the initial data $w_0(0)$ from (3.47), we arrive at the following Schrödinger–Poisson system

$$
\begin{cases}
i\partial_t w_0(t) = \frac{1}{2}\Delta w_0(t) + \phi_0(t)\begin{pmatrix} u_0(t) \\ -v_0(t)\end{pmatrix}, \quad u_0(0) = \begin{pmatrix} 0 \\ 2\psi_{I,0}^- \end{pmatrix}, \quad v_0(0) = \begin{pmatrix} 2\psi_{I,0}^+ \\ 0 \end{pmatrix}, \\
-\Delta\phi_0 = \frac{1}{4}\big(|u_0|^2 + |v_0|^2 \big) = \rho_0.
\end{cases}
\tag{3.49}
$$

Decomposing $u_0 = \begin{pmatrix} u_0^+ \\ u_0^- \end{pmatrix}$ and $v_0 = \begin{pmatrix} v_0^+ \\ v_0^- \end{pmatrix}$, respectively, into upper and lower components (see also (2.42)), we observe that $u_0^+(t) = 0 = v_0^-(t)$ are vanishing for all times t since the potential $\phi_0(t,x)$ is scalar and multiplicative. Therefore, the special structure of the initial data in (3.49) is preserved for all times t, i.e.

$$u_0(t) = \begin{pmatrix} 0 \\ u_0^-(t) \end{pmatrix}, \quad v_0(t) = \begin{pmatrix} v_0^+(t) \\ 0 \end{pmatrix} \qquad \text{for all } t. \tag{3.50}$$

Furthermore, from this structure we conclude

$$u_0 \cdot v_0 = 0, \quad u_0 \overline{\boldsymbol{\alpha}_j u_0} = 0 \quad \text{and} \quad \overline{v_0 \boldsymbol{\alpha}_j} v_0 = 0 \quad \text{for } j = 1, \ldots, d,$$

where we exploited the hermitian property of the matrices $\boldsymbol{\alpha}_j$ for $j = 1,2,3$ from (1.19). The Dirac matrices $\boldsymbol{\alpha}_j$ for $j = 1,2,3$ are given in (1.21). In particular, due to (3.39), we thus obtain

$$\boldsymbol{J}_{-1}^{(0,0)}(t) \equiv 0 \quad \text{and} \quad \phi_0^{(\pm 2,0)}(t) \equiv 0 \qquad \text{vanish} \tag{3.51}$$

which allows to simplify $\mathbb{a}_0$ in (3.43) to (cf. (3.14))

$$\mathbb{a}_0(t,\varphi,\theta) = \widetilde{\mathbb{a}}_0(t,\varphi) = e^{i\varphi}\boldsymbol{a}_0(t) + C_{\mathbb{a}_0},$$

where as before in (3.14) we can choose $C_{\mathbb{a}_0} = 0$. Recall the identities $\mathbb{W}_j(t,\varphi,\theta) = e^{i\theta} w_j(t), j = 0,1$ from (3.43) and (3.46), respectively, and recall the decomposition of $\mathbb{J}_0^P$ from (3.39)

$$\begin{aligned}
\mathbb{J}_0^P(t,\varphi,\theta) =& \boldsymbol{J}_0^{0,0}(t) + e^{2i\theta}\boldsymbol{J}_0^{2,0}(t) + e^{-2i\theta}\boldsymbol{J}_0^{-2,0}(t), \\
\boldsymbol{J}_0^{0,0}(t) =& \frac{1}{2}\mathcal{P}_{\mathrm{df}}\left[\mathrm{Re}\left(u_0 \cdot \overline{\boldsymbol{\alpha}u_1} + \overline{v_0} \cdot \overline{\boldsymbol{\alpha}} v_1, \right)\right] \\
\boldsymbol{J}_0^{2,0}(t) =& \frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_0 \cdot \overline{\boldsymbol{\alpha}} v_1 + u_1 \cdot \overline{\boldsymbol{\alpha}} v_0\right], \\
\boldsymbol{J}_0^{-2,0}(t) =& \frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[\overline{v_1} \cdot \overline{\boldsymbol{\alpha}u_0} + \overline{v_0} \cdot \overline{\boldsymbol{\alpha}u_1}\right].
\end{aligned}$$

Plugging the latter identities into equation (3.44) for $\mathbb{W}_2$ and $\mathbb{a}_2$, we find

$$\begin{aligned}
(i\partial_\theta + 1)\mathbb{W}_2(t,\varphi,\theta) =& 0 \\
i\partial_\theta \mathbb{a}_2(t,\varphi,\theta) =& -\langle\nabla\rangle_0 (i\partial_\varphi + 1)\widetilde{\mathbb{a}}_1(t,\varphi) + \langle\nabla\rangle_0^{-1} \boldsymbol{J}_0^{(0,0)}(t) \\
& - ie^{i\varphi}\partial_t \boldsymbol{a}_0(t) \\
& + e^{2i\theta}\left(\frac{1}{2}\boldsymbol{J}_{-1}^{(2,0)}(t) + \langle\nabla\rangle_0^{-1}\boldsymbol{J}_0^{(2,0)}(t)\right) \\
& + e^{-2i\theta}\left(-\frac{1}{2}\boldsymbol{J}_{-1}^{(-2,0)}(t) + \langle\nabla\rangle_0^{-1}\boldsymbol{J}_0^{(-2,0)}(t)\right).
\end{aligned} \tag{3.52}$$

As in the previous steps, we eliminate that terms on the right hand side which lie in the kernel of the operator $i\partial_\theta$ and demand

$$\langle\nabla\rangle_0 (i\partial_\varphi + 1)\widetilde{\mathbb{a}}_1(t,\varphi) \stackrel{!}{=} \langle\nabla\rangle_0^{-1} \boldsymbol{J}_0^{(0,0)}(t) - ie^{i\varphi}\partial_t \boldsymbol{a}_0(t). \tag{3.53}$$

Next, by the same argument, since $e^{i\varphi}\partial_t \boldsymbol{a}_0(t)$ lies in the kernel of $\langle\nabla\rangle_0 (i\partial_\varphi + 1)$, we require

$$\partial_t \boldsymbol{a}_0(t) = 0,$$

which implies that $\boldsymbol{a}_0(t) = \boldsymbol{a}_0(0)$ is constant for all times t. Then similar as in the case of MKG, we have (cf. (3.21))

$$\mathbb{W}_0(t,\theta) = e^{i\theta} w_0(t), \qquad \mathfrak{a}_0(t,\varphi,\theta) = e^{i\varphi}\mathfrak{a}_{I,0} = e^{i\varphi}(A_{I,0} - i\,\langle\nabla\rangle_0^{-1} A'_{I,0}). \tag{3.54}$$

Note that by virtue of Remark 2.1, the operator $\langle\nabla\rangle_0^{-1}$ is well-defined on the spaces $\dot{H}^r$, in which we are especially interested. The latter will become more clear in the convergence analysis in Section 3.4 below. Note that for all $n \in \mathbb{N}_0$ we have $A_{I,n}, A'_{I,n} \in \mathbb{R}^d$. The identity $\mathbb{A}_0 = \frac{1}{2}(\mathfrak{a}_0 + \overline{\mathfrak{a}_0})$ then implies

$$\mathbb{A}_0(t,\varphi,\theta) = \cos(\varphi) A_{I,0} + \frac{\sin(\varphi)}{\langle\nabla\rangle_0} A'_{I,0}. \tag{3.55}$$

Plugging (3.54) into (3.53), together with (3.46), this justifies the ansatz (cf. (3.43))

$$\begin{aligned} \mathbb{W}_1(t,\varphi,\theta) =& e^{i\theta} w_1(t), \\ \mathfrak{a}_1(t,\varphi,\theta) = \widetilde{\mathfrak{a}}_1(t,\varphi) =& e^{i\varphi}\boldsymbol{a}_1^{(0,1)}(t) + \langle\nabla\rangle_0^{-2} \boldsymbol{J}_0^{(0,0)}(t). \end{aligned} \tag{3.56}$$

Then (3.52) reduces to the system

$$\begin{aligned} (i\partial_\theta + 1)\mathbb{W}_2(t,\varphi,\theta) =& 0, \\ i\partial_\theta \mathfrak{a}_2(t,\varphi,\theta) =& e^{2i\theta}\Big(\frac{1}{2}\boldsymbol{J}_{-1}^{(2,0)}(t) + \langle\nabla\rangle_0^{-1} \boldsymbol{J}_0^{(2,0)}(t)\Big) \\ &+ e^{-2i\theta}\Big(-\frac{1}{2}\boldsymbol{J}_{-1}^{(-2,0)}(t) + \langle\nabla\rangle_0^{-1} \boldsymbol{J}_0^{(-2,0)}(t)\Big). \end{aligned}$$

which allows solutions of the form

$$\begin{aligned} \mathbb{W}_2(t,\varphi,\theta) =& e^{i\theta}\widetilde{\mathbb{w}}_2^{(1)}(t,\varphi), \\ \mathfrak{a}_2(t,\varphi,\theta) =& \widetilde{\mathfrak{a}}_2^{(0)}(t,\varphi) - \frac{1}{2}e^{2i\theta}\Big(\frac{1}{2}\boldsymbol{J}_{-1}^{(2,0)}(t) + \langle\nabla\rangle_0^{-1} \boldsymbol{J}_0^{(2,0)}(t)\Big) \\ &+ \frac{1}{2}e^{-2i\theta}\Big(-\frac{1}{2}\boldsymbol{J}_{-1}^{(-2,0)}(t) + \langle\nabla\rangle_0^{-1} \boldsymbol{J}_0^{(-2,0)}(t)\Big). \end{aligned}$$

The coefficients $w_1 = w_1^{(1,0)}$, $\widetilde{\mathbb{w}}_2 = \widetilde{\mathbb{w}}_2^1$, $\boldsymbol{a}_1 = \boldsymbol{a}_1^{(0,1)}$ and $\widetilde{\mathfrak{a}}_2 = \widetilde{\mathfrak{a}}_2^{(0)}$ and higher order coefficients of $\mathbb{W}, \Phi, \mathfrak{a}, \mathbb{A}$ can be determined in successive steps by solving the equations arising at higher order of c^{-n}, see Section 3.3.3 below.

Gathering the results from (3.48), (3.49), (3.54) and (3.55) yields the following Schrödinger–Poisson system (cf. (3.30) for the case of MKG)

$$\begin{cases} i\partial_t w_0 =& \frac{1}{2}\Delta w_0(t) + \phi_0(t)\begin{pmatrix} u_0(t) \\ -v_0(t)\end{pmatrix}, \quad u_0(0) = \begin{pmatrix} 0 \\ 2\psi_{I,0}^- \end{pmatrix}, \quad v_0(0) = \begin{pmatrix} 2\overline{\psi_{I,0}^+} \\ 0 \end{pmatrix}, \\ -\Delta\phi_0 =& \frac{1}{4}\big(\,|u_0|^2 + |v_0|^2\,\big) = \rho_0, \\ \boldsymbol{a}_0(t) =& e^{ic\langle\nabla\rangle_0 t}\mathfrak{a}_{I,0}, \quad \mathfrak{a}_{I,0} = A_{I,0} - i\,\langle\nabla\rangle_0^{-1} A'_{I,0}, \\ \boldsymbol{\mathcal{A}}_0(t) =& \cos(c\,\langle\nabla\rangle_0\, t)A_{I,0} + \frac{\sin(c\,\langle\nabla\rangle_0\, t)}{\langle\nabla\rangle_0} A'_{I,0}, \end{cases}$$

with solutions $w_0 = (u_0, v_0)^\top$, ϕ_0, $\boldsymbol{a}_0)^\top$. The initial data $\psi_{I,0} = (\psi_{I,0}^+, \psi_{I,0}^-)^\top$, $A_{I,0}$ and $A'_{I,0}$ are the first terms in the MFE expansion of ψ_I, A_I, A'_I (cf. (3.9)). Furthermore, similar to (3.32), the terms

$$\psi_0(t) = \frac{1}{2}(e^{ic^2 t}u_0(t) + e^{-ic^2 t}\overline{v_0}(t)), \quad \phi_0(t), \quad \boldsymbol{\mathcal{A}}_0(t)$$

(at this point formally) $\mathcal{O}\left(c^{-1}\right)$ approximation bounds to the exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MD system (2.36). A rigorous convergence analysis of these approximations in low regularity spaces can be found in [70]. We collect rigorous convergence results in Theorem 4.8. Next, we briefly discuss the derivation of higher order terms. in the subsequent section.

3.3.3 Higher Order Terms for MD

Similar to Section 3.2.2, we can extend the procedure of the previous section in order to derive explicit formulas for the higher order MFE coefficients in (3.6)

$$\mathbb{W}_n(t,\varphi,\theta), \quad \Phi_n(t,\varphi,\theta) \quad \text{and} \quad \mathbb{a}_n(t,\varphi,\theta) \qquad \text{for } n \geq 1.$$

Thereby, we successively solve the equations arising at order c^{-n} for $n \geq 1$.

Order $c^{-n}, n \geq 1$: The terms of order $c^{-n}, n \geq 1$ obey the system (3.29). However, note that in case of MKG in Section 3.2.2 the terms $\mathbb{G}_n$ did vanish, whereas in our case we refer to the definition of $\mathbb{G}_n$ in (3.39). Also the coefficients $\mathbb{p}_n$ and $\mathbb{J}_n^P$ are different to the MKG case, see Section 3.3.1.

In the following, we briefly discuss the MFE coefficients $\mathbb{W}_1$ and Φ_1. Due to the relations in (3.54) and (3.56), respectively,

$$\mathbb{W}_0(t,\varphi,\theta) = e^{i\theta}(u_0(t), v_0(t))^\top \quad \text{and} \quad \mathbb{W}_1(t,\varphi,\theta) = e^{i\theta}w_1(t) = e^{i\theta}(u_1(t), v_1(t))^\top,$$

we deduce the following Poisson equation for Φ_1 from the multiscale system (3.29) together with the definition of $\mathbb{p}_1$ in (3.39)

$$\begin{aligned} -\Delta\Phi_1(t,\varphi,\theta) = \mathbb{p}_1(t,\varphi,\theta) =& \frac{1}{2}\operatorname{Re}\left(u_0(t)\cdot\overline{u_1}(t) + v_0(t)\cdot\overline{v_1}(t)\right) \\ &+ \frac{1}{4}e^{+2i\theta}\left(u_0(t)\cdot v_1(t) + u_1(t)\cdot v_0(t)\right) \\ &+ \frac{1}{4}e^{-2i\theta}\left(\overline{u_0}(t)\cdot\overline{v_1}(t) + \overline{u_1}(t)\cdot\overline{v_0}(t)\right). \end{aligned} \tag{3.57a}$$

This manifests in a decomposition of Φ_1 as

$$\Phi_1(t,\varphi,\theta) = \phi_1^{(0,0)}(t) + e^{2i\theta}\phi_1^{(2,0)}(t) + e^{-2i\theta}\phi_1^{(-2,0)}(t), \tag{3.57b}$$

where the potentials $\phi_1^{(j,0)}$ for $j = -2, 0, 2$ solve the Poisson equations

$$-\Delta\phi_1^{(j,0)}(t) = \rho_1^{(j,0)}(t) \qquad \text{for } j = -2, 0, 2, \tag{3.57c}$$

with $\rho_1^{(j,0)}$ for $j = -2, 0, 2$ given as

$$\begin{aligned} \rho_1^{(0,0)}(t) =& \frac{1}{2}\operatorname{Re}\left(u_0(t)\cdot\overline{u_1}(t) + v_0(t)\cdot\overline{v_1}(t)\right) =: \tilde{\rho}_1(t), \\ \rho_1^{(2,0)}(t) =& \frac{1}{4}\left(u_0(t)\cdot v_1(t) + u_1(t)\cdot v_0(t)\right) \quad \text{and} \\ \rho_1^{(-2,0)}(t) =& \overline{\rho_1^{(2,0)}}(t). \end{aligned} \tag{3.57d}$$

We use the notation $\tilde{\phi}_1 = \phi_1^{(0,0)}$ and $\rho_1 = \rho_1^{(0,0)}$ in the following. Furthermore, the terms of order c^{-1} admit that w_1 solves a Schrödinger–Poisson system (see [69, Theorem 1.4] for the second terms in case of nonlinear Klein–Gordon) similar to the case of MKG (cf. (3.28))

$$\begin{cases} i\partial_t w_1 = \frac{1}{2}\Delta w_1 + \phi_0 \begin{pmatrix} u_1 \\ -v_1 \end{pmatrix} + \tilde{\phi}_1 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix} + i\frac{1}{2}\sum_{j=1}^{d}(\partial_j \phi_0)\begin{pmatrix} \alpha_j u_0 \\ -\overline{\alpha_j} v_0 \end{pmatrix}, \\ -\Delta\tilde{\phi}_1 = \frac{1}{2}\operatorname{Re}\left(u_0 \cdot \overline{u_1} + v_0 \cdot \overline{v_1}\right) = \tilde{\rho}_1, \\ w_1(0) = w_{I,1}, \end{cases} \tag{3.58a}$$

where the initial data

$$w_{I,1} = \begin{pmatrix} (\mathcal{I}_4 - \boldsymbol{\beta})\psi_{I,1} \\ (\mathcal{I}_4 + \boldsymbol{\beta})\overline{\psi_{I,1}} \end{pmatrix} + \sum_{j=1}^{d} \begin{pmatrix} i\boldsymbol{\alpha}_j \partial_j \psi_{I,0} \\ i\overline{\boldsymbol{\alpha}_j}\partial_j \overline{\psi_{I,0}} \end{pmatrix} \quad \text{are given through (3.36).} \tag{3.58b}$$

3.3.4 Summary of the Asymptotic Approximation Results for MD

In the end of this section, we collect the (formal) results on the first terms of the expansion (3.6) of the exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ to the MD system (2.36) and $(w, \phi, \mathfrak{a})^\top$ to the MD first order system (3.3), respectively. Moreover, we substitute the time scales $\varphi(t) = ct\,\langle\nabla\rangle_0$ and $\theta(t) = c^2 t$ by their definitions in (3.5) and write

$$\begin{aligned} \psi_0(t) =& \Psi_0(t, \varphi(t), \theta(t)), \qquad \boldsymbol{\mathcal{A}}_0(t) = \mathbb{A}(t, \varphi(t), \theta(t)), \\ \mathfrak{a}_0(t) =& \mathbb{a}_0(t, \varphi(t), \theta(t)) = \widetilde{\mathbb{a}}_0(t, \varphi(t)) \end{aligned}$$

and similar for the remaining terms. Combining (3.7) and (3.14), we find

$$\psi_0(t) = \frac{1}{2}\left(e^{ic^2 t}u_0(t) + e^{-ic^2 t}\overline{v_0}(t)\right), \tag{3.59a}$$

where the non-oscillatory function $w_0 = (u_0, v_0)^\top$ together with the limit potential $\Phi_0 = \phi_0$ satisfy the Schrödinger–Poisson system (3.49). The terms $\boldsymbol{a}_0$ and $\boldsymbol{\mathcal{A}}_0$ are given by (3.54) and (3.55) respectively.

On a formal level, due to our ansatz (3.6), we thus have the (at first formal) approximation property $\psi = \psi_0 + \mathcal{O}\left(c^{-1}\right)$, and similar for the terms $\boldsymbol{\mathcal{A}}_0, \phi_0$. Solving the following Schrödinger–Poisson (3.59b) system in the nonrelativistic limit regime,

$$\begin{cases} i\partial_t w_0 = \frac{1}{2}\Delta w_0(t) + \phi_0(t)\begin{pmatrix} u_0(t) \\ -v_0(t) \end{pmatrix}, \quad u_0(0) = \begin{pmatrix} 0 \\ 2\psi_{I,0}^- \end{pmatrix}, \quad v_0(0) = \begin{pmatrix} 2\overline{\psi_{I,0}^+} \\ 0 \end{pmatrix}, \\ -\Delta\phi_0 = \frac{1}{4}\left(|u_0|^2 + |v_0|^2\right) =: \rho_0, \\ \boldsymbol{a}_0(t) = e^{ic\langle\nabla\rangle_0 t}\mathfrak{a}_{I,0}, \quad \mathfrak{a}_{I,0} = A_{I,0} - i\,\langle\nabla\rangle_0^{-1} A'_{I,0}, \\ \boldsymbol{\mathcal{A}}_0(t) = \cos(c\,\langle\nabla\rangle_0 t)A_{I,0} + \frac{\sin(c\,\langle\nabla\rangle_0 t)}{\langle\nabla\rangle_0}A'_{I,0}, \end{cases} \tag{3.59b}$$

where the initial data satisfies

$$\begin{aligned} \psi_I = (\psi_I^+, \psi_I^-)^\top \quad \text{with} \quad \psi_I^+ =& \psi_{I,0}^+ + \mathcal{O}\left(c^{-1}\right), \qquad \psi_I^- = \psi_{I,0}^- + \mathcal{O}\left(c^{-1}\right), \\ A_I =& A_{I,0} + \mathcal{O}\left(c^{-1}\right), \qquad A'_I = A'_{I,0} + \mathcal{O}\left(c^{-1}\right), \end{aligned} \tag{3.59c}$$

we thus obtain an approximation to the exact solution. More precisely, assuming boundedness of $\Psi_n, \mathbb{W}_n, \Phi_n, \mathbb{A}_n$ for all $n \in \mathbb{N}_0$ and for $t \in [0, T]$ in the sense of the H^r norm, we finally (formally) obtain the approximations

$$\begin{pmatrix} \psi(t) \\ \phi(t) \\ \boldsymbol{\mathcal{A}}(t) \end{pmatrix} = \begin{pmatrix} \psi_0(t) \\ \phi_0(t) \\ \boldsymbol{\mathcal{A}}_0(t) \end{pmatrix} + \mathcal{O}\left(c^{-1}\right). \tag{3.60}$$

For a rigorous convergence analysis of these approximations, we refer to [19, 22, 70] and also Theorem 3.4. Furthermore, we can improve this convergence for a $\mathcal{O}\left(c^{-N}\right)$ bound for $N \in \mathbb{N}$ in the sense of the H^r norm if we take into account additional higher order approximation terms in the expansion (3.6). The truncated expansions

$$\begin{aligned} \psi_\infty^{(N_1-1)} &= \psi_0 + c^{-1}\psi_1 + \cdots + c^{-(N_1-1)}\psi_{N_1-1} \\ \phi_\infty^{(N_2-1)} &= \phi_0 + c^{-1}\phi_1 + \cdots + c^{-(N_2-1)}\phi_{N_2-1} \qquad \text{for } N_1, N_2, N_3 \in \mathbb{N} \\ \boldsymbol{\mathcal{A}}_\infty^{(N_3-1)} &= \boldsymbol{\mathcal{A}}_0 + c^{-1}\boldsymbol{\mathcal{A}}_1 + \cdots + c^{-(N_3-1)}\boldsymbol{\mathcal{A}}_{N_3-1} \end{aligned} \tag{3.61a}$$

satisfy (formally, see [45, 69] for convergence bounds of higher order approximations for the case of nonlinear Klein–Gordon equations)

$$\begin{pmatrix} \psi(t) \\ \phi(t) \\ \boldsymbol{\mathcal{A}}(t) \end{pmatrix} = \begin{pmatrix} \psi_\infty^{(N_1-1)}(t) \\ \phi_\infty^{(N_2-1)}(t) \\ \boldsymbol{\mathcal{A}}_\infty^{(N_3-1)}(t) \end{pmatrix} + \mathcal{O}\left(\begin{pmatrix} c^{-N_1} \\ c^{-N_2} \\ c^{-N_3} \end{pmatrix} \right). \tag{3.61b}$$

Thus, in order to obtain a $\mathcal{O}\left(c^{-2}\right)$ convergence bound for an approximation to the exact solution $(\psi, \phi)^\top$ of the MD system (2.36) we proceed as follows. Additionally to (3.59), we also solve the system (3.58) for $w_1 = (u_1, v_1)^\top$ combined with the Poisson equations for $\phi_1^{(\pm 2,0)}$ given in (3.57), and then compute

$$\begin{aligned} \psi_1(t) &= \frac{1}{2}\left(e^{ic^2t}u_1(t) + e^{-ic^2t}\overline{v_1}(t)\right) \qquad \text{and} \\ \phi_1(t) &= \tilde{\phi}_1(t) + e^{2ic^2t}\phi_1^{(2,0)} + e^{-2ic^2t}\overline{\phi_1^{(2,0)}}(t). \end{aligned} \tag{3.62a}$$

More precisely, we solve (cf. (3.34a) and see [69, Theorem 1.4] for the second terms in case of nonlinear Klein–Gordon equations)

$$\begin{cases} i\partial_t w_1 = \frac{1}{2}\Delta w_1 + \phi_0 \begin{pmatrix} u_1 \\ -v_1 \end{pmatrix} + \tilde{\phi}_1 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix} + i\frac{1}{2}\sum_{j=1}^d (\partial_j \phi_0) \begin{pmatrix} \alpha_j u_0 \\ -\overline{\alpha_j} v_0 \end{pmatrix}, \\ -\Delta \tilde{\phi}_1 = \frac{1}{2}\operatorname{Re}\left(u_0 \cdot \overline{u_1} + v_0 \cdot \overline{v_1}\right) = \tilde{\rho}_1, \\ -\Delta \phi_1^{(2,0)} = \frac{1}{4}\left(u_0 \cdot v_1 + u_1 \cdot v_0\right) \\ w_1(0) = w_{I,1}, \end{cases} \tag{3.62b}$$

where the initial data

$$w_{I,1} = \begin{pmatrix} (\mathcal{I}_4 - \boldsymbol{\beta})\psi_{I,1} \\ (\mathcal{I}_4 + \boldsymbol{\beta})\overline{\psi_{I,1}} \end{pmatrix} + \sum_{j=1}^d \begin{pmatrix} i\boldsymbol{\alpha}_j \partial_j \psi_{I,0} \\ i\overline{\boldsymbol{\alpha}_j}\overline{\partial_j \psi_{I,0}} \end{pmatrix} \quad \text{are given through (3.36),} \tag{3.62c}$$

Then the (formal) convergence bounds hold

$$\begin{pmatrix} \psi(t) \\ \phi(t) \\ \boldsymbol{\mathcal{A}}(t) \end{pmatrix} = \begin{pmatrix} \psi_0(t) + c^{-1}\psi_1(t) \\ \phi_0(t) + c^{-1}\phi_1(t) \\ \boldsymbol{\mathcal{A}}_0(t) \end{pmatrix} + \begin{pmatrix} \mathcal{O}\left(c^{-2}\right) \\ \mathcal{O}\left(c^{-2}\right) \\ \mathcal{O}\left(c^{-1}\right) \end{pmatrix}. \tag{3.63}$$

Note, that within this thesis, we only focus on the rigorous convergence analysis of the first order asymptotic approximation terms $(\psi_0, \phi_0, \boldsymbol{\mathcal{A}}_0)^\top$ towards the exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MKG/MD system (2.20)/(2.36) in the nonrelativistic limit. These results are mainly based on the papers [21, 22, 70] in which the asymptotic behaviour of the above limit systems have been extensively studied in low-regularity spaces. Additionally, we underline the latter convergence bounds by numerical experiments in Chapter 5.

A rigorous convergence analysis for higher order asymptotic approximations in case of nonlinear Klein–Gordon can be found in [45, 69].

In the current section we carried out some formal (constructive) calculations in order to derive the first MFE coefficients of the expansion (3.6). The subsequent section shows that the latter coefficients indeed satisfy rigorous analytical convergence bounds of type (3.32) and (3.60), respectively.

3.4 Rigorous Convergence Analysis for the MKG/MD First Order Limit Approximation

This section is dedicated to rigorously prove the formal convergence bounds on the first MFE coefficients of (3.6), which we formally derived in the previous section. Big parts of the proof are based on [19–22, 70], in which rigorous convergence results in low regularity spaces have been proven. Note that also in [57] the authors investigated numerically the convergence of the MD limit approximation towards the solution of the MD system in the nonrelativistic limit, however no rigorous convergence proof has been given.

We use the following convention for the notation. Let $(w, \phi, \mathfrak{a})^\top$ be the exact solution of the MKG/MD first order system (3.3) and let $(w_0, \phi_0, \boldsymbol{a}_0)^\top$ be the exact solution of the nonrelativistic limit system (3.30b) and (3.59b), respectively, i.e.

$$\begin{cases} i\partial_t w_0 = \frac{1}{2}\Delta w_0(t) + \phi_0(t)\begin{pmatrix} u_0(t) \\ -v_0(t)\end{pmatrix}, & w_0(0) = w_{I,0} = (u_{I,0}, v_{I,0})^\top \\ -\Delta\phi_0 = \rho_0 = \begin{cases} -\frac{1}{4}\left(|u_0|^2 - |v_0|^2\right), & \text{in case of MKG,} \\ \frac{1}{4}\left(|u_0|^2 + |v_0|^2\right), & \text{in case of MD,}\end{cases} \\ \boldsymbol{a}_0(t) = e^{ic\langle\nabla\rangle_0 t}\mathfrak{a}_{I,0}, \quad \mathfrak{a}_{I,0} = A_{I,0} - i\langle\nabla\rangle_0^{-1} A'_{I,0} \\ \boldsymbol{\mathcal{A}}_0(t) = \cos(c\langle\nabla\rangle_0 t)A_{I,0} + \frac{\sin(c\langle\nabla\rangle_0 t)}{\langle\nabla\rangle_0}A'_{I,0}, \end{cases}$$

with initial data (see also (3.31))

$$\begin{cases} u_{I,0} = \psi_{I,0} - i\psi'_{I,0}, & v_{I,0} = \overline{\psi_{I,0}} - i\overline{\psi'_{I,0}} & \text{in case of MKG} \\ u_{I,0} = \psi_{I,0} - i\psi'_{I,0} = \begin{pmatrix} 0 \\ 2\psi^-_{I,0}\end{pmatrix}, & v_{I,0} = \overline{\psi_{I,0}} - i\overline{\psi'_{I,0}} = \begin{pmatrix} 2\overline{\psi^+_{I,0}} \\ 0\end{pmatrix} & \text{in case of MD.}\end{cases}$$

Then for $w = (u, v)^\top$ and $w_0 = (u_0, v_0)^\top$ we have due to (2.22) and (3.30a)

$$\psi(t) = \frac{1}{2}(u(t) + \overline{v}(t)), \qquad \boldsymbol{\mathcal{A}}(t) = \frac{1}{2}(\mathfrak{a}(t) + \overline{\mathfrak{a}}(t)) \quad \text{and}$$
$$\psi_0(t) = \frac{1}{2}(e^{ic^2t}u_0(t) + e^{-ic^2t}\overline{v_0}(t)).$$

Note that due to the local well-posedness results on the MKG and MD system from Propositions 2.4 and 2.7, respectively, the following Assumption 3.1 and Assumption 3.2 hold true. Local well-posedness results for nonlinear Schrödinger and Schrödinger-Poisson systems can be found in [23, 24, 84, 86] and [1, 2, 36, 67], respectively, and references therein.

Assumption 3.1 (Regularity of the Oscillatory Solution). *Let $r > d/2$ and $r' \geq 0$. Due to Proposition 2.4, we can assume that the MKG/MD first order systems (2.33) and (2.41) with solution*

$$(w, \phi, \mathfrak{a})^\top$$

are locally well-posed in $H^{r+r'} \times \dot{H}^{r+R+r'} \times \dot{H}^{r+r'}$ with

$$R = 1 \quad \text{in case of MKG and} \qquad R = 2 \quad \text{in case of MD},$$

i.e. for initial data $w_I \in H^{r+r'}, \mathfrak{a}_I \in \dot{H}^{r+r'}$ there exist constants $T_{r+r'} > 0$ and $\mathcal{M}^{r+r'} > 0$ independent of $c \geq 1$ such that for all $0 \leq t \leq T_{r+r'}$ and for all $c \geq 1$

$$\|w(t)\|_{r+r'} + \|\phi(t)\|_{r+r'+R,0} + \|\mathfrak{a}(t)\|_{r+r',0} \leq \mathcal{M}^{r+r'}.$$

In particular, for all $0 \leq t \leq T_{r+r'}$ and for all $c \geq 1$ we can establish the separate bounds

$$\|w(t)\|_{r+r'} \leq \mathcal{M}_w^{r+r'}, \qquad \|\mathfrak{a}(t)\|_{r+r',0} \leq \mathcal{M}_{\mathfrak{a}}^{r+r'},$$

with constants $\mathcal{M}_w^{r+r'}, \mathcal{M}_{\mathfrak{a}}^{r+r'} > 0$ independent of $c \geq 1$.

Assumption 3.2 (Regularity of the Limit Solution). *Let $r > d/2$ and $r' \geq 0$. We assume that the limit systems (3.30b) and (3.59b) with solution $(w_0, \phi_0, \boldsymbol{a}_0)^\top$ corresponding to the MKG/MD first order systems (2.33) and (2.41) are locally well-posed in $H^{r+r'} \times \dot{H}^{r+2+r'} \times \dot{H}^{r+r'}$ ([1, 2, 23, 24, 36, 67, 84, 86]), i.e. for initial data $w_{I,0} \in H^{r+r'}, \mathfrak{a}_{I,0} \in \dot{H}^{r+r'}$ there exist constants $T_{r+r'} > 0$ and $\mathcal{M}_\infty^{r+r'} > 0$ such that for all $0 \leq t \leq T_{r+r'}$*

$$\|w_0(t)\|_{r+r'} + \|\phi_0(t)\|_{r+r'+2,0} + \|\boldsymbol{a}_0(t)\|_{r+r',0} \leq \mathcal{M}_\infty^{r+r'}.$$

In particular, for all $0 \leq t \leq T_{r+r'}$ and for all $c \geq 1$ we can establish the separate bounds

$$\|w_0(t)\|_{r+r'} \leq \mathcal{M}_{w_0}^{r+r'}, \qquad \|\boldsymbol{a}_0(t)\|_{r+r',0} \leq \mathcal{M}_{\boldsymbol{a}_0}^{r+r'}.$$

with constants $\mathcal{M}_{w_0}^{r+r'}, \mathcal{M}_{\boldsymbol{a}_0}^{r+r'} > 0$ independent of $c \geq 1$.

Respecting the above assumptions, we now state Theorems 3.3 and 3.4 for the convergence of the MKG/MD system (2.20)/(2.36) to the corresponding limit system (3.30b) and (3.59b). These results have been proven before by Bechouche et al. in [21, 22] and also by Masmoudi and Nakanishi in [70]. Furthermore for the proof of Theorem 3.3 in the MKG case, see also the paper [63] by Krämer and Schratz.

Also recall the definition of the spaces H^r, $\dot{H}^r$ and $\mathcal{P}_{\text{df}} H^r$ in Definitions A.1, A.3 and A.13.

Theorem 3.3 (see [21, 63, 70] and also [69], MKG Limit Convergence). *Let $r > d/2$. Let the initial data of the MKG system (2.20) satisfy*

$$\psi_I, \psi_{I,0}, \psi_{I,1}, \psi_I', \psi_{I,0}', \psi_{I,1}' \in H^{r+4} \quad \text{and} \quad A_I, A_{I,0} \in \mathcal{P}_{\text{df}} H^{r+1}, \quad A_I', A_{I,0}' \in \mathcal{P}_{\text{df}} H^r \tag{3.65}$$

such that

$$\|\psi_I - \psi_{I,0}\|_{r+4} + \left\|\psi_I' - \psi_{I,0}'\right\|_{r+4} + \|A_I - A_{I,0}\|_{r+1} + \left\|A_I' - A_{I,0}'\right\|_r \leq K_I^1 c^{-1}$$

and additionally

$$\left\|\psi_I - (\psi_{I,0} + c^{-1}\psi_{I,1})\right\|_{r+4} + \left\|\psi'_I - (\psi'_{I,0} + c^{-1}\psi'_{I,1})\right\|_{r+4} \leq K_I^2 c^{-2},$$

where $K_I^1, K_I^2 > 0$ *do not depend on* c.

Then for all $t \in [0,T]$ *we obtain the convergence result*[①].

$$\begin{aligned}
\left\|w(t) - e^{ic^2t}w_0(t)\right\|_r &\leq K_{w_0}^{\text{MKG}}\Big(\|\psi_I - \psi_{I,0}\|_r + \left\|\psi'_I - \psi'_{I,0}\right\|_r + c^{-2}\Big),\\
\|\phi(t) - \phi_0(t)\|_{r+2,0} &\leq K_{\phi_0}^{\text{MKG}}\Big(\|\psi_I - \psi_{I,0}\|_r + \left\|\psi'_I - \psi'_{I,0}\right\|_r + c^{-2}\Big),\\
\|\mathfrak{a}(t) - \boldsymbol{a}_0(t)\|_{r,0} &\leq K_{\boldsymbol{a}_0}^{\text{MKG}} c^{-1},
\end{aligned}$$

where the constants $K_{w_0}^{\text{MKG}}, K_{\boldsymbol{a}_0}^{\text{MKG}}, K_{\phi_0}^{\text{MKG}}$ *only depend on* $\mathcal{M}_w^{r+4}, \mathcal{M}_{w_0}^{r+4}, \mathcal{M}_{\mathfrak{a}}^{r+1}, \mathcal{M}_{\boldsymbol{a}_0}^{r+1}$ *and on* d *and* T *but not on* c.

In particular this result shows that if additionally $\psi_{I,1}$ *and* $\psi'_{I,1}$ *asymptotically vanish, i.e. if*

$$\|\psi_I - \psi_{I,0}\|_r + \left\|\psi'_I - \psi'_{I,0}\right\|_r \leq K_2 c^{-2},$$

then we obtain an $\mathcal{O}\left(c^{-2}\right)$ *convergence bound for* w_0 *and* ϕ_0 *(cf. [69]), i.e.*

$$\left\|w(t) - e^{ic^2t}w_0(t)\right\|_r + \|\phi(t) - \phi_0(t)\|_{r+2,0} \leq c^{-2}\cdot K \cdot (K_{w_0}^{\text{MKG}} + K_{\phi_0}^{\text{MKG}}),$$

with constants $K, K_{w_0}^{\text{MKG}}, K_{\phi_0}^{\text{MKG}}$ *independent of* c.

Theorem 3.4 (see [22, 70], MD Limit Convergence)**.** *Let* $r > d/2$. *Let the initial data of the MD system* (2.36) *satisfy*

$$\psi_I, \psi_{I,0}, \psi_{I,1} \in H^{r+4} \quad \text{and} \quad A_I, A_{I,0} \in \mathcal{P}_{\text{df}}H^{r+1}, \quad A'_I, A'_{I,0} \in \mathcal{P}_{\text{df}}H^r$$

such that

$$\|\psi_I - \psi_{I,0}\|_{r+4} + \|A_I - A_{I,0}\|_{r+1} + \left\|A'_I - A'_{I,0}\right\|_r \leq K_I c^{-1},$$

where $K_I > 0$ *is independent of* c. *Then for all* $t \in [0,T]$ *we obtain the convergence result*

$$\begin{aligned}
\left\|w(t) - e^{ic^2t}w_0(t)\right\|_r &\leq K_{w_0}^{\text{MD}} c^{-1},\\
\|\phi(t) - \phi_0(t)\|_{r+2,0} &\leq K_{\phi_0}^{\text{MD}} c^{-1},\\
\|\mathfrak{a}(t) - \boldsymbol{a}_0(t)\|_{r,0} &\leq K_{\boldsymbol{a}_0}^{\text{MD}} c^{-1},
\end{aligned}$$

where the constants $K_{w_0}^{\text{MD}}, K_{\boldsymbol{a}_0}^{\text{MD}}, K_{\phi_0}^{\text{MD}}$ *only depend on* $\mathcal{M}_w^{r+4}, \mathcal{M}_{w_0}^{r+4}, \mathcal{M}_{\mathfrak{a}}^{r+1}, \mathcal{M}_{\boldsymbol{a}_0}^{r+1}$ *and on* d *and* T *but not on* c.

Before we prove this theorem we collect some auxiliary results. We carry out the analysis by considering Duhamel's formula (see for instance [85, Proposition 1.35] and also (A.20)) for the solution $(w, \phi, \mathfrak{a})^\top$ of the MKG first order system (2.33) and the MD first order system (2.41), respectively. We obtain

[①] Note that we can measure the convergence of ϕ_0 towards ϕ in $\dot{H}^{r+2}$, since due to the assumption (3.65) $\psi_I, \psi'_I \in H^{r+4}$ on the initial data of the MKG system (2.20), we have that $\phi(t) \in \dot{H}^{r+5}$ (see Proposition 2.4) rigorous error estimates for the corresponding asymptotic approximations by comparing the latter to the Duhamel solution $(e^{ic^2t}w_0, \phi_0, \boldsymbol{a}_0)^\top$ of the corresponding limit systems (3.30b) and (3.59b), respectively, respecting the corresponding oscillatory phases e^{ic^2t}.

Because the basic ideas for deriving these error bounds are very similar in both the MKG and MD case, we carry out the analysis for both systems simultaneously and point out the differences explicitly. Furthermore similar to the previous section we collect the MKG/MD first order systems (2.33) and (2.41) in the combined system (3.3), i.e.

$$\begin{cases} i\partial_t w = -c\langle\nabla\rangle_c w + F[w,\phi,\mathfrak{a}] + G[w,\phi,\mathfrak{a}], \qquad w(0) = w_I = \begin{pmatrix} \psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'} \end{pmatrix} \\ -\Delta\phi = \rho[w] \\ i\partial_t \mathfrak{a} = -c\langle\nabla\rangle_0 \mathfrak{a} + \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P[w,\mathfrak{a}], \qquad \mathfrak{a}(0) = \mathfrak{a}_I = A_I - i\langle\nabla\rangle_0^{-1} A_I'. \end{cases} \tag{3.66}$$

Analogously we collect the MKG/MD asymptotic systems (3.30b) and (3.59b) in the system

$$\begin{cases} i\partial_t w_0 = \frac{1}{2}\Delta w_0 + \phi_0 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix}, \qquad w_0(0) = w_{I,0} = \begin{pmatrix} \psi_{I,0} - i\psi_{I,0}' \\ \overline{\psi_{I,0} - i\psi_{I,0}'} \end{pmatrix}, \\ -\Delta\phi_0 = \rho_0, \\ \boldsymbol{a}_0(t) = e^{itc\langle\nabla\rangle_0}\mathfrak{a}_{I,0}, \quad \mathfrak{a}_{I,0} = A_{I,0} - i\langle\nabla\rangle_0^{-1} A_{I,0}'. \end{cases} \tag{3.67}$$

We point out that the main differences between the MKG case (see (2.33) and (3.30b)) and the MD case (see (2.41) and (3.59b)) basically are due to different definitions of the nonlinear terms $G, \rho, \boldsymbol{J}^P, \rho_0$ and also in the initial data w_I and $w_{I,0}$. However, the definition of F in terms of $w, \phi, \mathfrak{a}$ is the same in both cases, which allows us to transfer the main ideas for the error analysis between the two systems.

In the following, we illustrate the ideas for establishing the bounds on $\left\|w(t) - e^{ic^2t}w_0(t)\right\|_r$. The bound for $\|\mathfrak{a}(t) - \boldsymbol{a}_0(t)\|_r$ is based on similar techniques.

First we establish bounds of type

$$\left\|w(t) - e^{ic^2t}w_0(t)\right\|_r \leq \|w_I - w_{I,0}\|_r + c^{-2}K_1 + K_2\int_0^t \left\|w(s) - e^{ic^2s}w_0(s)\right\|_r ds,$$

where the constants $K_1, K_2 > 0$ are independent of c. Then Gronwall's Lemma (see for instance [85, Theorem 1.10] and also Lemma A.21) shows that

$$\left\|w(t) - e^{ic^2t}w_0(t)\right\|_r \leq \Big(\|w_I - w_{I,0}\|_r + c^{-2}K_1\Big)e^{tK_2}.$$

Due to the identities $w = (u,v)^\top$, $w_0 = (u_0, v_0)^\top$ and

$$\psi(t) = \frac{1}{2}\left(u(t) + \overline{v}(t)\right) \quad \text{and} \quad \psi_0(t) = \frac{1}{2}\left(e^{ic^2t}u_0(t) + e^{-ic^2t}\overline{v_0}(t)\right),$$

(see (2.22),(3.30a),(3.59a)), we have that

$$\|\psi(t) - \psi_0(t)\|_r \leq 2\left\|w(t) - e^{ic^2t}w_0(t)\right\|_r.$$

In particular, by the assumptions on the initial data we have in the MKG case for constants $\tilde{K}_1, \tilde{K}_2 > 0$ independent of c that

$$\|w_I - w_{I,0}\|_r \leq \tilde{K}_1 c^{-1} \qquad \text{if } \psi_{I,1}, \psi_{I,1}' \neq 0 \tag{3.68}$$

and

$$\|w_I - w_{I,0}\|_r \le \tilde{K}_2 c^{-2} \qquad \text{if } \psi_{I,1} = 0 = \psi'_{I,1} \text{ vanish.}$$

In the MD case we find the desired c^{-1} by establishing a bound on the initial data as in (3.68). This finally yields the assertion. The interested reader gets details of the proof in the following subsections.

3.4.1 Proof of the Limit Approximation Results Theorems 3.3 and 3.4

This section is based on the paper [63] by Krämer and Schratz in which a proof for the approximation results in case of MKG was already given. Additionally some ideas and parts of the proof are taken from [19–22, 70], see also [45]. In the latter papers the authors analysed the convergence of the limit systems (3.30b) and (3.59b), respectively, to the MKG/MD systems (2.20)/(2.36) in low regularity spaces, respecting the highly oscillatory phases e^{ic^2t}.

We apply Duhamel's perturbation formula (see for instance [85, Proposition 1.35] and also Proposition A.20) to the systems (3.66) and (3.67) which yields

$$\begin{aligned}
w(t) &= \mathcal{T}^{t}_{[c\langle\nabla\rangle_c]} w_I - i\int_0^t \mathcal{T}^{t-s}_{[c\langle\nabla\rangle_c]} \Big(F\big[w(s),\phi(s),\boldsymbol{\mathcal{A}}(s)\big] + G\big[w(s),\phi(s),\boldsymbol{\mathcal{A}}(s)\big]\Big) ds,\\
e^{ic^2t} w_0(t) &= \mathcal{T}^{t}_{[c^2-\frac12\Delta]} w_{I,0} - i\int_0^t \mathcal{T}^{t-s}_{[c^2-\frac12\Delta]} \left(\phi_0(s) e^{ic^2 s} \begin{pmatrix} u_0(s) \\ -v_0(s)\end{pmatrix} \right) ds,\\
\mathfrak{a}(t) &= \mathcal{T}^{t}_{[c\langle\nabla\rangle_0]} \mathfrak{a}_I - i\int_0^t \mathcal{T}^{t-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P\big[w(s),\mathfrak{a}(s)\big] ds,\\
\mathfrak{a}_0(t) &= \mathcal{T}^{t}_{[c\langle\nabla\rangle_0]} \mathfrak{a}_{I,0},
\end{aligned} \tag{3.69}$$

where we have used the notation from Lemma A.10, i.e.

$$\mathcal{T}^{t}_{[A]} \coloneqq e^{itA} \qquad \text{for } A \text{ being an operator of type } c\langle\nabla\rangle_c \tag{3.70}$$

which allows us to write $\mathcal{T}^{t}_{[c^2-\frac12\Delta]} \coloneqq e^{ic^2t}\mathcal{T}^{t}_{[-\frac12\Delta]}$. The definition of F in (2.33) and (2.41) admits to write

$$F[w,\phi,\mathfrak{a}] = \phi\begin{pmatrix} u \\ -v\end{pmatrix} + i\frac12 \langle\nabla\rangle_c^{-1} \begin{pmatrix} -(\mathfrak{a}+\overline{\mathfrak{a}})\cdot\nabla(u+\overline{v}) \\ (\mathfrak{a}+\overline{\mathfrak{a}})\cdot\nabla(\overline{u}+v)\end{pmatrix} + \mathcal{R}_F,$$

with a remainder term

$$\mathcal{R}_F \coloneqq -\frac12\big(\phi - \langle\nabla\rangle_c^{-1}\phi\langle\nabla\rangle_c\big)\begin{pmatrix} u-\overline{v} \\ \overline{u}-v\end{pmatrix} - \frac18 c^{-1}\langle\nabla\rangle_c^{-1}\begin{pmatrix} |\mathfrak{a}+\overline{\mathfrak{a}}|^2(u+\overline{v}) \\ |\mathfrak{a}+\overline{\mathfrak{a}}|^2(\overline{u}+v)\end{pmatrix},$$

which we already can bound in H^r by terms of order $\mathcal{O}\left(c^{-2}\right)$ as explained in the following. The application of the bilinear estimates from Lemma A.8 and the usage of Lemma A.11 shows that

$$\left\|\big(\phi - \langle\nabla\rangle_c^{-1}\phi\langle\nabla\rangle_c\big)w\right\|_r \le Kc^{-2}\|\phi\|_{r+2}\|w\|_{r+2}, \qquad \left\||\mathfrak{a}|^2 w\right\|_r \le K\|\mathfrak{a}\|_r^2\|w\|_r.$$

Therefore by Assumption 3.1 the remainder $\mathcal{R}_F$ satisfies for $s\le t\le T$ for some $T>0$

$$\|\mathcal{R}_F(s)\|_r \le c^{-2}K_{\mathcal{R}_F}\big(\mathcal{M}_w^{r+2},\mathcal{M}_{\mathfrak{a}}^r\big). \tag{3.72}$$

In the following, we may write $F(s), G(s), \boldsymbol{J}^P(s)$ instead of $F\big[w(s),\phi(s),\boldsymbol{\mathcal{A}}(s)\big]$, $G\big[w(s),\phi(s),\boldsymbol{\mathcal{A}}(s)\big]$ and $\boldsymbol{J}^P\big[w(s),\mathfrak{a}(s)\big]$, respectively. Furthermore, for easier notation we use the abbreviations

$$\mathfrak{e}_{w_0}(t) \coloneqq w(t) - e^{ic^2t}w_0(t) \qquad \text{and} \qquad \mathfrak{e}_{\mathfrak{a}_0}(t) \coloneqq \mathfrak{a}(t) - \mathfrak{a}_0(t).$$

Duhamel's formula (3.69) for w and w_0 yields that

$$
\begin{aligned}
\|\mathfrak{e}_{w_0}(t)\|_r \leq\ & \left\| \mathcal{T}^{t}_{[c\langle\nabla\rangle_c]} w_I - \mathcal{T}^{t}_{[c^2-\frac{1}{2}\Delta]} w_{I,0} \right\|_r \\
&+ \left\| \int_0^t \mathcal{T}^{t-s}_{[c\langle\nabla\rangle_c]} F(s) - \mathcal{T}^{t-s}_{[c^2-\frac{1}{2}\Delta]} \left(\phi_0(s) e^{ic^2 s} \begin{pmatrix} u_0(s) \\ -v_0(s) \end{pmatrix} \right) ds \right\|_r \\
&+ \left\| \int_0^t \mathcal{T}^{t-s}_{[c\langle\nabla\rangle_c]} G(s) ds \right\|_r .
\end{aligned}
$$

An application of the bound

$$
\left\| \mathcal{T}^{t}_{[c\langle\nabla\rangle_c]} \tilde{w} - \mathcal{T}^{t}_{[c^2-\frac{1}{2}\Delta]} \tilde{w}_0 \right\|_r \leq \|\tilde{w} - \tilde{w}_0\|_r + c^{-2} |t| \, \|\tilde{w}_0\|_{r+4} \quad \text{for } \tilde{w} \in H^r, \tilde{w}_0 \in H^{r+4} \tag{3.73}
$$

to the first and second integral term implies that

$$
\begin{aligned}
\|\mathfrak{e}_{w_0}(t)\|_r \leq\ & \|w_I - w_{I,0}\|_r + c^{-2} t \, \|w_{I,0}\|_{r+4} \\
&+ \left\| \int_0^t \mathcal{T}^{t-s}_{[c\langle\nabla\rangle_c]} \left(\phi(s) \begin{pmatrix} u(s) \\ -v(s) \end{pmatrix} \right) - \mathcal{T}^{t-s}_{[c^2-\frac{1}{2}\Delta]} \left(\phi_0(s) e^{ic^2 s} \begin{pmatrix} u_0(s) \\ -v_0(s) \end{pmatrix} \right) ds \right\|_r \\
&+ \left\| \int_0^t \mathcal{T}^{t-s}_{[c\langle\nabla\rangle_c]} \frac{1}{2} \langle\nabla\rangle_c^{-1} \begin{pmatrix} -(\mathfrak{a}(s) + \overline{\mathfrak{a}}(s)) \cdot \nabla(u(s) + \overline{v}(s)) \\ (\mathfrak{a}(s) + \overline{\mathfrak{a}}(s)) \cdot \nabla(\overline{u}(s) + v(s)) \end{pmatrix} ds \right\|_r \\
&+ \left\| \int_0^t \mathcal{T}^{t-s}_{[c\langle\nabla\rangle_c]} \mathcal{R}_F(s) ds \right\|_r \\
&+ \left\| \int_0^t \mathcal{T}^{t-s}_{[c\langle\nabla\rangle_c]} G(s) ds \right\|_r .
\end{aligned}
$$

Recall that by Lemma A.10 the operators $\mathcal{T}^{t}_{[c\langle\nabla\rangle_c]}$ and $\mathcal{T}^{t}_{[c^2-\frac{1}{2}\Delta]}$ are isometries in H^r. Hence, combining the latter inequality with the bounds of (3.72) and (3.73), this implies the following intermediate result

$$
\begin{aligned}
\|\mathfrak{e}_{w_0}(t)\|_r \leq\ & \|w_I - w_{I,0}\|_r \\
&+ c^{-2} t \, \|w_{I,0}\|_{r+4} + c^{-2} t K_{\mathcal{R}_F} + c^{-2} \int_0^t (t-s) \left\| \phi_0(s) \begin{pmatrix} u_0(s) \\ -v_0(s) \end{pmatrix} \right\|_{r+4} ds \\
&+ \int_0^t \left\| \phi(s) \begin{pmatrix} u(s) \\ -v(s) \end{pmatrix} - \phi_0(s) e^{ic^2 s} \begin{pmatrix} u_0(s) \\ -v_0(s) \end{pmatrix} \right\|_r ds \qquad (3.74a) \\
&+ \left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_c]} \langle\nabla\rangle_c^{-1} \begin{pmatrix} -(\mathfrak{a}(s) + \overline{\mathfrak{a}}(s)) \cdot \nabla(u(s) + \overline{v}(s)) \\ (\mathfrak{a}(s) + \overline{\mathfrak{a}}(s)) \cdot \nabla(\overline{u}(s) + v(s)) \end{pmatrix} ds \right\|_r \qquad (3.74b) \\
&+ \left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_c]} G(s) ds \right\|_r . \qquad (3.74c)
\end{aligned}
$$

Employing the definition of ϕ_0 in the limit systems (3.30b) and (3.59b) and applying the bilinear estimates Lemma A.8, we immediately obtain that

$$
c^{-2} \int_0^t s \left\| \phi_0(s) \begin{pmatrix} u_0(s) \\ -v_0(s) \end{pmatrix} \right\|_{r+4} ds \leq c^{-2} t^2 K \cdot (\mathcal{M}^{r+4}_{w_0})^3 . \tag{3.75}
$$

Similarly we have that

$$
\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0} \leq \|\mathfrak{a}_I - \mathfrak{a}_{I,0}\|_{r,0} + \left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P \left[w(s), \mathfrak{a}(s) \right] ds \right\|_{r,0} . \tag{3.76}
$$

We divide the further analysis into several parts. In the subsequent subsections the remaining integral terms (3.74a), (3.74b) and (3.74c) in the above estimate shall be bounded seperately in the subsequent subsections. We begin with an estimate for the term (3.74a).

Estimate for Term (3.74a)

Due to the bilinear estimate $\|uv\|_r \leq K\|u\|_r\|v\|_r$ (see Lemma A.8) we obtain for $\mathfrak{e}_{w_0}(t) := w(t) - e^{ic^2t}w_0(t)$

$$\left\|\phi(s)w(s) - \phi_0(s)e^{ic^2s}w_0(s)\right\|_r \leq \|\phi(s)-\phi_0(s)\|_{r,0}\|w(s)\|_r + \|\phi_0(s)\|_{r,0}\|\mathfrak{e}_{w_0}(s)\|_r\,. \tag{3.77}$$

Recall that

$$\rho = \begin{cases} -\frac{1}{4}\operatorname{Re}\big((u+\overline{v})c^{-1}\langle\nabla\rangle_c(\overline{u}-v)\big), & \text{given in (2.33) in case of MKG,}\\ \frac{1}{4}(|u|^2+|v|^2+2\operatorname{Re}(u\cdot v)), & \text{given in (2.41) in case of MD,}\end{cases}$$

and that

$$\rho_0 = \begin{cases} -\frac{1}{4}\big(|u_0|^2-|v_0|^2\big), & \text{given in (3.30b) in case of MKG,}\\ \frac{1}{4}\big(|u_0|^2+|v_0|^2\big), & \text{given in (3.59b) in case of MD.}\end{cases}$$

First we give an estimate for the MKG case. From the definition of the solution operator $\dot{\Delta}^{-1}$ (see Appendix A.4) to Poisson's equations

$$-\Delta\phi = \rho \qquad \text{and} \qquad -\Delta\phi_0 = \rho_0$$

and by the estimate on $\|\rho(s)-\rho_0(s)\|_{r,0}$ given in Proposition 3.5 for the MKG case we have

$$\begin{aligned}\|\phi(s)-\phi_0(s)\|_{r+2,0} &= \big\|\dot{\Delta}^{-1}(\rho(s)-\rho_0(s))\big\|_{r+2,0} \leq \|\rho(s)-\rho_0(s)\|_{r,0}\\ &\leq K\|\rho(s)-\rho_0(s)\|_r\\ &\leq c^{-2}K_\phi^1\big(\mathcal{M}_w^{r+2},\mathcal{M}_{w_0}^r\big) + K_\phi\big(\mathcal{M}_w^{r+1},\mathcal{M}_{w_0}^r\big)\|\mathfrak{e}_{w_0}(s)\|_r\,.\end{aligned} \tag{3.78}$$

Similarly, we establish the following bound in the MD case, exploiting the estimate on $\|\rho(s)-\rho_0(s)\|_{r,0}$ from Proposition 3.7

$$\|\phi(s)-\phi_0(s)\|_{r+2,0} \leq K_\phi\big(\mathcal{M}_w^r,\mathcal{M}_{w_0}^r\big)\|\mathfrak{e}_{w_0}(s)\|_r\,. \tag{3.79}$$

Thus, combining the bound in (3.77) with the bounds (3.78) and (3.79), respectively, in the MKG case as well as in the MD case, we obtain the bound

$$[\text{term (3.74a)}] \leq c^{-2}K^1_{(3.74a)}\big(\mathcal{M}_w^{r+2},\mathcal{M}_{w_0}^r\big) + K^2_{(3.74a)}\big(\mathcal{M}_w^r,\mathcal{M}_{w_0}^r\big)\int_0^t\|\mathfrak{e}_{w_0}(s)\|_r\,ds. \tag{3.80}$$

Note that the constants $K^1_{(3.74a)}$ and $K^2_{(3.74a)}$ only depend on the regularity of w and w_0 (see Assumption 3.1 and Assumption 3.2) and that $K^1_{(3.74a)} = 0$ in case of MD due to (3.79).

Next, we establish a bound on the integral term (3.74b).

Estimate for Term (3.74b)

The idea for estimating the integral term (3.74b), i.e.

$$\left\|\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_c]}\langle\nabla\rangle_c^{-1}\begin{pmatrix}-(\mathfrak{a}(s)+\overline{\mathfrak{a}}(s))\cdot\nabla(u(s)+\overline{v}(s))\\ (\mathfrak{a}(s)+\overline{\mathfrak{a}}(s))\cdot\nabla(\overline{u}(s)+v(s))\end{pmatrix}ds\right\|_r,$$

relies on "inserting zeros" and then applying integration by parts. More precisely, we expand the terms of type $\mathfrak{a}\cdot\nabla(u+\overline{v})$ by adding and subtracting additional terms such that

$$\langle\nabla\rangle_c^{-1}\Big(\mathfrak{a}\cdot\nabla(u+\overline{v})\Big) = \langle\nabla\rangle_c^{-1}\Big((\mathfrak{a}-\boldsymbol{a}_0)\cdot\nabla(u+\overline{v})\Big) \tag{3.81a}$$

$$+\langle\nabla\rangle_c^{-1}\Big(\boldsymbol{a}_0\cdot\nabla(u-e^{ic^2s}u_0+\overline{v}-e^{-ic^2s}\overline{v_0})\Big) \tag{3.81b}$$

$$+\langle\nabla\rangle_c^{-1}\Big(\boldsymbol{a}_0\cdot\nabla(e^{ic^2s}u_0+e^{-ic^2s}\overline{v_0})\Big). \tag{3.81c}$$

In the analysis of these terms, we repeatedly exploit that by Lemma A.10 the operator $\mathcal{T}^{t}_{[c\langle\nabla\rangle_c]}$ is an isometry in H^r. Furthermore, for the first and second of the three terms, (3.81a) and (3.81b), we use the estimates $\left\|\langle\nabla\rangle_c^{-1} w\right\|_r \le c^{-1}\|w\|_r$ for the first and $\left\|\langle\nabla\rangle_c^{-1} w\right\|_r \le K\|w\|_{r-1}$ for the second term (see Lemma A.5 and Lemma A.11 respectively). The application of the bilinear estimates $\|uv\|_{r-j}\le K\|u\|_r\|v\|_{r-j}, j=0,1$ from Lemma A.8 yields

$$\begin{aligned}\int_0^t\left\|\langle\nabla\rangle_c^{-1}\Big((\mathfrak{a}(s)-\boldsymbol{a}_0(s))\cdot\nabla(u(s)+\overline{v}(s))\Big)\right\|_r ds\\ \le c^{-1}K\mathcal{M}_w^{r+1}\int_0^t\|\mathfrak{a}(s)-\boldsymbol{a}_0(s)\|_{r,0}\,ds\end{aligned} \tag{3.82}$$

and

$$\begin{aligned}\int_0^t\left\|\langle\nabla\rangle_c^{-1}\Big(\boldsymbol{a}_0(s)\cdot\nabla(u(s)-e^{ic^2s}u_0(s)+\overline{v}(s)-e^{-ic^2s}\overline{v_0}(s))\Big)\right\|_r ds\\ \le K\mathcal{M}_{\boldsymbol{a}_0}^r\int_0^t\left\|w(s)-e^{ic^2s}w_0(s)\right\|_r ds.\end{aligned} \tag{3.83}$$

For the last term (3.81c), we prove that $\left\|\int_0^t\mathcal{T}^{-s}_{[c\langle\nabla\rangle_c]}(\text{term (3.81c)})ds\right\|_r\le Kc^{-2}$ via integration by parts, where we treat the terms involving $e^{ic^2s}u_0(s)$ and $e^{-ic^2s}\overline{v_0}(s)$ separately.

Using the notation $\mathcal{T}^t_{[c\langle\nabla\rangle_c]}=e^{itc\langle\nabla\rangle_c}$ (see (3.70)) we have that

$$e^{\pm ic^2s}\mathcal{T}^{-s}_{[c\langle\nabla\rangle_c]}=e^{is(\pm c^2-c\langle\nabla\rangle_c)}=\mathcal{T}^{s}_{[\pm c^2-c\langle\nabla\rangle_c]}.$$

According to Lemma A.11, we furthermore have that $\left\|(c^2+c\langle\nabla\rangle_c)^{-1}w\right\|_r\le Kc^{-2}\|w\|_r$ and that $\left\|(c^2-c\langle\nabla\rangle_c)w\right\|_r\le K\|w\|_{r+2}$. Thus, we can exploit that the integration of the term $\mathcal{T}^{s}_{[-c^2-c\langle\nabla\rangle_c]}$ with respect to s provides a factor of c^{-2} without losing regularity, and we make use of the fact that the operator $\partial_s(\mathcal{T}^{s}_{[+c^2-c\langle\nabla\rangle_c]})$ is bounded from H^{r+2} to H^r with respect to c.

More precisely, on the one hand, the term involving $e^{-ic^2s}\overline{v_0}(s)$ then becomes

$$\begin{aligned}&\int_0^t\mathcal{T}^{s}_{[-c^2-c\langle\nabla\rangle_c]}\langle\nabla\rangle_c^{-1}\Big(\boldsymbol{a}_0(s)\cdot\nabla\overline{v_0}(s)\Big)ds\\ &=\Big[i(c^2+c\langle\nabla\rangle_c)^{-1}\mathcal{T}^{s}_{[-c^2-c\langle\nabla\rangle_c]}\langle\nabla\rangle_c^{-1}\Big(\boldsymbol{a}_0(s)\cdot\nabla\overline{v_0}(s)\Big)\Big]_{s=0}^t\\ &\quad-i\int_0^t\mathcal{T}^{s}_{[-c^2-c\langle\nabla\rangle_c]}(c^2+c\langle\nabla\rangle_c)^{-1}\langle\nabla\rangle_c^{-1}\Big(\partial_s\boldsymbol{a}_0(s)\cdot\nabla\overline{v_0}(s)+\boldsymbol{a}_0(s)\cdot\nabla\partial_s\overline{v_0}(s)\Big)ds.\end{aligned}$$

Using that by (3.30b) and (3.59b), respectively, the derivatives $\partial_s\boldsymbol{a}_0$ and $\partial_s w_0$ satisfy

$$i\partial_s\boldsymbol{a}_0(s)=-c\langle\nabla\rangle_0\boldsymbol{a}_0(s)\quad\text{and}\quad i\partial_s w_0(s)=\frac{1}{2}\Delta w_0(s)+\phi_0(s)\begin{pmatrix}u_0(s)\\ v_0(s)\end{pmatrix}$$

and because of $\left\| c \langle \nabla \rangle_c^{-1} w \right\|_r \leq \|w\|_r$ (see Lemma A.11), we thus find

$$\begin{aligned} &\left\| \int_0^t \mathcal{T}^s_{[-c^2 - c\langle \nabla \rangle_c]} \langle \nabla \rangle_c^{-1} \Big(\boldsymbol{a}_0(s) \cdot \nabla \overline{v_0}(s) \Big) ds \right\|_r \\ &\leq c^{-2} K \cdot \Big(\mathcal{M}^r_{\boldsymbol{a}_0} \mathcal{M}^r_{w_0} + t \Big(\mathcal{M}^{r+1}_{\boldsymbol{a}_0} \mathcal{M}^{r+1}_{w_0} + \mathcal{M}^r_{\boldsymbol{a}_0} (\mathcal{M}^{r+2}_{w_0} + (\mathcal{M}^r_{w_0})^3) \Big) \Big). \end{aligned} \tag{3.84}$$

On the other hand, by integration of $\boldsymbol{a}_0(s)$ (see (3.30b) and (3.59b) respectively) we get

$$\begin{aligned} &\int_0^t \mathcal{T}^s_{[+c^2 - c\langle \nabla \rangle_c]} \langle \nabla \rangle_c^{-1} \Big(\boldsymbol{a}_0(s) \cdot \nabla u_0(s) \Big) ds \\ &= \Big[\mathcal{T}^s_{[+c^2 - c\langle \nabla \rangle_c]} \langle \nabla \rangle_c^{-1} \Big(\big((ic \langle \nabla \rangle_0)^{-1} \boldsymbol{a}_0(s) \big) \cdot \nabla u_0(s) \Big) \Big]_{s=0}^t \\ &\quad - i \int_0^t \mathcal{T}^s_{[+c^2 - c\langle \nabla \rangle_c]} (+c^2 - c \langle \nabla \rangle_c) \langle \nabla \rangle_c^{-1} \Big(\big((ic \langle \nabla \rangle_0)^{-1} \boldsymbol{a}_0(s) \big) \cdot \nabla u_0(s) \Big) ds \\ &\quad - \int_0^t \mathcal{T}^s_{[+c^2 - c\langle \nabla \rangle_c]} \langle \nabla \rangle_c^{-1} \big((ic \langle \nabla \rangle_0)^{-1} \boldsymbol{a}_0(s) \big) \cdot \nabla \partial_s u_0(s) \Big) ds. \end{aligned}$$

Exploiting that $\left\| c^{-1} \langle \nabla \rangle_c^{-1} w \right\|_r \leq c^{-2} \|w\|_r$, the latter can be bounded by

$$\begin{aligned} &\left\| \int_0^t \mathcal{T}^s_{[+c^2 - c\langle \nabla \rangle_c]} \langle \nabla \rangle_c^{-1} \Big(\boldsymbol{a}_0(s) \cdot \nabla u_0(s) \Big) ds \right\|_r \\ &\leq c^{-2} K \cdot \Big(\mathcal{M}^{r-1}_{\boldsymbol{a}_0} \mathcal{M}^{r+1}_{w_0} + t \Big(\mathcal{M}^{r+1}_{\boldsymbol{a}_0} \mathcal{M}^{r+3}_{w_0} + \mathcal{M}^{r-1}_{\boldsymbol{a}_0} (\mathcal{M}^{r+3}_{w_0} + (\mathcal{M}^{r+1}_{w_0})^3) \Big) \Big). \end{aligned} \tag{3.85}$$

Collecting the results in (3.82),(3.83), (3.84) and (3.85) and applying the triangle inequality, allows us to establish the bound

$$\begin{aligned} &[\text{term (3.74b)}] \\ &\leq c^{-2} K^1_{(3.74b)} (t, \mathcal{M}^{r+1}_{\boldsymbol{a}_0}, \mathcal{M}^{r+3}_{w_0}) + K^2_{(3.74b)} (\mathcal{M}^{r+1}_{w}) \int_0^t c^{-1} \|\mathfrak{e}_{\boldsymbol{a}_0}(s)\|_{r,0} \, ds \\ &\quad + K^3_{(3.74b)} (\mathcal{M}^r_{\boldsymbol{a}_0}) \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r \, ds, \end{aligned} \tag{3.86}$$

where the constants $K^2_{(3.74b)}, K^3_{(3.74b)}$ only depend on the regularity of $w, \boldsymbol{a}_0$ and w_0, and $K^1_{(3.74b)}$ additionally linearly on time t, see Assumption 3.1 and Assumption 3.2.

In a next step, we bound the last integral term (3.74c).

Estimate for Term (3.74c)

In case of MKG the term (3.74c) vanishes, since $G \equiv 0$ (see (2.33)). Therefore, considering the MKG system only, we may continue in the subsequent subsection.

In the MD case however, we observe that the nonlinear term G in (2.41) involves terms of type

$$\langle \nabla \rangle_c^{-1} \Big(\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{curl}}[\mathfrak{a}] + \mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\phi] + \frac{1}{2} \mathfrak{D}^{\boldsymbol{\alpha}}_0 [i \langle \nabla \rangle_0 (\mathfrak{a})] \Big) (u + \overline{v}).$$

Recall that by Definition 2.6 we have that for $\tilde{\mathfrak{a}}(x) = (\tilde{\mathfrak{a}}_1(x), \ldots, \tilde{\mathfrak{a}}_d(x))^\top \in \mathbb{C}^d$ and $\tilde{\phi}(x) \in \mathbb{C}$

$$\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{curl}}[\tilde{\mathfrak{a}}] = -\frac{1}{2} \sum_{\substack{j,k=1 \\ j\neq k}}^{d} \boldsymbol{\alpha}_j \boldsymbol{\alpha}_k [(\partial_j(\tilde{\mathfrak{a}}_k)) - (\partial_k(\tilde{\mathfrak{a}}_j))],$$

$$\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\tilde{\phi}] = \sum_{j=1}^{d} \boldsymbol{\alpha}_j(\partial_j \tilde{\phi}) \qquad \text{and} \qquad \mathfrak{D}^{\boldsymbol{\alpha}}_0[\tilde{\mathfrak{a}}] = \sum_{j=1}^{d} \boldsymbol{\alpha}_j(\tilde{\mathfrak{a}}_j).$$

The property $\left\| \langle \nabla \rangle_c^{-1} w \right\|_r \leq c^{-1} \|w\|_r$ for $w \in H^r$ from Lemma A.11 and the application of the bilinear estimate $\|uv\|_r \leq K \|u\|_r \|v\|_r$ for $u, v \in H^r$ from Lemma A.8, then immediately allows us to bound the term (3.74c), i.e.

$$\left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_c]} G(s) ds \right\|_r \leq c^{-1} t K \cdot \mathcal{M}^r_w \big(\mathcal{M}^{r+1}_{\mathfrak{a}} + (\mathcal{M}^r_w)^2\big) := c^{-1} K_G(t, \mathcal{M}^{r+1}_{\mathfrak{a}}, \mathcal{M}^r_w). \tag{3.87}$$

We now collect the bounds (3.80), (3.86) and (3.87), respectively on the corresponding integral terms in (3.74) and arrive at an intermediate result in the subsequent paragraph.

Intermediate Result

Plugging the bounds (3.80), (3.86) and (3.87), respectively, into the error estimate (3.74) above, we obtain

$$\begin{aligned} \|\mathfrak{e}_{w_0}(t)\|_r \leq \|w_I - w_{I,0}\|_r &+ c^{-1} K_G(t, \mathcal{M}^{r+1}_{\mathfrak{a}}, \mathcal{M}^r_w) \\ &+ c^{-2} K_{c^{-2}}(t, t^2, \mathcal{M}^{r+4}_{w_0}, \mathcal{M}^{r+2}_w, \mathcal{M}^{r+1}_{\boldsymbol{a}_0}, \mathcal{M}^r_{\mathfrak{a}}) \\ &+ K_{\text{int}}(\mathcal{M}^r_{w_0}, \mathcal{M}^r_w, \mathcal{M}^r_{\boldsymbol{a}_0}) \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r \, ds \\ &+ K^2_{(3.74b)}\big(\mathcal{M}^{r+1}_w\big) \int_0^t c^{-1} \|\mathfrak{e}_{\boldsymbol{a}_0}(s)\|_{r,0} \, ds, \end{aligned} \tag{3.88}$$

where the constant $K_{c^{-2}}$ depends on the constants $K^1_{(3.74a)}, K^1_{(3.74b)}$ and on additional constants in front of c^{-2} given in (3.74) and (3.75). The constant K_{int} depends on $K^2_{(3.74a)}, K^3_{(3.74b)}$. Recall that in case of MKG $K_G = 0$ vanishes, since $G \equiv 0$.

Observe that if we can bound the last integral in (3.88) such that

$$\int_0^t c^{-1} \|\mathfrak{e}_{\boldsymbol{a}_0}(s)\|_{r,0} \, ds \leq K(c^{-1} \|\mathfrak{a}_I - \mathfrak{a}_{I,0}\|_{r,0} + c^{-2} + \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r \, ds), \tag{3.89}$$

then Gronwall's Lemma (see for instance [85, Theorem 1.10] and also Lemma A.21) yields the desired results of Theorems 3.3 and 3.4, i.e.

$$\|\mathfrak{e}_{w_0}(t)\|_r \leq K \cdot \Big(\|w_I - w_{I,0}\|_r + c^{-1} K_G + \big(c^{-1} \|\mathfrak{a}_I - \mathfrak{a}_{I,0}\|_{r,0} + c^{-2}\big) \Big), \tag{3.90}$$

where K only depends on t and on the regularity of $w_0, w, \boldsymbol{a}_0, \mathfrak{a}$ (see Assumption 3.1 and Assumption 3.2).

We determine the bound of type (3.89) separately in the following subsections for MKG and for MD. We shall see in Section 3.4.2 below, that the final arguments in proving Theorem 3.3 underlie a straight forward calculation. Applying Gronwall's Lemma (see for instance [85, Theorem 1.10] and also Lemma A.21) to the term $\|\mathfrak{e}_{\boldsymbol{a}_0}\|_r$ immediately yields the desired bound (3.89) and thus also (3.90).

However, in the MD case (see Section 3.4.3 below), we need a bootstrap argument[2] to reach the bound of type (3.90). We proceed with the MKG case.

3.4.2 Final Arguments in Proving Theorem 3.3 (MKG Limit Approximation)

Let us first discuss the case of MKG. Recall that from (3.76)

$$\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0} \leq \|\mathfrak{a}_I - \mathfrak{a}_{I,0}\|_{r,0} + \left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P\left[w(s), \mathfrak{a}(s)\right] ds \right\|_{r,0}, \tag{3.91}$$

with $\boldsymbol{J}^P$ given in (2.33)

$$\boldsymbol{J}^P\left[w, \mathfrak{a}\right] = \mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i\frac{1}{4}(u+\overline{v})\nabla(\overline{u}+v)\right) - \frac{1}{c}\frac{1}{8}(\mathfrak{a}+\overline{\mathfrak{a}})\left|u+\overline{v}\right|^2\right].$$

Our aim is now to play back the error $\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0}$ for $\boldsymbol{a}_0$ to an error $\|\mathfrak{e}_{w_0}(t)\|_r$ in w_0, i.e.

$$\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0} \leq \|\mathfrak{a}_I - \mathfrak{a}_{I,0}\|_{r,0} + K\left(c^{-1} + \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r\, ds\right). \tag{3.92}$$

In proving a bound of this type for (3.91) we proceed as follows (see Lemma 3.6). We plug the identity

$$\boldsymbol{J}^P\left[w(s), \mathfrak{a}(s)\right] = \underbrace{\left(\boldsymbol{J}^P\left[w(s), \mathfrak{a}(s)\right] - \boldsymbol{J}^P\left[e^{ic^2 s}w_0(s), 0\right]\right)}_{=:(*)} + \underbrace{\boldsymbol{J}^P\left[e^{ic^2 s}w_0(s), 0\right]}_{=:(**)} \tag{3.93}$$

into (3.91). The integral term involving $(*)$ can be played back to $\int_0^t \|\mathfrak{e}_{w_0}(s)\|_r\, ds$. The remaining term involving $(**)$ can be bounded in $\mathcal{O}\left(c^{-1}\right)$ via integration by parts. This gives the bound (3.92). For details, see Lemma 3.6 below.

The bound (3.92) from Lemma 3.6 then allows us to derive the following estimate

$$\begin{aligned}\int_0^t c^{-1}\|\mathfrak{e}_{\boldsymbol{a}_0}(s)\|_{r,0}\, ds \leq & c^{-1}\, t\,\|\mathfrak{a}_I - \mathfrak{a}_{I,0}\|_{r,0} + c^{-2}\; K^1_{\mathfrak{a}}(t, \mathcal{M}^{r+2}_{w_0}, \mathcal{M}^r_w, \mathcal{M}^r_{\mathfrak{a}}) \\ & + c^{-1}\; tK_{\mathfrak{a}}(\mathcal{M}^r_w, \mathcal{M}^r_{w_0}) \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r\, ds),\end{aligned}$$

where the constants are given in Lemma 3.6. Here, we exploited that for a positive function $a(t)$ we have

$$\int_0^t\int_0^s a(\sigma)d\sigma ds \leq \int_0^t\int_0^t a(\sigma)d\sigma ds = t\int_0^t a(\sigma)d\sigma.$$

Therefore in case of MKG, the estimate in (3.88) reduces to

$$\|\mathfrak{e}_{w_0}(t)\|_r \leq K\cdot\left(c^{-2} + \|w_I - w_{I,0}\|_r + \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r\, ds\right), \tag{3.94}$$

since by assumption of Theorem 3.3 $\|\mathfrak{a}_I - \mathfrak{a}_{I,0}\|_{r,0} \leq Kc^{-1}$ and since by $G = 0$ also $K_G = 0$.

Recall that the initial data w_I and $w_{I,0}$ of the MKG first order system (3.66) and of the corresponding limit system (3.67), respectively, are given by

$$w_I = \begin{pmatrix}\psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'}\end{pmatrix} \quad\text{and}\quad w_{I,0} = \begin{pmatrix}\psi_{I,0} - i\psi_{I,0}' \\ \overline{\psi_{I,0} - i\psi_{I,0}'}\end{pmatrix}, \quad \text{respectively.}$$

[2] See for instance [85, Chapter 1.3] for a comprehensive explanation of a bootstrap argument, and also [44, Proof of Proposition IV.14] and Remark 3.13 below for particular applications of bootstrap arguments.

Applying the triangle inequality, this implies

$$\|w_I - w_{I,0}\|_r \le K\Big(\|\psi_I - \psi_{I,0}\|_r + \left\|\psi_I' - \psi_{I,0}'\right\|_r \Big),$$

where the constant K is independent of c. Now we are ready to collect all the results and state the final arguments in the proof of Theorem 3.3. Let $K_{w_0}^{\mathrm{MKG}}$, $K_{\boldsymbol{\mathfrak{a}}_0}^{\mathrm{MKG}}$ and $K_{\phi_0}^{\mathrm{MKG}}$ be constants only depending on T, $\mathcal{M}_{w_0}^{r+4}$, $\mathcal{M}_{w}^{r+2}$, $\mathcal{M}_{\boldsymbol{\mathfrak{a}}_0}^{r+1}$, $\mathcal{M}_{\boldsymbol{\mathfrak{a}}}^{r+1}$ for $t \in [0,T]$ but not on c. According to Assumption 3.1 and Assumption 3.2, we thus require the initial data of the MKG system (2.20) and (2.33) to satisfy $\psi_I, \psi_I' \in H^{r+4}$, $A_I \in \mathcal{P}_{\mathrm{df}} H^{r+1}$, $A_I' \in \mathcal{P}_{\mathrm{df}} H^r$, where

$$\mathcal{P}_{\mathrm{df}} H^r = \{A \in \dot{H}^r \quad \text{with} \quad \operatorname{div} A = 0\}, \qquad \text{see Definitions A.3 and A.13.}$$

The application of Gronwall's Lemma (see for instance [85, Theorem 1.10] and also Lemma A.21) to (3.94) finally yields

$$\|\mathfrak{e}_{w_0}(t)\|_r \le K_{w_0}^{\mathrm{MKG}} \cdot \left(\|\psi_I - \psi_{I,0}\|_r + \left\|\psi_I' - \psi_{I,0}'\right\|_r + c^{-2} \right). \tag{3.95a}$$

Therefore, if $\psi_{I,1}$ and $\psi_{I,1}'$ asymptotically vanish (see assumptions in Theorem 3.3), i.e. if

$$\|\psi_I - \psi_{I,0}\|_r + \left\|\psi_I' - \psi_{I,0}'\right\|_r \le K_2 c^{-2},$$

with K_2 independent of c, we obtain a $\mathcal{O}\left(c^{-2}\right)$ convergence bound for (3.95a). Otherwise, i.e. if we can only establish a bound

$$\|\psi_I - \psi_{I,0}\|_r + \left\|\psi_I' - \psi_{I,0}'\right\|_r \le K_1 c^{-1}$$

with K_1 independent of c, we obtain a $\mathcal{O}\left(c^{-1}\right)$ bound for (3.95a).

Moreover, Lemma 3.6 then immediately gives the error bound for $\mathfrak{e}_{\boldsymbol{a}_0}$

$$\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0} \le K_{\boldsymbol{a}_0}^{\mathrm{MKG}} \cdot c^{-1}. \tag{3.95b}$$

From (3.78) and from the estimate on $\|\mathfrak{e}_{w_0}(t)\|_r$ we deduce

$$\|\phi(t) - \phi_0(t)\|_{r+2,0} \le K_{\phi_0}^{\mathrm{MKG}} \cdot \left(\|\psi_I - \psi_{I,0}\|_r + \left\|\psi_I' - \psi_{I,0}'\right\|_r + c^{-2} \right). \tag{3.95c}$$

The inequalities (3.95) then finally prove Theorem 3.3. □

Next, we state the final arguments in proving Theorem 3.4 on the convergence of the limit system (3.59b) in case of MD.

3.4.3 Final Arguments in Proving Theorem 3.4 (MD Limit Approximation)

The final arguments in the convergence proof of Theorem 3.4 in the MD case are not as straight forward as in the MKG case. Due to the additional factor of c in the current density $\boldsymbol{J}^P$ given in (2.41), i.e.

$$\boldsymbol{J}^P = c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[(u + \overline{v})\overline{\boldsymbol{\alpha}}(\overline{u} + v)\right],$$

the analysis becomes more difficult since an expansion of $\boldsymbol{J}^P$ of type (3.93) does not allow us to follow the line of argumentation from above. More precisely, naively applying the latter ideas provides only a pessimistic bound given in Proposition 3.8, i.e.

$$\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0} \le \|\boldsymbol{\mathfrak{a}}_I - \boldsymbol{\mathfrak{a}}_{I,0}\|_{r,0} + K\left(c^{-1} + c\int_0^t \|\mathfrak{e}_{w_0}(s)\|_r \, ds \right). \tag{3.96}$$

Due to the additional factor of c in front of the integral term, in contrast to (3.92), this bound will not be sufficient to establish an $\mathcal{O}\left(c^{-1}\right)$ bound for $\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0}$ directly, but we establish a sufficient bound later on, which exploits the following results.

However, we observe that the bound (3.96) is at least sufficient to establish the desired $\mathcal{O}\left(c^{-1}\right)$ bound for $\|\mathfrak{e}_{w_0}(t)\|_r$ due to the intermediate results (3.88)–(3.90). This bound can thus be exploited in order to establish the corresponding bound for $\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_r$.

More precisely, in view of (3.96) we find

$$\int_0^t c^{-1}\|\mathfrak{e}_{\boldsymbol{a}_0}(s)\|_{r,0}\,ds \leq tc^{-1}\|\mathfrak{a}_I-\mathfrak{a}_{I,0}\|_{r,0}+K\cdot(c^{-2}+t\int_0^t\|\mathfrak{e}_{w_0}(s)\|_r\,ds).$$

Plugging this bound into the intermediate result on $\|\mathfrak{e}_{w_0}(t)\|_r$ in (3.88) and exploiting the assumption $\|w_I-w_{I,0}\|_r+\|\mathfrak{a}_I-\mathfrak{a}_{I,0}\|_{r,0}\leq \tilde{K}c^{-1}$ of Theorem 3.4 yields that

$$\|\mathfrak{e}_{w_0}(t)\|_r \leq K\cdot\left(c^{-1}+\int_0^t\|\mathfrak{e}_{w_0}(s)\|_r\,ds\right) \tag{3.97}$$

with a constant $K>0$ independent of c. The application of Gronwall's Lemma (see for instance [85, Theorem 1.10] and also Lemma A.21) to the latter inequality allows us now to prove the desired bounds on $\|\mathfrak{e}_{w_0}\|_r$ and $\|\phi(t)-\phi_0(t)\|_{r+2,0}$. Let $K_{w_0}^{\text{MD}}$, $K_{\phi_0}^{\text{MD}}$ and $K_{\boldsymbol{a}_0}^{\text{MD}}$ be constants only depending on T, $\mathcal{M}_{w_0}^{r+4}$, $\mathcal{M}_w^{r+2}$, $\mathcal{M}_{\boldsymbol{a}_0}^{r+1}$, $\mathcal{M}_{\mathfrak{a}}^{r+1}$ for $t\in[0,T]$ but not on c. Then (3.97) gives

$$\|\mathfrak{e}_{w_0}(t)\|_r \leq K_{w_0}^{\text{MD}}\cdot c^{-1}. \tag{3.98a}$$

From (3.79) we then obtain the desired $\mathcal{O}\left(c^{-1}\right)$ bound on the error

$$\|\phi(t)-\phi_0(t)\|_{r+2,0}\leq K_{\phi_0}^{\text{MD}}\cdot c^{-1}. \tag{3.98b}$$

We observe that the pessimistic bound (3.96) (see also Proposition 3.8) only allows that

$$\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0}\leq K(c^{-1}+c\int_0^t\|\mathfrak{e}_{w_0}(s)\|_r\,ds)\leq Kc^0,$$

i.e. Proposition 3.8 does not provide the desired convergence result on $\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0}$.

However, using that $\|\mathfrak{a}_I-\mathfrak{a}_{I,0}\|_{r,0}\leq Kc^{-1}$ and exploiting the $\mathcal{O}\left(c^{-1}\right)$ bound on $\|\mathfrak{e}_{w_0}(t)\|_r$ in (3.98a), we are able to show that (see Lemma 3.9)

$$\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0}\leq\|\mathfrak{a}_I-\mathfrak{a}_{I,0}\|_{r,0}+Kc^{-1}\leq K_{\boldsymbol{a}_0}^{\text{MD}}c^{-1}. \tag{3.98c}$$

In the proof of Lemma 3.9 we make use of the structure of $u_0=\begin{pmatrix}0\\u_0^-\end{pmatrix}$ and $v_0=\begin{pmatrix}v_0^+\\0\end{pmatrix}$ in the MD case (see (3.50)). Applying a similar decomposition to u and v, we deduce that

$$\|\mathfrak{e}_{w_0}(t)\|_r=\left\|u^+(t)\right\|_r+\left\|u^-(t)-e^{ic^2t}u_0^-(t)\right\|_r+\left\|v^+(t)-e^{ic^2t}v_0^+(t)\right\|_r+\left\|v^-(t)\right\|_r, \tag{3.99}$$

which in particular implies that the components u^+,v^- are $\mathcal{O}\left(c^{-1}\right)$ if $\|\mathfrak{e}_{w_0}(t)\|_r\leq Kc^{-1}$.

Moreover, we exploit the technique of "twisted variables" (see Chapter 4) which make use of the fact that by the estimate $\left\|(c^2-c\langle\nabla\rangle_c)w\right\|_r\leq K\|w\|_{r+2}$ from Lemma A.11 the term $\partial_s(e^{-ic^2t}w)=e^{-ic^2t}(-ic^2w+$

$\partial_s w$) is uniformly bounded with respect to $c \geq 1$ in H^{r+2}. The inequalities (3.98) then finally prove Theorem 3.4. □

For the interested reader we give now some auxiliary results in more detail in the subsequent subsection which have been used in the previous section to prove Theorems 3.3 and 3.4. In Section 3.5 below we continue with the construction of numerical schemes based on the convergence results from Theorems 3.3 and 3.4.

3.4.4 Auxiliary Results on the Limit Approximations

In this section we provide auxiliary and more technical results which have been used in proving Theorems 3.3 and 3.4 in the previous sections.

Because the charge density ρ and the current density $\boldsymbol{J}^P$ are defined differently in the MKG first order system (2.33) and in the MD first order system (2.41) we have different asymptotics in the nonrelativistic limit. Therefore, we prove some auxiliary results for MKG seperately from those for MD.

Auxiliary Results for the MKG Limit

Because the error $\|\phi - \phi_0\|_{r+2,0}$ of the scalar potentials is played back to the error of the charge densities $\|\rho - \rho_0\|_r$ in (3.78), we provide the following Proposition 3.5 on the asymptotics of ρ_0 to ρ, which depends on the convergence bound for $\|\mathfrak{e}_{w_0}(t)\|_r = \left\|w(t) - e^{ic^2 t} w_0(t)\right\|_r$. Moreover, we show in Lemma 3.6 that the error $\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0} = \|\mathfrak{a}(t) - \boldsymbol{a}_0(t)\|_{r,0}$ also depends on $\|\mathfrak{e}_{w_0}(t)\|_r$, which allows us to reduce (3.88) to

$$\|\mathfrak{e}_{w_0}(t)\|_r \leq K(\|w_I - w_{I,0}\|_r + c^{-2} + \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r \, ds).$$

Next, we apply Gronwall's Lemma (see for instance [85, Theorem 1.10] and also Lemma A.21) to the latter and obtain the bound $\|\mathfrak{e}_{w_0}(t)\|_r \leq K(\|w_I - w_{I,0}\|_r + c^{-2})$. With the aid of this bound and Lemma 3.6, we immediately find the desired $\mathcal{O}\left(c^{-1}\right)$ bound for $\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0}$.

Proposition 3.5 ([70], MKG ρ_0 Convergence)**.** *Let $r > d/2$. The charge densities*

$$\rho = -\frac{1}{4} \operatorname{Re}\left((u + \overline{v}) \frac{\langle \nabla \rangle_c}{c} (\overline{u} - v)\right) \quad \text{and} \quad \rho_0 = -\frac{1}{4}(|u_0|^2 - |v_0|^2)$$

given in the first order formulation (2.33) of the MKG system and in the corresponding limit system (3.30b), respectively, satisfy for all $s \in [0, T]$

$$\|\rho(s) - \rho_0(s)\|_r \leq c^{-2} K_\phi^1\left(\mathcal{M}_w^{r+2}, \mathcal{M}_{w_0}^r\right) + K_\phi^2\left(\mathcal{M}_w^{r+1}, \mathcal{M}_{w_0}^r\right) \|\mathfrak{e}_{w_0}(s)\|_r \,,$$

where the constants $\mathcal{M}_w^{r+2}, \mathcal{M}_{w_0}^r$ are given in Assumption 3.1 and Assumption 3.2.

Proof: In the following we omit the s dependence of u, u_0 for sake of simplicity. Let $s \in [0, T]$. Then we have

$$
\begin{aligned}
&\|\rho(s)-\rho_0(s)\|_r \\
&\leq \left\| \operatorname{Re}\left((u+\overline{v}) \frac{\langle\nabla\rangle_c}{c}(\overline{u}-v) - (e^{ic^2 s}u_0 + e^{-ic^2 s}\overline{v_0})(e^{-ic^2 s}\overline{u_0} - e^{ic^2 s}v_0) \right) \right\|_r \\
&\leq \left\| (u - e^{ic^2 s}u_0 + \overline{v} - e^{-ic^2 s}\overline{v_0}) \frac{\langle\nabla\rangle_c}{c}(\overline{u}-v) \right\|_r \\
&\quad + \left\| (e^{ic^2 s}u_0 + e^{-ic^2 s}\overline{v_0}) \frac{c\langle\nabla\rangle_c - c^2}{c^2}(\overline{u}-v) \right\|_r \\
&\quad + \left\| (e^{ic^2 s}u_0 + e^{-ic^2 s}\overline{v_0})(\overline{u} - e^{-ic^2 s}\overline{u_0} - (v - e^{ic^2 s}v_0)) \right\|_r \\
&\leq K_\phi^2(\mathcal{M}_w^{r+1}, \mathcal{M}_{w_0}^r) \left\| w(s) - e^{ic^2 s}w_0(s) \right\|_r + c^{-2}K_\phi^1(\mathcal{M}_w^{r+2}, \mathcal{M}_{w_0}^r),
\end{aligned}
$$

where the last inequality follows from the bilinear estimates in Lemma A.8 and from the properties of the operator $\langle\nabla\rangle_c$ in Lemma A.11. This finishes the proof. □

Lemma 3.6 ([70], MKG $\boldsymbol{a}_0$ Convergence)**.** *Let $r > d/2$. The current density corresponding to the MKG first order system (2.33) reads*

$$
\boldsymbol{J}^P[w, \mathfrak{a}] = \mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i\frac{1}{4}(u+\overline{v})\nabla(\overline{u}+v) \right) - \frac{1}{c}\frac{1}{8}(\mathfrak{a}+\overline{\mathfrak{a}})\,|u+\overline{v}|^2 \right].
$$

Let $\mathfrak{a}$ be the solution of (2.33) and $\boldsymbol{a}_0$ the corresponding limit approximation given in (3.30b). The error $\mathfrak{e}_{\boldsymbol{a}_0}(t) := \mathfrak{a}(t) - \boldsymbol{a}_0(s)$ satisfies

$$
\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0} \leq \|\mathfrak{a}_I - \mathfrak{a}_{I,0}\|_{r,0} + \left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P[w(s), \mathfrak{a}(s)]\,ds \right\|_{r,0},
$$

where

$$
\begin{aligned}
\left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P[w(s), \mathfrak{a}(s)]\,ds \right\|_{r,0} \leq & c^{-1}K_{\mathfrak{a}}^1(t, \mathcal{M}_{w_0}^{r+2}, \mathcal{M}_w^r, \mathcal{M}_{\mathfrak{a}}^r) \\
& + K_{\mathfrak{a}}(\mathcal{M}_w^r, \mathcal{M}_{w_0}^r) \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r\,ds.
\end{aligned}
$$

Proof: The first term follows from the triangle inequality and the isometry property of $\mathcal{T}^t_{[c\langle\nabla\rangle_0]}$ in $\dot{H}^r$. It remains to estimate the integral term. Therefore define $\boldsymbol{J}_0(t) := \boldsymbol{J}^P[e^{ic^2 t}w_0(t), 0]$. Then

$$
\begin{aligned}
&\left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P[w(s), \mathfrak{a}(s)]\,ds \right\|_{r,0} \\
&\leq \int_0^t \left\| \langle\nabla\rangle_0^{-1} (\boldsymbol{J}^P[w(s), \mathfrak{a}(s)] - \boldsymbol{J}_0(s)) \right\|_{r,0} ds + \left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}_0(s)\,ds \right\|_{r,0}.
\end{aligned}
\tag{3.100}
$$

Because

$$
\begin{aligned}
&\boldsymbol{J}^P[w, 0] - \boldsymbol{J}_0 \\
&= \mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i(u - e^{ic^2 t}u_0 + \overline{v} - e^{-ic^2 t}\overline{v_0})\nabla(\overline{u}+v) \right) \right] \\
&\quad + \mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i(e^{ic^2 t}u_0 + e^{-ic^2 t}\overline{v_0})\nabla(\overline{u} - e^{-ic^2 t}\overline{u_0} + v - e^{ic^2 t}v_0) \right) \right],
\end{aligned}
$$

and because by Proposition A.14 the projection satisfies $\|\mathcal{P}_{\mathrm{df}}[w]\|_{r',0} \leq \|w\|_{r',0}$ for $r' > 0$, the first integral term can be bounded by

$$c^{-1}tK \cdot \mathcal{M}^r_{\mathfrak{a}}(\mathcal{M}^r w)^2 + \int_0^t \left\| \langle\nabla\rangle_0^{-1} \left(\boldsymbol{J}^P\left[w(s),0\right] - \boldsymbol{J}_0(s)\right)\right\|_{r,0} ds$$
$$\leq c^{-1}tK \cdot \mathcal{M}^r_{\mathfrak{a}}(\mathcal{M}^r_w)^2 + K(\mathcal{M}^r_w + \mathcal{M}^r_{w_0}) \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r \, ds,$$

where the second inequality follows from $\left\|\langle\nabla\rangle_0^{-1} w\right\|_{r,0} \leq \|w\|_{r-1,0} \leq \|w\|_{r-1}$ and the bilinear estimate $\|uv\|_{r-1} \leq K\|u\|_{r-1}\|v\|_r$ (see Lemma A.5 and Lemma A.8).

Neglecting in the difference term $\boldsymbol{J}^P[w,0] - \boldsymbol{J}_0$ the presence of the bounded projection operator $\mathcal{P}_{\mathrm{df}}$ (see Proposition A.14) and of the real part Re, then the second integral on the right hand side of (3.100) is of the form

$$\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \left(u_0(s)\nabla\overline{u_0}(s) + \overline{v_0}(s)\nabla v_0(s)\right)ds \tag{3.101a}$$
$$+ \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \left(e^{2ic^2 s}(u_0(s)\nabla v_0(s)) + e^{-2ic^2 s}(\overline{u_0}(s)\overline{\nabla v_0}(s)\right)ds. \tag{3.101b}$$

Applying integration by parts to these integrals, where in (3.101a) we integrate $\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}$ using that $\partial_s w_0$ is bounded with respect to c, and in (3.101b) we integrate $e^{\pm 2ic^2 s}$ exploiting that

$$c^{-2}\left((\partial_s \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]})w_0(s) + \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}\partial_s w_0(s)\right) \quad \text{is} \quad \mathcal{O}\left(c^{-1}\right),$$

we thus obtain

$$\left\|\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}_0(s)ds\right\|_{r,0}$$
$$\leq c^{-1}K\Big((\mathcal{M}^r_{w_0})^2 + t\big(\mathcal{M}^{r+1}_{w_0}(\mathcal{M}^{r+2}_{w_0} + (\mathcal{M}^{r+1}_{w_0})^3)\big)\Big).$$

Therefore, we establish the following bound for (3.100)

$$c^{-1}\left(K^1_{\mathfrak{a}}(\mathcal{M}^r_{w_0}) + tK^2_{\mathfrak{a}}(\mathcal{M}^{r+2}_{w_0}, \mathcal{M}^r_{\mathfrak{a}}, \mathcal{M}^r_w)\right) + K_{\mathfrak{a}}(\mathcal{M}^r_w, \mathcal{M}^r_{w_0}) \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r \, ds,$$

which yields the assertion. □

We now proceed with some auxiliary results for the convergence of the MD limit system.

Auxiliary Results for the MD Limit

Similar to Proposition 3.5, the following Proposition 3.7 allows us to play back the error of the potential $\|\phi - \phi_0\|_{r+2,0}$ to the error of the charge densities $\|\rho - \rho_0\|_r$ in (3.79).

Then we give an error estimate for $\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0}$ in Proposition 3.8, which is rather pessimistic but sufficient to at first show a $\mathcal{O}\left(c^{-1}\right)$ bound for $\|\mathfrak{e}_{w_0}(t)\|_r$. This is due to the fact that then (3.88) reduces to

$$\|\mathfrak{e}_{w_0}(t)\|_r \leq K(\|w_I - w_{I,0}\|_r + c^{-1} + \int_0^t \|\mathfrak{e}_{w_0}(s)\|_r \, ds),$$

such that again by Gronwall's Lemma (see for instance [85, Theorem 1.10] and also Lemma A.21) we obtain $\|\mathfrak{e}_{w_0}(t)\|_r \leq Kc^{-1}$. Exploiting this $\mathcal{O}\left(c^{-1}\right)$ convergence bound on $\mathfrak{e}_{w_0}$, the particular structure of u_0, v_0 in (3.50) and the technique of "twisted variables" (see Chapter 4), we are able to show a better bound on $\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0}$ in Lemma 3.9 which finally yields $\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0} \leq Kc^{-1}$.

Proposition 3.7 ([70], MD ρ_0 Convergence)**.** *Let $r > d/2$. The charge densities*

$$\rho = \frac{1}{4}(|u|^2 + |v|^2) \quad \text{and} \quad \rho_0 = \frac{1}{4}(|u_0|^2 + |v_0|^2)$$

given in the first order formulation (2.41) of the MD system and in the corresponding limit system (3.59b), respectively, satisfy for all $s \in [0,T]$

$$\|\rho(s) - \rho_0(s)\|_r \le K_\phi\big(\mathcal{M}_w^r, \mathcal{M}_{w_0}^r\big)\, \|\mathfrak{e}_{w_0}(s)\|_r\,,$$

where the constants $\mathcal{M}_w^r, \mathcal{M}_{w_0}^r$ are given in Assumption 3.1 and Assumption 3.2.

Proof: The difference between ρ and ρ_0 can be played back to the differences $|u|^2 - |u_0|^2$ and $|v|^2 - |v_0|^2$. We have

$$|u|^2 - |u_0|^2 = (u - e^{ic^2 s}u_0)\overline{u} + e^{ic^2 s}u_0)(\overline{u} - e^{-ic^2 s}\overline{u_0})$$

and analogously for v and v_0. Thus, the inequality

$$\|\rho(s) - \rho_0(s)\|_r \le K_\phi\big(\mathcal{M}_w^r, \mathcal{M}_{w_0}^r\big) \left\| w(s) - e^{ic^2 s} w_0(s) \right\|_r$$

finishes the proof. □

Proposition 3.8 ([70], MD $\boldsymbol{a}_0$ Pessimistic Convergence Bound)**.** *Let $r > d/2$. The current density corresponding to the MD first order system (2.41) reads*

$$\boldsymbol{J}^P[w] = c\frac{1}{4}\mathcal{P}_{df}\left[(u + \overline{v})\overline{\boldsymbol{\alpha}}(\overline{u} + v)\right].$$

Let $\mathfrak{a}$ be the solution of (2.41) and $\boldsymbol{a}_0$ the corresponding limit approximation given in (3.59b). The error $\mathfrak{e}_{\boldsymbol{a}_0}(t) := \mathfrak{a}(t) - \boldsymbol{a}_0(s)$ satisfies

$$\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0} \le \|\mathfrak{a}_I - \mathfrak{a}_{I,0}\|_{r,0} + \left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P\big[w(s), \mathfrak{a}(s)\big]\, ds \right\|_{r,0},$$

where

$$\begin{aligned}\left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P\big[w(s)\big]\, ds \right\|_{r,0} \le & c^{-1} K^1_{\mathfrak{a}}(t, \mathcal{M}^{r+4}_{w_0}) \\ & + K_{\mathfrak{a}}(\mathcal{M}_w^r, \mathcal{M}_{w_0}^r) \int_0^t c\, \|\mathfrak{e}_{w_0}(s)\|_r\, ds.\end{aligned}$$

Note that the integral in the last inequality differs from the inequality in Lemma 3.6 by a factor of c.

Proof: The first term follows from the triangle inequality and the isometry property of $\mathcal{T}^{t}_{[c\langle\nabla\rangle_0]}$ in $\dot{H}^r$. It remains to estimate the integral term.

Therefore define $\boldsymbol{J}_0(t) := \boldsymbol{J}^P[e^{ic^2 t}w_0(t)]$. Then

$$\begin{aligned}&\left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P\big[w(s)\big]\, ds \right\|_{r,0} \\ &\le \int_0^t \left\| \langle\nabla\rangle_0^{-1} (\boldsymbol{J}^P\big[w(s)\big] - \boldsymbol{J}_0(s)) \right\|_{r,0} ds + \left\| \int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} \boldsymbol{J}_0(s) ds \right\|_{r,0}.\end{aligned} \tag{3.102}$$

Because

$$\begin{aligned}
&\boldsymbol{J}^P[w]-\boldsymbol{J}_0\\
&=c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[(u-e^{ic^2t}u_0+\overline{v}-e^{-ic^2t}\overline{v_0})\overline{\boldsymbol{\alpha}}(\overline{u}+v)\right]\\
&\quad+c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[(e^{ic^2t}u_0+e^{-ic^2t}\overline{v_0})\overline{\boldsymbol{\alpha}}(\overline{u}-e^{-ic^2t}\overline{u_0}+v-e^{ic^2t}v_0)\right]
\end{aligned}$$

and because by Proposition A.14 the projection satisfies $\|\mathcal{P}_{\mathrm{df}}[w]\|_{r',0}\leq\|w\|_{r',0}$ for $r'\geq 0$, the first integral term is bounded by

$$cK\cdot(\mathcal{M}_w^r+\mathcal{M}_{w_0}^r)\int_0^t\|\mathfrak{e}_{w_0}(s)\|_r\,ds,$$

where the second inequality follows from $\left\|\langle\nabla\rangle_0^{-1}w\right\|_{r,0}\leq\|w\|_{r-1,0}\leq\|w\|_{r-1}$ and the bilinear estimate $\|uv\|_{r-1}\leq K\|u\|_{r-1}\|v\|_r$ (see Lemma A.5 and Lemma A.8).

Neglecting in $\boldsymbol{J}^P[w]-\boldsymbol{J}_0$ the presence of the projection operator $\mathcal{P}_{\mathrm{df}}$ and of the real part Re, the second integral on the right hand side of (3.102) is of the form

$$c\int_0^t\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}\langle\nabla\rangle_0^{-1}\big(u_0(s)\overline{\boldsymbol{\alpha}}\overline{u_0}(s)+\overline{v_0}(s)\overline{\boldsymbol{\alpha}}v_0(s)\big)ds \tag{3.103a}$$

$$+c\int_0^t\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}\langle\nabla\rangle_0^{-1}\big(e^{2ic^2s}(u_0(s)\overline{\boldsymbol{\alpha}}v_0(s))+e^{-2ic^2s}(\overline{u_0}(s)\overline{\boldsymbol{\alpha}}\overline{v_0}(s))\big)ds. \tag{3.103b}$$

The particular structure of $u_0=\begin{pmatrix}0\\u_0^-\end{pmatrix}$ and $v_0=\begin{pmatrix}v_0^+\\0\end{pmatrix}$ (see (3.50)) admits that the first integral (3.103a) vanishes since

$$u_0\overline{\boldsymbol{\alpha}}\overline{u_0}=\begin{pmatrix}0\\u_0^-\end{pmatrix}\cdot\begin{pmatrix}0_2&\overline{\boldsymbol{\sigma}}\\\overline{\boldsymbol{\sigma}}&0_2\end{pmatrix}\begin{pmatrix}0\\\overline{u_0^-}\end{pmatrix}=0=\overline{v_0}\overline{\boldsymbol{\alpha}}v_0.$$

Applying integration by parts to the second integral (3.103b), we exploit that integrating $e^{\pm ic^2s}$ yields

$$\begin{aligned}
&c\int_0^t\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}\langle\nabla\rangle_0^{-1}e^{2ic^2s}\big(u_0(s)\overline{\boldsymbol{\alpha}}v_0(s)\big)ds\\
=&\left[\frac{c}{2ic^2}e^{2ic^2s}\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}\langle\nabla\rangle_0^{-1}\left(u_0(s)\overline{\boldsymbol{\alpha}}v_0(s)\right)\right]_{s=0}^t\\
&-\int_0^t\frac{c}{2ic^2}e^{2ic^2s}\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}\langle\nabla\rangle_0^{-1}\partial_s\big(u_0(s)\overline{\boldsymbol{\alpha}}v_0(s)\big)ds\\
&-\int_0^t\frac{-c^2}{2c^2}e^{2ic^2s}\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}\big(u_0(s)\overline{\boldsymbol{\alpha}}v_0(s)\big)ds.
\end{aligned}$$

Another integration by parts applied to the last integral, shows that by integrating once more the term e^{2ic^2s} gives the desired c^{-1} bound for (3.103b) in H^r. More precisely, we have that

$$\begin{aligned}
&\left\|\int_0^t\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}\langle\nabla\rangle_0^{-1}\boldsymbol{J}_0(s)ds\right\|_{r,0}\\
&\leq c^{-1}K^1_{\mathfrak{a}}(t,\mathcal{M}^{r+4}_{w_0}).
\end{aligned}$$

Therefore, we establish the following bound for (3.102)

$$c^{-1}K^1_{\mathfrak{a}}(t,\mathcal{M}^{r+4}_{w_0})+K_{\mathfrak{a}}(\mathcal{M}^r_w,\mathcal{M}^r_{w_0})\int_0^t c\,\|\mathfrak{e}_{w_0}(s)\|_r\,ds,$$

which gives the assertion. □

Lemma 3.9 ([70], MD $\boldsymbol{a}_0$ Convergence under Condition of $\mathcal{O}\left(c^{-1}\right)$ Convergence of w_0)**.** *Let $r > d/2$. The current density corresponding to the MD first order system (2.41) reads*

$$\boldsymbol{J}^P[w] = c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[(u+\overline{v})\overline{\boldsymbol{\alpha}}(\overline{u}+v)\right].$$

Let $\mathfrak{a}$ be the solution of (2.41) and $\boldsymbol{a}_0$ the corresponding limit approximation given in (3.59b). The error $\mathfrak{e}_{\boldsymbol{a}_0}(t) := \mathfrak{a}(t) - \boldsymbol{a}_0(s)$ satisfies

$$\|\mathfrak{e}_{\boldsymbol{a}_0}(t)\|_{r,0} \leq \|\mathfrak{a}_I - \mathfrak{a}_{I,0}\|_{r,0} + \left\|\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}\langle\nabla\rangle_0^{-1}\boldsymbol{J}^P\left[w(s),\mathfrak{a}(s)\right]ds\right\|_{r,0},$$

where

$$\left\|\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}\langle\nabla\rangle_0^{-1}\boldsymbol{J}^P\left[w(s),\mathfrak{a}(s)\right]ds\right\|_{r,0} \leq K(t,\mathcal{M}^{r+2}_{w_0},\mathcal{M}^{r+2}_{w},\mathcal{M}^{r}_{\mathfrak{a}},K^{\mathrm{MD}}_{w_0})\cdot c^{-1},$$

with a constant K depending on time t, on the regularity of $w_0, w, \mathfrak{a}$ (see Assumption 3.1 and Assumption 3.2) and on the constant $K^{\mathrm{MD}}_{w_0}$ given in (3.98).

Proof: Neglecting the projection $\mathcal{P}_{\mathrm{df}}$ which is uniformly bounded in H^r (see Proposition A.14) and the factor $\frac{1}{4}$, we can expand $\boldsymbol{J}^P$ as

$$c(u+\overline{v})\overline{\boldsymbol{\alpha}}(\overline{u}+v) = c\big(u\overline{\boldsymbol{\alpha}}\overline{u} + \overline{v}\overline{\boldsymbol{\alpha}}v + u\overline{\boldsymbol{\alpha}}v + \overline{v}\overline{\boldsymbol{\alpha}}\overline{u}\big).$$

Considering the decomposition $u = (u^+,u^-)^\top$ and $v = (v^+,v^-)^\top$ into upper and lower components, the structure of the matrices $\boldsymbol{\alpha}$ (see (1.21)) admits that

$$u\overline{\boldsymbol{\alpha}}\overline{u} + \overline{v}\overline{\boldsymbol{\alpha}}v = u^+\overline{\boldsymbol{\sigma}}\overline{u^-} + u^-\overline{\boldsymbol{\sigma}}\overline{u^+} + \overline{v^+}\overline{\boldsymbol{\sigma}}v^- + \overline{v^-}\overline{\boldsymbol{\sigma}}v^+ \tag{3.104a}$$

$$u\overline{\boldsymbol{\alpha}}v + \overline{v}\overline{\boldsymbol{\alpha}}\overline{u} = u^+\overline{\boldsymbol{\sigma}}v^- + \overline{v^-}\overline{\boldsymbol{\sigma}}\overline{u^+} \tag{3.104b}$$

$$+ u^-\overline{\boldsymbol{\sigma}}v^+ + \overline{v^+}\overline{\boldsymbol{\sigma}}\overline{u^-}. \tag{3.104c}$$

In the proof we repeatedly make use of the bounds from (3.99)

$$\left\|u^+\right\|_r + \left\|v^-\right\|_r \leq K^{\mathrm{MD}}_{w_0}\cdot c^{-1} \tag{3.105a}$$

and

$$\left\|u^-(t) - e^{ic^2t}u_0^-(t)\right\|_r + \left\|v^+(t) - e^{ic^2t}v_0^+(t)\right\|_r \leq K^{\mathrm{MD}}_{w_0}\cdot c^{-1}, \tag{3.105b}$$

where $K^{\mathrm{MD}}_{w_0}$ is the constant given in (3.98a).

Moreover, we use the technique of "twisted variables" (see Chapter 4) which shows that $\partial_s(e^{-ic^2s}w(s))$ is uniformly bounded in H^r with respect to c if w solves the MKG or MD first order system (2.33) or (2.41).

In view of the decomposition $w = (u^+,u^-,v^+,v^-)^\top$ and in view of the local well-posedness result on w from Proposition 2.7, this implies that

$$\text{if} \quad \|z(s)\|_r \leq Kc^{-1} \quad \text{then also} \quad \left\|\partial_s(e^{-ic^2s}z(s))\right\|_r \leq Kc^{-1} \quad \text{for } z\in\{u^+,v^-\}. \tag{3.106}$$

Taking into account the first of the terms in (3.104a) we find with

$$u^+\overline{\boldsymbol{\sigma}}\overline{u^-} = u^+\overline{\boldsymbol{\sigma}}(\overline{u^-} - e^{-ic^2s}\overline{u_0^-}) + u^+\overline{\boldsymbol{\sigma}}(e^{-ic^2s}\overline{u_0^-})$$

that

$$\begin{aligned}
&\left\|\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} cu^+(s)\overline{\boldsymbol{\sigma}}\overline{u^-}(s)ds\right\|_{r,0} \\
\leq & tc \sup_{s\in[0,T]} \left\|u^+(s)\right\|_r \left\|u^-(s) - e^{ic^2 s}u_0^-(s)\right\|_r \\
&+ \left\|\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} c\Big(e^{-ic^2 s}u^+(s)\Big)\overline{\boldsymbol{\sigma}}\overline{u_0^-}(s)ds\right\|_{r,0}.
\end{aligned}$$

Applying integration by parts to the last integral term and integrating $\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}$ we obtain a factor c^{-1}. Recall that by (3.105) we have $\|u^+\|_r \leq Kc^{-1}$ and that by (3.106) also $\left\|\partial_s(e^{-ic^2 s}u^+(s))\right\|_r \leq Kc^{-1}$ holds. Then the c-independence of $\partial_s u_0^-(s)$ yields the $\mathcal{O}\left(c^{-1}\right)$ bound for the first term $u^+\overline{\boldsymbol{\sigma}}\overline{u^-}$ in (3.104a). The remaining terms of (3.104a) can be estimated analogously.

The bound $\|u^+\|_r + \|v^-\|_r \leq K_{w0}^{\mathrm{MD}} \cdot c^{-1}$ from above immediately gives the desired $\mathcal{O}\left(c^{-1}\right)$ for the terms (3.104b).

Consider now the first term in (3.104c). We have

$$\begin{aligned}
&\left\|\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} cu^-(s)\overline{\boldsymbol{\sigma}}v^+(s)ds\right\|_{r,0} \\
=&\left\|\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} e^{2ic^2 s}c\Big(e^{-ic^2 s}u^-(s)\Big)\overline{\boldsymbol{\sigma}}\Big(e^{-ic^2 s}v^+(s)\Big)ds\right\|_{r,0}.
\end{aligned}$$

From the same arguments as before on the twisted variables we observe that

$$\partial_s\bigg(\Big(e^{-ic^2 s}u^-(s)\Big)\overline{\boldsymbol{\sigma}}\Big(e^{-ic^2 s}v^+(s)\Big)\bigg)$$

is uniformly bounded with respect to c in H^r. Integration by parts then yields, integrating $e^{2ic^2 s}$, that

$$\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} e^{2ic^2 s}c\Big(e^{-ic^2 s}u^-(s)\Big)\overline{\boldsymbol{\sigma}}\Big(e^{-ic^2 s}v^+(s)\Big)ds \tag{3.107a}$$

$$=\left[\frac{c}{2ic^2}\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}u^-(s)\overline{\boldsymbol{\sigma}}v^+(s)\right]_{s=0}^t \tag{3.107b}$$

$$-\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} \langle\nabla\rangle_0^{-1} e^{2ic^2 s}\frac{c}{2ic^2}\partial_s\bigg(\Big(e^{-ic^2 s}u^-(s)\Big)\overline{\boldsymbol{\sigma}}\Big(e^{-ic^2 s}v^+(s)\Big)\bigg)ds \tag{3.107c}$$

$$-\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}e^{2ic^2 s}\frac{c^2}{2ic^2}\Big(e^{-ic^2 s}u^-(s)\Big)\overline{\boldsymbol{\sigma}}\Big(e^{-ic^2 s}v^+(s)\Big)ds. \tag{3.107d}$$

Note that since $\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}$ is an isometry in H^r (and thus in particular in $\dot{H}^r$), the first two terms (3.107b) and (3.107c) satisfy a $\mathcal{O}\left(c^{-1}\right)$ bound in the sense of the $\dot{H}^r$ norm, i.e.

$$\|\text{term (3.107b)}\|_{r,0} + \|\text{term (3.107c)}\|_{r,0} \leq Kc^{-1},$$

where the constant K only depends on t and on the constants $\mathcal{M}_w^{r+1}, \mathcal{M}_{\mathfrak{a}}^r$ (see Assumption 3.1) but not on c. In order to find a $\mathcal{O}\left(c^{-1}\right)$ bound also for the last term (3.107d), we apply integration by parts another time to (3.107d). Note that we regain the term (3.107d) from the full integral term (3.107a) via the application of the operator $\frac{\langle\nabla\rangle_0}{2ic}$. Thus, applying integration by parts once more and omitting the constant $1/(2i)$, the term (3.107d) becomes

$$\begin{aligned}
&\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} e^{2ic^2 s}\left(e^{-ic^2 s}u^-(s)\right)\overline{\boldsymbol{\sigma}}\left(e^{-ic^2 s}v^+(s)\right)ds\\
=&\left[\frac{1}{2ic^2}\langle\nabla\rangle_0\,\mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]}u^-(s)\overline{\boldsymbol{\sigma}}v^+(s)\right]_{s=0}^t\\
&-\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} e^{2ic^2 s}\frac{1}{2ic^2}\partial_s\left(\left(e^{-ic^2 s}u^-(s)\right)\overline{\boldsymbol{\sigma}}\left(e^{-ic^2 s}v^+(s)\right)\right)ds\\
&-\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_0]} e^{2ic^2 s}\frac{\langle\nabla\rangle_0}{2ic}\left(e^{-ic^2 s}u^-(s)\right)\overline{\boldsymbol{\sigma}}\left(e^{-ic^2 s}v^+(s)\right)ds.
\end{aligned}$$

We observe that the latter can now also be bounded in $\mathcal{O}\left(c^{-1}\right)$ in the sense of the $\dot{H}^r$ norm, i.e.

$$\|\text{term } (3.107\text{b})\|_{r,0} + \|\text{term } (3.107\text{c})\|_{r,0} + \|\text{term } (3.107\text{d})\|_{r,0} \le Kc^{-1},$$

where the constant K only depends on t and on the constants $\mathcal{M}_w^{r+2}, \mathcal{M}_{\mathfrak{a}}^r$ (see Assumption 3.1) but not on c. This yields the desired $\mathcal{O}\left(c^{-1}\right)$ bound.

The second term $\overline{v^+}\overline{\boldsymbol{\sigma}}\overline{u^-}$ in (3.104c) is treated similary. We simply replace in (3.107a) the term

$$e^{2ic^2 s}c\left(e^{-ic^2 s}u^-(s)\right)\overline{\boldsymbol{\sigma}}\left(e^{-ic^2 s}v^+(s)\right)$$

by the term

$$e^{-2ic^2 s}c\left(e^{ic^2 s}\overline{v^+}(s)\right)\overline{\boldsymbol{\sigma}}\left(e^{ic^2 s}\overline{u^-}(s)\right)$$

and follow the line of argumentation from above.

This finishes the proof. □

We now proceed with the construction of numerical schemes in the nonrelativistic limit regime in the subsequent section.

3.5 Construction of Numerical Schemes in the Nonrelativistic Limit Regime

This section is based on [44, 45, 65, 66] and on the paper [63] by Krämer and Schratz. The reader may in particular pay attention to the paragraphs “Existing Work” and “Our Contribution” below.

In this section, our aim is to construct efficient and robust numerical schemes for the highly oscillatory MKG/MD first order systems (3.3) in the nonrelativistic limit regime, i.e. for $c \gg 1$. Thereby, we exploit the convergence of the MKG/MD systems to the corresponding c independent Schrödinger–Poisson (SP) limit systems (3.30b) and (3.59b), respectively (see Theorems 3.3 and 3.4), i.e. the convergence of the solution $(w, \phi, \mathfrak{a})^\top$ of the MKG/MD first order system in time (3.3) towards $(e^{ic^2 t}w_0, \phi_0, \boldsymbol{a}_0)^\top$, where the functions $w_0 = (u_0, v_0)^\top$, ϕ_0 and $\boldsymbol{a}_0$ solve the SP limit system

$$\begin{cases} i\partial_t w_0 = \frac{1}{2}\Delta w_0 + \phi_0 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix}, & w_0(0) = w_{I,0} = \begin{pmatrix} \psi_{I,0} - i\psi'_{I,0} \\ \overline{\psi_{I,0} - i\psi'_{I,0}} \end{pmatrix}, \\ -\Delta\phi_0 = \rho_0 = \begin{cases} -\frac{1}{4}\left(|u_0|^2 - |v_0|^2\right) & \text{in case of MKG (see (3.30b))}, \\ \frac{1}{4}\left(|u_0|^2 + |v_0|^2\right) & \text{in case of MD (see (3.59b))}, \end{cases} \\ \boldsymbol{a}_0(t) = e^{ic\langle\nabla\rangle_0 t}\mathfrak{a}_{I,0}. \end{cases} \tag{3.108}$$

Note that in particular by (3.59b) in case of Maxwell–Dirac we have that $\psi'_{I,0} = 0$ and that

$$w_{I,0} = (u_{I,0}, v_{I,0})^\top \quad \text{with} \quad u_{I,0} = \begin{pmatrix} 0 \\ 2\psi^-_{I,0} \end{pmatrix} \quad \text{and} \quad v_{I,0} = \begin{pmatrix} 2\overline{\psi^+_{I,0}} \\ 0 \end{pmatrix}$$

according to the decomposition $\psi_{I,0} = (\psi^+_{I,0}, \psi^-_{I,0})^\top$ (see (2.42)). Furthermore, recall that ([70], see also Theorems 3.3 and 3.4)

$$\psi = \psi_0 + \mathcal{O}\left(c^{-1}\right) \qquad \text{with} \qquad \psi_0(t) = \frac{1}{2}(e^{ic^2 t}u_0(t) + e^{-ic^2 t}\overline{v_0}(t)).$$

The basis for constructing efficient numerical time integration methods in the nonrelativistic limit regime then relies on numerically solving the SP limit system (3.108) above. We therefore apply a suitable numerical time integration scheme of order p (see Definition A.17 and Lemma A.19) to the above system.

The resulting semi-discrete scheme then satisfies convergence bounds of order $\mathcal{O}\left(c^{-1} + \tau^p\right)$. We observe that this method is convergent of order p in time for all $c \gg 1$ with $\tau^p \gtrsim c^{-1}$. In particular, we thus obtain a good approximation to the exact solution if c is large.

In our case we choose an exponential Strang splitting scheme ([44, 65]) of classical order $p = 2$ for the solution of the SP system (3.108). For the analysis of the corresponding semi-discrete scheme we refer to [65]. In the latter paper, Lubich used the technique of Lie derivatives (see [52, Chapter III.5] or [44, Chapter IV.1]) in order to show that the Strang splitting method applied to nonlinear Schrödinger and Schrödinger–Poisson systems for $x \in \mathbb{R}^3$ satisfies error bounds of order $\mathcal{O}\left(\tau^2\right)$ in $L^2 = H^0(\mathbb{R}^3)$ if the initial data and thus the solution for all times t is in $H^4(\mathbb{R}^3)$. This result can be easily extended to error bounds of order $\mathcal{O}\left(\tau^2\right)$ in H^r if the initial data is in H^{r+4} on the torus $\mathbb{T}^d$ for $r > d/2$ (see [44]).

In the subsequent paragraph we gather results which already exist in the literature and point out our contribution explicitly.

Existing Work

Note that in case of Maxwell–Klein–Gordon we successfully published a paper [63], in which we proposed and analysed a scheme for efficiently solving the MKG system in the nonrelativistic limit regime. The latter scheme is based on an exponential Strang splitting method combined with Fourier space discretization techniques (see [44, 45, 65, 66]) for the numerical solution of the Schrödinger Poisson (SP) limit system (3.30b) corresponding to the MKG system (2.20). In constructing our method within [63] we followed the ideas given in [45] for the case of nonlinear Klein–Gordon equations. We considered the system on a finite time interval $[0, T]$ and on the torus $\mathbb{T}^d = [-\pi, \pi]^d$. Moreover, we have shown that the application of this method, with time step τ and M grid points in space, yields numerical convergence bounds of order $\mathcal{O}\left(c^{-2} + \tau^2 + M^{-r'}\right)$ ([63, Theorem 2], compare to Theorem 3.15 below), where r' and the constants in the bounds only depend on T and on the regularity of the exact solution, but not on c . Within this section we elaborate the ideas for the construction of the latter method in more detail.

Also note that in [57] the authors already proposed a familiar method for the approximate solution of the Maxwell–Dirac system in the nonrelativistic limit regime. However, the numerical convergence of this method has only been proven heuristically in [57] by numerical experiments. The authors did not give a rigorous error estimate.

Our Contribution

Thus our contribution within this section is to elaborate the ideas for the construction of the method proposed and analysed in [63] in more detail. Furthermore, we give rigorous numerical error bounds for the Strang splitting method applied to the SP limit system (3.59b) in case of MD. We collect the numerical approximation results of the latter methods in Theorem 3.15 below.

First we begin with the description of the Strang splitting time integration scheme applied to the SP system (3.108).

3.5.1 Time Discretization of the SP Limit System for w_0

This section is based on [44, 65]. Further convergence results for time-splitting methods applied to nonlinear Schrödinger and Schrödinger–Poisson systems can be found in [8, 25–28, 38, 43, 46, 49] and references therein. We carry out the numerical time integration of the Schrödinger-Poisson system (3.108) with an exponential Strang splitting method as in [65]. Thus we naturally split the SP system

$$\begin{cases} i\partial_t w_0 = \frac{1}{2}\Delta w_0 + \phi_0 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix}, & w_0(0) = w_{I,0} = (u_{I,0}, v_{I,0})^\top \\ -\Delta\phi_0 = \rho_0[u_0, v_0] \begin{cases} -\frac{1}{4}(|u_0|^2 - |v_0|^2), & \text{in case of MKG, see (3.30b)}, \\ \frac{1}{4}(|u_0|^2 + |v_0|^2), & \text{in case of MD, see (3.59b)}, \end{cases} \end{cases} \tag{3.109}$$

where the initial data

$$w_{I,0} = \begin{cases} \begin{pmatrix} \psi_{I,0} - i\psi'_{I,0} \\ \overline{\psi_{I,0} - i\psi'_{I,0}} \end{pmatrix} & \text{for MKG is given through (3.9)}, \\ \begin{pmatrix} (\mathcal{I}_4 - \boldsymbol{\beta})\psi_{I,0} \\ \overline{(\mathcal{I}_4 + \boldsymbol{\beta})\psi_{I,0}} \end{pmatrix} = \begin{pmatrix} (\ 0\ , 2\psi^-_{I,0})^\top \\ \overline{(2\psi^+_{I,0},\ 0\ )^\top} \end{pmatrix} & \text{for MD is given through (3.36) and (3.37)}, \end{cases}$$

into the kinetic part

$$i\partial_t w_0(t) = \frac{1}{2}\Delta w_0(t), \quad w_0(0) = \tilde{w}_I \tag{w_0.I}$$

and the potential part

$$\begin{cases} i\partial_t w_0(t) = \phi_0(t)\begin{pmatrix} u_0(t) \\ -v_0(t) \end{pmatrix}, & w_0(0) = \tilde{w}_I \\ -\Delta\phi_0(t) = \rho_0(t) \end{cases} \tag{w_0.II}$$

for given initial data $\tilde{w}_I = (\tilde{u}_I, \tilde{v}_I)^\top$. Observe that within the second subproblem (w_0.II) the modulus of u_0, v_0 is constant over time since ϕ_0 is a real scalar potential, i.e.

$$\begin{aligned}\partial_t |u_0(t)|^2 =&(\partial_t u_0(t)) \cdot \overline{u_0}(t) + u_0(t) \cdot (\overline{\partial_t u_0}(t))\\ =&(-i\phi_0(t)u_0(t)) \cdot \overline{u_0}(t) + u_0(t) \cdot (i\phi_0(t)\overline{u_0}(t)) = 0\end{aligned}$$

and similar for v_0. This immediately implies that in the time evolution of (w_0.II) also $\phi_0(t) = \phi_0(0)$ is constant over time.

In the following, we denote the exact solutions of the subproblems (w_0.I) and (w_0.II) by the flows $\varphi^t_{w_0.\mathrm{I}}$ and $\varphi^t_{w_0.\mathrm{II}}$, respectively (see Definition A.16). The notation $\mathcal{T}^{\,t}_{[-\frac{1}{2}\Delta]} = e^{-it\frac{1}{2}\Delta}$ (see (3.70)) thus allows us to write

$$\varphi^\tau_{w_0.\mathrm{I}}(\tilde{w}_I(x)) = e^{-i\tau\frac{1}{2}\Delta}\tilde{w}_I(x) = \mathcal{T}^{\,\tau}_{[-\frac{1}{2}\Delta]}\tilde{w}_I(x) \tag{3.110a}$$

and (see Appendix A.3 for the definition of $\dot{\Delta}^{-1}$)

$$\varphi^\tau_{w_0.\mathrm{II}}(\tilde{w}_I(x)) = \begin{pmatrix} e^{-i\int_0^\tau \phi_0(s,x)ds}\tilde{u}_I(x) \\ e^{+i\int_0^\tau \phi_0(s,x)ds}\tilde{v}_I(x)\end{pmatrix} = \begin{pmatrix} e^{-i\tau\phi_0(0,x)}\tilde{u}_I(x) \\ e^{+i\tau\phi_0(0,x)}\tilde{v}_I(x)\end{pmatrix}, \quad \phi_0(0) = -\dot{\Delta}^{-1}\rho_0[\tilde{u}_I, \tilde{v}_I]. \tag{3.110b}$$

We observe that the evaluation of $\varphi^\tau_{w_0.\mathrm{II}}(\tilde{w}_I(x))$ involves only pointwise multiplications in space and thus can be carried out very efficiently. The application of Fourier pseudo-spectral techniques for the spatial discretization of $\mathcal{T}^{\,\tau}_{[-\frac{1}{2}\Delta]}$ allows to compute the flow $\varphi^\tau_{w_0.\mathrm{I}}(\tilde{w}_I(x))$ exactly in time. We discuss these techniques in Section 3.5.3 below.

The Strang splitting approximation to the exact flow $\varphi^{t_n}_{w_0}(w_0(0)) = \varphi^{t_n}_{w_0.\mathrm{I}+w_0.\mathrm{II}}(w_0(0))$ of the SP system (3.109) at time $t_n = n\tau, n = 0, 1, 2, \ldots, T/\tau$ with time step size τ is then given by

$$\Bigg(\underbrace{\varphi^{\tau/2}_{w_0.\mathrm{I}} \circ \varphi^{\tau}_{w_0.\mathrm{II}} \circ \varphi^{\tau/2}_{w_0.\mathrm{I}}}_{=:\Phi^\tau_{w_0,\mathrm{Strang}}}\Bigg)^n (w_0(0)) = \left(\Phi^\tau_{w_0,\mathrm{Strang}}\right)^n(w_0(0)) = w_0^n \approx \varphi^{t_n}_{w_0}(w_0(0)). \tag{3.110c}$$

Note that $\Phi^\tau_{w_0,\mathrm{Strang}}$ provides a semidiscrete time integration scheme, i.e. the approximations $w_0^n = w_0^n(x)$ are still depending on the space variable $x \in \mathbb{T}^d$. The discretization in space and the fully-discrete scheme shall be discussed in the subsequent sections.

Based on [65, Theorem 2.1] we state the following Corollary 3.10 on the numerical approximation of the Strang splitting scheme (3.110).

Corollary 3.10 ([44, Proposition IV.6 and Remark IV.7], see also [65, Theorem 2.1])**.** *Let $r > d/2$. Suppose that the exact solution $w_0(t)$ to the SP system (3.109) is in H^{r+4} for $t \in [0,T]$. Then the numerical solution w_0^n to (3.109) given by the scheme (3.110) with time step size $\tau > 0$ satisfies*

$$\|w_0(t_n) - w_0^n\|_r \le K\big(\mathcal{M}^{r+4}_{w_0}\big)\tau^2, \qquad \textit{for } T_n = n\tau \le T.$$

Proof: For the proof, see [65, Theorem 2.1] and also [44, Proposition IV.6 and Remark IV.7]. □

Similar results for the Lie splitting method

$$\Bigg(\underbrace{\varphi^{\tau}_{w_0.\mathrm{II}} \circ \varphi^{\tau}_{w_0.\mathrm{I}}}_{=:\Phi^{\tau}_{w_0,\mathrm{Lie}}}\Bigg)^n (w_0(0)) = \left(\Phi^{\tau}_{w_0,\mathrm{Lie}}\right)^n (w_0(0)) \approx \varphi^{t_n}_{w_0}(w_0(0))$$

and the Strang splitting method (3.110) applied to the cubic nonlinear Schrödinger equation on the torus $\mathbb{T}^d$ — simply replace ϕ_0 in (3.109) and (w_0.II) by $|w_0|^2$ — have been shown in [44, Proposition IV.6 and Remark IV.7]. The Lie splitting then admits global error bounds of order $\mathcal{O}(\tau)$ whereas the Strang splitting allows error bounds of order $\mathcal{O}(\tau^2)$, respectively. Note that later in Chapter 5 we underline the second order error bound for the latter Strang splitting scheme by numerical experiments.

Later, in Theorem 3.15 we show that these schemes admit convergence bounds towards the exact solutions w and ϕ of the MKG/MD first order systems in time (2.33)/(2.41) of order $\mathcal{O}\left(c^{-1} + \tau^p\right)$, where $p = 1$ in case of the Lie splitting $\Phi^{\tau}_{w_0,\mathrm{Lie}}$ and $p = 2$ in case of the Strang splitting scheme $\Phi^{\tau}_{w_0,\mathrm{Strang}}$, respectively.

Note that according to higher order limit approximations (see (3.35) and (3.63)), we can (formally) improve the convergence in c by additionally numerically solving a SP system for a function w_1 with a suitable time integration scheme up to bounds of order $\mathcal{O}\left(c^{-2} + \tau^p\right)$. Recall that by (3.34a) for the case of MKG and by (3.62b) for the case of MD, we have that for

$$\delta_{\mathrm{MD}} = 0 \quad \text{in case of MKG and} \quad \delta_{\mathrm{MD}} = 1 \quad \text{in case of MD} \tag{3.111a}$$

the functions w_1, $\tilde{\phi}_1$ and $\phi_1^{(2,0)}$ satisfy

$$\begin{cases} i\partial_t w_1 = \frac{1}{2}\Delta w_1 + \phi_0 \begin{pmatrix} u_1 \\ -v_1 \end{pmatrix} + \tilde{\phi}_1 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix} + \delta_{\mathrm{MD}} i \frac{1}{2} \sum_{j=1}^{d} (\partial_j \phi_0) \begin{pmatrix} \boldsymbol{\alpha}_j u_0 \\ -\overline{\boldsymbol{\alpha}_j} v_0 \end{pmatrix}, \\ -\Delta \tilde{\phi}_1 = \tilde{\rho}_1 = \begin{cases} \frac{1}{2}\mathrm{Re}\,(-u_0 \cdot \overline{u_1} + v_0 \cdot \overline{v_1}) & \text{in case of MKG,} \\ \frac{1}{2}\mathrm{Re}\,(\ \ u_0 \cdot \overline{u_1} + v_0 \cdot \overline{v_1}) & \text{in case of MD,} \end{cases} \\ -\Delta \phi_1^{(2,0)} = \rho_1^{(2,0)} = \begin{cases} 0 & \text{in case of MKG,} \\ \frac{1}{4}(u_0 \cdot v_1 + u_1 \cdot v_0) & \text{in case of MD,} \end{cases} \\ w_1(0) = w_{I,1} = (u_{I,1}, v_{I,1})^{\top}, \end{cases} \tag{3.111b}$$

where the initial data

$$w_{I,1} = \begin{cases} \begin{pmatrix} \psi_{I,1} - i\psi'_{I,1} \\ \overline{\psi_{I,1} - i\psi'_{I,1}} \end{pmatrix} & \text{for MKG is given through (3.9),} \\ \begin{pmatrix} (\mathcal{I}_4 - \boldsymbol{\beta})\psi_{I,1} \\ (\mathcal{I}_4 + \boldsymbol{\beta})\overline{\psi_{I,1}} \end{pmatrix} + \sum_{j=1}^{d} \begin{pmatrix} i\boldsymbol{\alpha}_j \partial_j \psi_{I,0} \\ \overline{i\boldsymbol{\alpha}_j \partial_j \psi_{I,0}} \end{pmatrix} & \text{for MD is given through (3.36).} \end{cases} \tag{3.111c}$$

Recall that (formally, see [70] and also (3.35) and (3.63) in Sections 3.2.4 and 3.3.4, respectively),

$$\psi = \psi_0 + c^{-1}\psi_1 + \mathcal{O}\left(c^{-2}\right)$$

with

$$\begin{aligned} \psi_0(t) &= \frac{1}{2}(e^{ic^2 t} u_0(t) + e^{-ic^2 t}\overline{v_0}(t)) \quad \text{and} \\ \psi_1(t) &= \frac{1}{2}(e^{ic^2 t} u_1(t) + e^{-ic^2 t}\overline{v_1}(t)). \end{aligned}$$

Furthermore, note that by (3.62)

$$\phi_1(t) = \tilde{\phi}_1(t) + e^{2ic^2t}\phi_1^{(2,0)} + e^{-2ic^2t}\overline{\phi_1^{(2,0)}}(t). \tag{3.112}$$

In the subsequent subsection we construct a Strang splitting scheme for numerically solving the latter system (3.111).

3.5.2 Time Discretization of the SP System for the Second Term w_1

Based on [44, 65], we construct a Strang splitting scheme for the numerical time integartion of (3.111) by splitting the system, similar to before, into the following subproblems for given initial data $\tilde{w}_I = (\tilde{u}_I, \tilde{v}_I)^\top$

$$i\partial_t w_1 = \frac{1}{2}\Delta w_1, \quad w_1(0) = \tilde{w}_I \quad \text{with solution} \quad \varphi^\tau_{w_1.\mathrm{I}}(\tilde{w}_I) = e^{-i\frac{1}{2}\tau\Delta}\tilde{w}_I \tag{w_1.I}$$

and

$$i\partial_t w_1 = \phi_0 \begin{pmatrix} u_1 \\ -v_1 \end{pmatrix}, \quad w_1(0) = \tilde{w}_I \quad \text{with solution} \quad \varphi^\tau_{w_1.\mathrm{II}}(\tilde{w}_I) = \begin{pmatrix} e^{-i\int_0^\tau \phi_0(s)ds}\tilde{u}_I \\ e^{+i\int_0^\tau \phi_0(s)ds}\tilde{v}_I \end{pmatrix} \tag{w_1.II}$$

and

$$i\partial_t w_1 = i\delta_{\mathrm{MD}}\frac{1}{2}\sum_{j=1}^d (\partial_j\phi_0)\begin{pmatrix} \boldsymbol{\alpha}_j u_0 \\ -\overline{\boldsymbol{\alpha}_j} v_0 \end{pmatrix} := i\delta_{\mathrm{MD}} G_{w_1}[w_0, \phi_0], \quad w_1(0) = \tilde{w}_I \tag{w_1.III}$$

with solution (recall that by (3.111a) $\delta_{\mathrm{MD}} = 0$ in case of MKG and $\delta_{\mathrm{MD}} = 1$ in case of MD)

$$\varphi^\tau_{w_1.\mathrm{III}}(\tilde{w}_I) = \tilde{w}_I + \delta_{\mathrm{MD}}\int_0^\tau G_{w_1}[w_0(s), \phi_0(s)]ds, \tag{3.113}$$

and the last subproblem using the solution operator $\dot{\Delta}^{-1}$ (see (A.4)) in order to write $\tilde{\phi}_1$ in terms of w_0 and w_1, i.e.

$$i\partial_t w_1 = \left(\frac{1}{2}\dot{\Delta}^{-1}\,\mathrm{Re}\left((-1)^{\delta_{\mathrm{MD}}} u_0 \cdot \overline{u_1} - v_0 \cdot \overline{v_1}\right)\right)\begin{pmatrix} u_0 \\ -v_0 \end{pmatrix}, \quad w_1(0) = \tilde{w}_I \tag{w_1.IV}$$

with solution $\varphi^\tau_{w_1.\mathrm{IV}}(\tilde{w}_I)$, which is specified in (3.115) below. Note that we discuss the numerical approximations to the integral terms in (w_1.II) and (3.113) later in this section.

Because the right hand side of (w_1.IV) involves the complex conjugate $\overline{w_1}$ of the solution, we consider the latter subproblem (w_1.IV) in its real and imaginary parts of w_0 and w_1, respectively, similar to [45, Example 2]. More precisely, if we define the mapping

$$T : \mathbb{C}^m \to \mathbb{R}^{2m} \quad \text{with} \quad T(Z) = (\mathrm{Re}\,(Z)\,, \mathrm{Im}\,(Z))^\top$$

and its inverse by

$$T^{-1} : \mathbb{R}^{2m} \to \mathbb{C}^m \quad \text{with} \quad T^{-1}((\alpha, \beta)^\top) = \alpha + i\beta, \text{ where } \alpha, \beta \in \mathbb{R}^m,$$

and if we set

$$(\alpha_j, \beta_j)^\top := T(u_j) \quad \text{and} \quad (\eta_j, \xi_j)^\top := T(v_j) \quad \text{for} \quad j = 0, 1, \tag{3.114}$$

we collect the variables (3.114) in the vectors

$$\mathcal{Y}_0 = (\alpha_0, \beta_0, \eta_0, \xi_0)^\top \qquad \text{and} \qquad \mathcal{Y}_1 = (\alpha_1, \beta_1, \eta_1, \xi_1)^\top, \quad \text{respectively.}$$

By comparison of real and imaginary parts in (w_1.IV) we obtain the system

$$\begin{aligned}\partial_t \mathcal{Y}_1 =& \frac{1}{2}\Big(\dot{\Delta}^{-1}\left((-1)^{\delta_{\text{MD}}}(\alpha_0\cdot\alpha_1+\beta_0\cdot\beta_1)-(\eta_0\cdot\eta_1+\xi_0\cdot\xi_1)\right)\Big)\begin{pmatrix}\beta_0\\-\alpha_0\\-\xi_0\\\eta_0\end{pmatrix}\\ =:& H[\mathcal{Y}_1;\mathcal{Y}_0], \qquad \mathcal{Y}_1(0)=(T(\tilde{u}_I),T(\tilde{v}_I))^\top\end{aligned}$$

with solution

$$\mathfrak{T}\circ\varphi^\tau_{w_1.\text{IV}}(\tilde{w}_I) := \begin{pmatrix}T(u_1(\tau))\\T(v_1(\tau))\end{pmatrix} = \mathcal{Y}_1(\tau)=\mathcal{Y}_1(0)+\int_0^\tau H[\mathcal{Y}_1(s);\mathcal{Y}_0(s)]ds, \tag{3.115}$$

where we set for $u=\alpha+i\beta,\ v=\eta+i\xi\in\mathbb{C}^m$ and $\alpha,\beta,\eta,\xi\in\mathbb{R}^m$

$$\begin{aligned}\mathfrak{T}:\mathbb{C}^{2m}\to\mathbb{R}^{2m} \quad &\text{with} \quad \mathfrak{T}\Big((u,v)^\top\Big)=\begin{pmatrix}T(u)\\T(v)\end{pmatrix}=\begin{pmatrix}(\alpha,\beta)^\top\\(\eta,\xi)^\top\end{pmatrix}\\ \mathfrak{T}^{-1}:\mathbb{R}^{2\cdot 2m}\to\mathbb{C}^{2m} \quad &\text{with} \quad \mathfrak{T}^{-1}\Big((\alpha,\beta,\eta,\xi)^\top\Big)=\begin{pmatrix}T^{-1}((\alpha,\beta)^\top)\\T^{-1}((\beta,\xi)^\top)\end{pmatrix}=\begin{pmatrix}u\\v\end{pmatrix}.\end{aligned}$$

We approximate the integral terms in the exact flows $\varphi^\tau_{w_1.\text{II}}$ and $\varphi^\tau_{w_1.\text{III}}$ given in (w_1.II) and (3.113), respectively, by the second order accurate trapezoidal rule (also called Crank-Nicolson method, see for instance [33, Chapter 10.2 and 12.7]), i.e. we obtain the numerical flows

$$\begin{aligned}\Phi^\tau_{w_1.\text{II}}(w_1^n) :=& \begin{pmatrix}e^{-i\frac{\tau}{2}(\phi_0^n+\phi_0^{n+1})}\tilde{u}_I\\ e^{+i\frac{\tau}{2}(\phi_0^n+\phi_0^{n+1})}\tilde{v}_I\end{pmatrix} \approx \varphi^\tau_{w_1.\text{II}}(w_1^n)\\ \Phi^\tau_{w_1.\text{III}}(w_1^n) :=& \tilde{w}_I+\frac{\tau}{2}\delta_{\text{MD}}\Big(G_{w_1}[w_0^n,\phi_0^n]+G_{w_1}[w_0^{n+1},\phi_0^{n+1}]\Big)\approx\varphi^\tau_{w_1.\text{III}}(w_1^n),\end{aligned} \tag{3.116a}$$

where we assume that the approximations $w_0^{\tilde{n}},\phi_0^{\tilde{n}}$ to $w_0(t_{\tilde{n}}),\phi_0(t_{\tilde{n}})$ for $\tilde{n}\in\{n,n+1\}$ satisfy second order error bounds in time and where by (3.111a) $\delta_{\text{MD}}=0$ in case of MKG and $\delta_{\text{MD}}=1$ in case of MD).

For the approximation of the flow $\mathfrak{T}\circ\varphi^\tau_{w_1.\text{IV}}$, given in (3.115) we use the following modified second order accurate method of Heun ([17, Chapter 8.1.3 and 8.1.8)])

$$\begin{aligned}\mathcal{Y}_1^{n+\frac{1}{2}} =& \mathcal{Y}_1^n+\tau H[\mathcal{Y}_1^n;\mathcal{Y}_0^n]\\ \mathcal{Y}_1^{n+1}=\Phi^\tau_{w_1.\text{IV}}(\mathcal{Y}_1^n) =& \mathcal{Y}_1^n+\frac{\tau}{2}\Big(H[\mathcal{Y}_1^n;\mathcal{Y}_0^n]+H[\mathcal{Y}_1^{n+\frac{1}{2}};\mathcal{Y}_0^{n+1}]\Big)\approx\mathfrak{T}\circ\varphi^\tau_{w_1.\text{IV}}(w_1^n).\end{aligned} \tag{3.116b}$$

This yields

$$\mathfrak{T}^{-1}\circ\Phi^\tau_{w_1.\text{IV}}\circ\mathfrak{T}(w_1^n)\approx\varphi^\tau_{w_1.\text{IV}}(w_1^n). \tag{3.116c}$$

Gathering the exact flow $\varphi^\tau_{w_1.\text{I}}$ of subproblem (w_1.I) and the numerical flows $\Phi^\tau_{w_1.\text{II}}$, $\Phi^\tau_{w_1.\text{III}}$ and $\mathfrak{T}^{-1}\circ\Phi^\tau_{w_1.\text{IV}}\circ\mathfrak{T}$ given in (3.116) corresponding to subproblems (w_1.II), (w_1.III) and (w_1.IV), respectively, we are ready to formulate a second order Strang splitting method for the numerical solution of the problem (3.111), i.e.

$$\begin{aligned}w_1^{n+1} =& \Phi^\tau_{w_1,\text{Strang}}(w_1^n)\\ :=& \varphi^{\tau/2}_{w_1.\text{I}}\circ\Phi^{\tau/2}_{w_1.\text{II}}\circ\Phi^{\tau/2}_{w_1.\text{III}}\circ\mathfrak{T}^{-1}\circ\Phi^\tau_{w_1.\text{IV}}\circ\mathfrak{T}\circ\Phi^{\tau/2}_{w_1.\text{III}}\circ\Phi^{\tau/2}_{w_1.\text{II}}\circ\varphi^{\tau/2}_{w_1.\text{I}}(w_1^n).\end{aligned} \tag{3.117a}$$

If we suppose that $w_1^{n+1}\approx w_1(t_{n+1})$, i.e. that the latter scheme provides an approximation to the exact solution of (3.111) we obtain an approximation ϕ_1^{n+1} to $\phi_1(t_{n+1})$ by numerically solving

$$-\Delta\tilde{\phi}_1^{n+1}=\tilde{\rho}_1^{n+1}\approx\tilde{\rho}_1(t_{n+1}), \qquad -\Delta\phi_1^{(2,0),n+1}=\rho_1^{(2,0),n+1}\approx\rho_1^{(2,0)}(t_{n+1}), \tag{3.117b}$$

such that according to (3.112)

$$\phi_1^{n+1} = \tilde{\phi}_1^{n+1} + e^{2ic^2 t_{n+1}} \phi_1^{(2,0),n+1} + e^{-2ic^2 t_{n+1}} \overline{\phi_1^{(2,0),n+1}} \approx \phi_1(t_{n+1}). \tag{3.117c}$$

Note that for stepping from w_1^n to w_1^{n+1} this scheme uses second order accurate numerical approximations w_0^n, w_0^{n+1}, ϕ_0^n, ϕ_0^{n+1} to the solutions $w_0(\sigma)$, $\phi_0(\sigma)$ at time $\sigma = t_n$ and $\sigma = t_{n+1}$, respectively, of the SP system (3.109) (see (3.116)).

Because the numerical flows $\Phi^t_{w_1.\mathrm{II}}$, $\Phi^t_{w_1.\mathrm{III}}$, $\Phi^t_{w_1.\mathrm{IV}}$ given in (3.116) are second order accurate approximations to the exact flows corresponding to subproblems (w_1.II), (w_1.III) and (w_1.IV), respectively, one can show that the Strang splitting scheme (3.117) satisfies global error bounds of order $\mathcal{O}\left(\tau^2\right)$ (see [52, Chapter II.5] and [44, Proposition IV.6 and Remark IV.7] and also Corollary 3.10 above), i.e.

$$w_1(t_n) = w_1^n + \mathcal{O}\left(\tau^2\right). \tag{3.118}$$

The interested reader may exploit similar techniques as in the proof of [44, Proposition IV.6 and Remark IV.7] and also Corollary 3.10 in order to prove the $\mathcal{O}\left(\tau^2\right)$ bound (3.118). Our numerical experiments in Chapter 5 underline this error bound.

In the subsequent section we discuss the discretization in space of the SP system (3.109).

3.5.3 Space Discretization of the SP Limit System

This section is based on [44] and on [30, 48, 49, 66, 88]. For the discretization in space of the spatial differential operators ∂_ℓ, $\ell = 1, \ldots, d$, Δ and $\langle \nabla \rangle_c$ on the torus $\mathbb{T}^d = [-\pi, \pi]^d$, we choose Fourier pseudo-spectral methods. We explain the idea behind this method at the example of $d = 1$ and follow [44, Chapter III and Chapter IV.4]. Even though the proofs in this section will be given only for $d = 1$, all the results remain valid also for higher dimensions $d \geq 1$.

Spatial Discretization with Fourier techniques

Let $d = 1$ and let $u \in H^r(\mathbb{T}^1)$ be a periodic function on the torus $\mathbb{T}^1 = [-\pi, \pi]^1$. Then its Fourier series expansion reads

$$u(x) = \sum_{k \in \mathbb{Z}^1} \widehat{u}_k e^{ik \cdot x} \quad \text{with} \quad \widehat{u}_k = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^1} u(x) e^{-ik \cdot x} dx. \tag{3.119}$$

Now define the set $\mathcal{Z}_M \subset \mathbb{Z}$ by

$$\mathcal{Z}_M := \begin{cases} \{-R, \ldots, R-1\}, & \text{if } M = 2R \in \mathbb{N} \text{ is even}, \\ \{-R, \ldots, R\}, & \text{if } M = 2R+1 \in \mathbb{N} \text{ is odd}, \end{cases}$$

and associate the equidistant discretization of $\mathbb{T}^1$ as

$$x_j = j \cdot \frac{2\pi}{M} \quad \text{with} \quad j \in \mathcal{Z}_M. \tag{3.120}$$

Furthermore define the discrete Fourier transform $\mathcal{F}_M : \mathbb{C}^M \to \mathbb{C}^M$ and its inverse such that for all $j \in \mathcal{Z}_M$ and $k \in \mathcal{Z}_M$ respectively

$$(\widehat{v^M})_k = (\mathcal{F}_M v^M)_k = \frac{1}{M} \sum_{j \in \mathcal{Z}_M} v_j^M e^{-ij \cdot x_k} \quad \text{and} \quad (v^M)_j = (\mathcal{F}_M^{-1} \widehat{v^M})_j = \sum_{k \in \mathcal{Z}_M} (\widehat{v^M})_k e^{ik \cdot x_j}.$$

Let $U = (U_j)_{j\in\mathcal{Z}_M}$ with $U_j = u(x_j)$ be the vector, containing the exact evaluation of u in the grid points x_j. We observe that applying $\mathcal{F}_M$ to U can be associated with an approximation to the Fourier integral $\widehat{u}_k$ from (3.119) by the trapezoidal rule in the nodes x_j such that

$$\widehat{U^M} = \mathcal{F}_M U \approx (\widehat{u}_k)_{k\in\mathcal{Z}_M}.$$

For the definition of the trapezoidal quadrature rule, see [17, Chapter 6.1]. Then $U^M := \mathcal{F}_M^{-1}\widehat{U^M}$ can be seen as an approximation to the truncated Fourier series expansion of u given in (3.119), i.e.

$$u(x_j) - \sum_{k\notin\mathcal{Z}_M} \widehat{u}_k e^{ik\cdot x_j} = \sum_{k\in\mathcal{Z}_M} \widehat{u}_k e^{ik\cdot x_j} \approx \sum_{k\in\mathcal{Z}_M} (\widehat{U^M})_k e^{ik\cdot x_j} = (U^M)_j \qquad \text{for } j\in\mathcal{Z}_M. \tag{3.121}$$

Moreover we may extend the finite vector $(\widehat{U^M})_k$ with $k\in\mathcal{Z}_M$ to a sequence by zeros for indices outside of $\mathcal{Z}_M$, i.e.

$$(\widehat{U^M})_k = 0 \quad \text{for } k\notin\mathcal{Z}_M. \tag{3.122}$$

With the aid of [44, Lemma IV.13] we thus show that for the infinite sequence $\widehat{U} := (\widehat{u}_k)_{k\in\mathbb{Z}}$ — note that the index set is $\mathbb{Z}$ and not $\mathcal{Z}_M$ here— the following Lemma 3.11 holds. For the definition of the spaces ℓ_r^m see Definition A.6.

Lemma 3.11 ([44, Lemma IV.13], see also [88])**.** *Let $r\geq 0$ and let $s,s'\in\mathbb{R}$ such that $s'-s>d/2$. Furthermore let $u\in H^{r+s'}$. Then*

$$\left\|\widehat{U}-\widehat{U^M}\right\|_{\ell_r^2} \leq \left\|\widehat{U}-\widehat{U^M}\right\|_{\ell_r^1} \leq K\cdot M^{-s}\left\|\widehat{U}\right\|_{\ell_{r+s}^1} \leq K\cdot M^{-s}\left\|\widehat{U}\right\|_{\ell_{r+s'}^2}.$$

Therefore, the accuracy of the approximation with the presented Fourier techniques only depend on the regularity of u. Recall, that for all $r'\in\mathbb{R}$ the space $\ell_{r'}^2$ can be identified with the space $H^{r'}(\mathbb{T}^d)$ and vice versa (see Definition A.6).

Proof (see [44, Lemma IV.13])*:* The last inequality is a consequence of the embeddings $\ell_{r+s'}^2\subset\ell_{r+s}^1\subset\ell_{r+s}^2$ from Proposition A.7. The first inequality is a consequence of $\langle k\rangle^r|z_k|\leq\|z\|_{\ell_r^1}\sum_{k\in\mathbb{Z}^d}$ for all $k\in\mathbb{Z}$ and

$$\|z\|_{\ell_r^2}^2 = \sum_{k\in\mathbb{Z}^d}\langle k\rangle^{2r}|z_k|^2 \leq \|z\|_{\ell_r^1}\sum_{k\in\mathbb{Z}^d}\langle k\rangle^r|z_k| = \|z\|_{\ell_r^1}^2.$$

Because $\widehat{U^M}$ is a finite dimensional vector, we have that according to (3.121)

$$\left\|\widehat{U}-\widehat{U^M}\right\|_{\ell_r^1} \leq \sum_{k\notin\mathcal{Z}_M}\langle k\rangle^r\left|\widehat{U}_k\right| + \sum_{k\in\mathcal{Z}_M}\langle k\rangle^r\left|\widehat{U}_k-(\widehat{U^M})_k\right|.$$

Thus, according to the proof of [44, Lemma IV.13], the crucial point in proving the second inequality is to find a bound for the first term in the latter estimate. We have that

$$\sum_{k\notin\mathcal{Z}_M}\langle k\rangle^r\left|\widehat{U}_k\right| = M^{-s}\sum_{k\notin\mathcal{Z}_M}\langle k\rangle^r M^s\left|\widehat{U}_k\right|.$$

Note that for $k\in\mathcal{Z}_M$, we have $|k|\geq|M/2-1|$. Hence, we find a constant K such that

$$\begin{aligned}\sum_{k\notin\mathcal{Z}_M}\langle k\rangle^r\left|\widehat{U}_k\right| &= M^{-s}\sum_{k\notin\mathcal{Z}_M}\langle k\rangle^r M^s\left|\widehat{U}_k\right| \leq K\cdot M^{-s}\sum_{k\notin\mathcal{Z}_M}\langle k\rangle^{r+s}\left|\widehat{U}_k\right|\\ &\leq K\cdot M^{-s}\left\|\widehat{U}\right\|_{\ell_r^1}.\end{aligned}$$

For the second term, we use the aliasing formula (see [66, Proof of Theorem III.1.7])

$$\widehat{U^M}_k = \sum_{a\in\mathbb{Z}} \widehat{U}_{k+aM} = \widehat{U}_k + \sum_{a\in\mathbb{Z}\setminus 0} \widehat{U}_{k+aM}.$$

Then

$$\begin{aligned}\sum_{k\in\mathcal{Z}_M} \langle k\rangle^r \left|\widehat{U}_k - (\widehat{U^M})_k\right| &\leq \sum_{k\in\mathcal{Z}_M} \langle k\rangle^r \sum_{a\in\mathbb{Z}\setminus 0} \left|\widehat{U}_{k+aM}\right| \\ &\leq M^{-s} \sum_{a\in\mathbb{Z}\setminus 0} \sum_{k\in\mathcal{Z}_M} \langle k+aM\rangle^r M^s \left|\widehat{U}_{k+aM}\right|.\end{aligned}$$

Because $M \leq K \cdot \langle k+aM\rangle$ for $k \in \mathcal{Z}_M$ and $|a| > 0$ and some constant K, this finishes the proof. □

As a consequence of Lemma 3.11 we state the following remark.

Remark 3.12 ([44])**.** *Note that if s, s' satisfy the conditions of Lemma 3.11 and if $u \in H^{r+m+s'}$ for some $m \in \mathbb{R}$ such that $r+m \geq 0$, then the error of the space approximation remains $\mathcal{O}(M^{-s})$ in the sense of the H^{r+m} norm, i.e.*

$$\left\|\widehat{U} - \widehat{U^M}\right\|_{\ell^2_{r+m}} \leq K \cdot M^{-s} \left\|\widehat{U}\right\|_{\ell^2_{r+m+s'}}.$$

However, if u is not smooth enough we only obtain a weaker convergence in M, i.e.

$$\text{if } u \in H^{r+s'}, \text{ then} \quad \left\|\widehat{U} - \widehat{U^M}\right\|_{\ell^2_{r+m}} \leq K \cdot M^{-(s-m)} \left\|\widehat{U}\right\|_{\ell^2_{r+s'}}.$$

This result allows us to formulate a Fourier pseudo-spectral method for the approximation of spatial operators like the Laplace operator Δ and the operator $\langle\nabla\rangle_c$ in the following subsection.

Fourier Pseudo-Spectral Method for the Discretization of Spatial Operators

The following results are based on [44]. Consider the Fourier series expansion of $u(x)$ in (3.119). Applying for example ∂_x^m for $m \in \mathbb{N}_0$ to u then results in

$$\partial_x^m u(x_j) = \sum_{k\in\mathbb{Z}} (ik)^m \hat{u}_k e^{ik\cdot x_j} \approx: \sum_{k\in\mathcal{Z}_M} (ik)^m (\widehat{U^M})_k e^{ik\cdot x_j} =: (\partial_{x,M}^m U^M)_j,$$

with $x_j = j \cdot 2\pi/M$ for $j \in \mathcal{Z}_M$ given in (3.120). The index M in the derivative denotes that we consider the discrete operator $\partial_{x,M}^m$.

With the above identities, we have $\widehat{\Delta_M}(k) = (\widehat{\Delta_M})_k = -|k|^2$ and

$$\widehat{\langle\nabla\rangle_{c,M}}(k) = (\widehat{\langle\nabla\rangle_{c,M}})_k = \sqrt{|k|^2 + c^2}.$$

Note that from Lemma 3.11 we can deduce the following. Let $r \geq 0$ and let $s' - s > d/2$. If $u \in H^{r+2+s'}$ then

$$\left\|\Delta u - \Delta_M U^M\right\|_r \leq \left\|u - U^M\right\|_{r+2} \leq K \cdot M^{-s} \|\Delta u\|_{r+s'} \leq K \cdot M^{-s} \|u\|_{r+2+s'}.$$

In the subsequent subsection we analyse the numerical error of the semi-discretization in space of the SP system (3.108), exploiting the results from above.

Space Approximation Result for the Schrödinger–Poisson system

This section is based on [44] and [66, Chapter III.1.3]. In order to discretize the Schrödinger–Poisson system (3.109) in space we follow the idea presented in [44, Chapter III.6]. We therefore apply a Fourier pseudo-spectral collocation method (see also [66, Chapter III.1.3]) which is defined as follows. Find a trigonometric polynomial

$$w_0^M(t,x) = \sum_{k\in\mathcal{Z}_M} (w_0^M)_k(t) e^{ik\cdot x},$$

which satisfies the Schrödinger–Poisson system (3.109) in the grid points. More precisely, for all times $t \in [0,T]$ and for all $j \in \mathcal{Z}_M$, the solution $w_0^M = (u_0^M, v_0^M)^\top$ satisfies

$$\begin{cases} i\partial_t w_0^M(t,x_j) = \frac{1}{2}\Delta_M w_0^M(t,x_j) + \phi_0^M(t,x_j)\begin{pmatrix} u_0^M(t,x_j) \\ -v_0^M(t,x_j)\end{pmatrix}, \\ -\Delta_M \phi_0^M(t,x_j) = \rho_0^M(t,x_j), \\ w_0^M(0,x_j) = w_0(0,x_j), \end{cases} \tag{3.123}$$

with $x_j = j \cdot 2\pi/M$ for $j \in \mathcal{Z}_M$ given in (3.120). Assume that $w_0(0) \in H^{r+s'}$. Note that from (3.121) and Lemma 3.11 ([44, Lemma IV.13]) we thus have for $s \in \mathbb{R}$ with $s' - s > d/2$

$$\left\| w_0(0) - w_0^M(0) \right\|_r \leq K \cdot M^{-s} \left\| w_0(0) \right\|_{r+s'}. \tag{3.124}$$

For simplicity, we leave out the spatial argument x_j in the following. Duhamel's formula from Proposition A.20 allows us to write the solution of the semi-discrete SP system (3.123) as

$$w_0^M(t) = e^{-i\Delta_M t/2} w_0^M(t) + \int_0^t e^{-i\Delta_M(t-s)/2}\phi_0^M(s)\begin{pmatrix} u_0^M(s) \\ -v_0^M(s)\end{pmatrix} ds,$$

where, motivated by $(\widehat{\Delta_M})_k = -|k|^2$ for $k \in \mathcal{Z}_M$, we define

$$\widehat{(e^{-it\Delta_M})}_k := e^{-it(-|k|^2)}.$$

We now compare the discretization $w_0^M(t)$ with the exact solution

$$w_0(t) = e^{-i\Delta t/2} w_0(t) + \int_0^t e^{-i\Delta(t-s)/2}\phi_0(s)\begin{pmatrix} u_0(s) \\ -v_0(s)\end{pmatrix} ds.$$

Exploiting the bilinear estimates $\|uv\|_r \leq K \|u\|_r \|v\|_r$ for $r > d/2$ from Lemma A.8, a simple fixed point argument allows us to find a constant $\mathcal{M}_{w_0}^{r+s'}$ such that $\|w_0(t)\|_{r+s'} \leq \mathcal{M}_{w_0}^{r+s'}$ for all $t \leq T$ (see Assumption 3.2 for definition of the constants $\mathcal{M}_{w_0}^{r+s'}$).

Considering (3.122), we have that $(\widehat{w_0^M})_k(t) = 0$ for $k \notin \mathcal{Z}_M$ and thus $e^{-i\Delta_M t/2} w_0^M = e^{-i\Delta t/2} w_0^M$. By the isometry property of $e^{-i\Delta t/2}$ in Lemma A.10 and by another application of the bilinear estimates from Lemma A.8, we obtain [44, Proof of Proposition IV.14]

$$\left\| w_0(t) - w_0^M(t) \right\|_r \leq \left\| w_0(0) - w_0^M(0) \right\|_r + K \int_0^t \left\| w_0(s) - w_0^M(s) \right\|_r ds \tag{3.125}$$

as long as

$$\left\| w_0^M(t) \right\|_r \leq 2\mathcal{M}_{w_0}^{r+s'} \tag{3.126}$$

is bounded. Note that the constant K depends on $\sup_{s\in[0,t]} \left\|w_0^M(t)\right\|_r$ and on the bound in (3.126), but can be chosen independently of M. We proceed with the application of Lemma 3.11 and (3.124), and find

$$\left\|w_0(t) - w_0^M(t)\right\|_r \leq K_0 \cdot M^{-s} \left\|w_0(0)\right\|_{r+s'} + K \int_0^t \left\|w_0(s) - w_0^M(s)\right\|_r ds, \quad \text{for all } t \in [0,T]$$

with constants $K_0, K > 0$ independent of M. Then, Gronwall's Lemma (see for instance [85, Theorem 1.10] and also Lemma A.21) shows that

$$\left\|w_0(t) - w_0^M(t)\right\|_r \leq \underbrace{\left(K_1 \cdot M^{-s} \cdot e^{K_2 T}\right)}_{\leq 1, \text{ for } M \geq M_0 \text{ sufficiently large}} \underbrace{\left\|w_0(0)\right\|_{r+s'}}_{\leq \mathcal{M}_{w_0}^{r+s'}}. \tag{3.127}$$

In a next step, we observe from the latter relation (3.127)

$$\begin{aligned} \left\|w_0^M(t)\right\|_r &\leq \left\|w_0(t)\right\|_r + \left\|w_0^M(t) - w_0(t)\right\|_r \\ &\leq \mathcal{M}_{w_0}^{r+s'} \cdot \left(1 + K_1 \cdot M^{-s} \cdot e^{K_2 T}\right) \leq 2\mathcal{M}_{w_0}^{r+s'} \end{aligned} \tag{3.128}$$

for $t \in [0,T]$ if $M \geq M_0$ is sufficiently large. Note that a bootstrap argument ([44, Proposition IV.14], see also [85, Chapter 1.3]) allows us to repeatedly apply equations (3.125)-(3.128) (see Remark 3.13 below). This finally proves Proposition 3.14 on the spatial approximation error of $w_0^M(t)$ for all $t \in T$.

Remark 3.13 (See [85, Chapter 1.3], A bootstrap argument)**.** *The latter estimate in* (3.128)*, i.e.*

$$\left\|w_0^M(t)\right\|_r \leq 2\mathcal{M}_{w_0}^{r+s'},$$

allows us to formulate the following bootstrap argument[3]*. Initially at $t = 0$, we choose $M \geq M_0$ sufficiently large such that*

$$\left(1 + K_1 \cdot M^{-s} \cdot e^{K_2 T}\right) \leq 2.$$

Then (3.128) *shows that $\left\|w_0^M(0)\right\|_r \leq 2\mathcal{M}_{w_0}^{r+s'}$ holds initially. Now let $\epsilon > 0$ be arbitrary small. Hence, from continuity in time of w_0 and w_0^M, we deduce that equations* (3.125)*-*(3.128) *hold true for $t = \epsilon$. Finally, iteratively increasing $t \curvearrowright t + \epsilon$ up to $t = T$ we can repeatedly apply equations* (3.125)*-*(3.128)*.*

From the above observations we immediately obtain the following Proposition 3.14, which is an adaption of [44, Proposition IV.14].

Proposition 3.14 ([44, Proposition IV.14], Collocation Error)**.** *Fix $r > d/2$ and let s', s such that $s' - s > d/2$. Furthermore assume that the exact solution to the Schrödinger–Poisson system* (3.109) *satisfies $\left\|w_0(t)\right\|_{r+s'} \leq \mathcal{M}_{w_0}^{r+s'}$ for all $t \in [0,T]$. Furthermore let $w_0^M(0)$ be the discrete initial data given in* (3.123)*. Then there exist constants $K_1, K_2 > 0$ and $M_0 > 0$ depending on $\mathcal{M}_{w_0}^{r+s'}$, s', s and T such that for $M \geq M_0$ and for all $t \in [0,T]$*

$$\left\|w_0(t) - w_0^M(t)\right\|_r \leq K_1 \cdot M^{-s} \cdot e^{K_2 T} \left\|w_0(0)\right\|_{r+s'}.$$

[3] See for instance [85, Chapter 1.3] for a comprehensive explanation of a bootstrap argument, and also [44, Proof of Proposition IV.14] and Remark 3.13 below for particular applications of bootstrap arguments.

We focussed in this section on the case $d = 1$. The results also hold true in higher dimensions (see [44, Chapters III and IV]). We only need to replace ∂_x by the partial derivatives $\partial_{x^\ell}, \ell = 1, \ldots, d$ and the corresponding Fourier multipliers (ik) by (ik^ℓ), where $\mathcal{K} := (k^1, \ldots, k^d)^\top \in \mathcal{Z}_M^d$ with $\mathcal{Z}_M := \{-M/2, \ldots, M/2-1\} \subset \mathbb{Z}$. Moreover the symbol for Δ_M becomes

$$\widehat{\Delta_M} = \Big(-\left(\left|k^1\right|^2 + \cdots + \left|k^d\right|^2\right)\Big)_{\mathcal{K} \in \mathcal{Z}_M^d}.$$

We furthermore denote by $x_j \in \mathbb{T}^d$ for $j \in \mathcal{Z}_M^d$ the vector

$$x_j = (x_{j_1}, \ldots, x_{j_d})^\top, \quad j = (j_1, \ldots, j_d)^\top \in \mathcal{Z}_M^d, \quad \text{which means that each } j_\ell \in \mathcal{Z}_M. \tag{3.129a}$$

In particular, we set

$$x_{j_\ell} = j_\ell \cdot \frac{2\pi}{M} \quad \text{for} \quad j_\ell \in \mathcal{Z}_M. \tag{3.129b}$$

Similarly we discretize the operator $\langle \nabla \rangle_0$ in space which has already a diagonal structure in the continuous setting. For $c \in \mathbb{R}$ fixed we have by Definition A.2 the Fourier representation of $\langle \nabla \rangle_c$ as

$$(\widehat{\langle \nabla \rangle_c})_k = \sqrt{|k|^2 + c^2}, \quad \text{for all } k \in \mathbb{Z}^d.$$

Also in the discrete setting, using the techniques from above, we obtain a diagonal structure, replacing $\mathbb{Z}^d$ by $\mathcal{Z}_M^d$, i.e.

$$\langle \nabla \rangle_c \boldsymbol{a}_0(t, x_j) \approx \langle \nabla \rangle_{c,M} \boldsymbol{a}_0(t, x_j) = \sum_{k \in \mathcal{Z}_M^d} \sqrt{|k|^2 + c^2}\, (\widehat{\boldsymbol{a}_0^M}(t))_k e^{ik \cdot x_j}, \qquad j \in \mathcal{Z}_M^d.$$

In particular, the technique presented in this section allows us to easily solve the Poisson problem

$$-\Delta \phi_0 = \rho_0, \quad \rho_0 \in H^r,$$

if we are looking for a solution $\phi_0 \in \dot{H}^{r+2}$. Recall that we defined the solution operator $\dot{\Delta}^{-1} : H^r \to \dot{H}^{r+2}$ in Fourier space according to (A.4) as

$$(\widehat{\dot{\Delta}^{-1}})_k = \begin{cases} 0, & k = 0, \\ -|k|^{-2}, & k \in \mathbb{Z}^d \setminus \{0\}. \end{cases} \tag{3.130}$$

Then its discrete version $\dot{\Delta}_M^{-1}$ is defined analogously for $k \in \mathcal{Z}_M^d$ and we obtain $\phi_0^M = -\dot{\Delta}_M^{-1} \rho_0^M$.

In the subsequent section we combine the results on the time discretization from Section 3.5.1 with the results on the space discretization from Section 3.5.3 in order to obtain a fully discrete time integration scheme for the SP system (3.108).

3.5.4 Full Discretization of the SP Limit System

In this section we restate the convergence result from [44, Theorem IV.17] on the fully discrete Strang splitting Fourier pseudo-spectral scheme for solving the SP system (3.108) numerically. In the following let $0 < \tau < 1$ be a time step and let $M > 0$ be a number of grid points in each direction for the discretization of $\mathbb{T}^d$. Furthermore let

$t_n = n\tau$ with $n = 0, 1, 2, \ldots, T/\tau$ be a discretization of the interval $[0, T]$ and let

x_j with $j \in \mathcal{Z}_M^d$ be the discrete grid on $\mathbb{T}^d$ according to (3.129).

Then for a function $z : [0, T] \times \mathbb{T}^d \to \mathbb{C}^m$ with $m \in \mathbb{N}$ we use the notation

$$\left(z^{n,M}\right)_j :\approx z(t_n, x_j) \quad \text{for } j \in \mathcal{Z}_M^d.$$

Using this notation, we denote by $w_0^{n,M} := (u_0^{n,M}, v_0^{n,M})^\top$, $\phi_0^{n,M}$ and $\boldsymbol{a}_0^{n,M}$ the solutions to the fully discrete SP system (3.131) obtained with the exponential Strang splitting method $\Phi^\tau_{w_0,\text{Strang}}$ with time step τ (see (3.110)) combined with the Fourier space discretization techniques with $M \in \mathbb{N}$ grid points of the previous Section 3.5.3. The fully discrete SP system corresponding to (3.108) reads

$$\begin{cases} i\partial_t w_0^{n,M} = \frac{1}{2}\Delta_M w_0^{n,M} + \phi_0^{n,M}\begin{pmatrix} u_0^{n,M} \\ -v_0^{n,M}\end{pmatrix}, \qquad w_0^M(0) = w_{I,0}^M \\ -\Delta_M \phi_0^{n,M} = \rho_0^{n,M} = \begin{cases} -\frac{1}{4}\left(\left|u_0^{n,M}\right|^2 - \left|v_0^{n,M}\right|^2\right) & \text{in case of MKG (see (3.30b))}, \\ \frac{1}{4}\left(\left|u_0^{n,M}\right|^2 + \left|v_0^{n,M}\right|^2\right) & \text{in case of MD (see (3.59b))}, \end{cases} \\ \boldsymbol{a}_0^{n,M} = e^{ic\langle\nabla\rangle_{0,M} t_n}\mathfrak{a}_{I,0}^M. \end{cases} \tag{3.131}$$

For the numerical solution of the discrete Poisson equation $-\Delta_M \phi_0^{n,M} = \rho_0^{n,M}$ see (3.130).

Combining the convergence result in Corollary 3.10, on the exponential Strang splitting time discretization from Section 3.5.1, with the approximation properties in Proposition 3.14 of the Fourier pseudo-spectral space discretization techniques from the previous Section 3.5.3, we obtain a fully-discrete time integration scheme for numerically solving the Schrödinger–Poisson limit system (3.109). This method then satisfies numerical error bounds of order $\mathcal{O}\left(\tau^2 + M^{-r_1'}\right)$ where M is the number of grid points in each direction and where r_1' depends on the regularity of the solution $w_0(t_n)$. Therefore denoting by $w_0^{n,M} \approx \left(w_0(t_n, x_j)\right)_{j\in\mathcal{Z}_M^d}$ the fully discrete approximation to w_0 we have

$$\left\|w_0^{n,M} - w_0(t_n)\right\|_r \le K(\mathcal{M}_{w_0}^{r+4}) \cdot (\tau^2 + M^{-r_1'}).$$

Equation (3.108) shows that we have an explicit formula for $\boldsymbol{a}_0(t)$ for every $t \in [0, T]$, i.e.

$$\boldsymbol{a}_0(t_n) = e^{i\langle\nabla\rangle_0 t_n}\mathfrak{a}_{I,0}.$$

Therefore we do not have any time discretization error for $\boldsymbol{a}_0(t_n)$ such that $\boldsymbol{a}_0(t_n) = \boldsymbol{a}_0^n$. But the discretization in space of the operator $\langle\nabla\rangle_0$ leads to an error

$$\left\|\boldsymbol{a}_0^{n,M} - \boldsymbol{a}_0(t_n)\right\|_{r,0} \le K \cdot M^{-r_2'},$$

where r_2' depends on the regularity of $\boldsymbol{a}_0(t_n)$.

In the subsequent section we prove rigorous numerical approximation results for the convergence of the numerical limit approximation

$$\begin{pmatrix}\psi_0^{n,M} \\ \phi_0^{n,M} \\ \boldsymbol{\mathcal{A}}_0^{n,M}\end{pmatrix} \quad \text{towards the exact solution} \quad \begin{pmatrix}\psi(t_n, x_j) \\ \phi(t_n, x_j) \\ \boldsymbol{\mathcal{A}}(t_n, x_j)\end{pmatrix} \quad \text{in the regime } c \gg 1$$

for both the MKG and the MD system (2.20) and (2.36), respectively, in the space $H^r \times \dot{H}^{r+2} \times \dot{H}^r$, where

$$\psi_0^{n,M} := \frac{1}{2}\left(e^{ic^2 t_n}u_0^{n,M} + e^{-ic^2 t_n}\overline{v_0}^{n,M}\right) \qquad \text{and} \qquad \boldsymbol{\mathcal{A}}_0^{n,M} = \frac{1}{2}(\boldsymbol{a}_0^{n,M} + \overline{\boldsymbol{a}_0^{n,M}}).$$

3.6 Error Bounds for the Numerical Limit Approximations

In this section we collect the results of the previous subsections and state the main approximation result in Theorem 3.15. Note that we have proven the results on the MKG case in the paper [63] by Krämer and Schratz, whereas the numerical convergence results for the case of Maxwell–Dirac have not been proven before. Furthermore, note that in [57] the authors heuristically verified these convergence bounds in the MD case only by numerical experiments but no rigorous analysis has been given in the latter paper. In addition the proof of Theorem 3.15 below allows to prove similar bounds for higher order limit approximations (see Sections 3.2.3 and 3.3.3).

Exploiting the findings of the previous subsections, we are able to formulate the following main Theorem 3.15 on the convergence of the numerical limit approximation

$$\psi_0^{n,M} := \frac{1}{2}\left(e^{ic^2t_n}u_0^{n,M} + e^{-ic^2t_n}\overline{v_0}^{n,M}\right), \quad \phi_0^{n,M} \quad \text{and} \quad \boldsymbol{\mathcal{A}}_0^{n,M} = \frac{1}{2}(\boldsymbol{a}_0^{n,M} + \overline{\boldsymbol{a}_0^{n,M}}),$$

towards the exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MKG/MD system (2.20)/(2.36), respectively. Note that $(w_0^{n,M}, \phi_0^{n,M}, \boldsymbol{a}_0^{n,M})^\top$ denotes the numerical solution of the discrete SP system (3.131). For the case of MKG, see the paper [63, Theorem 2] by Krämer and Schratz.

Theorem 3.15 (Convergence of the MKG/MD Numerical Limit Approximations)**.** *Let $\epsilon > 0$ be arbitrarily small and fix $r_1, r_2, r > d/2$. Furthermore let $\psi_I, \psi_I' \in H^{r+r_1'}(\mathbb{T}^d)$ and $A_I, A_I' \in H^{r+r_2'}(\mathbb{T}^d)$ with $r_1' = \max\{4, r_1 + d/2 + \epsilon\}$ and $r_2' = \max\{1, r_2 + d/2 + \epsilon\}$. Then there exist $T, C, M_0, \tau_0 > 0$ such that the following holds: Let us define the numerical approximation of the the first-order approximation term $\psi_0(t)$ at time $t_n = n\tau$ through*

$$\psi_0^{n,M} := \frac{1}{2}\left(e^{ic^2t_n}u_0^{n,M} + e^{-ic^2t_n}\overline{v_0}^{n,M}\right),$$

where $w_0^{n,M} = (u_0^{n,M}, v_0^{n,M})^\top$ denotes the numerical approximation to the solution $w_0(t_n)$ of the limit system (3.108) obtained by the Fourier pseudo-spectral Strang splitting scheme (3.110) (see Sections 3.5.1 and 3.5.3) with time step $\tau \le \tau_0$ and $M \ge M_0$ grid points in space (and thus a mesh size $h \le h_0$ for some $h_0 > 0$). Furthermore, let $\phi_0^{n,M}$ denote the numerical approximation to $\phi_0(t_n)$ given through the discrete Poisson equation

$$-\Delta_M \phi_0^{n,M} := \rho_0^{n,M} = \begin{cases} -\quad \frac{1}{4}(\left|u_0^{n,M}\right|^2 - \left|v_0^{n,M}\right|^2), & \text{in case of MKG, see (3.30b)}, \\ \quad \frac{1}{4}(\left|u_0^{n,M}\right|^2 + \left|v_0^{n,M}\right|^2), & \text{in case of MD, see (3.59b)}. \end{cases}$$

Also let

$$\begin{aligned} \boldsymbol{\mathcal{A}}_0^{n,M} =& \frac{1}{2}(\boldsymbol{a}_0^{n,M} + \overline{\boldsymbol{a}_0^{n,M}}) \\ =& \cos\left(ct_n\langle\nabla\rangle_{0,M}\right) A_I^M + \left(c\langle\nabla\rangle_{0,M}\right)^{-1} \sin\left(ct_n\langle\nabla\rangle_{0,M}\right) c{A_I'}^M \end{aligned}$$

and

$$\begin{aligned} \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_0^{n,M} =& \frac{1}{2} i\langle\nabla\rangle_{0,M}(\boldsymbol{a}_0^{n,M} - \overline{\boldsymbol{a}_0^{n,M}}) \\ =& -c\langle\nabla\rangle_{0,M} \sin\left(ct_n\langle\nabla\rangle_{0,M}\right) A_I^M + \cos\left(ct_n\langle\nabla\rangle_{0,M}\right) c{A_I'}^M \end{aligned}$$

denote the numerical approximation to $\boldsymbol{\mathcal{A}}_0(t_n)$ and $\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_0(t_n)$, respectively, where $A_I^M, {A_I'}^M$ are the evaluations of A_I and A_I' in the grid points.

Furthermore choose $\delta_1, \delta_2 \in \{0,1\}$ *according to the convergence bound*

$$\left\| w(t) - e^{ic^2 t} w_0(t) \right\|_r = \mathcal{O}\left(\delta_1 c^{-1} + \delta_2 c^{-2}\right) \quad \text{from Theorems 3.3 and 3.4.}$$

Note that in case of MKG (cf. Theorem 3.3) we have

$$\begin{aligned} &\delta_1 = 1 \quad \text{and} \quad \delta_2 = 0 \qquad \text{if } \|\psi_I - \psi_{I,0}\|_{r+4} + \left\|\psi_I' - \psi_{I,0}'\right\|_{r+4} \leq K c^{-1} \text{ and} \\ &\delta_1 = 0 \quad \text{and} \quad \delta_2 = 1 \qquad \text{if } \|\psi_I - \psi_{I,0}\|_{r+4} + \left\|\psi_I' - \psi_{I,0}'\right\|_{r+4} \leq K c^{-2}. \end{aligned} \tag{3.133a}$$

In case of MD (cf. Theorem 3.4) we have

$$\delta_1 = 1 \quad \text{and} \quad \delta_2 = 0 \qquad \text{if } \|\psi_I - \psi_{I,0}\|_{r+4} + \left\|\psi_I' - \psi_{I,0}'\right\|_{r+4} \leq K c^{-1} \tag{3.133b}$$

Then, we obtain the following convergence bounds of the numerical solution $(\psi_0^{n,M}, \phi_0^{n,M}, \boldsymbol{\mathcal{A}}_0^{n,M})$ *towards the exact solution* $(\psi(t_n,x), \phi(t_n,x), \boldsymbol{\mathcal{A}}(t_n,x))^\top$ *of the MKG/MD systems* (2.20) *and* (2.36)*, respectively, for all* $t_n \in [0,T]$ *and for all* $c \geq 1$ *:*

$$\begin{aligned} \left\|\psi(t_n) - \psi_0^{n,M}\right\|_r + \left\|\phi(t_n) - \phi_0^{n,M}\right\|_{r+2,0} &\leq K_{w_0}^{num}\left(\tau^2 + M^{-r_1} + \delta_1 c^{-1} + \delta_2 c^{-2}\right), \\ \left\|\boldsymbol{\mathcal{A}}(t_n) - \boldsymbol{\mathcal{A}}_0^{n,M}\right\|_{r,0} + c^{-1}\left\|\partial_t \boldsymbol{\mathcal{A}}(t_n) - \partial_t \boldsymbol{\mathcal{A}}_0^{n,M}\right\|_{r-1,0} &\leq K_{\boldsymbol{\mathfrak{a}}_0}^{num}\left(\qquad M^{-r_2} + c^{-1}\right), \end{aligned}$$

where the constants $K_{w_0}^{num}$ *and* $K_{\boldsymbol{\mathfrak{a}}_0}^{num}$ *only depend on* $\mathcal{M}_w^{r+4}, \mathcal{M}_{w_0}^{r+4}, \mathcal{M}_{\boldsymbol{\mathfrak{a}}}^{r+1}, \mathcal{M}_{\boldsymbol{\mathfrak{a}}_0}^{r+1}$ *and on* d *and* T *but not on* c*,* M *or* τ*.*

Note that in [45] for the case of the nonlinear Klein–Gordon equation, the authors have shown a $\mathcal{O}\left(\tau^2 + c^{-2}\right)$ convergence bound for initial data satisfying bounds similar to the second line of (3.133a).

Remark 3.16 ([45, 69])**.** *Similar to [45, Theorem 4] for the case of the cubic Klein–Gordon equation, the results of this Theorem 3.15 can be extended to higher order limit approximations (cf. Section 3.2.3 and Section 3.2.4), i.e. for* $N_1, N_2, N_3 \in \mathbb{N}$

$$\begin{aligned} \psi_\infty^{(N_1-1)} &:= \psi_0 + c^{-1}\psi_1 + \cdots + c^{-(N_1-1)}\psi_{N_1-1} \\ \phi_\infty^{(N_2-1)} &:= \phi_0 + c^{-1}\phi_1 + \cdots + c^{-(N_2-1)}\phi_{N_2-1} \\ \boldsymbol{\mathcal{A}}_\infty^{(N_3-1)} &:= \boldsymbol{\mathcal{A}}_0 + c^{-1}\boldsymbol{\mathcal{A}}_1 + \cdots + c^{-(N_3-1)}\boldsymbol{\mathcal{A}}_{N_3-1}. \end{aligned}$$

These higher order limit approximations allow analytical convergence bounds of order $\mathcal{O}\left(c^{-N_j}\right)$*,* $j = 1,2,3$ *(cf. Theorems 3.3 and 3.4), i.e.*

$$\begin{aligned} &\left\|\psi(t) - \psi_\infty^{(N_1-1)}(t)\right\|_r + \left\|\phi(t) - \phi_\infty^{(N_2-1)}(t)\right\|_{r+2,0} + \left\|\boldsymbol{\mathcal{A}}(t) - \boldsymbol{\mathcal{A}}_\infty^{(N_3-1)}(t)\right\|_{r,0} \\ &\leq K_{N_1} c^{-N_1} + K_{N_2} c^{-N_2} + K_{N_3} c^{-N_3}, \end{aligned}$$

where the constants K_{N_j} *only depends on the regularity of* $\psi, \phi, \boldsymbol{\mathcal{A}}$ *and the corresponding limit approximations but not on* c *(see also [45, 69]). Successively numerical solving the additionally arising partial differential equations for the higher order terms by similar time integration techniques of order* p *as described above, we reach numerical convergence of order* $\mathcal{O}\left(c^{-N_j} + \tau^p + M^{-\tilde{r}}\right)$*,* $j = 1,2,3$*, where* $\tilde{r}$ *depends on the regularity of the exact solution of the MKG/MD system* (2.20)/(2.36) *and on the regularity of the exact solution of the higher order approximation terms.*

We proceed with the proof of Theorem 3.15.

Proof (of Theorem 3.15)*:* Recall the identities

$$\psi(t) = \frac{1}{2}\left(e^{ic^2t}u(t) + e^{-ic^2t}\overline{v}(t)\right) \quad \text{and} \quad \boldsymbol{\mathcal{A}}(t) = \frac{1}{2}(\mathfrak{a}(t) + \overline{\mathfrak{a}}(t))$$

in (2.22) and (2.39), respectively, which directly transfer to

$$\psi_0(t) = \frac{1}{2}\left(e^{ic^2t}u_0(t) + e^{-ic^2t}\overline{v_0}(t)\right) \quad \text{and} \quad \boldsymbol{\mathcal{A}}_0(t) = \frac{1}{2}(\boldsymbol{a}_0(t) + \overline{\boldsymbol{a}_0}(t))$$

via (3.7). We furthermore obtain from (2.39) that

$$\partial_t\boldsymbol{\mathcal{A}}(t) = i\frac{1}{2}\left\langle\nabla\right\rangle_0(\mathfrak{a}(t) - \overline{\mathfrak{a}}(t)) \quad \text{and} \quad \partial_t\boldsymbol{\mathcal{A}}_0(t) = i\frac{1}{2}\left\langle\nabla\right\rangle_0(\boldsymbol{a}_0(t) - \overline{\boldsymbol{a}_0}(t)).$$

Then we immediately obtain by triangle inequality that

$$\begin{aligned}\left\|\psi(t_n) - \psi_0^{n,M}\right\|_r &\le \|\psi(t_n) - \psi_0(t_n)\|_r + \|\psi_0(t_n) - \psi_0^n\|_r + \left\|\psi_0^n - \psi_0^{n,M}\right\|_r \\ &\le \underbrace{\left\|w(t_n) - e^{ic^2t}w_0(t_n)\right\|_r}_{=\mathcal{O}(\delta_1c^{-1}+\delta_2c^{-2})} + \underbrace{\|w_0(t_n) - w_0^n\|_r}_{=\mathcal{O}(\tau^2)} + \underbrace{\left\|w_0^n - w_0^{n,M}\right\|_r}_{=\mathcal{O}(M^{-r_1})}.\end{aligned} \tag{3.134}$$

The first term can now be estimated by the results on the analyitical approximation in the nonrelativistic limit and provides the c^{-1} term according to Theorems 3.3 and 3.4. The second term corresponds to the error of the time discretization and provides the τ^2 term due to Corollary 3.10. Similarly, the last term gives the spatial approximation error which can be estimated by the M^{-r_1} term according to Proposition 3.14. The term $\left\|\phi(t_n) - \phi_0^{n,M}\right\|_{r+2,0}$ is estimated in the same way, exploiting (3.78) and Propositions 3.5 and 3.7, respectively.

From Theorems 3.3 and 3.4 and due to Proposition 3.14, exploiting that $\boldsymbol{a}_0(t_n) = \boldsymbol{a}_0^n$, we have

$$\begin{aligned}\left\|\boldsymbol{\mathcal{A}}(t_n) - \boldsymbol{\mathcal{A}}_0^{n,M}\right\|_{r,0} &\le \|\mathfrak{a}(t_n) - \boldsymbol{a}_0(t_n)\|_{r,0} + \left\|\boldsymbol{a}_0^n - \boldsymbol{a}_0^{n,M}\right\|_{r,0} \\ &= \mathcal{O}\left(c^{-1} + M^{-r_2}\right).\end{aligned}$$

Similarly we find

$$\begin{aligned}c^{-1}\left\|\partial_t\boldsymbol{\mathcal{A}}(t_n) - \partial_t\boldsymbol{\mathcal{A}}_0^{n,M}\right\|_{r-1,0} &\le \left\|\left\langle\nabla\right\rangle_0\mathfrak{a}(t_n) - \left\langle\nabla\right\rangle_{0M}\boldsymbol{a}_0^{n,M}\right\|_{r-1,0} \\ &\le \|\mathfrak{a}(t_n) - \boldsymbol{a}_0(t_n)\|_{r,0} + \left\|\left\langle\nabla\right\rangle_0\boldsymbol{a}_0^n - \left\langle\nabla\right\rangle_{0M}\boldsymbol{a}_0^{n,M}\right\|_{r-1,0} \\ &= \mathcal{O}\left(c^{-1} + M^{-r_2}\right).\end{aligned}$$

The constants can all be chosen independent of c, τ and M and depend only on the constants $\mathcal{M}_w^{r+r_1'}$, $\mathcal{M}_{w_0}^{r+r_1'}$, $\mathcal{M}_{\mathfrak{a}}^{r+r_2'}$, $\mathcal{M}_{\boldsymbol{a}_0}^{r+r_2'}$ and on d and T. □

The latter Theorem 3.15 shows that numerical time integration schemes, based on the asymptotic behaviour of the exact solution of the MKG/MD systems yield good results in the highly oscillatory nonrelativistic regime where c is very large. Though, we observe that the numerical accuracy of this method is limited by the asymptotic convergence rate $\mathcal{O}\left(c^{-N}\right)$ of the corresponding limit solution. Thus, they are efficient in regimes $c \gg 1$, where $\tau^p \gtrsim c^{-N}$ for a given time step τ.

In the next chapter, based on the technique of “twisted variables” ([18]) we construct uniformly accurate time integration schemes which allow error bounds of order $\mathcal{O}(\tau)$ independent of the large parameter c. These schemes thus perform well in highly to slowly oscillatory regimes.

CHAPTER

FOUR

TWISTED VARIABLES — UNIFORMLY ACCURATE TIME INTEGRATION SCHEMES

In this chapter, we construct and analyse uniformly accurate numerical time integration schemes for Maxwell–Klein–Gordon and Maxwell–Dirac systems. Due to error bounds of order $\mathcal{O}(\tau)$ independent of c, these schemes perform well in highly to slowly oscillatory regimes. In the construction, we thereby exploit the idea of "twisted variables" which has been introduced recently in [18] as a basis for the construction of uniformly accurate time integration schemes of arbitrary high order p in time for nonlinear Klein–Gordon (KG) equations. Within this chapter, we proceed as follows. In Section 4.1, we transform the highly oscillatory MKG/MD first order systems (2.33)/(2.41) into "twisted systems" with slowly varying solutions. These "twisted systems" together with a splitting idea then form the basis for the construction of uniformly accurate time integration schemes in Section 4.2. We shall analyse the latter schemes in Section 4.3 and collect the convergence results in Theorems 4.7 and 4.8.

Before we apply these ideas to our Maxwell–Klein–Gordon and Maxwell–Dirac systems, let us give a rough overview of the "twisted variables" and their advantages. In [18], the authors considered nonlinear Klein–Gordon equations of type

$$\partial_{tt}\psi = -c^2 \langle\nabla\rangle_c^2 \psi + c^2 f[\psi] \qquad \text{where} \qquad \overline{f[\psi]} = f[\overline{\psi}]. \tag{4.1}$$

Rewriting the latter as a first order system in time ([18, 45, 63, 69, 70]) of type (cf. Section 2.1.4)

$$i\partial_t w = -c\langle\nabla\rangle_c w + c\langle\nabla\rangle_c^{-1}\tilde{F}[w] \qquad \text{with} \qquad \tilde{F}[w] = \Big(f[\tfrac{1}{2}(u+\overline{v})], f[\tfrac{1}{2}(\overline{u}+v)]\Big)^\top. \tag{4.2}$$

with solution $w = (u, v)^\top$ satisfying $\psi = \frac{1}{2}(u+\overline{v})$, the technique of "twisted variables" ([18]) now follows the ansatz of "twisting" the variable w by a simple variable transform, i.e. we introduce

$$\text{the "twisted variables"} \qquad w_*(t) = e^{-ic^2 t} w(t).$$

These variables allow us to transform the system (4.2) with the highly oscillatory solution w

into a "twisted system" with a **slowly varying** solution w_*.

In [18], based on the latter "twisted system", the authors constructed uniformly accurate time integration schemes of numerical order p in time, independent of the paramater c. In this chapter, we mainly follow the ideas of the paper [18] in order to construct time integration schemes for the MKG/MD systems (2.20)/(2.36) which yield

$$\text{first order error bounds in time uniformly in} \qquad c \in [1, \infty).$$

Note that uniformly accurate time integration schemes for Klein–Gordon and Dirac type systems have already been proposed also in [11–14]. However, in contrast to the construction of the schemes in the latter papers, the construction of uniformly accurate schemes based on the concept of "twisted variables" allows us to easily increase the numerical order p in time of the method.

As far as we know, there exists, no literature which treats the construction and analysis of uniformly accurate schemes for Maxwell–Klein–Gordon and Maxwell–Dirac systems. Our contribution in this chapter is to adapt the technique of "twisted variables" from [18] to the case of the MKG/MD system (2.20)/(2.36). In the construction of our scheme we combine the latter ideas with a splitting ansatz. Note that due to the strong nonlinear coupling between ψ, ϕ and $\boldsymbol{\mathcal{A}}$ the construction and analysis in case of MKG and MD is much more involved than in [18]. Based on the resulting first order "twisted system" with bounded right hand side (see (4.15) below), we construct and analyse an exponential time integration scheme which is uniformly first order accurate in time and does not suffer from any time step restriction. Note that exponential integrators for nonlinear evolution equations have been originally proposed and analysed in [55]. We give more insight in exponential integrators in Section 4.2.1 below.

The numerical time integration methods proposed and analysed in [18] for nonlinear Klein–Gordon equations of type (4.1) are uniformly accurate in time for all $c \geq 0$, i.e. for a given time step τ these methods allow numerical error bounds of order $\mathcal{O}(\tau^p)$ independent of c. Therefore, they allow good numerical approximations also in the intermediate regime $1 \ll c \lesssim \tau^{-p}$, where the paramater c is too large to apply standard methods for the time integration of Klein–Gordon and Dirac type systems due to severe time step restrictions $\tau \lesssim c^{-2}$ (see [9, 10, 15, 16, 51]), and where c is too small to apply the methods based on the asymptotic expansion of the exact solution (cf. Chapter 3 and see [18, 45]). Recall that for the latter methods, the error of the numerical approximation is bounded in $\mathcal{O}\left(c^{-N} + \tau^p\right)$ for fixed $N \in \mathbb{N}$ in the sense of the H^r norm (cf. Theorem 3.15), i.e.

$$\text{error} = \underbrace{\text{asymptotic approximation error}}_{=\mathcal{O}(c^{-N})} + \underbrace{\text{numerical error}}_{=\mathcal{O}(\tau^p)}.$$

Therefore, the reachable accuracy is limited from below through the asymptotic approximation bound of order $\mathcal{O}\left(c^{-N}\right)$.

The goal in this chapter is to adapt the ideas of the "twisted variables" to the Maxwell–Klein–Gordon and Maxwell–Dirac systems (2.20) and (2.36), respectively and to construct a uniformly accurate and stable time integration method for all $c \geq 1$.

Recall that we can rewrite the Maxwell–Klein–Gordon and Maxwell–Dirac systems (2.20) and (2.36), respectively, with solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ as first order systems in time of type (2.33) in the case of MKG and (2.41) in the case of MD, respectively, with solution $(w, \phi, \mathfrak{a})^\top$ (see also [21, 22, 70]), i.e.

$$\begin{cases} i\partial_t w = -c\langle\nabla\rangle_c w + F[w,\phi,\mathfrak{a}] + \delta_{\text{MD}} G[w,\phi,\mathfrak{a}], & w(0) = w_I = \begin{pmatrix} \psi_I - i\psi_I' \\ \overline{\psi_I - i\psi_I'} \end{pmatrix} \\ -\Delta\phi = \rho[w] & \\ i\partial_t \mathfrak{a} = -c\langle\nabla\rangle_0 \mathfrak{a} + \langle\nabla\rangle_0^{-1} \boldsymbol{J}^P[w,\mathfrak{a}], & \mathfrak{a}(0) = \mathfrak{a}_I = A_I - i\langle\nabla\rangle_0^{-1} A_I', \end{cases} \tag{4.3a, 4.3b}$$

where $\delta_{\text{MD}} = 0$ in case of MKG (cf. (2.33)) and $\delta_{\text{MD}} = 1$ in case of MD (cf. (2.41)). Furthermore, we have the identities $w = (u, v)^\top$ and

$$\psi = \frac{1}{2}(u + \overline{v}) \quad \text{and} \quad \boldsymbol{\mathcal{A}} = \frac{1}{2}(\mathfrak{a} + \overline{\mathfrak{a}}). \tag{4.3c}$$

Recall that from (2.33) in the MKG case and from (2.41) in the MD case, respectively, we have

$$\begin{aligned} F[w,\phi,\mathfrak{a}] &= \phi\begin{pmatrix} u \\ -v \end{pmatrix} - \frac{1}{2}\left(\phi - \langle\nabla\rangle_c^{-1}\phi\langle\nabla\rangle_c\right)\begin{pmatrix} u - \overline{v} \\ \overline{u} - v \end{pmatrix} \\ &\quad - \frac{1}{8}c^{-1}\langle\nabla\rangle_c^{-1}\begin{pmatrix} |\mathfrak{a}+\overline{\mathfrak{a}}|^2(u+\overline{v}) \\ |\mathfrak{a}+\overline{\mathfrak{a}}|^2(\overline{u}+v) \end{pmatrix} + i\frac{1}{2}\langle\nabla\rangle_c^{-1}\begin{pmatrix} -(\mathfrak{a}+\overline{\mathfrak{a}})\cdot\nabla(u+\overline{v}) \\ (\mathfrak{a}+\overline{\mathfrak{a}})\cdot\nabla(\overline{u}+v) \end{pmatrix}, \\ G[w,\phi,\mathfrak{a}] &= i\frac{1}{2}\langle\nabla\rangle_c^{-1}\begin{pmatrix} \left(\frac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{curl}}[\mathfrak{a}+\overline{\mathfrak{a}}] + \mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\phi] + \frac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_0[i\langle\nabla\rangle_0(\mathfrak{a}-\overline{\mathfrak{a}})]\right)(u+\overline{v}) \\ -\left(\frac{1}{2}\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\text{curl}}[\mathfrak{a}+\overline{\mathfrak{a}}] + \mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\text{div}}[\phi] + \frac{1}{2}\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_0[i\langle\nabla\rangle_0(\mathfrak{a}-\overline{\mathfrak{a}})]\right)(\overline{u}+v) \end{pmatrix}, \end{aligned} \tag{4.3d}$$

and

$$\begin{aligned} \rho[w] &= \begin{cases} -\frac{1}{4}\operatorname{Re}\left((u+\overline{v})c^{-1}\langle\nabla\rangle_c(\overline{u}-v)\right) & \text{in case of MKG,} \\ \frac{1}{4}(|u|^2 + |v|^2 + 2\operatorname{Re}(u\cdot v)) & \text{in case of MD,} \end{cases} \\ \boldsymbol{J}^P[w,\mathfrak{a}] &= \begin{cases} \mathcal{P}_{\text{df}}\left[\operatorname{Re}\left(i\frac{1}{4}(u+\overline{v})\nabla(\overline{u}+v)\right) - \frac{1}{c}\frac{1}{8}(\mathfrak{a}+\overline{\mathfrak{a}})|u+\overline{v}|^2\right] & \text{in case of MKG,} \\ c\frac{1}{4}\mathcal{P}_{\text{df}}\left[(u+\overline{v})\overline{\boldsymbol{\alpha}}(\overline{u}+v)\right] & \text{in case of MD.} \end{cases} \end{aligned} \tag{4.3e}$$

The main challenge in numerically solving these systems lies in the numerical solution of the equation (4.3a) for the variables $w = (u, v)^\top$. This can already be seen in the linear case where the nonlinearities $F = G = 0$ vanish, i.e. for w satisfying

$$i\partial_t w = -c\langle\nabla\rangle_c w, \quad w(0) = w_I, \tag{4.4}$$

with given initial data w_I, as the linear operator $-c\langle\nabla\rangle_c$ triggers the highly oscillatory behaviour of w due to the phase e^{ic^2t} in the solution (see also Chapter 3).

This motivates the ansatz of writing

$$w(t) = e^{ic^2t} w_*(t) \tag{4.5}$$

for some smooth function $w_* = (u_*, v_*)^\top$ determined later. In particular, the identity (4.3c) admits the representation

$$\psi(t,x) = \psi_*(t,x) := \frac{1}{2}(e^{ic^2t}u_*(t,x) + e^{-ic^2t}v_*(t,x)). \tag{4.6}$$

Plugging the ansatz (4.5) for w into the above linear equation (4.4), we have on the one hand

$$i\partial_t w(t) = i\partial_t\left(e^{ic^2t}w_*(t)\right) = e^{ic^2t}\left(-c^2 w_*(t) + i\partial_t w_*(t)\right) \tag{4.7a}$$

and on the other hand

$$i\partial_t w(t) = -c\langle\nabla\rangle_c w(t) = e^{ic^2 t}\left(-c\langle\nabla\rangle_c w_*(t)\right). \tag{4.7b}$$

Therefore, the "twisted variables" w_* in the linear case satisfy the system

$$i\partial_t w_*(t) = -(c\langle\nabla\rangle_c - c^2)w_*(t), \quad w_*(0) = w(0) = w_I, \tag{4.8}$$

which motivates the definition of the operator

$$\mathcal{L}_c \coloneqq c\langle\nabla\rangle_c - c^2.$$

The big advantage in numerically solving the system (4.8) for w_* instead of (4.4) for w and respecting the relation $w(t) = e^{ic^2 t}w_*(t)$ from (4.5) now relies on the uniform boundedness for all $c \in \mathbb{R}$ of the operator (cf. Lemma A.11 and [18])

$$\mathcal{L}_c : H^{r+2} \to H^r.$$

Therefore, the solution

$$w_*(t) = e^{it\mathcal{L}_c}w_*(0) \quad \text{of the system} \quad i\partial_t w_*(t) = -\mathcal{L}_c w_*(t) \quad \text{with} \quad w_*(0) = w_I$$

is only slowly varying. We recover the highly oscillatory phase of the solution w of (4.4) by multiplying w_* with $e^{ic^2 t}$, i.e.

$$w(t) = e^{ic^2 t}w_*(t) = e^{ic^2 t}e^{it\mathcal{L}_c}w_*(0) = e^{itc\langle\nabla\rangle_c}w_I.$$

In the subsequent section we exploit these ideas in order to derive the "twisted system" corresponding to the nonlinear first order system in time (4.3), which allows us to construct a uniformly accurate time integration scheme for MKG and MD systems.

4.1 The "Twisted System" for MKG/MD

This section is based on [18]. Our aim in this section is to derive a "twisted system" corresponding to the first order system (4.3) above. We therefore exploit the ansatz from (4.5) and twist the variable w by the oscillatory phase $e^{ic^2 t}$, i.e.

$$w(t) = e^{ic^2 t}w_*(t),$$

and plug it into (4.3). Note that due to Remark 4.1, it is sufficient to only twist the variable w in the system (4.3), since the structure of the system allows to deal with derivatives of $\mathfrak{a}$ of order $\mathcal{O}(c\langle\nabla\rangle_0\,\mathfrak{a})$. Thus it is not necessary to also "twist" the variable $\mathfrak{a}$. Though, for numerical implementation issues we may slightly manipulate the equation (4.3b). We thereby modify the wave equations for $\boldsymbol{\mathcal{A}}$ in the original MKG/MD systems (2.20b)/(2.38b) in such a way that we insert and subtract an additional linear term $\gamma^2\boldsymbol{\mathcal{A}}$. More precisely, we consider

$$\partial_{tt}\boldsymbol{\mathcal{A}} = -c^2(-\Delta + \frac{\gamma^2}{c^2})\boldsymbol{\mathcal{A}} + \gamma^2\boldsymbol{\mathcal{A}} + c\mathcal{P}_{\text{df}}[\boldsymbol{J}] \quad \text{for } \gamma \in [0,1].$$

Introducing the operator $\langle\nabla\rangle_{\gamma/c} = (-\Delta + \frac{\gamma^2}{c^2})^{1/2}$ and making, analogously to Section 2.1.4 and Section 2.2.2, the ansatz $\mathfrak{a}^\gamma = \boldsymbol{\mathcal{A}} - i\langle\nabla\rangle_{\gamma/c}^{-1}c^{-1}\partial_t\boldsymbol{\mathcal{A}}$, we have as before $\boldsymbol{\mathcal{A}} = \frac{1}{2}(\mathfrak{a}^\gamma + \overline{\mathfrak{a}^\gamma})$. Furthermore $\mathfrak{a}^\gamma$

then satisfies

$$\begin{aligned} i\partial_t \mathfrak{a}^\gamma =& - c \langle \nabla \rangle_{\gamma/c} \mathfrak{a}^\gamma + \langle \nabla \rangle_{\gamma/c}^{-1} \left(\frac{\gamma^2}{2c} (\mathfrak{a}^\gamma + \overline{\mathfrak{a}^\gamma}) + \boldsymbol{J}^P[w, \mathfrak{a}^\gamma] \right), \\ \mathfrak{a}^\gamma(0) =& A_I - i \langle \nabla \rangle_{\gamma/c}^{-1} A_I', \qquad \gamma \in [0,1], \end{aligned} \tag{4.9}$$

which for $\gamma = 0$ coincides with (2.33c) and (2.41b), respectively. In the following, we use the notation

$$\mathfrak{a}_*^\gamma = \mathfrak{a}^\gamma \qquad \text{and} \qquad \boldsymbol{\mathcal{A}}_* = \frac{1}{2}(\mathfrak{a}_*^\gamma + \overline{\mathfrak{a}_*^\gamma}) \tag{4.10a}$$

and observe similar to (2.39), that

$$\partial_t \boldsymbol{\mathcal{A}}_* = i \frac{1}{2} c \langle \nabla \rangle_{\gamma/c} \left(\mathfrak{a}_*^\gamma - \overline{\mathfrak{a}_*^\gamma} \right). \tag{4.10b}$$

Replacing w in the nonlinear problem (4.3a) with the twisted variables $w = e^{ic^2 t} w_*$, we obtain the transformed (“twisted”) system for w_*

$$i\partial_t w_*(t) = - \mathcal{L}_c w_* + e^{-ic^2 t} \left(F[e^{ic^2 t} w_*, \phi, \mathfrak{a}_*^\gamma] + G[e^{ic^2 t} w_*, \phi, \mathfrak{a}_*^\gamma] \right), \qquad w_*(0) = w_I. \tag{4.11}$$

Note that the phase $e^{-ic^2 t}$ in front of the nonlinear terms F and G is due to an identity similar to (4.7). More precisely, on the one hand we have

$$i\partial_t w(t) = i\partial_t \left(e^{ic^2 t} w_*(t) \right) = e^{ic^2 t} \left(-c^2 w_*(t) + i\partial_t w_*(t) \right)$$

and on the other hand

$$i\partial_t w(t) = -c \langle \nabla \rangle_c w(t) = e^{ic^2 t} \left(-c \langle \nabla \rangle_c w_*(t) \right) + F[e^{ic^2 t} w_*, \phi, \mathfrak{a}_*^\gamma] + G[e^{ic^2 t} w_*, \phi, \mathfrak{a}_*^\gamma].$$

In a next step, plugging $w(t) = e^{ic^2 t} w_*(t)$ into the definition of the nonlinear densities ρ and $\boldsymbol{J}^P$ given in (4.3e), we observe the following expansion in terms of different phases $e^{jic^2 t}$ for $j = -2, 0, 2$, i.e.

$$\begin{aligned} \rho =& \rho[e^{ic^2 t} w_*] = \rho_*^0[w_*] + e^{2ic^2 t} \rho_*^2[w_*] + e^{-2ic^2 t} \rho_*^{-2}[w_*], \\ \phi = \phi_*^{\text{tot}} =& \phi_*^0 + e^{2ic^2 t} \phi_*^2 + e^{-2ic^2 t} \phi_*^{-2}, \quad -\Delta \phi_*^j = \rho_*^j[w_*], j = -2, 0, 2 \\ \boldsymbol{J}^P =& \boldsymbol{J}^P[e^{ic^2 t} w_*, \mathfrak{a}_*^\gamma] = \boldsymbol{J}_*^{P,0}[w_*, \mathfrak{a}_*^\gamma] + e^{2ic^2 t} \boldsymbol{J}_*^{P,2}[w_*, \mathfrak{a}_*^\gamma] + e^{-2ic^2 t} \boldsymbol{J}_*^{P,-2}[w_*, \mathfrak{a}_*^\gamma]. \end{aligned} \tag{4.13}$$

Details on this expansion are given separately for the MKG case and the MD case, respectively, in Sections 4.1.1 and 4.1.2 below. Note that because ϕ is a real valued potential and because $\boldsymbol{J}^P$ is a real valued current, we have the relations $\rho_*^{-2} = \overline{\rho_*^2}$ and thus $\phi_*^{-2} = \overline{\phi_*^2}$ and $\boldsymbol{J}_*^{P,-2} = \overline{\boldsymbol{J}_*^{P,2}}$, respectively.

A short calculation shows that exploiting the ansatz $w(t) = e^{ic^2 t} w_*(t)$ and the expansion (4.13) of $\phi = \phi_*^{\text{tot}}$ allows us to expand the nonlinear terms $F[w, \phi, \mathfrak{a}_*^\gamma]$ and $G[w, \phi, \mathfrak{a}_*^\gamma]$ given in (4.3d) as follows

$$\begin{aligned} e^{-ic^2 t} F[e^{ic^2 t} w_*, \phi, \mathfrak{a}_*^\gamma] =& F_*^0 + e^{2ic^2 t} F_*^2 + e^{-2ic^2 t} F_*^{-2} + e^{-4ic^2 t} F_*^{-4}, \\ e^{-ic^2 t} G[e^{ic^2 t} w_*, \phi, \mathfrak{a}_*^\gamma] =& G_*^0 + e^{2ic^2 t} G_*^2 + e^{-2ic^2 t} G_*^{-2} + e^{-4ic^2 t} G_*^{-4}. \end{aligned} \tag{4.14a}$$

More precisely the terms $F_*^m = F_*^m[w_*, \phi_*^0, \phi_*^2, \mathfrak{a}]$ and $G_*^m = G_*^m[w_*, \phi_*^0, \phi_*^2, \mathfrak{a}], m = -4, -2, 0, 2$ depend on the variables w_*, ϕ^0_*, ϕ^2_* and $\mathfrak{a}^\gamma_*$ and read

$$
\begin{aligned}
F^0_* =& \frac{1}{2}\Big(\phi^0_* + \langle\nabla\rangle_c^{-1}\phi^0_*\langle\nabla\rangle_c\Big)\begin{pmatrix} u_* \\ -v_*\end{pmatrix} + \frac{1}{2}\Big(\phi^2_* - \langle\nabla\rangle_c^{-1}\phi^2_*\langle\nabla\rangle_c\Big)\begin{pmatrix} \overline{v_*} \\ -\overline{u_*}\end{pmatrix}\\
&+ \langle\nabla\rangle_c^{-1}\Bigg(-\frac{1}{8c}\Bigg(\Big|\mathfrak{a}^\gamma_* + \overline{\mathfrak{a}^\gamma_*}\Big|^2\begin{pmatrix} u_* \\ v_*\end{pmatrix}\Bigg) - \frac{i}{2}\begin{pmatrix} (\mathfrak{a}^\gamma_* + \overline{\mathfrak{a}^\gamma_*})\cdot\nabla u_* \\ -(\mathfrak{a}^\gamma_* + \overline{\mathfrak{a}^\gamma_*})\cdot\nabla v_*\end{pmatrix}\Bigg)\\
F^2_* =& \frac{1}{2}\Big(\phi^2_* + \langle\nabla\rangle_c^{-1}\phi^2_*\langle\nabla\rangle_c\Big)\begin{pmatrix} u_* \\ -v_*\end{pmatrix}\\
F^{-2}_* =& \frac{1}{2}\Big(\overline{\phi^2_*} + \langle\nabla\rangle_c^{-1}\overline{\phi^2_*}\langle\nabla\rangle_c\Big)\begin{pmatrix} u_* \\ -v_*\end{pmatrix} + \frac{1}{2}\Big(\phi^0_* - \langle\nabla\rangle_c^{-1}\phi^0_*\langle\nabla\rangle_c\Big)\begin{pmatrix} \overline{v_*} \\ -\overline{u_*}\end{pmatrix}\\
&+ \langle\nabla\rangle_c^{-1}\Bigg(-\frac{1}{8c}\Bigg(\Big|\mathfrak{a}^\gamma_* + \overline{\mathfrak{a}^\gamma_*}\Big|^2\begin{pmatrix} \overline{v_*} \\ \overline{u_*}\end{pmatrix}\Bigg) - \frac{i}{2}\begin{pmatrix} (\mathfrak{a}^\gamma_* + \overline{\mathfrak{a}^\gamma_*})\cdot\nabla \overline{v_*} \\ -(\mathfrak{a}^\gamma_* + \overline{\mathfrak{a}^\gamma_*})\cdot\nabla \overline{u_*}\end{pmatrix}\Bigg)\\
F^{-4}_* =& \frac{1}{2}\Big(\overline{\phi^2_*} - \langle\nabla\rangle_c^{-1}\overline{\phi^2_*}\langle\nabla\rangle_c\Big)\begin{pmatrix} \overline{v_*} \\ -\overline{u_*}\end{pmatrix}.
\end{aligned}
\tag{4.14b}
$$

Furthermore, for $\delta_{\text{MD}} = 0$ in case of MKG and $\delta_{\text{MD}} = 1$ in case of MD we obtain (cf. (4.3))

$$
\begin{aligned}
G^0_* =& i\frac{1}{2}\delta_{\text{MD}}\langle\nabla\rangle_c^{-1}\Bigg(\begin{pmatrix} \Big(\frac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{curl}}[\mathfrak{a}^\gamma_* + \overline{\mathfrak{a}^\gamma_*}] + \mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\phi^0_*] + \frac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_0[i\langle\nabla\rangle_{\gamma/c}(\mathfrak{a}^\gamma_* - \overline{\mathfrak{a}^\gamma_*})]\Big)\cdot u_* \\ -\Big(\frac{1}{2}\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\text{curl}}[\mathfrak{a}^\gamma_* + \overline{\mathfrak{a}^\gamma_*}] + \mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\text{div}}[\phi^0_*] + \frac{1}{2}\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_0[i\langle\nabla\rangle_{\gamma/c}(\mathfrak{a}^\gamma_* - \overline{\mathfrak{a}^\gamma_*})]\Big)\cdot v_*\end{pmatrix}\\
&+ \begin{pmatrix} \Big(\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\phi^2_*]\Big)\cdot\overline{v_*} \\ -\Big(\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\text{div}}[\phi^2_*]\Big)\cdot\overline{u_*}\end{pmatrix}\Bigg),\\
G^2_* =& i\frac{1}{2}\delta_{\text{MD}}\langle\nabla\rangle_c^{-1}\begin{pmatrix} \Big(\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\phi^2_*]\Big)\cdot u_* \\ -\Big(\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\text{div}}[\phi^2_*]\Big)\cdot v_*\end{pmatrix},\\
G^{-2}_* =& i\frac{1}{2}\delta_{\text{MD}}\langle\nabla\rangle_c^{-1}\Bigg(\begin{pmatrix} \Big(\frac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{curl}}[\mathfrak{a}^\gamma_* + \overline{\mathfrak{a}^\gamma_*}] + \mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\phi^0_*] + \frac{1}{2}\mathfrak{D}^{\boldsymbol{\alpha}}_0[i\langle\nabla\rangle_{\gamma/c}(\mathfrak{a}^\gamma_* - \overline{\mathfrak{a}^\gamma_*})]\Big)\cdot \overline{v_*} \\ -\Big(\frac{1}{2}\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\text{curl}}[\mathfrak{a}^\gamma_* + \overline{\mathfrak{a}^\gamma_*}] + \mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\text{div}}[\phi^0_*] + \frac{1}{2}\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_0[i\langle\nabla\rangle_{\gamma/c}(\mathfrak{a}^\gamma_* - \overline{\mathfrak{a}^\gamma_*})]\Big)\cdot \overline{u_*}\end{pmatrix}\\
&+ \begin{pmatrix} \Big(\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\overline{\phi^2_*}]\Big)\cdot u_* \\ -\Big(\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\text{div}}[\overline{\phi^2_*}]\Big)\cdot v_*\end{pmatrix}\Bigg),\\
G^{-4}_* =& i\frac{1}{2}\delta_{\text{MD}}\langle\nabla\rangle_c^{-1}\begin{pmatrix} \Big(\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\overline{\phi^2_*}]\Big)\cdot \overline{v_*} \\ -\Big(\mathfrak{D}^{\overline{\boldsymbol{\alpha}}}_{\text{div}}[\overline{\phi^2_*}]\Big)\cdot \overline{u_*}\end{pmatrix}.
\end{aligned}
\tag{4.14c}
$$

In particular this implies that in case of the MKG system $G^m_* \equiv 0$, for $m = -4, -2, 0, 2$. Recall that by Definition 2.6 we have that for $\tilde{\mathfrak{a}}(x) = (\tilde{\mathfrak{a}}_1(x), \dots, \tilde{\mathfrak{a}}_d(x))^\top \in \mathbb{C}^d$ and $\tilde{\phi}(x) \in \mathbb{C}$

$$
\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{curl}}[\tilde{\mathfrak{a}}] = -\frac{1}{2}\sum_{\substack{j,k=1\\ j\neq k}}^{d}\boldsymbol{\alpha}_j\boldsymbol{\alpha}_k[(\partial_j(\tilde{\mathfrak{a}}_k)) - (\partial_k(\tilde{\mathfrak{a}}_j))],
$$

$$
\mathfrak{D}^{\boldsymbol{\alpha}}_{\text{div}}[\tilde{\phi}] = \sum_{j=1}^{d}\boldsymbol{\alpha}_j(\partial_j\tilde{\phi}) \qquad \text{and} \qquad \mathfrak{D}^{\boldsymbol{\alpha}}_0[\tilde{\mathfrak{a}}] = \sum_{j=1}^{d}\boldsymbol{\alpha}_j(\tilde{\mathfrak{a}}_j).
$$

In the following we collect the indices $m = -4, -2, 0, 2$ in the index set $I_m = \{-4, -2, 0, 2\}$. Moreover, we may also write for $m \in I_m$ and $j = 0, 2$

$$\begin{aligned}
F_*^m(t) =& F_*^m[w_*(t), \mathfrak{a}_*^\gamma(t)] = F_*^m[w_*(t), \phi_*^0(t), \phi_*^2(t), \mathfrak{a}_*^\gamma(t)], \\
G_*^m(t) =& G_*^m[w_*(t), \mathfrak{a}_*^\gamma(t)] = G_*^m[w_*(t), \phi_*^0(t), \phi_*^2(t), \mathfrak{a}_*^\gamma(t)], \\
\rho_*^j(t) =& \rho_*^j[w_*(t)], \\
\boldsymbol{J}_*^{P,j}(t) =& \boldsymbol{J}_*^{P,j}[w_*(t), \mathfrak{a}_*^\gamma(t)],
\end{aligned}$$

where ρ_*^j, $\boldsymbol{J}_*^{P,j}$ will be given later in Sections 4.1.1 and 4.1.2. Gathering the equation for $\mathfrak{a}_*^\gamma$ (4.9), the equation for w_* (4.11) and the expansion of the nonlinear terms (4.14), we formulate the "twisted system" corresponding to the MKG and MD first order systems (2.33) and (2.41), respectively, for $x \in \mathbb{T}^d$ and $t \in [0, T]$ as

$$\begin{cases}
i\partial_t w_* = - \mathcal{L}_c w_* + \left(F_*^0 + G_*^0\right) + e^{2ic^2t}\left(F_*^2 + G_*^2\right) + e^{-2ic^2t}\left(F_*^{-2} + G_*^{-2}\right) \\
\qquad\qquad + e^{-4ic^2t}\left(F_*^{-4} + G_*^{-4}\right), \\
-\Delta\phi_*^j = \rho_*^j, \quad j = 0, 2 \\
i\partial_t \mathfrak{a}_*^\gamma = - c\langle\nabla\rangle_{\gamma/c}\mathfrak{a}_*^\gamma + \langle\nabla\rangle_{\gamma/c}^{-1}\left(\frac{\gamma^2}{2c}(\mathfrak{a}_*^\gamma + \overline{\mathfrak{a}_*^\gamma}) + \boldsymbol{J}_*^{P,0} + e^{2ic^2t}\boldsymbol{J}_*^{P,2} + e^{-2ic^2t}\overline{\boldsymbol{J}_*^{P,2}}\right), \\
w_*(0) = w(0), \quad \mathfrak{a}_*^\gamma(0) = \mathfrak{a}^\gamma(0) \\
F_*^m, G_*^m, m \in I_m \quad \text{as defined in (4.14)}, \quad I_m = \{-4, -2, 0, 2\}, \\
\left.\begin{array}{r} \rho_*^j, j = 0, 2 \\ \boldsymbol{J}_*^{P,j}, j = 0, 2 \end{array}\right\} \text{as defined in (4.17) for MKG and (4.18) for MD.}
\end{cases} \tag{4.15}$$

Note that $\mathcal{P}_{\mathrm{df}}H^r \subset \dot{H}^r$ (see Definition A.13) for all $r \geq 1$. Thus, combining the local well-posedness result from Proposition 4.2 for $r > d/2$ with Corollary A.15 on the zero mode of the solution $\mathfrak{a}_*^\gamma(t)$ for all times $t \in [0, T]$, we deduce that

$$\text{if } A_I \in \mathcal{P}_{\mathrm{df}}H^r, A_I' \in \mathcal{P}_{\mathrm{df}}H^{r-1}, \text{ then } \mathfrak{a}_I \in \mathcal{P}_{\mathrm{df}}H^r.$$

In particular, the zero Fourier mode of the solution $\mathfrak{a}_*^\gamma(t)$ of (4.15) satisfies by Corollary A.15

$$\left(\widehat{\mathfrak{a}_*^\gamma(t)}\right)_0 = 0 \qquad \text{for all } t \in [0, T].$$

At the end of this subsection we give a short remark on the derivatives of w_* and $\mathfrak{a}_*^\gamma$.

Remark 4.1 (A Remark on $\mathfrak{a}_*^\gamma$). *Recall that our aim is to construct a uniformly accurate method for $c \geq 1$ for the MKG/MD system, which is based on the "twisted system" (4.15). Following the paper [18], the basis for such methods is the uniform boundedness in H^r with respect to c of the time derivative of the right hand side nonlinear terms in (4.15). More precisely, we require bounds*

$$\|F_*^m(t+s) - F_*^m(t)\|_r + \|G_*^m(t+s) - G_*^m(t)\|_r \leq |s| \left(K_{F_*^m}^2 + K_{G_*^m}^2\right) \tag{4.16}$$

for $m = -4, -2, 0, 2$ with constants $K_{F_*^m}^2, K_{G_*^m}^2 > 0$ independent of c. In view of the term $c\langle\nabla\rangle_{\gamma/c}\mathfrak{a}_*^\gamma$ in the equation for $\mathfrak{a}_*^\gamma$ in (4.15), it seems to be a hard task to establish these bounds independent of c. But fortunately, in Section 4.3.4, we are able to play back the bound (4.16) for F_*^m and G_*^m to the bound

$$\|w_*(t+s) - w_*(t)\|_r + c^{-1}\|\mathfrak{a}_*^\gamma(t+s) - \mathfrak{a}_*^\gamma(t)\|_r \leq |s| K_{w_*, \mathfrak{a}_*^\gamma},$$

with a constant $K_{w_*,\mathfrak{a}_*^\gamma} > 0$ independent of c but depending on $\|w_*\|_{r+2}$ and on $\|\mathfrak{a}_*^\gamma\|_{r+1}$. Due to bounds $\left\|\langle\nabla\rangle_c^{-1} w\right\|_{r'} \leq c^{-1}\|w\|_{r'}$ for all $w \in H^{r'}$ from Lemma A.11, the factor of c^{-1} in the latter term is provided by the operator $\langle\nabla\rangle_c^{-1}$ in front of each term in F_*^m and G_*^m involving $\mathfrak{a}_*^\gamma$.

Next, for the interested reader, we give explicit formulas for the densities ρ_*^j and $\boldsymbol{J}_*^{P,j}$, $j = 0, 2$ from (4.15) in the subsequent subsections, starting off with the terms in the MKG case, followed by the terms in the MD case. Afterwards, we state a local well-posedness result on the system (4.15). We carry out the construction of the uniformly accurate time integration scheme in Section 4.2 below.

4.1.1 Nonlinear Terms in case of MKG

Note that in case of MKG we have $G = 0$ and thus also $G_*^m = 0, m = -4, -2, 0, 2$. Replacing w and $\mathfrak{a}$ by the variables $e^{ic^2t}w_*$ and $\mathfrak{a}_*^\gamma$ in (cf. the MKG first order system (2.33))

$$\begin{aligned}\rho[w] =& -\frac{1}{4}\operatorname{Re}\left((u+\overline{v})c^{-1}\langle\nabla\rangle_c(\overline{u}-v)\right),\\ \boldsymbol{J}^P[w,\mathfrak{a}] =& \mathcal{P}_{\mathrm{df}}\left[\operatorname{Re}\left(i\frac{1}{4}(u+\overline{v})\nabla(\overline{u}+v)\right) - \frac{1}{c}\frac{1}{8}(\mathfrak{a}+\overline{\mathfrak{a}})\,|u+\overline{v}|^2\right],\end{aligned}$$

then yields the decomposition (4.13), where the charge densities $\rho_*^j = \rho_*^j[w_*]$, $j = 0, 2$ and the current densities $\boldsymbol{J}_*^{P,j} = \boldsymbol{J}_*^{P,j}[w_*, \mathfrak{a}_*^\gamma]$, $j = 0, 2$ read

$$\begin{aligned}\rho_*^0[w_*] =& -\frac{1}{4c}\operatorname{Re}\left(u_*\langle\nabla\rangle_c\overline{u_*} - \overline{v_*}\langle\nabla\rangle_c v_*\right),\\ \rho_*^2[w_*] =& -\frac{1}{8c}\left(-u_*\langle\nabla\rangle_c v_* + v_*\langle\nabla\rangle_c u_*\right),\\ \boldsymbol{J}_*^{P,0}[w_*,\mathfrak{a}_*^\gamma] =& \mathcal{P}_{\mathrm{df}}\left[i\frac{1}{8}\left(u_*\nabla\overline{u_*} - \overline{u_*}\nabla u_* + \overline{v_*}\nabla v_* - v_*\nabla\overline{v_*}\right) - \frac{1}{8c}(\mathfrak{a}_*^\gamma + \overline{\mathfrak{a}_*^\gamma})(|u_*|^2 + |v_*|^2)\right],\\ \boldsymbol{J}_*^{P,2}[w_*,\mathfrak{a}_*^\gamma] =& \mathcal{P}_{\mathrm{df}}\left[i\frac{1}{8}\left(u_*\nabla v_* - v_*\nabla u_*\right) - \frac{1}{8c}(\mathfrak{a}_*^\gamma + \overline{\mathfrak{a}_*^\gamma})(u_*v_*)\right].\end{aligned} \tag{4.17a}$$

The potentials ϕ_*^0, ϕ_*^2 are solutions to Poisson's equations

$$-\Delta\phi_*^0 = \rho_*^0 \qquad \text{and} \qquad -\Delta\phi_*^2 = \rho_*^2. \tag{4.17b}$$

4.1.2 Nonlinear Terms in case of MD

Similarly, the charge and current density (cf. MD first order system (2.41))

$$\begin{aligned}\rho[w] =& \frac{1}{4}(|u|^2 + |v|^2 + 2\operatorname{Re}(u\cdot v)),\\ \boldsymbol{J}^P[w] =& c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[(u+\overline{v})\overline{\boldsymbol{\alpha}}(\overline{u}+v)\right]\end{aligned}$$

are decomposed according to (4.13) with

$$\begin{aligned}\rho_*^0[w_*] =& \frac{1}{4}\left(|u_*|^2 + |v_*|^2\right),\\ \rho_*^2[w_*] =& \frac{1}{4}u_*\cdot v_*,\\ \boldsymbol{J}_*^{P,0}[w_*] =& c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_*\overline{\boldsymbol{\alpha}u_*} + \overline{v_*\boldsymbol{\alpha}}v_*\right],\\ \boldsymbol{J}_*^{P,2}[w_*] =& c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_*\overline{\boldsymbol{\alpha}}v_*\right].\end{aligned} \tag{4.18a}$$

This yields the Poisson equations

$$-\Delta\phi_*^0 = \rho_*^0 \qquad \text{and} \qquad -\Delta\phi_*^2 = \rho_*^2. \tag{4.18b}$$

4.1.3 Local Well-Posedness of the Twisted System

The local well-posedness results of this section are based on [19–22, 34, 35, 70, 71, 79, 80]. According to the latter papers, the MKG/MD first order system in time (4.15) with solution $(w, \phi, \mathfrak{a})^\top$ is locally well-posed in $H^r \times \dot{H}^{r+r'} \times \dot{H}^r$ independent of c (see also Propositions 2.4 and 2.7), where

$$r' = 1 \quad \text{in case of MKG and} \quad r' = 2 \quad \text{in case of MD.}$$

From the relation $w(t) = e^{ic^2 t} w_*(t)$ we thus immediately obtain the following local well-posedness result for the "twisted system" (4.15).

Proposition 4.2 ([21, 22, 34, 62, 70, 79], see also Propositions 2.4 and 2.7)**.** *Let $c > 0$ and let $r > d/2$. Let the initial data*

$$\begin{cases} \text{of the MKG system (2.20) satisfy} \quad (\psi_I, \psi_I', A_I, A_I')^\top \in H^r \times H^r \times \dot{H}^r \times \dot{H}^{r-1} \text{ or} \\ \text{of the MD system (2.36) satisfy} \quad (\psi_I, A_I, A_I')^\top \in H^r \times \dot{H}^r \times \dot{H}^{r-1}, \end{cases}$$

respectively. Then there exist constants $T_r^*, B_r^* > 0$ such that the solution $(w_*, \phi_*^0, \phi_*^2, \mathfrak{a}_*)^\top$ of the MKG/MD first order "twisted system" in time (4.15) satisfies (cf. Propositions 2.4 and 2.7)

$$\begin{cases} \|w_*(t)\|_r + \left\|\phi_*^0(t)\right\|_{r+1,0} + \left\|\phi_*^2(t)\right\|_{r+1,0} + \|\mathfrak{a}_*(t)\|_{r,0} & \leq B_r^* \quad \text{in case of MKG} \\ \|w_*(t)\|_r + \left\|\phi_*^0(t)\right\|_{r+2,0} + \left\|\phi_*^2(t)\right\|_{r+2,0} + \|\mathfrak{a}_*(t)\|_{r,0} & \leq B_r^* \quad \text{in case of MD} \end{cases}$$

for all $t \in [0, T_r^*]$.

Proof (see also [21, 22, 34, 62, 70, 79] and references therein)*:* The proof is an immediate consequence of the identities

$$w(t) = e^{ic^2 t} w_*(t), \quad \phi(t) = \phi_*^{\text{tot}}(t) = \phi_*^0(t) + e^{2ic^2 t}\phi_*^2(t) + e^{-2ic^2 t}\overline{\phi_*^2}(t) \quad \text{and}$$
$$\frac{1}{2}(\mathfrak{a}_*^\gamma(t) + \overline{\mathfrak{a}_*^\gamma}(t)) = \boldsymbol{\mathcal{A}}(t) = \frac{1}{2}(\mathfrak{a}(t) + \overline{\mathfrak{a}}(t))$$

together with Propositions 2.4 and 2.7, where $(w, \phi, \mathfrak{a})^\top$ solves the MKG/MD first order system in time (2.33)/(2.41). Due to the definition of ϕ_*^j for $j = 0, 2$ as the solution of a Poisson equation of type (4.17b) and (4.18b), respectively, we can establish bounds for $j = 0, 2$ (see also the proof of Propositions 2.4 and 2.7)

$$\begin{cases} \left\|\phi_*^j(t)\right\|_{r+1,0} \leq \left\|\dot{\Delta}^{-1}\rho_*^j(t)\right\|_{r+1,0} \leq \left\|\rho_*^j(t)\right\|_{r-1,0} & \\ \qquad \leq K \|w_*(t)\|_r \left\|c^{-1}\langle\nabla\rangle_c w_*\right\|_{r-1} \leq K \|w_*(t)\|_r^2 & \text{in case of MKG,} \\ \left\|\phi_*^j(t)\right\|_{r+2,0} \leq \left\|\dot{\Delta}^{-1}\rho_*^j(t)\right\|_{r+2,0} \leq \left\|\rho_*^j(t)\right\|_{r,0} & \\ \qquad \leq K \|w_*(t)\|_r^2 & \text{in case of MD} \end{cases} \tag{4.19}$$

with constants K independent of c. Thereby we exploit results from Lemma A.11 on the operator $\langle\nabla\rangle_c$ and we exploit bilinear Sobolev product estimates from Lemma A.8. This finishes the proof. □

We proceed with the construction of uniformly accurate time integration scheme based on the "twisted variables".

4.2 Construction of Uniformly Accurate Schemes

In this section, based on [18], we construct a numerical time integration scheme which exploits the idea of "twisted variables". Due to the strong nonlinear coupling between the solutions w_*, $\mathfrak{a}_*^\gamma$ and ϕ_*^0, ϕ_*^2 the construction is much more involved than in of nonlinear Klein–Gordon equations. To overcome this challenge we combine the idea from [18] of applying exponential integrators to the "twisted system" (4.15) with a splitting ansatz. For an overview of classical exponential integrators, see [55]. Because most of the ideas and results in this section are very similar in case of Maxwell–Klein–Gordon and Maxwell–Dirac systems, we carry out the construction such that it applies up to small changes for both systems. If at some point particular considerations for MKG or MD are necessary, we remark them explicitly. In particular recall the different nonlinear terms G_*^m, ρ_*^j, $\boldsymbol{J}_*^{P,j}$ for $m = -4, -2, 0, 2$ and $j = 0, 2$ in both cases ($G_*^m = 0$ for MKG), see (4.14) and Sections 4.1.1 and 4.1.2. In both systems the structure of F_*^m is the same.

Due to $0 \leq \gamma \leq 1$, we have $0 \leq \gamma/c \leq 1$ for all $c \geq 1$, i.e. the operator $\langle\nabla\rangle_{\gamma/c}$ and its inverse satisfy the following bounds for $a \in \dot{H}^{r+1}$ according to Lemma A.5, i.e. $\left\|\langle\nabla\rangle_{\gamma/c}\, a\right\|_r \leq K \left\|a\right\|_{r+1}$ and

$$\left\|\langle\nabla\rangle_{\gamma/c}^{-1}\, a\right\|_{r,0} \leq \left\|\langle\nabla\rangle_{\gamma/c}^{-1}\, a\right\|_{r,0} \leq \left\|a\right\|_{r-1} \leq K \left\|a\right\|_{r-1,0}.$$

The "twisted system" (4.15) allows us to construct time integration scheme based on the "twisted variables" which have numerical order p in time uniformly in c. More precisely, if we apply these methods to the (4.15) with time step τ, then at time $t_n = n\tau$, $n = 0, 1, 2, \dots, T/\tau$ the numerical approximation $(w_*^n, \mathfrak{a}_*^{\gamma,n})^\top \approx (w_*(t_n), \mathfrak{a}_*^\gamma(t_n))^\top$ satisfies error bounds of type

$$\left\|w_*^n - w_*(t_n)\right\|_r + \left\|\mathfrak{a}_*^{\gamma,n} - \mathfrak{a}_*^\gamma(t_n)\right\|_{r,0} \leq K\tau^p$$

with a constant $K > 0$ independent of c. Within this thesis we focus on the construction of a uniformly accurate method of order $p = 1$ in time. However, similar to [18] this construction extends to arbitrary high order $p \in \mathbb{N}$. We proceed in the subsequent subsection.

4.2.1 First Order in Time Uniformly Accurate Time Integration Scheme

In this section we exploit ideas from [18, 55] and construct an exponential uniformly accurate splitting integrator for our "twisted system" (4.15). A comprehensive overview about exponential integrators can be found in the review article [55] by Hochbruck and Ostermann. Let us illustrate the construction of an exponential integration scheme (see [9, 10, 16, 18, 54, 55]) at the example of a nonlinear Schrödinger equation. Because the leading operator $\mathcal{L}_c = c\langle\nabla\rangle_c - c^2$ in our "twisted system" (4.15) essentially behaves like the second order Laplace operator Δ (see Lemma A.11), the ideas for the construction in this particular example can be transferred to our setting.

Example 4.3 ([18], see also [9, 10, 16, 54, 55])**.** *Let $r > d/2$. Consider the cubic nonlinear Schrödinger (NLS) equation for $x \in \mathbb{T}^d$ and $t \in [0, T]$ equipped with periodic boundary conditions, i.e.*

$$i\partial_t u = \Delta u + \alpha\left|u\right|^2 u, \quad u(0) = u_I \in H^r(\mathbb{T}^d), \quad \alpha \in \mathbb{R}. \tag{4.20}$$

We collect the nonlinearity of the latter system in $g[u] := -i\alpha |u|^2 u$. *Then Duhamel's formula (see for instance [85, Proposition 1.35] and also Proposition A.20) yields that for* $t_n \in [0,T]$ *and* $\tau > 0$ *we have*

$$u(t_n+\tau) = e^{-i\tau\Delta}u(t_n) + \int_0^\tau e^{-i(\tau-s)\Delta} g[u(t_n+s)]ds. \tag{4.21}$$

Observe that adding zeros in terms of $g[u(t_n)]$ *yields*

$$\begin{aligned} u(t_n+\tau) =& e^{-i\tau\Delta}u(t_n) + \int_0^\tau e^{-i(\tau-s)\Delta} g[u(t_n)]ds \\ &+ \int_0^\tau e^{-i(\tau-s)\Delta}\Big(g[u(t_n+s)] - g[u(t_n)]\Big)ds. \end{aligned}$$

If we define the method

$$\Phi^\tau_{\text{exp},1}[u(t_n)] := e^{-i\tau\Delta}u(t_n) + \int_0^\tau e^{-i(\tau-s)\Delta} g[u(t_n)]ds, \tag{4.22}$$

we obtain by the triangle inequality

$$\left\|u(t_n+\tau) - \Phi^\tau_{\text{exp},1}[u(t_n)]\right\|_r \le \left\|\int_0^\tau e^{-i(\tau-s)\Delta}\Big(g[u(t_n+s)] - g[u(t_n)]\Big)ds\right\|_r. \tag{4.23}$$

The claim is now, that the method $\Phi^\tau_{\text{exp},1}$ *is first order accurate in time. Therefore, we show that the local error*[1] *(4.23) of* $\Phi^\tau_{\text{exp},1}$ *satisfies an* $\mathcal{O}(\tau^2)$ *bound with a constant independent of* τ *and that the method* $\Phi^\tau_{\text{exp},1}$ *is stable*[2] *to perturbations in the data, i.e. for* $u(t_n), u^n \in H^r$ *we have that*

$$\left\|\Phi^\tau_{\text{exp},1}[u(t_n)] - \Phi^\tau_{\text{exp},1}[u^n]\right\|_r \le e^{L\tau}\left\|u(t_n) - u^n\right\|_r,$$

with a constant L *only depending on* $\|u(t_n)\|_r$ *and* $\|u^n\|_r$. *The latter is easy to verify by using the isometry property (4.25) of* $e^{it\Delta}$ *in* H^r *(see Lemma A.10) together with the bilinear product estimates in* H^r *for* $r > d/2$ *from Lemma A.8. The crucial point, in proving the first order convergence of the method* $\Phi^\tau_{\text{exp},1}$, *thus relies on establishing the local error bound*

$$[\text{term } (4.23)] \le K\tau^2 \quad \text{with a constant } K \text{ independent of } \tau.$$

To show this bound, we firstly establish a bound of type

$$\|g[u(t_n+s)] - g[u(t_n)]\|_r \le K|s| \quad \text{with a constant } K \text{ independent of } \tau, \tag{4.24}$$

exploiting a bound similar to Lemma 4.11, i.e.

$$\left\|e^{-is\Delta}u(t_n)\right\|_r = \|u(t_n)\|_r \quad \text{and} \quad \left\|(e^{-is\Delta}-1)u(t_n)\right\|_r \le |s|\,\|u\|_{r+2} \tag{4.25}$$

and using that (similar to [18, Lemma 5]) Duhamel's formula (4.21) implies together with the bilinear estimates from Lemma A.8

$$\begin{aligned} \|u(t_n+s) - u(t_n)\|_r &\le |s|\,\|u(t_n)\|_{r+2} + |s| \sup_{\xi\in[0,s]} \|g[u(t_n+\xi)]\|_r \\ &\le |s|\left(\|u(t_n)\|_{r+2} + |\alpha| \sup_{\xi\in[0,s]} \|u(t_n+\xi)\|_r^3\right). \end{aligned}$$

[1] See Definition A.17 for the local error of time integration schemes.
[2] See Definition A.18 for the stability of time integration schemes.

This immediately yields the desired bound for the time derivative of g in (4.24), with K only depending on $\sup_{\xi\in[0,T]} \|u(\xi)\|_{r+2}$. Secondly, another application of the triangle inequality to (4.23) together with the isometry property (4.25), then implies the $\mathcal{O}\left(\tau^2\right)$ local error bound.

We have seen that due to the bound (4.23) the term (4.22) describes an approximative solution of the NLS (4.20). In the following, we describe a corresponding exponential integration scheme in more detail.

Recall that from (4.22) we have

$$\Phi^{\tau}_{\text{exp},1}[u(t_n)] = e^{-i\tau\Delta}\left(u(t_n) + \int_0^{\tau} e^{is\Delta} ds\ g[u(t_n)]\right).$$

The remaining integral term can be integrated exactly — considering the operator $e^{is\Delta}$ in Fourier space (see Lemma A.10) — and we obtain the following first order exponential integrator for the NLS (4.20)

$$u^{n+1} = \Phi^{\tau}_{\text{exp},1}[u^n] := e^{-i\tau\Delta}\Big(u^n + \tau\varphi_1(i\tau\Delta)\ g[u^n]\Big) \quad \text{with} \quad \varphi_1(i\tau\Delta) = \frac{e^{i\tau\Delta}-1}{i\tau\Delta},$$

where the φ_j functions ([55]) are given in Definition A.22.

The first order approach can be extended to higher order exponential integrators (see [55]). Here we are interested in a particular type of exponential integrator (see for instance [18]).

Note that as described in [18, Section 4.1], we can increase the order of convergence of the method $\Phi^{\tau}_{\text{exp},1}$ with order $p = 1$ easily by recursively plugging in Duhamel's formula (4.21) into itself, i.e.

$$u(t_n+\tau) = e^{-i\tau\Delta}u(t_n) + \int_0^{\tau} e^{-i(\tau-s)\Delta} g\left[e^{-is\Delta}u(t_n) + \int_0^{s} e^{-i(s-\sigma)\Delta} g[u(t_n+\sigma)]d\sigma\right] ds.$$

Thus, we obtain a second order accurate method $\Phi^{\tau}_{\text{exp},2}$ via

$$u^{n+1} = \Phi^{\tau}_{\text{exp},2}[u^n] := e^{-i\tau\Delta}\left(u^n + \int_0^{\tau} e^{is\Delta} g\left[e^{-is\Delta}\left(u^n + \int_0^{s} e^{i\sigma\Delta} d\sigma\ g[u^n] ds\right)\right]\right),$$

which involves higher order φ_j functions with $j \geq 1$ ([55], see also Definition A.22).

Higher order methods $\Phi^{\tau}_{\text{exp},p}$ with $p \in \mathbb{N}$ can be constructed recursively in a similar way. ◇

The latter example has shown that the basis of exponential integrators ([55]) for the NLS (4.20) relies on Duhamel's formula (4.21) for its solution u. Furthermore, we have seen that a crucial point in the analysis of the resulting scheme is the boundedness of the time derivative of the nonlinearity g in (4.24).

Let us focus on the construction of uniformly accurate in c time integration schemes for the MKG and MD systems. We already pointed out, that the twisted first order systems (4.15) have structure, similar to the NLS (4.20). In particular, this is due to the essential behaviour of the operator $\mathcal{L}_c = c\left\langle\nabla\right\rangle_c - c^2$ applied to $w_* \in H^{r+2}$ similar to the Laplace operator Δ applied to $w_* \in H^{r+2}$. More precisely, we have (see Lemma A.11)

$$\left\|\mathcal{L}_c w_*\right\|_r \leq \frac{1}{2}\left\|w_*\right\|_{r+2}, \qquad \text{for all } c \in \mathbb{R}.$$

see [18, Lemma 3] and Lemma A.11. Following the ideas in [18] and Example 4.3, we thus need to establish uniform bounds of type (4.24) for the derivatives of F_*^m, G_*^m which are independent of c. We combine the construction with a splitting idea for the system (4.15).

Consider a discretization of the interval $t \in [0,T]$ with a time step size $\tau > 0$ such that $t_n = n\tau$, $n = 0, 1, 2, \ldots, T/\tau$. In the following, we use the notation $\mathcal{T}^{\tau}_{[\mathcal{L}_c]} := \exp(i\tau\mathcal{L}_c)$ (see (3.70)).

Recall Duhamel's perturbation formula (cf. Proposition A.20) for the solution $(w_*, \mathfrak{a}_*^\gamma)^\top$ of (4.15)

$$\begin{aligned}
w_*(t_n+\tau) =& \mathcal{T}^{\tau}_{[\mathcal{L}_c]} w_*(t_n) - i \int_0^\tau \mathcal{T}^{\tau-s}_{[\mathcal{L}_c]} \sum_{m\in I_m} e^{mic^2(t_n+s)} \left(F_*^m(t_n+s) + G_*^m(t_n+s)\right) ds,\\
\mathfrak{a}_*^\gamma(t_n+\tau) =& \mathcal{T}^{\tau}_{[c\langle\nabla\rangle_{\gamma/c}]} \mathfrak{a}_*^\gamma(t_n)\\
& - i \langle\nabla\rangle^{-1}_{\gamma/c} \int_0^\tau \mathcal{T}^{\tau-s}_{[c\langle\nabla\rangle_{\gamma/c}]} \Bigg(\frac{\gamma^2}{2c}\left(\mathfrak{a}_*^\gamma(t_n+s) + \overline{\mathfrak{a}_*^\gamma}(t_n+s)\right)\\
&\qquad + \boldsymbol{J}_*^{P,0}(t_n+s)\\
&\qquad + e^{+2ic^2(t_n+s)} \boldsymbol{J}_*^{P,2}(t_n+s)\\
&\qquad + e^{-2ic^2(t_n+s)} \overline{\boldsymbol{J}_*^{P,2}}(t_n+s)\Bigg) ds,
\end{aligned} \tag{4.26}$$

where $I_m = \{-4,-2,0,2\}$. In order to numerically handle the strong nonlinear coupling between w_* and $\mathfrak{a}_*$ in (4.15), we split the system (4.15) into the subproblems

$$\begin{cases}
i\partial_t w_* = -\mathcal{L}_c w_* + \left(F_*^0 + G_*^0\right) + e^{2ic^2t}\left(F_*^2 + G_*^2\right) + e^{-2ic^2t}\left(F_*^{-2} + G_*^{-2}\right)\\
\qquad\qquad + e^{-4ic^2t}\left(F_*^{-4} + G_*^{-4}\right),\\
-\Delta\phi_*^j = \rho_*^j, \quad j=0,2\\
i\partial_t \mathfrak{a}_*^\gamma = 0, \quad \text{given initial data} \quad w_*(0), \quad \mathfrak{a}_*^\gamma(0)
\end{cases} \tag{4.27a}$$

and

$$\begin{cases}
i\partial_t w_* = 0\\
i\partial_t \mathfrak{a}_*^\gamma = -c\langle\nabla\rangle_{\gamma/c}\mathfrak{a}_*^\gamma + \langle\nabla\rangle^{-1}_{\gamma/c}\left(\frac{\gamma^2}{2c}(\mathfrak{a}_*^\gamma + \overline{\mathfrak{a}_*^\gamma}) + \boldsymbol{J}_*^{P,0} + e^{2ic^2t}\boldsymbol{J}_*^{P,2} + e^{-2ic^2t}\overline{\boldsymbol{J}_*^{P,2}}\right),\\
\qquad \text{given initial data} \quad w_*(0), \quad \mathfrak{a}_*^\gamma(0),
\end{cases} \tag{4.27b}$$

with

$$F_*^m, G_*^m, m\in I_m \quad \text{and} \quad \boldsymbol{J}_*^{P,j}, j=0,2 \qquad \text{given explicitly in (4.14) and (4.17)/(4.18).}$$

In the following paragraphs we derive a numerical scheme for the solution of subproblem (4.27a) first and afterwards for subproblem (4.27b).

Numerical Solution of Subproblem (4.27a)

Note that Duhamels's formula (see Proposition A.20) corresponding to subproblem (4.27a) reads in the notation $I_m = \{-4,-2,0,2\}$ ((cf. (4.26))

$$\begin{cases}
w_*(t_n+\tau) = \mathcal{T}^{\tau}_{[\mathcal{L}_c]} w_*(t_n) - i \int_0^\tau \mathcal{T}^{\tau-s}_{[\mathcal{L}_c]} \sum_{m\in I_m} e^{mic^2(t_n+s)} \big(F_*^m[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n)]\\
\qquad\qquad + G_*^m[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n)] \big) ds,\\
\mathfrak{a}_*^\gamma(t_n+\tau) = \mathfrak{a}_*^\gamma(t_n).
\end{cases} \tag{4.28}$$

Having a closer look at the nonlinearities F_*^m and G_*^m given in (4.14), we observe that the terms involving $\mathfrak{a}_*^\gamma$ come together with the operator $\langle\nabla\rangle_c^{-1}$. Exploiting the bounds of type $\left\|\langle\nabla\rangle_c^{-1} w\right\|_r \le c^{-1}\|w\|_r$ from Lemma A.11 allows us to establish uniform bounds in c on the time derivative of $F_*^m + G_*^m$ in Section 4.3.4.

This means, that the nonlinearities F_*^m and G_*^m are only slowly varying in time, which is discussed in more detail in Remark 4.1. More precisely, in Duhamel's formula (4.26) above, we have (cf. (4.76))

$$\begin{aligned} &F_*^m[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n+s)] + G_*^m[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n+s)] \\ =&F_*^m[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)] + G_*^m[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)] + \mathcal{O}(s), \end{aligned} \tag{4.29}$$

These bounds are discussed in more detail later on in Section 4.3.4. Furthermore, due to Lemma 4.11 the operator $\mathcal{T}_{[\mathcal{L}_c]}^{-s}$ is a smooth perturbation of the identity from H^{r+2} to H^r, i.e.

$$\text{for } w \in H^{r+2} \text{ we have} \quad \left\| (\mathcal{T}_{[\mathcal{L}_c]}^{-s} - 1)w \right\|_r \leq \frac{1}{2}|s| \, \|w\|_{r+2}.$$

We thus carry out the construction of our scheme for the integration of w_* by simply

- "freezing" the nonlinearities F_*^m, G_*^m at time t_n in (4.28) (cf. (4.29)),
- substituting $\mathcal{T}_{[\mathcal{L}_c]}^{-s}$ in the integral term in (4.28) by the identity and
- integrating the remaining integral terms $\int_0^\tau e^{mic^2 s} ds = \tau\varphi_1(mic^2\tau)$ in (4.28) exactly in time (see Definition A.22 and [55] for definition of the φ_j funtions).

Note that for according to Definition A.22 we have $\varphi_1(z) = (e^z - 1)/z$ for $z \in \mathbb{C}$. The scheme for numerically solving subproblem (4.27a) then reads

$$\Psi_{w_*}^\tau[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)] := \begin{pmatrix} \Phi_{w_*}^\tau\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right] \\ \mathfrak{a}_*^\gamma(t_n) \end{pmatrix}, \tag{4.30a}$$

where in the notation $I_m = \{-4, -2, 0, 2\}$ the numerical flow $\Phi_{w_*}^\tau$ is defined as

$$\begin{aligned} &\Phi_{w_*}^\tau\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right] \\ &= \mathcal{T}_{[\mathcal{L}_c]}^\tau \Big(w_*(t) - i \sum_{m \in I_m} \tau\varphi_1(mic^2\tau) e^{mic^2 t_n} \big(F_*^m[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)] \\ &\qquad\qquad + G_*^m[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)]\big)\Big). \end{aligned} \tag{4.30b}$$

Note that for $m \in I_m$ the nonlinearities F_*^m, G_*^m are given explicitly in (4.14), and that for MKG we have $G_*^m = 0$ (cf. (2.41)). Next, we derive a similar scheme for the solution of subproblem (4.27b).

Numerical Solution of Subproblem (4.27b)

We proceed with the construction of a scheme for the solution of subproblem (4.27b), similar to (4.30). Duhamel's formula corresponding to the second subproblem (4.27b) reads

$$\begin{cases} w_*(t_n+\tau) = w_*(t_n), \\ \mathfrak{a}_*^\gamma(t_n+\tau) = \mathcal{T}_{[c\langle\nabla\rangle_{\gamma/c}]}^\tau \mathfrak{a}_*^\gamma(t_n) \\ \qquad - i\,\langle\nabla\rangle_{\gamma/c}^{-1} \displaystyle\int_0^\tau \mathcal{T}_{[c\langle\nabla\rangle_{\gamma/c}]}^{\tau-s} \Big(\frac{\gamma^2}{2c}(\mathfrak{a}_*^\gamma(t_n+s) + \overline{\mathfrak{a}_*^\gamma}(t_n+s)) \\ \qquad\qquad + \boldsymbol{J}_*^{P,0}[w_*(t_n), \mathfrak{a}_*^\gamma(t_n+s)] \\ \qquad\qquad + e^{+2ic^2(t_n+s)} \boldsymbol{J}_*^{P,2}[w_*(t_n), \mathfrak{a}_*^\gamma(t_n+s)] \\ \qquad\qquad + e^{-2ic^2(t_n+s)} \overline{\boldsymbol{J}_*^{P,2}}[w_*(t_n), \mathfrak{a}_*^\gamma(t_n+s)] \Big) ds. \end{cases} \tag{4.31}$$

Recall from Sections 4.1.1 and 4.1.2, that the currents $\boldsymbol{J}_*^{P,j}$, $j=-2,0,2$ are different in the case of MKG and MD, i.e. in case of MKG we have (see Section 4.1.1)

$$\begin{aligned}\boldsymbol{J}_*^{P,0}[w_*,\mathfrak{a}_*^\gamma] =& \mathcal{P}_{\mathrm{df}}\left[i\frac{1}{8}\left(u_*\nabla\overline{u_*}-\overline{u_*}\nabla u_*+\overline{v_*}\nabla v_*-v_*\nabla\overline{v_*}\right)-\frac{1}{8c}(\mathfrak{a}_*^\gamma+\overline{\mathfrak{a}_*^\gamma})(|u_*|^2+|v_*|^2)\right],\\ \boldsymbol{J}_*^{P,2}[w_*,\mathfrak{a}_*^\gamma] =& \mathcal{P}_{\mathrm{df}}\left[i\frac{1}{8}\left(u_*\nabla v_*-v_*\nabla u_*\right)-\frac{1}{8c}(\mathfrak{a}_*^\gamma+\overline{\mathfrak{a}_*^\gamma})(u_*v_*)\right],\end{aligned}$$

and in case of MD we have (see Section 4.1.2)

$$\begin{aligned}\boldsymbol{J}_*^{P,0}[w_*] =& c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_*\overline{\boldsymbol{\alpha}u_*}+\overline{v_*}\boldsymbol{\alpha}v_*\right],\\ \boldsymbol{J}_*^{P,2}[w_*] =& c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_*\overline{\boldsymbol{\alpha}}v_*\right].\end{aligned} \tag{4.32}$$

Firstly, we observe that due to Duhamel's formula (4.31) and due to the bound (cf. (4.73) and Lemmas 4.11 and A.10)

$$\left\|\langle\nabla\rangle_{\gamma/c}^{-1}c^{-1}\left(e^{ics\langle\nabla\rangle_{\gamma/c}}\mathfrak{a}_*^\gamma(t_n)-\mathfrak{a}_*^\gamma(t_n)\right)\right\|_{r,0}\le|s|\,\|\mathfrak{a}_*^\gamma(t_n)\|_{r,0}$$

we have the following bound on the derivatives of $\mathfrak{a}_*^\gamma$ within subproblem (4.27b)

$$\langle\nabla\rangle_{\gamma/c}^{-1}\frac{\gamma^2}{c}\mathfrak{a}_*^\gamma(t_n+s)=\langle\nabla\rangle_{\gamma/c}^{-1}\frac{\gamma^2}{c}\mathfrak{a}_*^\gamma(t_n)+\mathcal{O}(s) \tag{4.33}$$

in the sense of the $\dot{H}^r$ norm. The latter bound can be established in the MKG case as well as in the MD case. Note that the idea of freezing $\boldsymbol{J}_*^{P,j}$ for $j=0,2$ yields different bounds in the MKG case as in the MD case. We thus distinguish between the two cases in the following.

The MKG case: Freezing $\boldsymbol{J}_*^{P,j}$ for $j=0,2$ at time t_n, the bound (4.33) together with the bilinear Sobolev product estimates from Lemma A.8 provide the bound

$$\boldsymbol{J}_*^{P,j}[w_*(t_n+s),\mathfrak{a}_*^\gamma(t_n+s)]=\boldsymbol{J}_*^{P,j}[w_*(t_n),\mathfrak{a}_*^\gamma(t_n)]+\mathcal{O}(s)$$

in the sense of the $\dot{H}^r$ norm. Later in Section 4.3, we combine this result with (4.29) to show first order convergence bounds uniformly in c of our method.

The MD case: However, applying the previous standard estimates in the MD case in $\dot{H}^r$ to $\boldsymbol{J}_*^{P,j}$ for $j=0,2$ (we omit the second argument in $\boldsymbol{J}_*^{P,j}$) yields bounds of type

$$\boldsymbol{J}_*^{P,j}[w_*(t_n)+\mathcal{O}(s)]=\boldsymbol{J}_*^{P,j}[w_*(t_n)]+\mathcal{O}(cs)$$

which are not independent of c. Thus, freezing $\boldsymbol{J}_*^{P,j}$ at time t_n does not directly yield c-independent numerical approximation bounds. Despite that within this thesis for **general Maxwell–Dirac initial data**, we have not been able to prove global first order convergence bounds uniformly in c for the method constructed in this chapter, the results of our numerical experiments in Section 5.4 do not show any c-dependence. Note that respecting the findings given in Remark 4.4 below, we can set up conditions on the initial data of the MD system (2.36), see Assumption 4.5. More precisely, according to the decomposition (2.42) of the initial data ψ_I into upper and lower components ψ_I^+,ψ_I^-, we assume that

$$\psi_I=(\psi_I^+,\psi_I^-)^\top \quad \text{satisfies} \quad \left(\psi_I^-\overline{\boldsymbol{\sigma}}\overline{\psi_I^+}\right)=\mathcal{O}\left(c^{-1}\right). \tag{4.34}$$

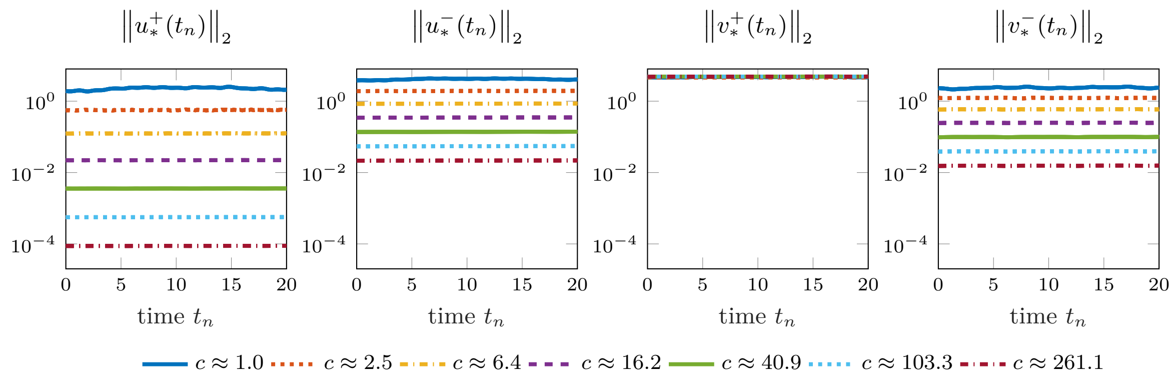


Figure 4.1: (MD, Simulation of the H^2 norm of $w_*(t_n) = (u_*^+(t_n), u_*^-(t_n), v_*^+(t_n), v_*^-(t_n))^\top$). With the special choice of initial data according to Assumption 4.5 for the MD system (2.36) (or the reduced MD system (2.37), respectively) we observe in our numerical simulation for $d = 2$ that $v_*^+(t_n) = \mathcal{O}(1)$ and $u_*^+(t_n) = \mathcal{O}\left(c^{-1}\right)$ for all $t_n \in [0, 20]$. The latter can be seen from the second from left semilogarithmic plot since the lines corresponding to $\left\|u_*^-(t_n)\right\|_2$ for values $c = 1.59^{2\ell}, \ell = 0, 1, \ldots, 6$ are equidistant. This allows us to bound $u_*^- \overline{\boldsymbol{\sigma}} \overline{v_*^+}$ in $\mathcal{O}(1)$ in the sense of the H^2 norm. Thus $\boldsymbol{J}_*^{P,2} = \mathcal{O}(1)$, see (4.36). The numerical approximation to the solution w_* of the MD first order system (2.41) at time $t_n = n\tau, n = 1, \ldots, 20/\tau$ for the time step $\tau \approx 0.004$ is obtained via the "twisted" time integration scheme Ψ_*^τ (with $\gamma = 1$) given in (4.39) with initial data corresponding to Experiment 5.3 (see Section 5.4) which satisfy Assumption 4.5.

Due to Remark 4.4, these assumptions combined with the local well-posedness results from Proposition 4.2, allow us to establish the bounds $\boldsymbol{J}_*^{P,j}(t) = \mathcal{O}(1)\,,\ j = 0, 2$ uniformly in c for all $t \in [0, T]$. Then, freezing $\boldsymbol{J}_*^{P,j}$ at time t_n yields the following approximation bound independent of c

$$\boldsymbol{J}_*^{P,j}[w_*(t_n) + \mathcal{O}(s)] = \boldsymbol{J}_*^{P,j}[w_*(t_n)] + \mathcal{O}(s)\,. \tag{4.35}$$

The proof of the uniform first order convergence of our scheme for general initial data might be interesting future research.

We gather the additional assumptions (4.34) on the initial data of the MD system (2.36) in Assumption 4.5 below.

Remark 4.4. *Consider the definition of* $\boldsymbol{J}_*^{P,j}$ *in* (4.32) *in the case of Maxwell–Dirac . According to* (2.42) *the solution* $w_* = (u_*, v_*)^\top = (u_*^+, u_*^-, v_*^+, v_*^-)^\top$ *obeys the following structure in the sense of the* H^r *norm*

$$\begin{aligned} u_*^+(t) &= \mathcal{O}\left(c^{-1}\right), & v_*^+(t) &= \mathcal{O}\left(\overline{\psi^+(t)}\right), \\ u_*^-(t) &= \mathcal{O}\left(\psi^-(t)\right), & v_*^-(t) &= \mathcal{O}\left(c^{-1}\right), \end{aligned} \qquad \text{for all times } t.$$

Assuming that $\psi^\pm(t) = \mathcal{O}(1)$ *we deduce from the latter that*

$$\boldsymbol{J}_*^{P,0} = c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_*^+ \overline{\boldsymbol{\sigma}} \overline{u_*^-} + u_*^- \overline{\boldsymbol{\sigma}} \overline{u_*^+} + \overline{v_*^+} \overline{\boldsymbol{\sigma}} v_*^- + \overline{v_*^-} \overline{\boldsymbol{\sigma}} v_*^+\right] = \mathcal{O}(1)\,.$$

Therefore, the argumentation in (4.35) *can be applied to* $\boldsymbol{J}_*^{P,0}$ *and we find*

$$\boldsymbol{J}_*^{P,0}[w_*(t_n) + \mathcal{O}(s)] = \boldsymbol{J}_*^{P,j}[w_*(t_n)] + \mathcal{O}(s)\,.$$

In view of the decomposition

$$\begin{aligned} \boldsymbol{J}_*^{P,2} =& c\frac{1}{4}\mathcal{P}_{\text{df}}\left[u_*^+\overline{\boldsymbol{\sigma}}v_*^- + u_*^-\overline{\boldsymbol{\sigma}}v_*^+\right] = \underbrace{c\frac{1}{4}\mathcal{P}_{\text{df}}\left[u_*^+\overline{\boldsymbol{\sigma}}v_*^-\right]}_{=:\boldsymbol{J}_*^{P,2,ok}} + \underbrace{c\frac{1}{4}\mathcal{P}_{\text{df}}\left[u_*^-\overline{\boldsymbol{\sigma}}v_*^+\right]}_{=:\boldsymbol{J}_*^{P,2,c}} \\ =& \mathcal{O}\left(1 + c\big(\psi^-\overline{\boldsymbol{\sigma}}\overline{\psi^+}\big)\right), \end{aligned} \tag{4.36}$$

the term $\boldsymbol{J}_*^{P,2,ok} = \mathcal{O}(1)$ is uniformly bounded with respect to c. However, in order to establish uniform boundedness of $\boldsymbol{J}_*^{P,2}$, the remaining term $\boldsymbol{J}_*^{P,2,c} = \mathcal{O}\left(c\big(\psi^-\overline{\boldsymbol{\sigma}}\overline{\psi^+}\big)\right)$ requires to set up the condition on the components $\psi^\pm$ of the exact solution $\psi = (\psi^+,\psi^-)^\top$ to satisfy $\psi^-\overline{\boldsymbol{\sigma}}\overline{\psi^+} = \mathcal{O}(c^{-1})$. Thus, the argumentation (4.35) on $\boldsymbol{J}_*^{P,j}$ applies only in the special case where the initial data

$$\psi_I = (\psi_I^+,\psi_I^-)^\top \quad \text{satisfies} \quad \big(\psi_I^-\overline{\boldsymbol{\sigma}}\overline{\psi_I^+}\big) = \mathcal{O}\left(c^{-1}\right), \qquad \text{see Fig. 4.1.}$$

Such a restriction has already been used in [22, Theorem 1.3] in order to obtain a better convergence of the nonrelativistic limit approximation (see (3.59) in Chapter 3) in low regularity spaces by assuming that $\psi_I^- = \mathcal{O}\left(c^{-1}\right)$.

We collect this particular choice of Maxwell–Dirac initial data in the following Assumption 4.5.

Assumption 4.5. *Let $r > d/2$ and let $r' \geq 0$. We assume that the initial data $\psi(0) = \psi_I = (\psi_I^+,\psi_I^-)^\top$ of the Maxwell–Dirac system (2.36) satisfies*

$$\left\|\psi_I^-\overline{\boldsymbol{\sigma}}\overline{\psi_I^+}\right\|_{r+r'} \leq Kc^{-1}$$

with a constant K independent of c.

Fortunately, promising numerical experiments in Section 5.4 suggest that our scheme is uniformly convergent also for initial data violating the latter Assumption 4.5.

Even though there are challenges in proving convergence bounds uniformly in c of our method in case of MD with general initial data, we proceed with the construction of our method for both cases. Note that in case of MD with initial data satisfying Assumption 4.5 and in case of MKG, the construction and the analysis of our method is rigorous. Since we have not been able within this thesis for general initial data in case of MD to prove uniform convergence bounds, the construction in this case is only formal but admits also first order convergence bounds uniformly in c in our numerical experiments in Section 5.4.

We come back to the construction of a method for solving subproblem (4.27b). Respecting the above considerations, the idea for the construction follows the same ideas as before. We thus

- "freeze" the terms $\boldsymbol{J}_*^{P,j}$ for $j = -2, 0, 2$ as well as the terms $\mathfrak{a}_*^\gamma$ at time t_n in the integral in (4.31) and to
- integrate the remaining integral terms $\int_0^t \mathcal{T}^{-s}_{[c\langle\nabla\rangle_{\gamma/c}]} e^{jic^2 s} ds = \tau\varphi_1\Big(i\tau(jc^2 - c\langle\nabla\rangle_{\gamma/c})\Big)$ exactly in time (see Definition A.22 and [55] for definition of the φ_j funtions).

Recall that according to Definition A.2, the Fourier symbol of $\langle\nabla\rangle_{\gamma/c} = \left(-\Delta + \gamma^2/c^2\right)^{1/2}$ is given by

$$\left(\widehat{\langle\nabla\rangle_{\gamma/c}}\right)_k = \left(|k|^2 + \gamma^2/c^2\right)^{1/2} \qquad \text{for all } k \in \mathbb{Z}^d. \tag{4.37}$$

This allows us to evaluate $\varphi_1\Big(i\tau(jc^2 - c\langle\nabla\rangle_{\gamma/c})\Big)$ in its Fourier representation.

The resulting scheme for numerically solving of subproblem (4.27b) is based on Duhamel's formula (4.31) above and reads

$$\Psi^\tau_{\mathfrak{a}_*}[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)] := \begin{pmatrix} w_*(t_n) \\ \Phi^\tau_{\mathfrak{a}_*}\left[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)\right] \end{pmatrix}, \tag{4.38a}$$

where we define the numerical flow $\Phi^\tau_{\mathfrak{a}_*}$ as

$$\begin{aligned}
&\Phi^\tau_{\mathfrak{a}_*}\left[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)\right] \\
&= \mathcal{T}^\tau_{[c\langle\nabla\rangle_{\gamma/c}]}\Bigg(\mathfrak{a}^\gamma_*(t_n) - i\tau\langle\nabla\rangle^{-1}_{\gamma/c}\Bigg\{ \\
&\qquad \varphi_1\left(i\tau \quad (-c\langle\nabla\rangle_{\gamma/c})\right)\Bigg(\frac{\gamma^2}{2c}(\mathfrak{a}^\gamma_*(t_n) + \overline{\mathfrak{a}^\gamma_*}(t_n)) \\
&\qquad\qquad + \boldsymbol{J}^{P,0}_*[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)]\Bigg) \\
&\qquad + \varphi_1\left(i\tau(+2c^2 - c\langle\nabla\rangle_{\gamma/c})\right)e^{+2ic^2t_n}\boldsymbol{J}^{P,2}_*[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)] \\
&\qquad + \varphi_1\left(i\tau(-2c^2 - c\langle\nabla\rangle_{\gamma/c})\right)e^{-2ic^2t_n}\overline{\boldsymbol{J}^{P,2}_*}[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)]\Bigg\}\Bigg).
\end{aligned} \tag{4.38b}$$

Note that the currents $\boldsymbol{J}^{P,j}_*$, $j = 0, 2$ are given explicitly for the case of MKG in (4.17) and for the case of MD in (4.18), respectively. Next, we combine the solutions of the subproblems (4.27a) and (4.27b) in the subsequent subsection by a simple splitting idea.

A First Order in Time Uniformly Accurate in c "Twisted" Scheme

Employing a simple splitting idea, we combine the numerical flow $\Psi^\tau_{w_*}$ given in (4.30) for the numerical solution of subproblem (4.27a) with the numerical flow $\Psi^\tau_{\mathfrak{a}_*}$ given in (4.38) for the numerical solution of subproblem (4.27b) as follows. Firstly, we compute the numerical flow $\Psi^\tau_{w_*}$ corresponding to subproblem (4.27a) and afterwards we use the numerical result in order to compute the numerical flow $\Psi^\tau_{\mathfrak{a}^\gamma_*}$ corresponding to subproblem (4.27b). Starting from an approximation $(w^n_*, \mathfrak{a}^{\gamma,n}_*)^\top$ to the exact solution $(w_*(t_n), \mathfrak{a}^\gamma_*(t_n))^\top$, we thus obtain an

$$\text{approximation} \quad (w^{n+1}_*, \mathfrak{a}^{\gamma,n+1}_*)^\top \quad \text{to} \quad (w_*(t_{n+1}), \mathfrak{a}^\gamma_*(t_{n+1}))^\top.$$

Exploiting (4.13) and solving the Poisson equations (4.40) for $\phi^{0,n+1}_*$ and $\phi^{2,n+1}_*$, we obtain a numerical approximation to the potential $\phi(t_{n+1}) = \phi^{\text{tot}}_*(t_{n+1})$. More precisely, we numerically approximate the exact solution $(\psi(t_{n+1}), \phi(t_{n+1}), \boldsymbol{\mathcal{A}}(t_{n+1}))^\top$ of the MKG/MD system (2.20)/(2.36) via

$$\psi^{n+1}_* = \frac{1}{2}\left(e^{ic^2t_{n+1}}u^{n+1}_* + e^{-ic^2t_{n+1}}\overline{v^{n+1}_*}\right) \quad \text{and} \quad \boldsymbol{\mathcal{A}}^{n+1}_* = \frac{1}{2}(\mathfrak{a}^{\gamma,n+1}_* + \overline{\mathfrak{a}^{\gamma,n+1}_*}), \tag{4.39a}$$

and $\phi^{\text{tot},n+1}_*$, where $w^{n+1}_* = (u^{n+1}_*, v^{n+1}_*)^\top$, $\phi^{\text{tot},n+1}_*$ and $\mathfrak{a}^{\gamma,n+1}_*$ are given through the resulting scheme for the solution of the full "twisted system" (4.15), i.e.

$$\begin{cases} \begin{pmatrix} w^{n+1}_* \\ \mathfrak{a}^{\gamma,n+1}_* \end{pmatrix} = \Psi^\tau_*[w^n_*, \mathfrak{a}^{\gamma,n}_*] := \Psi^\tau_{\mathfrak{a}_*} \circ \Psi^\tau_{w_*}[w^n_*, \mathfrak{a}^{\gamma,n}_*] = \begin{pmatrix} \Phi^\tau_{w_*}\left[w^n_*, \mathfrak{a}^{\gamma,n}_*\right] \\ \Phi^\tau_{\mathfrak{a}_*}\left[w^{n+1}_*, \mathfrak{a}^{\gamma,n}_*\right] \end{pmatrix}, \\ \phi^{\text{tot},n+1}_* = \phi^{0,n+1}_* + e^{2ic^2t_{n+1}}\phi^{2,n+1}_* + e^{-2ic^2t_{n+1}}\overline{\phi^{2,n+1}_*}, \end{cases} \tag{4.39b}$$

where $\Phi^\tau_{w_*}$ and $\Phi^\tau_{\mathfrak{a}_*}$ are given in (4.30) and (4.38), respectively, as

$$\begin{aligned}
&\Phi^\tau_{w_*}\left[w^n_*, \mathfrak{a}^{\gamma,n}_*\right] = \mathcal{T}^\tau_{[\mathcal{L}_c]}\Big(w^n_* - i\sum_{m\in I_m}\tau\varphi_1(mic^2\tau)e^{mic^2t_n}\big(\,F^m_*[w^n_*, \mathfrak{a}^{\gamma,n}_*] + G^m_*[w^n_*, \mathfrak{a}^{\gamma,n}_*]\big)\Big),\\
&\Phi^\tau_{\mathfrak{a}_*}\left[w^{n+1}_*, \mathfrak{a}^{\gamma,n}_*\right]\\
&= \mathcal{T}^\tau_{[c\langle\nabla\rangle_{\gamma/c}]}\Big(\mathfrak{a}^{\gamma,n}_* - i\tau\langle\nabla\rangle^{-1}_{\gamma/c}\Big\{\ \varphi_1\left(i\tau\qquad(-c\langle\nabla\rangle_{\gamma/c})\right)\Big(\ \frac{\gamma^2}{2c}(\mathfrak{a}^{\gamma,n}_* + \overline{\mathfrak{a}^{\gamma}_*}(t_n))\\
&\qquad\qquad + \boldsymbol{J}^{P,0}_*[w^{n+1}_*, \mathfrak{a}^{\gamma,n}_*]\Big)\\
&\qquad + \varphi_1\left(i\tau(+2c^2 - c\langle\nabla\rangle_{\gamma/c})\right)e^{+2ic^2t_n}\boldsymbol{J}^{P,2}_*[w^{n+1}_*, \mathfrak{a}^{\gamma,n}_*]\\
&\qquad + \varphi_1\left(i\tau(-2c^2 - c\langle\nabla\rangle_{\gamma/c})\right)e^{-2ic^2t_n}\overline{\boldsymbol{J}^{P,2}_*}[w^{n+1}_*, \mathfrak{a}^{\gamma,n}_*]\Big\}\Big),
\end{aligned}\tag{4.39c}$$

with $I_m = \{-4, -2, 0, 2\}$. We define the nonlinearities

$$F^m_*, G^m_*, m \in I_m \quad \text{and} \quad \boldsymbol{J}^{P,j}_*, j = 0, 2 \qquad \text{explicitly in (4.14) and (4.17)/(4.18)} \tag{4.39d}$$

and the approximations $\phi^{0,n}_*$ and $\phi^{2,n}_*$ to $\phi^j_*(t_n)$ for $j = 0, 2$

for the case of MKG according to (4.17) as the solutions to Poisson's equations

$$\begin{aligned}
-\Delta\phi^{0,n}_* &= -\frac{1}{4c}\operatorname{Re}\left(u^n_*\langle\nabla\rangle_c\overline{u^n_*} - \overline{v^n_*}\langle\nabla\rangle_c v^n_*\right),\\
-\Delta\phi^{2,n}_* &= -\frac{1}{8c}\left(-u^n_*\langle\nabla\rangle_c v^n_* + v^n_*\langle\nabla\rangle_c u^n_*\right),
\end{aligned}\tag{4.40a}$$

and for the case of MD according to (4.18) as the solutions to Poisson's equations

$$\begin{aligned}
-\Delta\phi^{0,n}_* &= \frac{1}{4}\left(|u^n_*|^2 + |v^n_*|^2\right),\\
-\Delta\phi^{2,n}_* &= \frac{1}{4}u^n_*\cdot v^n_*.
\end{aligned}\tag{4.40b}$$

The currents $\boldsymbol{J}^{P,j}_*$, $j = 0, 2$ are given explicitly for the case of MKG in (4.17) and for the case of MD in (4.18). Furthermore, note that in the MKG case $G^m_* = 0$, see (4.15). The φ_1 function is given via Definition A.22 as

$$\varphi_1(z) = (e^z - 1)/z \quad \text{and satisfies} \quad \int_0^\tau e^{i\omega s}ds = \tau\varphi_1(i\omega\tau) \quad \text{for all } \omega \in \mathbb{R}.$$

In particular, due to Proposition A.32 and with the aid of the Fourier representation (4.37) of $\langle\nabla\rangle_{\gamma/c}$, we have

$$\left\|\varphi_1\left(i\tau(mc^2 - \ell c\langle\nabla\rangle_{\gamma/c})\right)w\right\|_r \leq \|w\|_r \qquad \text{for all } m, \ell \in \mathbb{Z} \text{ and all } w \in H^r.$$

Within this thesis we focus on methods which are first order accurate in time uniformly in c. Thus, in Section 4.3 we establish the following uniform bounds for our numerical scheme Ψ^τ_* given in (4.39), i.e.

$$\left\|\begin{pmatrix} w_*(t_{n+1})\\ \mathfrak{a}^\gamma_*(t_{n+1})\end{pmatrix} - \begin{pmatrix} w^{n+1}_*\\ \mathfrak{a}^{\gamma,n+1}_*\end{pmatrix}\right\|_r \leq K\tau$$

with a constant K independent of c. Though, we roughly sketch the idea for the construction of higher order schemes in the subsequent subsection.

Higher Order in Time Uniformly Accurate Schemes Based on "Twisted Variables"

The scheme of the previous section can be easily extended to higher order uniformly accurate methods which allow error bounds of order $\mathcal{O}(\tau^p)$ for $p \in \mathbb{N}$. Recall that we based our construction on freezing the slowly varying nonlinear terms at time t_n in Duhamel's formula (4.26)

$$\begin{aligned} w_*(t_n+\tau) =& \mathcal{T}^{\tau}_{[\mathcal{L}_c]} w_*(t_n) - i \int_0^\tau \mathcal{T}^{\tau-s}_{[\mathcal{L}_c]} \sum_{m \in I_m} e^{mic^2(t_n+s)} \left(F_*^m(t_n+s) + G_*^m(t_n+s) \right) ds, \\ \mathfrak{a}_*^\gamma(t_n+\tau) =& \mathcal{T}^{\tau}_{[c\langle\nabla\rangle_{\gamma/c}]} \mathfrak{a}_*^\gamma(t_n) \\ & - i \langle\nabla\rangle_{\gamma/c}^{-1} \int_0^\tau \mathcal{T}^{\tau-s}_{[c\langle\nabla\rangle_{\gamma/c}]} \Bigg(\frac{\gamma^2}{2c} \left(\mathfrak{a}_*^\gamma(t_n+s) + \overline{\mathfrak{a}_*^\gamma}(t_n+s) \right) \\ & \qquad + \qquad \boldsymbol{J}_*^{P,0}(t_n+s) \\ & \qquad + e^{+2ic^2(t_n+s)} \boldsymbol{J}_*^{P,2}(t_n+s) \\ & \qquad + e^{-2ic^2(t_n+s)} \overline{\boldsymbol{J}_*^{P,2}}(t_n+s) \Bigg) ds, \end{aligned} \tag{4.41}$$

where $I_m = \{-4, -2, 0, 2\}$ and where we use the notation for $m \in I_m$, $j = 0, 2$

$$\begin{aligned} F_*^m(t_n+s) =& F_*^m[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n+s)] = F_*^m[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)] + \mathcal{O}(s), \\ G_*^m(t_n+s) =& G_*^m[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n+s)] = G_*^m[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)] + \mathcal{O}(s), \\ \boldsymbol{J}_*^{P,j}(t_n+s) =& \boldsymbol{J}_*^{P,j}[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n+s)] = \boldsymbol{J}_*^{P,j}[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)] + \mathcal{O}(s)\,^{③}. \end{aligned} \tag{4.42}$$

We integrated the remaining integral terms exactly using the φ_j functions ([55], see also Definition A.22). If we aim to construct higher order uniformly accurate methods of order $p \in \mathbb{N}$, we recursively plug in Duhamel's formula (4.41) into itself as described in Example 4.3 above. In other words, we recursively substitute $w_*(t_n+s)$ and $\mathfrak{a}_*^\gamma(t_n+s)$ in the nonlinearity $F_*^m[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n+s)]$ (and similar in $G_*^m, \boldsymbol{J}_*^{P,j}$) with its corresponding Duhamel representation (4.41) and use the bound from Lemma 4.11

$$\left\| (\mathcal{T}^{-s}_{[\mathcal{L}_c]} - 1) w \right\|_r \leq \frac{1}{2} |s| \, \|w\|_{r+2} \, .$$

We repeatedly apply this procedure $p \in \mathbb{N}$ times, and at stage p "freeze" the nonlinearities $F_*^m, G_*^m, \boldsymbol{J}_*^{P,j}$ according to (4.42). Then, we exploit the $\mathcal{O}(s_\ell)$ approximation bound (4.42), where s_ℓ, $\ell = 1, \ldots, p$ is the integration variable at stage ℓ. The resulting scheme then shows local error bounds of order

$$\mathcal{O}\left(\int_0^\tau \int_0^{s_1} \int_0^{s_2} \cdots \int_0^{s_{p-1}} s_p ds_p \cdots ds_2 ds_1 \right) = \mathcal{O}\left(\tau^{p+1}\right).$$

We proceed in the Sections 4.2.2 and 4.2.3 with the space and the full discretization of our time integration scheme Ψ_*^τ given in (4.39).

4.2.2 Space Discretization

For the space discretization, we choose a Fourier pseudo-spectral collocation method ([44, 66]) as presented in Section 3.5.3. Only the terms involving derivatives are computed in Fourier space. We evaluate all nonlinear terms in physical space.

③Note Remark 4.4 and Assumption 4.5 on some peculiarities in case of MD

4.2.3 Fully-Discrete Scheme

In the notation of Section 3.5.4 we denote the fully-discretized numerical approximation with the superscript ^{n,M}, i.e. $w_*^{n,M} \approx \big(w_*(t_n, x_j)\big)_{j\in\mathcal{Z}_M^d}$ where $\mathcal{Z}_M$ is defined in Section 3.5.3. We thus define the fully discrete method by

$$\begin{cases} \begin{pmatrix} w_*^{n+1,M} \\ \mathfrak{a}_*^{\gamma,n+1,M} \end{pmatrix} &= \Psi_*^{\tau,M}[w_*^{n,M}, \mathfrak{a}_*^{\gamma,n,M}] = \begin{pmatrix} \Phi_{w_*}^{\tau,M}\left[w_*^{n,M}, \mathfrak{a}_*^{\gamma,n,M}\right] \\ \Phi_{\mathfrak{a}_*}^{\tau,M}\left[w_*^{n+1,M}, \mathfrak{a}_*^{\gamma,n,M}\right] \end{pmatrix}, \\ \phi_*^{\mathrm{tot},n+1,M} &= \phi_*^{0,n+1,M} + e^{2ic^2 t_{n+1}} \phi_*^{2,n+1,M} + e^{-2ic^2 t_{n+1}} \overline{\phi_*^{2,n+1,M}} \end{cases} \tag{4.43a}$$

where $\Psi_*^{\tau,M}$ and $\Phi_{w_*}^{\tau,M}, \Phi_{\mathfrak{a}_*}^{\tau,M}$ are the numerical flows defined in (4.39), combined with the Fourier pseudo-spectral space discretization techniques for the spatial differential operators described in Sections 3.5.3 and 4.2.2 above (see also ([44, 66]). We finally obtain a numerical approximation to the exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MKG/MD system (2.20)/(2.36) at time t_n via

$$\begin{aligned} \psi_*^{n,M} &= \frac{1}{2}\left(e^{ic^2 t_n} u_*^{n,M} + e^{-ic^2 t_n} \overline{v_*^{n,M}}\right), \\ \boldsymbol{\mathcal{A}}_*^{n,M} &= \frac{1}{2}\left(\mathfrak{a}_*^{\gamma,n,M} + \overline{\mathfrak{a}_*^{\gamma,n,M}}\right), \end{aligned} \tag{4.43b}$$

respecting the relations from (4.3c),(4.5), (4.6) and (4.10)

$$\begin{aligned} w(t_n) &= (u(t_n), v(t_n))^\top = e^{ic^2 t_n}(u_*(t_n), v_*(t_n))^\top, \\ \psi(t_n) &= \frac{1}{2}(u(t_n) + \overline{v}(t_n)) = \psi_*(t_n) = \frac{1}{2}(e^{ic^2 t_n} u_*(t_n) + e^{-ic^2 t_n}\overline{v_*}(t_n)), \\ \boldsymbol{\mathcal{A}}(t_n) &= \boldsymbol{\mathcal{A}}_*(t_n) = \frac{1}{2}(\mathfrak{a}_*^\gamma(t_n) + \overline{\mathfrak{a}_*^\gamma}(t_n)). \end{aligned} \tag{4.44}$$

Furthermore, for $j = 0, 2$ the fully discrete potentials $\phi_*^{j,n+1,M}$ are solutions to the discrete Poisson equations (cf. (4.40) and the end of Section 3.5.3)

for the case of MKG according to (4.17)

$$\begin{aligned} -\Delta_M \phi_*^{0,n,M} &= -\frac{1}{4c}\operatorname{Re}\left(u_*^{n,M}\langle\nabla\rangle_c \overline{u_*^{n,M}} - \overline{v_*^{n,M}}\langle\nabla\rangle_c v_*^{n,M}\right), \\ -\Delta_M \phi_*^{2,n,M} &= -\frac{1}{8c}\left(-u_*^{n,M}\langle\nabla\rangle_c v_*^{n,M} + v_*^{n,M}\langle\nabla\rangle_c u_*^{n,M}\right), \end{aligned}$$

and for the case of MD according to (4.18)

$$\begin{aligned} -\Delta_M \phi_*^{0,n,M} &= \frac{1}{4}\left(\left|u_*^{n,M}\right|^2 + \left|v_*^{n,M}\right|^2\right), \\ -\Delta_M \phi_*^{2,n,M} &= \frac{1}{4} u_*^{n,M} \cdot v_*^{n,M}. \end{aligned}$$

The discrete solution operator $\dot{\Delta}_M^{-1}$ for discrete Poisson equations of type

$$-\Delta_M \tilde{\phi}^M = \tilde{\rho}^M \quad \text{such that} \quad \tilde{\phi}^M = -\dot{\Delta}_M^{-1}\tilde{\rho}^M$$

is given in (3.130), respecting the restriction of $\mathbb{Z}^d$ to the bounded index set $\mathcal{Z}_M^d$ (see Section 3.5.3).

In the subsequent section, we analyse the numerical error of the scheme (4.43).

4.3 Error Analysis of the "Twisted Scheme"

In this section, we prove first order in time error bounds for our fully discrete time integration scheme $\Psi_*^{\tau,M}$ given in (4.43) which are independent of the large parameter c. Note that for Maxwell–Klein–Gordon and Maxwell–Dirac systems there exists (as far as we know) no literature which proposed and analysed a scheme of type (4.43) before. Though, as our scheme is based on the ideas from [18] for the case of the nonlinear Klein–Gordon equation, we may exploit these ideas and the results therein within this section. Furthermore, the book [44] provides important techniques for the analysis of numerical schemes for time-dependent Schrödinger-type systems.

Before we start with the error analysis of the "twisted scheme" (4.39), we make assumptions on the regularity of w_* and $\mathfrak{a}_*^\gamma$ in Assumption 4.6. Note that these assumptions hold true due to Proposition 4.2.

Assumption 4.6 (Regularity of the twisted solution). *Let $r > d/2$ and $r' \geq 0$. We assume that the twisted system (4.15) with solution*

$$(w_*, \phi_*^{tot}, \mathfrak{a}_*^\gamma)^\top$$

are locally well-posed in

$$\begin{cases} H^{r+r'} \times \dot{H}^{r+1+r'} \times \dot{H}^{r+r'} & \text{in case of MKG,} \\ H^{r+r'} \times \dot{H}^{r+2+r'} \times \dot{H}^{r+r'} & \text{in case of MD,} \end{cases}$$

i.e. for initial data $w_*(0) \in H^{r+r'}$, $\mathfrak{a}_*^\gamma(0) \in \dot{H}^{r+r'}$ there exist constants $T_{r+r'} > 0$ and $\mathcal{M}_*^{r+r'} > 0$ such that for all $0 \leq t \leq T_{r+r'}$

$$\begin{cases} \|w_*(t)\|_{r+r'} + \|\phi_*^{tot}(t)\|_{r+r'+1,0} + \|\mathfrak{a}_*^\gamma(t)\|_{r+r',0} \leq \mathcal{M}_*^{r+r'}. & \text{in case of MKG,} \\ \|w_*(t)\|_{r+r'} + \|\phi_*^{tot}(t)\|_{r+r'+2,0} + \|\mathfrak{a}_*^\gamma(t)\|_{r+r',0} \leq \mathcal{M}_*^{r+r'} & \text{in case of MD.} \end{cases}$$

In particular, for all $0 \leq t \leq T_{r+r'}$ we can establish the separate bounds

$$\|w_*(t)\|_{r+r'} \leq \mathcal{M}_{w_*}^{r+r'}, \qquad \|\mathfrak{a}_*^\gamma(t)\|_{r+r',0} \leq \mathcal{M}_{\mathfrak{a}_*}^{r+r'},$$

with constants $\mathcal{M}_{w_*}^{r+r'}, \mathcal{M}_{\mathfrak{a}_*}^{r+r'} > 0$ independent of $c \geq 1$.

Exploiting these assumptions and using the notation $\mathcal{M}_{w_*}^{r+r'}, \mathcal{M}_{\mathfrak{a}_*}^{r+r'}$ for the bounds of the exact twisted solution $(w_*(t), \mathfrak{a}_*^\gamma(t))^\top$ in $H^{r+r'} \times \dot{H}^{r+r'}$ with $r > d/2$ and $r' \geq 0$, we formulate the following theorems on the uniform in c convergence of the fully discrete scheme $\Psi_*^{\tau,M}$ given in (4.43). First we state a theorem for the case of MKG and afterwards we formulate the result corresponding to the case of MD. For the case of MD we respect the particular Assumption 4.5 on the initial data of the MD system, i.e. we assume that in case of MD

$$\psi_I = (\psi_I^+, \psi_I^-)^\top \quad \text{satisfies} \quad \left(\psi_I^- \overline{\boldsymbol{\sigma}} \overline{\psi_I^+}\right) = \mathcal{O}\left(c^{-1}\right).$$

Recall that we set up this Assumption 4.5 as a consequence of the challenges in the analysis below, which we discussed before in Remark 4.1. Let us provide the theorem for the MKG case.

Theorem 4.7 (Convergence of the "twisted scheme" for MKG). *Fix $r_1, r_2, r > d/2$ and $\epsilon > 0$ arbitrarily small. Furthermore, let $r_j' = \max\{2, r_j + d/2 + \epsilon\}$ for $j = 1, 2$. Let the initial data of the MKG system*

(2.20) *satisfy* $\psi_I, \psi_I' \in H^{r+r_1'}$ *and* $A_I, A_I' \in \dot{H}^{r+r_2'}$ *and let* $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ *be the solution to the MKG system* (2.20).

Then there exist constants $T, K_*^{\text{MKG}}, M_0, \tau_0 > 0$ *such that the following holds: Let us define the numerical approximations to* $\psi(t_n)$ *and to* $\boldsymbol{\mathcal{A}}(t_n)$ *at time* $t_n = n\tau \in [0, T]$ *through*

$$\psi_*^{n,M} := \frac{1}{2}\left(e^{ic^2 t_n} u_*^{n,M} + e^{-ic^2 t_n} \overline{v_*^{n,M}}\right), \quad \boldsymbol{\mathcal{A}}_*^{n,M} := \frac{1}{2}\left(\mathfrak{a}_*^{\gamma,n,M} + \overline{\mathfrak{a}_*^{\gamma,n,M}}\right),$$
$$\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_*^{n,M} := \frac{1}{2} i \langle \nabla \rangle_{\gamma/c,M}\left(\mathfrak{a}_*^{\gamma,n,M} - \overline{\mathfrak{a}_*^{\gamma,n,M}}\right),$$

where $w_*^{n,M} := (u_*^{n,M} + \overline{v_*^{n,M}})^\top$ *and* $\mathfrak{a}_*^{\gamma,n,M}$ *denote the numerical approximations to* $w_*(t_n)$ *and* $\mathfrak{a}_*^\gamma(t_n)$ *obtained with the fully discrete uniformly first order in time scheme* $\Psi_*^{\tau,M}$ *(i.e. the time integration method defined by* (4.43) *combined with a Fourier pseudo-spectral space discretization as in Section 3.5.3) with time step* $\tau \le \tau_0$ *and* $M \ge M_0$ *grid points in space, i.e.*

$$(w_*^{n,M}, \mathfrak{a}_*^{\gamma,n,M})^\top := \Psi_*^{\tau,M}[w_*^{n-1,M}, \mathfrak{a}_*^{\gamma,n-1,M}].$$

Furthermore let us denote the numerical approximation to $\phi(t_n) = \phi_*^{\text{tot}}(t_n)$ *by*

$$\phi_*^{\text{tot},n,M} = \phi_*^{0,n,M} + e^{2ic^2 t_n}\phi_*^{2,n,M} + e^{-2ic^2 t_n}\overline{\phi_*^{2,n,M}},$$

with $\phi_*^{j,n,M}$ *for* $j = 0, 2$ *satisfying the discrete Poisson equations similar as in Theorems 3.3 and 3.4 (see* (4.17) *for the definition of* ϕ_*^j*)*

$$-\Delta_M \phi_*^{0,n,M} = -\frac{1}{4c}\operatorname{Re}\left(u_*^{n,M}\langle\nabla\rangle_{c,M}\overline{u_*^{n,M}} - \overline{v_*^{n,M}}\langle\nabla\rangle_{c,M} v_*^{n,M}\right)$$
$$-\Delta_M \phi_*^{2,n,M} = -\frac{1}{8c}\left(-u_*^{n,M}\langle\nabla\rangle_{c,M} v_*^{n,M} + v_*^{n,M}\langle\nabla\rangle_{c,M} u_*^{n,M}\right).$$

Then, we find the following first order error bound in time

$$\left\|\psi_*^{n,M} - \psi(t_n)\right\|_r + \left\|\phi_*^{\text{tot},n,M} - \phi(t_n)\right\|_{r+1,0}$$
$$+ \left\|\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_*^{n,M} - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n)\right\|_{r-1,0} + \left\|\boldsymbol{\mathcal{A}}_*^{n,M} - \boldsymbol{\mathcal{A}}(t_n)\right\|_{r,0} \le K_*^{\text{MKG}}\left(\tau + M^{-r_3}\right),$$

which holds uniformly for all $c \ge 1$. *Thereby, we choose* $r_3 := \min\{r_1, r_2\}$. *The constant* K_*^{MKG} *only depends on* $\mathcal{M}_{w_*}^{r+r_1'}, \mathcal{M}_{\mathfrak{a}_*}^{r+r_2'}, T$ *but not on* c.

Next we formulate the Theorem 4.8 on the uniform in c first order in time numerical convergence bound of the fully discrete method (4.43) in case of MD, respecting the Assumption 4.5 on the initial data.

Theorem 4.8 (Convergence of the "twisted scheme" for MD)**.** *Fix* $r_1, r_2, r > d/2$ *and* $\epsilon > 0$ *arbitrarily small. Furthermore, let* $r_j' = \max\{2, r_j + d/2 + \epsilon\}$ *for* $j = 1, 2$. *Let the initial data to the MD system* (2.20) *satisfy* $\psi_I \in H^{r+r_1'}$, *Assumption 4.5 on the particular choice of the initial data, i.e.*

$$\psi_I = (\psi_I^+, \psi_I^-)^\top \quad \text{satisfies} \quad \left\|\psi_I^- \overline{\boldsymbol{\sigma}}\,\overline{\psi_I^+}\right\|_r \le Kc^{-1}$$

with a constant K *independent of* c, *and let* $A_I, A_I' \in \dot{H}^{r+r_2'}$. *Moreover, let* $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ *be the solution to the MD system* (2.36).

Then there exist constants $T, K_*^{\text{MD}}, M_0, \tau_0 > 0$ such that the following holds: Let us define the numerical approximations to $\psi(t_n)$ and to $\boldsymbol{\mathcal{A}}(t_n)$ at time $t_n = n\tau \in [0, T]$ through

$$\psi_*^{n,M} := \frac{1}{2}\left(e^{ic^2t_n}u_*^{n,M} + e^{-ic^2t_n}\overline{v_*^{n,M}}\right), \quad \boldsymbol{\mathcal{A}}_*^{n,M} := \frac{1}{2}\left(\mathfrak{a}_*^{\gamma,n,M} + \overline{\mathfrak{a}_*^{\gamma,n,M}}\right),$$
$$\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_*^{n,M} := \frac{1}{2}i\langle\nabla\rangle_{\gamma/c,M}\left(\mathfrak{a}_*^{\gamma,n,M} - \overline{\mathfrak{a}_*^{\gamma,n,M}}\right)$$

where $w_*^{n,M} := (u_*^{n,M} + \overline{v_*^{n,M}})^\top$ and $\mathfrak{a}_*^{\gamma,n,M}$ denote the numerical approximations to $w_*(t_n)$ and $\mathfrak{a}_*^\gamma(t_n)$ obtained with the fully discrete uniformly first order in time scheme $\Psi_*^{\tau,M}$ with time step $\tau \leq \tau_0$ and $M \geq M_0$ grid points in space, i.e.

$$(w_*^{n,M}, \mathfrak{a}_*^{\gamma,n,M})^\top := \Psi_*^{\tau,M}[w_*^{n-1,M}, \mathfrak{a}_*^{\gamma,n-1,M}].$$

Furthermore, let us denote the numerical approximation to $\phi(t_n)$ by

$$\phi_*^{\text{tot},n,M} = \phi_*^{0,n,M} + e^{2ic^2t_n}\phi_*^{2,n,M} + e^{-2ic^2t_n}\overline{\phi_*^{2,n,M}}$$

with $\phi_*^{j,n,M}$ for $j = 0, 2$ satisfying the discrete Poisson equations similar as in Theorems 3.3 and 3.4 (see (4.17) for the definition of ϕ_*^j), i.e.

$$-\Delta_M\phi_*^{0,n,M} = \frac{1}{4}\left(\left|u_*^{n,M}\right|^2 + \left|v_*^{n,M}\right|^2\right)$$
$$-\Delta_M\phi_*^{2,n,M} = \frac{1}{4}u_*^{n,M}\cdot v_*^{n,M}.$$

Then we find the following uniform first order error bound in time

$$\left\|\psi_*^{n,M} - \psi(t_n)\right\|_r + \left\|\phi_*^{\text{tot},n,M} - \phi(t_n)\right\|_{r+2,0}$$
$$+ \left\|\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_*^{n,M} - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n)\right\|_{r-1,0} + \left\|\boldsymbol{\mathcal{A}}_*^{n,M} - \boldsymbol{\mathcal{A}}(t_n)\right\|_{r,0} \leq K_*^{\text{MD}}\left(\tau + M^{-r_3}\right),$$

which holds uniformly for all $c \geq 1$. Thereby, we choose $r_3 := \min\{r_1, r_2\}$. The constant K_*^{MD} only depends on $\mathcal{M}_{w_*}^{r+2}, \mathcal{M}_{\mathfrak{a}_*}^{r+2}, T$ but not on c.

Before we prove these theorems, let us give a short remark on future research in the case where the initial data of the MD system (2.36) violate Assumption 4.5.

Remark 4.9. *For general initial data in case of MD, which do not satisfy Assumption 4.5, our numerical experiments also show a numerical first order convergence. Therefore, our local error and stability analysis within this thesis may not be sharp enough to prove the general uniform first order convergence. In future research, we may apply different techniques (summation by parts, energy techniques) for proving the uniform first order convergence of our method applied to the MD system (2.36) with initial data violating Assumption 4.5.*

Actually, using the techniques from this thesis it is possible to prove first order convergence in case of MD with ***general initial*** *data by setting up a CFL (**C**ourant-**F**riedrichs-**L**ewy) condition on the time step τ which allows time steps $\tau = \mathcal{O}\left(c^{-1}\right)$ in order to ensure stability (see Section 4.3.2).*

We prove these theorems similarly to the proof of Theorems 3.3 and 3.4. Recall from (4.43b) and (4.44) together with (4.10), that in the notation $\psi(t_n) = \psi_*(t_n)$ and $\boldsymbol{\mathcal{A}}(t_n) = \boldsymbol{\mathcal{A}}_*(t_n)$ we have

$$\begin{aligned}
\psi_*(t_n) =& \frac{1}{2}(e^{ic^2t_n}u_*(t_n) + e^{-ic^2t_n}\overline{v_*}(t_n)),\\
\boldsymbol{\mathcal{A}}_*(t_n) =& \frac{1}{2}\Big(\mathfrak{a}_*^\gamma(t_n) + \overline{\mathfrak{a}_*^\gamma}(t_n)\Big),\\
\partial_t\boldsymbol{\mathcal{A}}_*(t_n) =& i\frac{1}{2}c\left\langle\nabla\right\rangle_{\gamma/c}\Big(\mathfrak{a}_*^\gamma(t_n) - \overline{\mathfrak{a}_*^\gamma}(t_n)\Big)
\end{aligned}$$

and

$$\begin{aligned}
\psi_*^{n,M} =& \frac{1}{2}\left(e^{ic^2t_n}u_*^{n,M} + e^{-ic^2t_n}\overline{v_*^{n,M}}\right),\\
\boldsymbol{\mathcal{A}}_*^{n,M} =& \frac{1}{2}\left(\mathfrak{a}_*^{\gamma,n,M} + \overline{\mathfrak{a}_*^{\gamma,n,M}}\right),\\
\partial_t\boldsymbol{\mathcal{A}}_*^{n,M} =& i\frac{1}{2}c\left\langle\nabla\right\rangle_{\gamma/c}\left(\mathfrak{a}_*^{\gamma,n,M} - \overline{\mathfrak{a}_*^{\gamma,n,M}}\right).
\end{aligned}$$

Exploiting these identities, we can decompose the error of the full scheme into a space approximation error of our scheme of order $\mathcal{O}\left(M^{-\tilde{r}}\right)$, $\tilde{r}\in\{r_1,r_2\}$ (semi-discretization in space, see [44] and also Proposition 3.14 from Section 3.5.3) and a time integration error of our scheme of order $\mathcal{O}(\tau)$ (semi-discretization in time).Within this section, we shall focus on the time integration error. More precisely, similar to (3.134) we decompose the error for $R=1$ in case of MKG and $R=2$ in case of MD (see also Proposition 4.2) as

$$\begin{aligned}
&\left\|\psi_*^{n,M} - \psi(t_n)\right\|_r + \left\|\phi_*^{\mathrm{tot},n,M} - \phi(t_n)\right\|_{r+R,0}\\
&\leq K_{w_*}\Bigg(\underbrace{\left\|w_*^{n,M} - w_*^n\right\|_r}_{=\mathcal{O}(M^{-r_1})} + \underbrace{\left\|w_*^n - w_*(t_n)\right\|_r}_{=\mathcal{O}(\tau)}\Bigg)
\end{aligned}\tag{4.47a}$$

and

$$\begin{aligned}
&\left\|\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_*^{n,M} - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n)\right\|_{r-1} + \left\|\boldsymbol{\mathcal{A}}_*^{n,M} - \boldsymbol{\mathcal{A}}(t_n)\right\|_{r,0}\\
&\leq K_{\mathfrak{a}_*}\Bigg(\underbrace{\left\|\mathfrak{a}_*^{\gamma,n,M} - \mathfrak{a}_*^{\gamma,n}\right\|_{r,0}}_{=\mathcal{O}(M^{-r_2})} + \underbrace{\left\|\mathfrak{a}_*^{\gamma,n} - \mathfrak{a}_*^\gamma(t_n)\right\|_r}_{=\mathcal{O}(\tau)}\Bigg),
\end{aligned}\tag{4.47b}$$

where the constants $K_{w_*}, K_{\mathfrak{a}_*}$ only depend on the regularity of w_* and $\mathfrak{a}_*^\gamma$, but not on c nor on τ and M. Here we used in (4.47a) that as long as $w_*^{n,M}, w_*(t_n)\in H^r$, we can play back the error of $\phi_*^{\mathrm{tot},n,M}$ in H^{r+R} to the error of $w_*^{n,M}$ in H^r (cf. (4.19)), exploiting bounds on $\left\|uc^{-1}\left\langle\nabla\right\rangle_c v\right\|_r \leq K\left\|u\right\|_r\left\|v\right\|_r$ in case of MKG and bounds on $\left\|uv\right\|_{r-1}\leq K\left\|u\right\|_r\left\|v\right\|_r$ in case of MD for $u,v\in H^r$ from Lemmas A.8 and A.11, i.e.

$$\left\|\phi_*^{\mathrm{tot},n,M} - \phi(t_n)\right\|_{r+R,0}\leq K\left\|w_*^{n,M} - w_*(t_n)\right\|_r,$$

where the constant K is independent of c and only depends on $\left\|w_*^{n,M}\right\|_r$ and $\left\|w_*(t_n)\right\|_r$. We immediatlely obtain the respective $\mathcal{O}\left(M^{-\tilde{r}}\right)$ bounds for $\tilde{r}\in\{r_1,r_2\}$ from the space discretization error bounds in Section 3.5.3. In the following, we focus on proving the uniform $\mathcal{O}(\tau)$ time integration error bound.

The time integration error at time t_{n+1} obeys the decomposition

$$\begin{aligned}
&\left\|\begin{pmatrix} w_*(t_{n+1})\\ \mathfrak{a}_*^\gamma(t_{n+1})\end{pmatrix} - \Psi_*^\tau[w_*^n,\mathfrak{a}_*^{\gamma,n}]\right\|_r\\
&\leq \underbrace{\left\|\begin{pmatrix} w_*(t_{n+1})\\ \mathfrak{a}_*^\gamma(t_{n+1})\end{pmatrix} - \Psi_*^\tau[w_*(t_n),\mathfrak{a}_*^\gamma(t_n)]\right\|_r}_{=:d_*^{n+1},\quad\text{local error}} + \underbrace{\left\|\Psi_*^\tau[w_*(t_n),\mathfrak{a}_*^\gamma(t_n)] - \Psi_*^\tau[w_*^n,\mathfrak{a}_*^{\gamma,n}]\right\|_r}_{=:\mathcal{S}_*^n,\quad\text{stability}}.
\end{aligned}\tag{4.48}$$

Based on [44, Definition II.7], the first term in the latter inequality can be associated with the local error of Ψ_*^τ (see Definition A.17) whereas the second term is linked to the stability of the method (see Definition A.18). By "local error" we denote the error of the method after performing one step with step size τ starting from exact initial data. According to [44, Definition II.7] (see also Definition A.17), the method Ψ_*^τ is (consistent) of order $p = 1$, if the (local error) $\leq K\tau^2$ for a constant K independent of τ.

By "stability" we mean that the method Ψ_*^τ is stable under perturbations of the initial data. According to [44, Definition II.7] (see also Definition A.18), the method Ψ_*^τ is stable, if for data w_1, w_2, a_1, a_2 we find a constant $L > 0$ such that

$$\|\Psi_*^\tau[w_1, a_1] - \Psi_*^\tau[w_2, a_2]\|_r \leq e^{L\tau}\big(\|w_1 - w_2\|_r + \|a_1 - a_2\|_{r,0} \big),$$

where L is independent of c and only depends on $\|w_j\|_r$ and $\|a_j\|_{r,0}$ for $j = 1, 2$.

Recall that by (4.39) our method is defined through

$$\Psi_*^\tau[w_*^n, \mathfrak{a}_*^{\gamma,n}] = \begin{pmatrix} \Phi_{w_*}^\tau\left[w_*^n, \mathfrak{a}_*^{\gamma,n}\right] \\ \Phi_{\mathfrak{a}_*}^\tau\left[w_*^{n+1}, \mathfrak{a}_*^{\gamma,n}\right] \end{pmatrix}.$$

Exploiting the definition of $\left\|(u,v)^\top\right\|_r = \|u\|_r + \|v\|_r$ for $u, v \in H^r$ (see Definition A.1) and plugging Ψ_*^τ into (4.48), the local error term reads

$$\begin{aligned} d_*^{n+1} =& \left\|w_*(t_{n+1}) - \Phi_{w_*}^\tau\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right]\right\|_r \\ &+ \left\|\mathfrak{a}_*^\gamma(t_{n+1}) - \Phi_{\mathfrak{a}_*}^\tau\left[\Phi_{w_*}^\tau[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)]), \mathfrak{a}_*^\gamma(t_n)\right]\right\|_{r,0}, \end{aligned}$$

and similarly the stability term is given by

$$\begin{aligned} \mathcal{S}_*^n =& \left\|\Phi_{w_*}^\tau\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right] - \Phi_{w_*}^\tau\left[w_*^n, \mathfrak{a}_*^{\gamma,n}\right]\right\|_r \\ &+ \left\|\Phi_{\mathfrak{a}_*^\gamma}^\tau\left[\Phi_{w_*}^\tau\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right], \mathfrak{a}_*^\gamma(t_n)\right] - \Phi_{\mathfrak{a}_*}^\tau\left[\Phi_{w_*}^\tau\left[w_*^n, \mathfrak{a}_*^{\gamma,n}\right], \mathfrak{a}_*^{\gamma,n}\right]\right\|_{r,0}. \end{aligned} \tag{4.49}$$

Recall that our aim is to prove a global first order bound in time uniformly in c for the global error term (4.48), i.e.

$$[\text{term } (4.48)] \leq K\tau$$

with a constant K independent of c. In order to achieve this goal, we firstly show a local error bound of order $p = 1$ in Section 4.3.1 for the term d_*^{n+1}

$$d_*^{n+1} \leq K_{\text{loc}}\tau^2 \quad \text{for all } n \geq 0 \text{ with } K_{\text{loc}} > 0 \text{ independent of } c, n \text{ and } \tau. \tag{4.50}$$

Secondly in Section 4.3.2 we establish a stability bound on the term $\mathcal{S}_*^n$. Exploiting (4.48), we obtain

$$\begin{aligned} \mathcal{S}_*^n \leq& e^{\tau L_{\text{stab}}}\left\|\begin{pmatrix} w_*(t_n) \\ \mathfrak{a}_*^\gamma(t_n) \end{pmatrix} - \Psi_*^\tau[w_*^{n-1}, \mathfrak{a}_*^{\gamma,n-1}]\right\|_r \quad \text{for all } n \geq 1 \\ \leq& e^{L_{\tau\text{stab}}}\left(d_*^n + \mathcal{S}_*^{n-1}\right) \end{aligned} \tag{4.51}$$

with $L_{\text{stab}} > 0$ independent of c, n and τ. In particular L_{stab} depends on $\|w_*(t_n)\|_r$, $\|\mathfrak{a}_*^\gamma(t_n)\|_{r,0}$, $\|w_*^n\|_r$ and on $\|\mathfrak{a}_*^{\gamma,n}\|_{r,0}$. Note that $\mathcal{S}_*^0 = 0$, if we start our method from exact initial data, i.e. $w_*^0 = w_*(0)$ and $\mathfrak{a}_*^{\gamma,0} = \mathfrak{a}_*^\gamma(0)$.

In Section 4.3.3, we combine the uniform local error bound (4.50) on d_*^{n+1} with the uniform stability bound (4.51) on $\mathcal{S}_*^n$ in order to obtain a global first order error bound uniformly in c of our method. More precisely, we resolve the recursion from (4.48), i.e.

$$\begin{aligned}
&\left\| \begin{pmatrix} w_*(t_{n+1}) \\ \mathfrak{a}_*^\gamma(t_{n+1}) \end{pmatrix} - \Psi_*^\tau[w_*^n, \mathfrak{a}_*^{\gamma,n}] \right\|_r \\
\leq & d_*^{n+1} + \mathcal{S}_*^n \leq d_*^{n+1} + e^{L_{\text{stab}}\tau}\left(d_*^n + \mathcal{S}_*^{n-1}\right) \\
\leq & K \cdot K_{\text{loc}}\tau^2 \sum_{j=0}^{n} e^{j\tau L_{\text{stab}}} \leq \tau K \cdot K_{\text{loc}}\big((n+1)\tau\big)e^{(n\tau)L_{\text{stab}}} \\
\leq & \tau K \cdot T K_{\text{loc}} e^{T L_{\text{stab}}},
\end{aligned}$$

which holds uniformly in c for all $t_{n+1} \in [0, T]$. The constants $K, K_{\text{loc}}, L_{\text{stab}} > 0$ can be chosen independent of c.

We proceed with establishing the local error bound (4.50) in the subsequent Section 4.3.1.

4.3.1 Local Time Integration Error of the "Twisted Scheme"

Our aim is now to show that the local error of Ψ_*^τ is of order $p = 1$ uniformly in c, i.e. we show that

$$\left\| w_*(t_{n+1}) - \Phi_{w_*}^\tau\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right] \right\|_r \tag{4.52a}$$

$$+ \left\| \mathfrak{a}_*^\gamma(t_{n+1}) - \Phi_{\mathfrak{a}_*}^\tau\left[\Phi_{w_*}^\tau[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)]), \mathfrak{a}_*^\gamma(t_n)\right] \right\|_{r,0} \leq K\tau^2 \tag{4.52b}$$

with a constant K independent of c. In this section, we only sketch the proof of the local error bound but omit lengthy details here. The interested reader may refer to Section 4.3.4 for more details.

Recall Duhamel's formula (4.26) for the exact solution of (4.15)

$$\begin{aligned}
w_*(t_n + \tau) =& \mathcal{T}_{[\mathcal{L}_c]}^\tau w_*(t_n) - i \int_0^\tau \mathcal{T}_{[\mathcal{L}_c]}^{\tau-s} \sum_{m \in I_m} e^{mic^2(t_n+s)} \left(F_*^m(t_n+s) + G_*^m(t_n+s)\right) ds, \\
\mathfrak{a}_*^\gamma(t_n + \tau) =& \mathcal{T}_{[c\langle\nabla\rangle_{\gamma/c}]}^\tau \mathfrak{a}_*^\gamma(t_n) \\
& - i \langle\nabla\rangle_{\gamma/c}^{-1} \int_0^\tau \mathcal{T}_{[c\langle\nabla\rangle_{\gamma/c}]}^{\tau-s} \Bigg(\frac{\gamma^2}{2c}\left(\mathfrak{a}_*^\gamma(t_n+s) + \overline{\mathfrak{a}_*^\gamma}(t_n+s)\right) \\
& \qquad + \boldsymbol{J}_*^{P,0}(t_n+s) \\
& \qquad + e^{+2ic^2(t_n+s)}\boldsymbol{J}_*^{P,2}(t_n+s) \\
& \qquad + e^{-2ic^2(t_n+s)}\overline{\boldsymbol{J}_*^{P,2}}(t_n+s)\Bigg) ds,
\end{aligned} \tag{4.53}$$

where $I_m = \{-4, -2, 0, 2\}$ and where we define the nonlinearities

$$F_*^m, G_*^m, m \in I_m \quad \text{and} \quad \boldsymbol{J}_*^{P,j}, j = 0, 2 \qquad \text{explicitly in (4.14) and (4.17)/(4.18).}$$

Furthermore our method Ψ_*^τ is defined in (4.39) as

$$\begin{cases}
\begin{pmatrix} w_*^{n+1} \\ \mathfrak{a}_*^{\gamma,n+1} \end{pmatrix} = \Psi_*^\tau[w_*^n, \mathfrak{a}_*^{\gamma,n}] := \Psi_{\mathfrak{a}_*}^\tau \circ \Psi_{w_*}^\tau[w_*^n, \mathfrak{a}_*^{\gamma,n}] = \begin{pmatrix} \Phi_{w_*}^\tau\left[w_*^n, \mathfrak{a}_*^{\gamma,n}\right] \\ \Phi_{\mathfrak{a}_*}^\tau\left[w_*^{n+1}, \mathfrak{a}_*^{\gamma,n}\right] \end{pmatrix}, \\
\phi_*^{\text{tot},n+1} = \phi_*^{0,n+1} + e^{2ic^2 t_{n+1}}\phi_*^{2,n+1} + e^{-2ic^2 t_{n+1}}\overline{\phi_*^{2,n+1}},
\end{cases} \tag{4.54a}$$

where $\Phi^\tau_{w_*}$ and $\Phi^\tau_{\mathfrak{a}_*}$ are given in (4.30) and (4.38), respectively, as

$$\Phi^\tau_{w_*}\left[w^n_*, \mathfrak{a}^{\gamma,n}_*\right] = \mathcal{T}^\tau_{[\mathcal{L}_c]}\Big(w^n_* - i\sum_{m\in I_m}\tau\varphi_1(mic^2\tau)e^{mic^2t_n}\big(F^m_*[w^n_*,\mathfrak{a}^{\gamma,n}_*] + G^m_*[w^n_*,\mathfrak{a}^{\gamma,n}_*]\big)\Big),$$

$$\begin{aligned}&\Phi^\tau_{\mathfrak{a}_*}\left[w^{n+1}_*, \mathfrak{a}^{\gamma,n}_*\right]\\ &= \mathcal{T}^\tau_{[c\langle\nabla\rangle_{\gamma/c}]}\Big(\mathfrak{a}^{\gamma,n}_* - i\tau\langle\nabla\rangle^{-1}_{\gamma/c}\Big\{\ \varphi_1\big(i\tau\quad(-c\langle\nabla\rangle_{\gamma/c})\big)\Big(\frac{\gamma^2}{2c}(\mathfrak{a}^{\gamma,n}_* + \overline{\mathfrak{a}^{\gamma}_*}(t_n))\\ &\qquad + \boldsymbol{J}^{P,0}_*[w^{n+1}_*,\mathfrak{a}^{\gamma,n}_*]\Big)\\ &\qquad + \varphi_1\big(i\tau(+2c^2 - c\langle\nabla\rangle_{\gamma/c})\big)e^{+2ic^2t_n}\boldsymbol{J}^{P,2}_*[w^{n+1}_*,\mathfrak{a}^{\gamma,n}_*]\\ &\qquad + \varphi_1\big(i\tau(-2c^2 - c\langle\nabla\rangle_{\gamma/c})\big)e^{-2ic^2t_n}\overline{\boldsymbol{J}^{P,2}_*}[w^{n+1}_*,\mathfrak{a}^{\gamma,n}_*]\Big\}\Big).\end{aligned} \tag{4.54b}$$

We start off by establishing a bound for the local error term (4.52a).

Estimate on the Local Error Term (4.52a)

Beginning with an estimate for the first term (4.52a), we apply the bound

$$\left\|\left(e^{-is\mathcal{L}_c} - 1\right)w\right\|_r \le \frac{1}{2}|s|\,\|w\|_{r+2} \qquad \text{(see [18, Lemma 4] and also Lemma 4.11)}$$

to the difference terms

$$\begin{aligned}&\mathcal{T}^{-s}_{[\mathcal{L}_c]}F^m_*[w_*(t_n+s),\mathfrak{a}^\gamma_*(t_n+s)] - F^m_*[w_*(t_n),\mathfrak{a}^\gamma_*(t_n)]\\ =&\mathcal{T}^{-s}_{[\mathcal{L}_c]}\Big(F^m_*[w_*(t_n+s),\mathfrak{a}^\gamma_*(t_n+s)] - F^m_*[w_*(t_n),\mathfrak{a}^\gamma_*(t_n)]\Big)\\ &+\big(\mathcal{T}^{-s}_{[\mathcal{L}_c]} - 1\big)F^m_*[w_*(t_n),\mathfrak{a}^\gamma_*(t_n)],\end{aligned}$$

and similarly for G^m_* arising from Duhamel's formula (4.53) and from the definition of $\Phi^\tau_{w_*}$ in (4.54). In the notation

$$F^m_*(t_n+s) = F^m_*[w_*(t_n+s),\mathfrak{a}^\gamma_*(t_n+s)] \quad\text{and}\quad F^m_*(t_n+s) = F^m_*[w_*(t_n),\mathfrak{a}^\gamma_*(t_n)]$$

and similarly for G^m_*, this immediately provides the bound

$$\begin{aligned}&\left\|w_*(t_n+\tau) - \Phi^\tau_{w_*}\left[w_*(t_n),\mathfrak{a}^\gamma_*(t_n)\right]\right\|_r\\ \le&4\max_{m\in I_m}\Big(\frac{1}{2}\tau^2\|F^m_*(t_n)\|_{r+2} + \int_0^\tau \|F^m_*(t_n+s) - F^m_*(t_n)\|_r\,ds\\ &+\frac{1}{2}\tau^2\|G^m_*(t_n)\|_{r+2} + \int_0^\tau \|G^m_*(t_n+s) - G^m_*(t_n)\|_r\,ds\Big),\end{aligned} \tag{4.55}$$

where $I_m = \{-4,-2,0,2\}$. Thanks to the bounds from (4.74) in Section 4.3.4

$$\|w_*(t_n+s) - w_*(t_n)\|_{r+r_1'} + c^{-1}\|\mathfrak{a}^\gamma_*(t_n+s) - \mathfrak{a}^\gamma_*(t_n)\|_{r+r_2',0} \le |s|\,K, \tag{4.56}$$

with $r > d/2$, $r_1', r_2' \ge 0$, we obtain the bounds on F^m_*, G^m_* according to (4.76)

$$\|F^m_*(t_n)\|_{r+2} \le K^1_{F^m_*} \quad\text{and}\quad \|F^m_*(t_n+s) - F^m_*(t_n)\|_r \le |s|\,K^2_{F^m_*}, \tag{4.57}$$

and similarly for G_*^m with constants $K^\ell_{F_*^m}$ and $K^\ell_{G_*^m}$, $\ell = 1, 2$ only depending on the spatial regularity of w_* and $\mathfrak{a}_*^\gamma$ but not on c nor on s. We plug the bounds (4.57) into (4.55) and simply integrate $\int_0^\tau sds = \tau^2/2$ in (4.55). This yields the desired local error bound on (4.55), i.e.

$$\left\| w_*(t_n+\tau) - \Phi^\tau_{w_*}\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right] \right\|_r \le \tau^2 K^{\mathrm{MKG/MD}}_{w_*,\mathrm{loc}} \tag{4.58}$$

with a constant $K^{\mathrm{MKG}}_{w_*,\mathrm{loc}}$ depending on $\mathcal{M}^{r+2}_{w_*}, \mathcal{M}^{r+1}_{\mathfrak{a}_*}$ in case of MKG, and a constant $K^{\mathrm{MD}}_{w_*,\mathrm{loc}}$ depending on $\mathcal{M}^{r+2}_{w_*}, \mathcal{M}^{r+2}_{\mathfrak{a}_*}$ in case of MD. These bounds are given later on in more detail in (4.74) and (4.76). In both cases the constants can be chosen independently of c.

In the subsequent paragraph we establish bounds on the second local error term (4.52b).

Estimate on the Local Error Term (4.52b)

In order to bound the second term in (4.52)

$$\left\| \mathfrak{a}_*^\gamma(t_n+\tau) - \Phi^\tau_{\mathfrak{a}_*}\left[\Phi^\tau_{w_*}\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right], \mathfrak{a}_*^\gamma(t_n)\right] \right\|_{r,0}$$

we first focus on the case of MKG.

The MKG case: Recall that $\boldsymbol{J}_*^{P,j}$ for $j = 0, 2$ is defined in the MKG case as (see (4.17))

$$\begin{aligned}
\boldsymbol{J}_*^{P,0}[w_*, \mathfrak{a}_*^\gamma] =& \mathcal{P}_{\mathrm{df}}\left[i\frac{1}{8}\left(u_*\nabla\overline{u_*} - \overline{u_*}\nabla u_* + \overline{v_*}\nabla v_* - v_*\nabla\overline{v_*}\right) - \frac{1}{8c}(\mathfrak{a}_*^\gamma + \overline{\mathfrak{a}_*^\gamma})(|u_*|^2 + |v_*|^2)\right],\\
\boldsymbol{J}_*^{P,2}[w_*, \mathfrak{a}_*^\gamma] =& \mathcal{P}_{\mathrm{df}}\left[i\frac{1}{8}\left(u_*\nabla v_* - v_*\nabla u_*\right) - \frac{1}{8c}(\mathfrak{a}_*^\gamma + \overline{\mathfrak{a}_*^\gamma})(u_* v_*)\right].
\end{aligned}$$

From the bilinear estimates in Lemma A.8 we deduce that for pairs (w_1, a_1) and (w_2, a_2) in $H^r \times \dot{H}^r$, we have

$$\left\| \langle\nabla\rangle^{-1}_{\gamma/c}\left(\boldsymbol{J}_*^{P,j}[w_1, a_1] - \boldsymbol{J}_*^{P,j}[w_2, a_2]\right) \right\|_{r,0} \le K(\|w_1 - w_2\|_r + c^{-1}\|a_1 - a_2\|_{r,0})$$

with a constant K depending only on $\|w_\ell\|_r, \|a_\ell\|_{r,0}, \ell = 1, 2$ but independent of c.

Now let

$$\tilde{w_*}^{n+1} := \Phi^\tau_{w_*}[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)].$$

In view of (4.56) and the local error bound (4.58) on $\Phi^\tau_{w_*}$, we thus obtain for $s \in [0, \tau]$ and $j = 0, 2$

$$\begin{aligned}
&\left\| \langle\nabla\rangle^{-1}_{\gamma/c}\left(\boldsymbol{J}_*^{P,j}[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n+s)] - \boldsymbol{J}_*^{P,j}[\tilde{w_*}^{n+1}, \mathfrak{a}_*^\gamma(t_n)]\right) \right\|_{r,0}\\
\le& \left\| \langle\nabla\rangle^{-1}_{\gamma/c}\left(\boldsymbol{J}_*^{P,j}[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n+s)] - \boldsymbol{J}_*^{P,j}[w_*(t_n+\tau), \mathfrak{a}_*^\gamma(t_n)]\right) \right\|_{r,0}\\
&+ \left\| \langle\nabla\rangle^{-1}_{\gamma/c}\left(\boldsymbol{J}_*^{P,j}[w_*(t_n+\tau), \mathfrak{a}_*^\gamma(t_n)] - \boldsymbol{J}_*^{P,j}[\tilde{w_*}^{n+1}, \mathfrak{a}_*^\gamma(t_n)]\right) \right\|_{r,0}\\
\le& K_1 \cdot (\|w_*(t_n+s) - w_*(t_n+\tau)\|_r + c^{-1}\|\mathfrak{a}_*^\gamma(t_n+s) - \mathfrak{a}_*^\gamma(t_n)\|_{r,0})\\
&+ K_2\left\| w_*(t_n+\tau) - \Phi^\tau_{w_*}[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)] \right\|_r\\
\le& K \cdot (\tau + \tau^2).
\end{aligned} \tag{4.59}$$

The constant K has a similar dependence on the regularity of w_* and $\mathfrak{a}_*^\gamma$ as $K^{\mathrm{MKG}}_{w_*,\mathrm{loc}}$ from (4.58) but it is independent of c. In the following we may also use the notation

$$\boldsymbol{J}_*^{P,j}(t_n+s) = \boldsymbol{J}_*^{P,j}[w_*(t_n+s), \mathfrak{a}_*^\gamma(t_n+s)].$$

Next, we exploit that by Lemma A.10 the operator $\mathcal{T}^{-s}_{[c\langle\nabla\rangle_{\gamma/c}]}$ is an isometry in $\dot{H}^r$ and we make use of the estimate on the derivatives of w_* and $c^{-1}\mathfrak{a}^\gamma_*$ in (4.56). Together with the previous inequality (4.59) and the bilinear estimates Lemma A.8 we obtain

$$\begin{aligned}
&\left\|\mathfrak{a}_*(t_n+\tau) - \Phi^\tau_{\mathfrak{a}_*}\left[\tilde{w_*}^{n+1}, \mathfrak{a}^\gamma_*(t_n)\right]\right\|_{r,0} \\
\leq &\int_0^\tau c^{-1}\gamma^2 \left\|\langle\nabla\rangle^{-1}_{\gamma/c}\left(\mathfrak{a}^\gamma_*(t_n+s) - \mathfrak{a}^\gamma_*(t_n)\right)\right\|_{r,0} ds \\
&+ \left\| \int_0^\tau \mathcal{T}^{-s}_{[c\langle\nabla\rangle_{\gamma/c}]} \langle\nabla\rangle^{-1}_{\gamma/c} \Big(\boldsymbol{J}^{P,0}_*(t_n+s) - \boldsymbol{J}^{P,0}_*[\tilde{w_*}^{n+1}, \mathfrak{a}^\gamma_*(t_n)] \right. \\
&\qquad + e^{2ic^2(t_n+s)}\left(\boldsymbol{J}^{P,2}_*(t_n+s) - \boldsymbol{J}^{P,2}_*[\tilde{w_*}^{n+1}, \mathfrak{a}^\gamma_*(t_n)]\right) \\
&\qquad \left. + e^{-2ic^2(t_n+s)}\left(\overline{\boldsymbol{J}^{P,2}_*}(t_n+s) - \overline{\boldsymbol{J}^{P,2}_*}[\tilde{w_*}^{n+1}, \mathfrak{a}^\gamma_*(t_n)]\right)\Big) ds \right\|_{r,0} \\
\leq & K\tau^2
\end{aligned} \tag{4.60}$$

with a constant K depending only on $\mathcal{M}^{r+2}_{w_*}, \mathcal{M}^{r+1}_{\mathfrak{a}_*}$.

Gathering the results in (4.58) and (4.60) we thus finally obtain the local error bound of our method on the term (4.52), i.e.

$$\begin{aligned}
&\left\|w_*(t_n+\tau) - \Phi^\tau_{w_*}\left[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)\right]\right\|_r \\
&+ \left\|\mathfrak{a}^\gamma_*(t_n+\tau) - \Phi^\tau_{\mathfrak{a}_*}\left[\Phi^\tau_{w_*}[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)], \mathfrak{a}^\gamma_*(t_n)\right]\right\|_{r,0} \leq K^{\mathrm{MKG}}_{*,\mathrm{loc}}\tau^2
\end{aligned} \tag{4.61}$$

with a constant independent of c. The constant $K^{\mathrm{MKG}}_{*,\mathrm{loc}}$ depends on $\mathcal{M}^{r+2}_{w_*}, \mathcal{M}^{r+1}_{\mathfrak{a}_*}$.

Next, we consider the case of MD, respecting Assumption 4.5 on the initial data of the MD system (2.36).

The MD case under Assumption 4.5: Recall Assumption 4.5 on the initial data ψ_I of the MD system[④] (2.36), i.e.

$$\psi_I = (\psi^+_I, \psi^-_I)^\top \quad \text{satisfies} \quad \left\|\psi^-_I \overline{\boldsymbol{\sigma}} \overline{\psi^+_I}\right\|_r \leq Kc^{-1},$$

with a constant K independent of c. Furthermore recall that $\boldsymbol{J}^{P,j}_*$ for $j = 0, 2$ is given in case of MD by (4.18) as

$$\begin{aligned}
\boldsymbol{J}^{P,0}_*[w_*] =& c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_*\overline{\boldsymbol{\alpha}}\overline{u_*} + \overline{v_*}\overline{\boldsymbol{\alpha}}v_*\right], \\
\boldsymbol{J}^{P,2}_*[w_*] =& c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_*\overline{\boldsymbol{\alpha}}v_*\right].
\end{aligned}$$

According to (2.42) the structure of $w_* = (u_*, v_*)^\top = (u^+_*, u^-_*, v^+_*, v^-_*)^\top$ admits that in the sense of the H^r norm for all times t

$$\begin{aligned}
u^+_*(t) =& \mathcal{O}\left(c^{-1}\right), & v^+_*(t) =& \mathcal{O}\left(\overline{\psi^+}(t)\right), \\
u^-_*(t) =& \mathcal{O}\left(\psi^-(t)\right), & v^-_*(t) =& \mathcal{O}\left(c^{-1}\right).
\end{aligned}$$

In view of Remark 4.4, we thus have in the sense of the H^r norm

$$\boldsymbol{J}^{P,0}_* = c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u^+_*\overline{\boldsymbol{\sigma}}\overline{u^-_*} + u^-_*\overline{\boldsymbol{\sigma}}\overline{u^+_*} + \overline{v^+_*}\overline{\boldsymbol{\sigma}}v^-_* + \overline{v^-_*}\overline{\boldsymbol{\sigma}}v^+_*\right] = \mathcal{O}(1)$$

[④]Note that due to Remark 4.4, for MD initial data violating Assumption 4.5, the term (4.62) is $\mathcal{O}(c)$. In that case, the error bounds (4.60) and (4.63) are not uniformly in c (see also Remark 4.9 above).

and

$$\begin{aligned}\boldsymbol{J}_*^{P,2} =& c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_*^+\overline{\boldsymbol{\sigma}}v_*^- + u_*^-\overline{\boldsymbol{\sigma}}v_*^+\right] = \underbrace{c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_*^+\overline{\boldsymbol{\sigma}}v_*^-\right]}_{=:\boldsymbol{J}_*^{P,2,\mathrm{ok}}} + \underbrace{c\frac{1}{4}\mathcal{P}_{\mathrm{df}}\left[u_*^-\overline{\boldsymbol{\sigma}}v_*^+\right]}_{=:\boldsymbol{J}_*^{P,2,c}} \\ =& \mathcal{O}(1).\end{aligned} \tag{4.62}$$

Under this assumption we have that $\boldsymbol{J}_*^{P,j}$ is $\mathcal{O}(1)$ for $j = 0, 2$. We thus carry out the local error analysis in the MD case very similar to the MKG case. Due to the estimate (4.56) for MD, we find

$$\begin{aligned}&\left\|w_*(t_n+\tau) - \Phi_{w_*}^\tau\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right]\right\|_r \\ &+ \left\|\mathfrak{a}_*(t_n+\tau) - \Phi_{\mathfrak{a}_*}^\tau\left[\Phi_{w_*}^\tau[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)], \mathfrak{a}_*^\gamma(t_n)\right]\right\|_{r,0} \le K_{*,\mathrm{loc}}^{\mathrm{MD}}\tau^2\end{aligned} \tag{4.63}$$

with a constant $K_{*,\mathrm{loc}}^{\mathrm{MD}}$ depending only on $\mathcal{M}_{w_*}^{r+2}, \mathcal{M}_{\mathfrak{a}_*}^{r+2}$.

In the subsequent section we derive stability bounds of type (4.51).

4.3.2 Stability Bound (Time Integration) of the “Twisted Scheme”

In this section, we prove a stability bound for our method

$$\Psi_*^\tau[w_*^n, \mathfrak{a}_*^{\gamma,n}] := \Psi_{\mathfrak{a}_*}^\tau \circ \Psi_{w_*}^\tau[w_*^n, \mathfrak{a}_*^{\gamma,n}] = \begin{pmatrix}\Phi_{w_*}^\tau\left[w_*^n, \mathfrak{a}_*^{\gamma,n}\right] \\ \Phi_{\mathfrak{a}_*}^\tau\left[w_*^{n+1}, \mathfrak{a}_*^{\gamma,n}\right]\end{pmatrix} \quad \text{given in (4.53)} \tag{4.64a}$$

with

$$\begin{aligned}&\Phi_{w_*}^\tau\left[w_*^n, \mathfrak{a}_*^{\gamma,n}\right] = \mathcal{T}_{[\mathcal{L}_c]}^\tau\left(w_*^n - i\sum_{m\in I_m}\tau\varphi_1(mic^2\tau)e^{mic^2t_n}\left(F_*^m[w_*^n, \mathfrak{a}_*^{\gamma,n}] + G_*^m[w_*^n, \mathfrak{a}_*^{\gamma,n}]\right)\right), \\ &\Phi_{\mathfrak{a}_*}^\tau\left[w_*^{n+1}, \mathfrak{a}_*^{\gamma,n}\right] \\ &= \mathcal{T}_{[c\langle\nabla\rangle_{\gamma/c}]}^\tau\Bigg(\mathfrak{a}_*^{\gamma,n} - i\tau\langle\nabla\rangle_{\gamma/c}^{-1}\Bigg\{\varphi_1\left(i\tau\left(-c\langle\nabla\rangle_{\gamma/c}\right)\right)\left(\frac{\gamma^2}{2c}(\mathfrak{a}_*^{\gamma,n} + \overline{\mathfrak{a}_*^\gamma}(t_n)) + \boldsymbol{J}_*^{P,0}[w_*^{n+1}, \mathfrak{a}_*^{\gamma,n}]\right) \\ &\qquad + \varphi_1\left(i\tau(+2c^2 - c\langle\nabla\rangle_{\gamma/c})\right)e^{+2ic^2t_n}\boldsymbol{J}_*^{P,2}[w_*^{n+1}, \mathfrak{a}_*^{\gamma,n}] \\ &\qquad + \varphi_1\left(i\tau(-2c^2 - c\langle\nabla\rangle_{\gamma/c})\right)e^{-2ic^2t_n}\overline{\boldsymbol{J}_*^{P,2}}[w_*^{n+1}, \mathfrak{a}_*^{\gamma,n}]\Bigg\}\Bigg)\end{aligned} \tag{4.64b}$$

with $m \in I_m = \{-4, -2, 0, 2\}$. The proof is based on the decompostion (4.49), i.e. our aim is to show

$$\begin{aligned}&\left\|\Phi_{w_*}^\tau\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right] - \Phi_{w_*}^\tau\left[w_*^n, \mathfrak{a}_*^{\gamma,n}\right]\right\|_r && (4.65a)\\ &+ \left\|\Phi_{\mathfrak{a}_*^\gamma}^\tau\left[\Phi_{w_*}^\tau\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right], \mathfrak{a}_*^\gamma(t_n)\right] - \Phi_{\mathfrak{a}_*}^\tau\left[\Phi_{w_*}^\tau\left[w_*^n, \mathfrak{a}_*^{\gamma,n}\right], \mathfrak{a}_*^{\gamma,n}\right]\right\|_{r,0} && (4.65b)\\ &\le \|w_*(t_n) - w_*^n\|_r + \|\mathfrak{a}_*^\gamma(t_n) - \mathfrak{a}_*^{\gamma,n}\|_{r,0} + \tau L_{*,\mathrm{stab}}^{\mathrm{MKG/MD}}\left(\|w_*(t_n) - w_*^n\|_r + \|\mathfrak{a}_*^\gamma(t_n) - \mathfrak{a}_*^{\gamma,n}\|_{r,0}\right) \\ &\le e^{\tau L_{*,\mathrm{stab}}^{\mathrm{MKG/MD}}}\left(\|w_*(t_n) - w_*^n\|_r + \|\mathfrak{a}_*^\gamma(t_n) - \mathfrak{a}_*^{\gamma,n}\|_{r,0}\right)\end{aligned}$$

with a constant $L_{*,\mathrm{stab}}^{\mathrm{MKG}}$ only depending on $\|w_*(t_n)\|_r$, $\|w_*^n\|_r$, $\|\mathfrak{a}_*^\gamma(t_n)\|_{r,0}$ and $\|\mathfrak{a}_*^{\gamma,n}\|_{r,0}$ but not on $c \ge 1$.

For sake of simplicity, in our analysis we may substitute the pairs $(w_*(t_n), \mathfrak{a}_*^\gamma(t_n))$ and $(w_*^n, \mathfrak{a}_*^{\gamma,n})$ with pairs (w_1, w_2) and (w_2, a_2). Moreover, we use the notation

$$F_*^m[w_*, \mathfrak{a}_*^\gamma] = F_*^m[w_*, \phi_*^0, \phi_*^2, \mathfrak{a}_*^\gamma] \quad \text{and} \quad G_*^m[w_*, \mathfrak{a}_*^\gamma] = G_*^m[w_*, \phi_*^0, \phi_*^2, \mathfrak{a}_*^\gamma]$$

for $m \in I_m$, where F_*^m, G_*^m are given explicitly in (4.14). Note that for MKG we have $G_*^m = 0$ (cf. (2.41)).

Firstly, we establish the bound on the term (4.65a) in the subsequent section. Afterwards, we derive a similar estimate for (4.65b).

A Bound on Term (4.65a)

Due to the isometry property of $\mathcal{T}^s_{[\mathcal{L}_c]}$ in H^r from Lemma A.10 , the term (4.65a) satisfies

$$\begin{aligned}&\left\|\Phi^\tau_{w_*}[w_1,a_1] - \Phi^\tau_{w_*}[w_2,a_2]\right\|_r \\ &\leq \|w_1-w_2\|_r + 4\tau \max_{m\in I_m}\left(\|F_*^m[w_1,a_1]-F_*^m[w_2,a_2]\|_r + \|G_*^m[w_1,a_1]-G_*^m[w_2,a_2]\|_r\right).\end{aligned} \tag{4.66}$$

The estimates on the operator $\langle\nabla\rangle_c$ in Lemma A.11 and the bilinear estimates from Lemma A.8 allow us to bound

$$\left\|\langle\nabla\rangle_c^{-1}\phi_*^j\langle\nabla\rangle_c w_*\right\|_r \leq K\left\|\phi_*^j\right\|_r\|w_*\|_r \quad \text{and} \quad \|u\cdot v\|_{r-r'} \leq K\|u\|_{r-r'}\|v\|_r$$

with $r' \in \{0,1\}$. According to (4.72) in (4.3.4) below, we divide F_*^m and G_*^m into their basic characteristic terms. Due to expansions of type

$$a_1\overline{a_1}w_1 - a_2\overline{a_2}w_2 = (a_1-a_2)\overline{a_1}w_1 + a_2(\overline{a_1}-\overline{a_2})w_1 + a_2\overline{a_2}(w_1-w_2),$$

the term (4.66) then obeys the stability bound

$$\left\|\Phi^\tau_{w_*}[w_1,a_1] - \Phi^\tau_{w_*}[w_2,a_2]\right\|_r \leq \|w_1-w_2\|_r + \tau L\big(\|w_1-w_2\|_r + \|a_1-a_2\|_{r,0}\big), \tag{4.67}$$

with a constant L only depending on $\|w_1\|_r, \|w_2\|_r, \|a_1\|_r, \|a_2\|_r$ but not on c.

In the subsequent paragraph we establish a stability bound on the second term (4.65b).

A Bound on Term (4.65b)

Recall that $\gamma \in [0,1]$ by (4.9). Thus, in the case of MKG and also in case of MD with initial data satisfying Assumption 4.5,[5] the term (4.65b) can be bounded as

$$\begin{aligned}&\left\|\Phi^\tau_{\mathfrak{a}_*^\gamma}[\tilde{w}_1,a_1] - \Phi^\tau_{\mathfrak{a}_*^\gamma}[\tilde{w}_2,a_2]\right\|_{r,0} \\ &\leq \|a_1-a_2\|_{r,0} + \tau\left(2\frac{\gamma^2}{c}\|a_1-a_2\|_{r,0} + 3\max_{j=0,2}\left\|\langle\nabla\rangle_{\gamma/c}^{-1}\left(\boldsymbol{J}_*^{P,j}[\tilde{w}_1,a_1] - \boldsymbol{J}_*^{P,j}[\tilde{w}_2,a_2]\right)\right\|_{r,0}\right) \\ &\leq \|a_1-a_2\|_{r,0} + \tau L\left(c^{-1}\|a_1-a_2\|_{r,0} + \|\tilde{w}_1-\tilde{w}_2\|_r\right),\end{aligned} \tag{4.68}$$

where the constant L depends on $\|\tilde{w}_1\|_r, \|\tilde{w}_2\|_r, \|a_1\|_r, \|a_2\|_r$ but not on c.

Replacing

$$w_1 = w_*(t_n), \quad a_1 = \mathfrak{a}_*^\gamma(t_n), \quad w_2 = w_*^n, \quad a_2 = \mathfrak{a}_*^{\gamma,n} \quad \text{in (4.67)},$$

$$\tilde{w}_1 = \Phi^\tau_{w_*}\left[w_*(t_n), \mathfrak{a}_*^\gamma(t_n)\right], \quad a_1 = \mathfrak{a}_*^\gamma(t_n), \quad \tilde{w}_2 = \Phi^\tau_{w_*}\left[w_*^n, \mathfrak{a}_*^{\gamma,n}\right], \quad a_2 = \mathfrak{a}_*^{\gamma,n} \quad \text{in (4.68)},$$

[5] Due to Remark 4.4, for MD initial data violating Assumption 4.5, the bound in (4.68) is not uniformly in c (see also Remark 4.9 above).

and exploiting once more the stability bound (4.67) in order to bound the term $\|\tilde{w}_1 - \tilde{w}_2\|_r$ in (4.68), we obtain the desired stability bound (4.65), i.e.

$$\begin{aligned} &\left\|\Phi^\tau_{w_*}\left[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)\right] - \Phi^\tau_{w_*}\left[w^n_*, \mathfrak{a}^{\gamma,n}_*\right]\right\|_r \\ &+ \left\|\Phi^\tau_{\mathfrak{a}^\gamma_*}\left[\Phi^\tau_{w_*}\left[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)\right], \mathfrak{a}^\gamma_*(t_n)\right] - \Phi^\tau_{\mathfrak{a}_*}\left[\Phi^\tau_{w_*}\left[w^n_*, \mathfrak{a}^{\gamma,n}_*\right], \mathfrak{a}^{\gamma,n}_*\right]\right\|_{r,0} \\ &\leq e^{\tau L^{\mathrm{MKG/MD}}_{*,\mathrm{stab}}}\left(\|w_*(t_n) - w^n_*\|_r + \|\mathfrak{a}^\gamma_*(t_n) - \mathfrak{a}^{\gamma,n}_*\|_{r,0}\right) \end{aligned} \tag{4.69}$$

with constants $L^{\mathrm{MKG}}_{*,\mathrm{stab}}, L^{\mathrm{MD}}_{*,\mathrm{stab}} > 0$ independent of c. The constants $L^{\mathrm{MKG}}_{*,\mathrm{stab}}, L^{\mathrm{MD}}_{*,\mathrm{stab}}$ may be different in case of MKG than in case of MD. In the subsequent section, we combine the local error results from Section 4.3.1 with the stability bounds derived in the current section.

4.3.3 Local to Global Time Integration Error of the "Twisted Scheme"

Define the error $\mathfrak{e}^n_*$ and the local error d^n_* (cf. (4.48)) of our method

$$\begin{pmatrix} w^n_* \\ \mathfrak{a}^{\gamma,n}_* \end{pmatrix} = \Psi^\tau_*\left[w^{n-1}_*, \mathfrak{a}^{\gamma,n-1}_*\right], \quad \text{given in (4.39) (see also also (4.64))}$$

at time t_n for all $n \geq 1$ by

$$\begin{aligned} \mathfrak{e}^n_* &:= \left\| \begin{pmatrix} w_*(t_n) \\ \mathfrak{a}^\gamma_*(t_n) \end{pmatrix} - \begin{pmatrix} w^n_* \\ \mathfrak{a}^{\gamma,n}_* \end{pmatrix} \right\|_r = \|w_*(t_n) - w^n_*\|_r + \|\mathfrak{a}^\gamma_*(t_n) - \mathfrak{a}^{\gamma,n}_*\|_{r,0}\,, \\ d^n_* &:= \left\| \begin{pmatrix} w_*(t_n) \\ \mathfrak{a}^\gamma_*(t_n) \end{pmatrix} - \Psi^\tau_*\left[w_*(t_{n-1}), \mathfrak{a}^\gamma_*(t_{n-1})\right] \right\|_r . \end{aligned}$$

Recall that the defect d^n_* can be associated with the local error (see Definition A.17) of the method Ψ^τ_* applied to exact initial data at time t_{n-1}. In (4.48) we have already seen that

$$\mathfrak{e}^{n+1}_* \leq d^{n+1}_* + \mathcal{S}^n_*,$$

where the stability term $\mathcal{S}^n_*$ for all $n \geq 0$ is given by (4.49) as

$$\mathcal{S}^n_* = \left\|\Psi^\tau_*\left[w_*(t_n), \mathfrak{a}^\gamma_*(t_n)\right] - \Psi^\tau_*\left[w^n_*, \mathfrak{a}^{\gamma,n}_*\right]\right\|_r \quad \text{and} \quad \mathcal{S}^0_* = 0.$$

In the previous sections, we established uniform bounds on the local error term d^{n+1}_* of our method Ψ^τ_* in (4.61) and (4.63), respectively, and we derived bounds for the stability term $\mathcal{S}^n_*$ in (4.69). More precisely, we derived the estimates

$$d^{n+1}_* \leq K^{\mathrm{MKG/MD}}_{*,\mathrm{loc}} \quad \text{and} \quad \mathcal{S}^n_* \leq e^{\tau L^{\mathrm{MKG/MD}}_{*,\mathrm{stab}}}\mathfrak{e}^n_*$$

which hold uniformly in c, i.e. the constants $K^{\mathrm{MKG/MD}}_{*,\mathrm{loc}}, L^{\mathrm{MKG/MD}}_{*,\mathrm{stab}}$ are independent of c but depend only on the regularity of $w_*(t_n), w^n_*, \mathfrak{a}^\gamma_*(t_n), \mathfrak{a}^{\gamma,n}_*$. We exploit these bounds in order to establish a global first order bound in time which holds uniformly in c. Note that we have

$$\mathfrak{e}^{n+1}_* \leq d^{n+1}_* + \mathcal{S}^n_* \leq \tau^2 K^{\mathrm{MKG/MD}}_{*,\mathrm{loc}} + e^{\tau L^{\mathrm{MKG/MD}}_{*,\mathrm{stab}}}\mathfrak{e}^n_*. \tag{4.70}$$

To resolve this error recursion we need boundedness of $\|w^n_*\|_r$ and $\|\mathfrak{a}^{\gamma,n}_*\|_{r,0}$ because of the explicit dependence of $L^{\mathrm{MKG}}_{*,\mathrm{stab}}$ on these norms (see (4.65)). Fortunately, we can ensure this condition by a simple induction argument: If $\left\|w^{n-1}_*\right\|_r + \left\|\mathfrak{a}^{\gamma,n-1}_*\right\|_{r,0} \leq M$ then from definition of Ψ^τ_* in (4.39) and due to the fact that $e^{imc^2 s}, m = -4, -2, 0, 2$ and $e^{i(jc^2 - c\langle\nabla\rangle_{\gamma/c})}, j = -2, 0, 2$ are isometries in H^r (see Lemma A.10) also $\|w_*^n\|_r + \|\mathfrak{a}_*^{\gamma,n}\|_{r,0} \leq K(M)$.

Resolving the recurrence (4.70), a bootstrap argument (see [44, Proof of Proposition IV.14] and also Remark 3.13) shows that the global error is globally of first order uniformly in c, i.e.

$$\mathfrak{e}_*^{n+1} = \left\| \begin{pmatrix} w_*(t_{n+1}) \\ \mathfrak{a}_*^\gamma(t_{n+1}) \end{pmatrix} - \begin{pmatrix} w_*^{n+1} \\ \mathfrak{a}_*^{\gamma,n+1} \end{pmatrix} \right\|_r \leq K_{*,\text{time}}^{\text{MKG/MD}} \tau.$$

In case of MKG the constant $K_{*,\text{time}}^{\text{MKG}}$ depends on T, $\mathcal{M}_{w_*}^{r+2}$ and $\mathcal{M}_{\mathfrak{a}_*}^{r+1}$ but can be chosen independent of c. In case of MD $K_{*,\text{time}}^{\text{MD}}$ depends on T, $\mathcal{M}_{w_*}^{r+2}$ and $\mathcal{M}_{\mathfrak{a}_*}^{r+2}$ but can be chosen independent of c.

This finally proves Theorems 4.7 and 4.8. □

Next, for the interested reader, we provide auxiliary results which we used in the previous sections for proving global convergence bounds of our schemes. Afterwards, in the subsequent chapter, we confirm the theoretical results of this thesis by numerical experiments.

4.3.4 Auxiliary Results and Bounds on the Derivatives of the Nonlinear Terms

Parts of this section are based on [18].

Firstly, we gather important properties of the operator $\mathcal{L}_c$ in Lemmas 4.10 and 4.11 below, which we have used in the previous sections for proving the global first order convergence in time uniformly in c of our time integration method Ψ_*^τ. Afterwards, we establish uniform bounds on the time derivatives of the solutions w_* and $\mathfrak{a}_*^\gamma$ of (4.15). More precisely, we show that for $r > d/2$ and $r' \geq 0$

$$\|w_*(t+s) - w_*(t)\|_{r+r'} + c^{-1} \|\mathfrak{a}_*^\gamma(t+s) - \mathfrak{a}_*^\gamma(t)\|_{r+r',0} \leq K_1 s$$

with a constant K_1 independent of c. We may exploit the latter bounds in proving uniform bounds on the time derivatives of F_*^m, G_*^m for $m = -4, -2, 0, 2$ (see (4.3d)) of type

$$\|F_*^m(t+s) - F_*^m(t)\|_r + \|G_*^m(t+s) - G_*^m(t)\|_r \leq K_2 s$$

with a constant K_2 independent of c.

Lemma 4.10 ([18, Lemma 3]). *The operator*

$$\mathcal{L}_c = c\,\langle\nabla\rangle_c - c^2$$

is uniformly bounded in H^{r+2} for all $c \geq 1$, i.e.

$$\|\mathcal{L}_c w\|_r \leq \frac{1}{2}\|w\|_{r+2}, \quad \forall w \in H^{r+2}.$$

Proof (see [18, Lemma 3])*:* This result has already been shown by Lemma A.11. □

Lemma 4.11 ([18, Lemma 4]). *For all $t \in \mathbb{R}$ and all $u \in H^{r+2}$ we have that*

$$\left\|e^{it\mathcal{L}_c}\right\|_r = 1 \quad \textit{and} \left\|\left(e^{-it\mathcal{L}_c} - 1\right)u\right\|_r \leq \frac{1}{2}|t|\,\|u\|_{r+2}.$$

Proof: The first assertion has been proven in Lemma A.10. The second assertion is an immediate consequence of the estimate $\left|e^{ix}-1\right| \leq |x|$ for all $x \in \mathbb{R}$ from Proposition A.32 together with the bound on $\mathcal{L}_c$ given in Lemma 4.10. Compare also to the proof of Lemma A.10. □

We proceed with bounds on the time derivatives of w_* and $\mathfrak{a}_*$. Afterwards, similar bounds shall be given for F_*^m, G_*^m for $m = -4, -2, 0, 2$.

Bounds on the Derivatives of w_* and $\mathfrak{a}_*$

Recall that Duhamel's formula (4.26) for the solution $(w_*, \mathfrak{a}_*^\gamma)^\top$ of the “twisted system” (4.15) reads in the notation $\mathcal{T}_{[A]}^s = e^{isA}$ (see (3.70))

$$\begin{aligned}
w_*(t_n+\tau) =& \mathcal{T}_{[\mathcal{L}_c]}^{\tau} w_*(t_n) - i\int_0^\tau \mathcal{T}_{[\mathcal{L}_c]}^{\tau-s} \sum_{m\in I_m} e^{mic^2(t_n+s)} \left(F_*^m(t_n+s) + G_*^m(t_n+s)\right) ds,\\
\mathfrak{a}_*^\gamma(t_n+\tau) =& \mathcal{T}_{[c\langle\nabla\rangle_{\gamma/c}]}^{\tau} \mathfrak{a}_*^\gamma(t_n)\\
&- i\langle\nabla\rangle_{\gamma/c}^{-1} \int_0^\tau \mathcal{T}_{[c\langle\nabla\rangle_{\gamma/c}]}^{\tau-s} \Bigg(\frac{\gamma^2}{2c}\left(\mathfrak{a}_*^\gamma(t_n+s) + \overline{\mathfrak{a}_*^\gamma}(t_n+s)\right)\\
&\qquad + \boldsymbol{J}_*^{P,0}(t_n+s)\\
&\qquad + e^{+2ic^2(t_n+s)}\boldsymbol{J}_*^{P,2}(t_n+s)\\
&\qquad + e^{-2ic^2(t_n+s)}\overline{\boldsymbol{J}_*^{P,2}}(t_n+s)\Bigg) ds
\end{aligned} \tag{4.71}$$

with $I_m = \{-4,-2,0,2\}$. Furthermore, note that the nonlinear terms $F_*^m, G_*^m, m \in I_m$ (see (4.3d)) are each composed of characteristic basic terms for $j = 0, 2$

$$\begin{aligned}
F_*^{m,1} :=& \left(\phi_*^j \pm \langle\nabla\rangle_c^{-1} \phi_*^j \langle\nabla\rangle_c\right) w_*\\
F_*^{m,2} :=& c^{-1}\langle\nabla\rangle_c^{-1}\left(\left|\mathfrak{a}_*^\gamma\right|^2 w_*\right)\\
F_*^{m,3} :=& \langle\nabla\rangle_c^{-1}\left(\mathfrak{a}_*^\gamma \cdot \nabla w_*\right),
\end{aligned} \tag{4.72a}$$

and

$$\begin{aligned}
G_*^{m,1} :=& \langle\nabla\rangle_c^{-1}\left(\mathfrak{D}_{\mathrm{curl}}^{\boldsymbol{\alpha}}[\mathfrak{a}_*^\gamma] w_*\right)\\
G_*^{m,2} :=& \langle\nabla\rangle_c^{-1}\left(\mathfrak{D}_{\mathrm{div}}^{\boldsymbol{\alpha}}[\phi_*^j] w_*\right)\\
G_*^{m,3} :=& \langle\nabla\rangle_c^{-1}\left(\mathfrak{D}_0^{\boldsymbol{\alpha}}[\langle\nabla\rangle_{\gamma/c}(\mathfrak{a}_*^\gamma)] w_*\right),
\end{aligned} \tag{4.72b}$$

where the $\mathfrak{D}^{\boldsymbol{\alpha}}$ terms are given in Definition 2.6 as

$$\mathfrak{D}_{\mathrm{curl}}^{\boldsymbol{\alpha}}[\tilde{\mathfrak{a}}] = -\frac{1}{2}\sum_{\substack{j,k=1\\ j\neq k}}^{d} \boldsymbol{\alpha}_j\boldsymbol{\alpha}_k[(\partial_j(\tilde{\mathfrak{a}}_k)) - (\partial_k(\tilde{\mathfrak{a}}_j))],$$

$$\mathfrak{D}_{\mathrm{div}}^{\boldsymbol{\alpha}}[\tilde{\phi}] = \sum_{j=1}^{d} \boldsymbol{\alpha}_j(\partial_j\tilde{\phi}) \qquad \text{and} \qquad \mathfrak{D}_0^{\boldsymbol{\alpha}}[\tilde{\mathfrak{a}}] = \sum_{j=1}^{d} \boldsymbol{\alpha}_j(\tilde{\mathfrak{a}}_j)$$

for some $\tilde{\mathfrak{a}}(x) = (\tilde{\mathfrak{a}}_1(x), \dots, \tilde{\mathfrak{a}}_d(x))^\top \in \mathbb{C}^d$ and $\tilde{\phi}(x) \in \mathbb{C}$.

Choosing $r > d/2$ and $r' \geq 0$, Lemma 4.11 yields the uniform estimate

$$\left\| \left(\mathcal{T}^s_{[\mathcal{L}_c]} - 1\right) w_* \right\|_{r+r'} \leq \frac{1}{2} |s| \, \|w_*\|_{r+r'+2} \quad \text{for all } w_* \in H^{r+r'+2} \text{ and } s \in \mathbb{R}.$$

Moreover, using the ideas from Lemma 4.11 leads to the nonuniform bound (cf. (4.33))

$$\left\| \left(\mathcal{T}^s_{[c\langle\nabla\rangle_{\gamma/c}]} - 1\right) \mathfrak{a}^\gamma_* \right\|_{r+r',0} \leq Kc \left\| \langle\nabla\rangle_{\gamma/c} \, \mathfrak{a}^\gamma_* \right\|_{r+r',0}, \tag{4.73}$$

with a constant K independent of c.

Exploiting the bilinear Sobolev product estimates from Lemma A.8 together with the bounds on the operator $\langle\nabla\rangle_c$ in Lemma A.11, based on Duhamel's formula (4.71) and on the terms (4.72) we can establish the bounds for $r > d/2$ and $r'_1, r'_2 \geq 0$

$$\|w_*(t+s) - w_*(t)\|_{r+r'_1} \leq |s| \left(\frac{1}{2} \|w_*(t)\|_{r+r'_1+2} + K_{F_*+G_*}\left(\mathcal{M}^{r+r'_1}_{w_*}, \mathcal{M}^{r+r'_1}_{\mathfrak{a}_*}\right)\right) \tag{4.74a}$$

$$\begin{aligned} \|\mathfrak{a}^\gamma_*(t+s) - \mathfrak{a}^\gamma_*(t)\|_{r+r'_2,0} \leq & Kc\,|s| \, \|\mathfrak{a}^\gamma_*(t)\|_{r+r'_2+1,0} + c\,|s| \, K_{\boldsymbol{J}^P_*}\left(\mathcal{M}^{r+r'_2}_{w_*}\right) \\ & + |s| \, K^2_{\mathfrak{a}_*}\left(\mathcal{M}^{r+r'_2}_{\mathfrak{a}_*}\right), \end{aligned} \tag{4.74b}$$

where the constants $K_{F_*+G_*}, K, K_{\boldsymbol{J}^P_*}, K^2_{\mathfrak{a}_*} > 0$ are independent of c and only depend on the spatial regularity of $w_*, \mathfrak{a}^\gamma_*$. The constants $\mathcal{M}^{\tilde{r}}_{w_*}, \mathcal{M}^{\tilde{r}}_{\mathfrak{a}_*} > 0$ for $\tilde{r} \geq 1$ are chosen according to Assumption 4.6 and correspond to the regularity of $w_* \in H^{\tilde{r}}$ and $\mathfrak{a}_* \in \dot{H}^{\tilde{r}}$, respectively. This yields a uniform bound for $r > d/2$ and $r'_1, r'_2 \geq 0$

$$\|w_*(t+s) - w_*(t)\|_{r+r'_1} + c^{-1} \|\mathfrak{a}^\gamma_*(t+s) - \mathfrak{a}^\gamma_*(t)\|_{r+r'_2,0} \leq K_1 |s| \tag{4.75}$$

with a constant K_1 independent of c.

Next, we shall exploit the bound (4.75) on the derivatives of w_* and $\mathfrak{a}^\gamma_*$ in proving uniform bounds on the derivatives of $F^m_*, G^m_*, m = -4, -2, 0, 2$.

Bounds on the Derivatives of F^m_* and G^m_*

In this section we establish bounds on the time derivatives F^m_* and G^m_*, $m \in I_m = \{-4, -2, 0, 2\}$ (see (4.72) for the basic characteristic terms in F^m_*, G^m_*) by playing the bound back to (4.75). We thus prove for $r > d/2$ and

$$r' := 0 \quad \text{in case of MKG} \quad (G^m_* = 0) \quad \text{and} \quad r' := 1 \quad \text{in case of MD}$$

that for all $m \in I_m$

$$\begin{aligned} & \|F^m_*(t+s) - F^m_*(t)\|_r + \|G^m_*(t+s) - G^m_*(t)\|_r \\ \leq & K(\mathcal{M}^{r+1}_{w_*}, \mathcal{M}^r_{\mathfrak{a}_*}) \Big(\|w_*(t+s) - w_*(t)\|_r + c^{-1} \|\mathfrak{a}^\gamma_*(t+s) - \mathfrak{a}^\gamma_*(t)\|_{r+r',0} \Big) \\ \leq & |s| \, K(\mathcal{M}^{r+2}_{w_*}, \mathcal{M}^{r+1+r'}_{\mathfrak{a}_*}) =: |s| \, (K^2_{F^m_*} + K^2_{G^m_*}), \end{aligned} \tag{4.76a}$$

where the last inequality follows from (4.74b) with a constant $K^2_{F^m_*} + K^2_{G^m_*}$ (see (4.57)) only depending on $\mathcal{M}^{r+2}_{w_*}$ and $\mathcal{M}^{r+r'+1}_{\mathfrak{a}_*}$ but independent of $c \geq 1$. Similarly, we establish the bound (cf. (4.57))

$$\|F^m_*(t)\|_{r+2} + \|G^m_*(t)\|_{r+2} \leq K^1_{F^m_*} + K^1_{G^m_*} \tag{4.76b}$$

with constants $K^1_{F^m_*}, K^1_{G^m_*}$ depending on $\mathcal{M}^{r+2}_{w_*}$ and $\mathcal{M}^{r+r'}_{\mathfrak{a}_*}$ but independent of $c \geq 1$.

Similar to (4.19), we prove the following bounds on ϕ^j_* for $j = 0, 2$ exploiting the bilinear estimate $\|uv\|_{r-r'} \leq K \|u\|_{r-r'} \|v\|_r$ from Lemma A.8 for $r' = 1$ in case of MKG and $r' = 0$ in case of MD. By virtue of the Poisson solution operator $\dot{\Delta}^{-1}$ given in Appendix A.3 we thus find

$$\begin{aligned}\left\|\phi^j_*(t+s) - \phi^j_*(t)\right\|_{r+2-r',0} \leq & \left\|\dot{\Delta}^{-1}\left(\rho^j_*(t+s) - \rho^j_*(t)\right)\right\|_{r+2-r',0} \\ \leq & K \cdot \mathcal{M}^r_{w_*} \left\|w_*(t+s) - w_*(t)\right\|_r .\end{aligned}$$

As a consequence from Lemma A.11, the latter bound allows us to estimate the time derivative of $F^{m,1}_*$ from (4.72) as

$$\left\|F^{m,1}_*(t+s) - F^{m,1}_*(t)\right\|_r \leq K_{F^{m,1}_*}(\mathcal{M}^r_{w_*}) \left\|w_*(t+s) - w_*(t)\right\|_r , \tag{4.77a}$$

with $K_{F^{m,1}_*}$ independent of c. In order to bound the term $\left\|F^{m,2}_*(t+s) - F^{m,2}_*(t)\right\|_r$, we consider

$$\begin{aligned}& \left|\mathfrak{a}^\gamma_*(t+s)\right|^2 w_*(t+s) - \left|\mathfrak{a}^\gamma_*(t)\right|^2 w_*(t) \\ =& \overline{\mathfrak{a}^\gamma_*(t+s)} w_*(t+s)\left(\mathfrak{a}^\gamma_*(t+s) - \mathfrak{a}^\gamma_*(t)\right) + \mathfrak{a}^\gamma_*(t) w_*(t+s)\left(\overline{\mathfrak{a}^\gamma_*(t+s)} - \overline{\mathfrak{a}^\gamma_*(t)}\right) \\ & + \left|\mathfrak{a}^\gamma_*(t)\right|^2 \left(w_*(t+s) - w_*(t)\right).\end{aligned} \tag{4.77b}$$

Exploiting the bilinear estimate $\left\|\langle\nabla\rangle_c^{-1}(uv)\right\|_r \leq K \|u\|_{r-1} \|v\|_r$ from Lemma A.8, yields

$$\begin{aligned}\left\|F^{m,2}_*(t+s) - F^{m,2}_*(t)\right\|_r \leq K_{F^{m,2}_*}(\mathcal{M}^r_{w_*}, \mathcal{M}^r_{\mathfrak{a}_*})\Big(& \left\|w_*(t+s) - w_*(t)\right\|_r \\ & + c^{-1} \left\|\mathfrak{a}^\gamma_*(t+s) - \mathfrak{a}^\gamma_*(t)\right\|_{r,0}\Big),\end{aligned} \tag{4.77c}$$

with $K_{F^{m,2}_*}$ independent of c. Similarly we find

$$\begin{aligned}\left\|F^{m,3}_*(t+s) - F^{m,3}_*(t)\right\|_r \leq K_{F^{m,3}_*}(\mathcal{M}^{r+1}_{w_*}, \mathcal{M}^r_{\mathfrak{a}_*})\Big(& \left\|w_*(t+s) - w_*(t)\right\|_r \\ & + c^{-1} \left\|\mathfrak{a}^\gamma_*(t+s) - \mathfrak{a}^\gamma_*(t)\right\|_{r,0}\Big),\end{aligned} \tag{4.77d}$$

and

$$\begin{aligned}\left\|G^{m,1}_*(t+s) - G^{m,1}_*(t)\right\|_r \leq & K_{G^{m,1}_*}(\mathcal{M}^r_{w_*}, \mathcal{M}^r_{\mathfrak{a}_*})\Big(\left\|w_*(t+s) - w_*(t)\right\|_r \\ & \qquad + c^{-1} \left\|\mathfrak{a}^\gamma_*(t+s) - \mathfrak{a}^\gamma_*(t)\right\|_{r+1,0}\Big), \\ \left\|G^{m,2}_*(t+s) - G^{m,2}_*(t)\right\|_r \leq & K_{G^{m,2}_*}(\mathcal{M}^r_{w_*})\Big(\left\|w_*(t+s) - w_*(t)\right\|_r \Big), \\ \left\|G^{m,3}_*(t+s) - G^{m,3}_*(t)\right\|_r \leq & K_{G^{m,3}_*}(\mathcal{M}^r_{w_*}, \mathcal{M}^r_{\mathfrak{a}_*})\Big(\left\|w_*(t+s) - w_*(t)\right\|_r \\ & \qquad + c^{-1} \left\|\mathfrak{a}^\gamma_*(t+s) - \mathfrak{a}^\gamma_*(t)\right\|_{r+1,0}\Big),\end{aligned} \tag{4.77e}$$

with constants $K_{F^{m,1}_*}, K_{G^{m,1}_*}, K_{G^{m,2}_*}, K_{G^{m,3}_*}$ independent of c.

Here we used again $\left\| \langle \nabla \rangle_c^{-1} w \right\|_r \leq c^{-1} \|w\|_r$ from Lemma A.11. Moreover, we exploited the bilinear Sobolev product estimates from Lemma A.8. Gathering the bounds in (4.77) we find the desired bound of type (4.76), i.e.

$$\|F_*^m(t+s) - F_*^m(t)\|_r + \|G_*^m(t+s) - G_*^m(t)\|_r \leq |s| \, (K_{F_*^m}^2 + K_{G_*^m}^2)$$

with constants $K_{F_*^m}^2, K_{G_*^m}^2$ independent of c.

We proceed with numerical experiments in the next chapter.

CHAPTER

FIVE

NUMERICAL EXPERIMENTS

In this chapter, we confirm the results of this thesis by numerical experiments. We thus underline the theoretical convergence bounds

$$\mathcal{O}\left(\tau^2 + c^{-N}\right) \quad \text{from Theorem 3.15}$$

on the numerical approximations to the exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MKG/MD systems (5.3)/(5.4) below. Recall that we obtained these approximations by exploiting the truncated asymptotic expansions (see (3.33) and (3.61), respectively)

$$\begin{pmatrix} \psi(t) \\ \phi(t) \\ \boldsymbol{\mathcal{A}}(t) \end{pmatrix} = \begin{pmatrix} \psi_\infty^{(N_1-1)}(t) \\ \phi_\infty^{(N_2-1)}(t) \\ \boldsymbol{\mathcal{A}}_\infty^{(N_3-1)}(t) \end{pmatrix} + \mathcal{O}\left(\begin{pmatrix} c^{-N_1} \\ c^{-N_2} \\ c^{-N_3} \end{pmatrix}\right) \qquad \text{for } N_1, N_2, N_3 \in \mathbb{N}.$$

We furthermore underline the uniformly first order in time convergence bounds

$$\mathcal{O}\left(\tau\right) \quad \text{uniformly in } c \text{ from Theorems 4.7 and 4.8}$$

of the numerical approximation in time of the exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MKG/MD systems (5.3)/(5.4) below, obtained with the uniformly accurate scheme given explicitly in (4.39) and (4.43)

$$\text{exploiting the “twisted variables”} \quad (w_* = (u_*, v_*), \phi_*^{\text{tot}}, \mathfrak{a}_*^\gamma)^\top, \quad \text{with}$$
$$\psi(t) = \psi_*(t) = \frac{1}{2}(e^{ic^2t}u_*(t) + e^{-ic^2t}\overline{v_*}(t)) \quad \text{and} \quad \boldsymbol{\mathcal{A}}(t) = \boldsymbol{\mathcal{A}}_*(t) = \frac{1}{2}(\mathfrak{a}_*^\gamma(t) + \overline{\mathfrak{a}_*^\gamma}(t)).$$

In our numerical experiments we focus on the case of

$$\text{space dimension} \qquad d = 2.$$

Because we have no analytic solutions of the MKG/MD system available, we need numerical reference solutions in order to test our time integration schemes. For this purpose, we construct exponential Gautschi-type ([9, 51, 54, 55]) reference schemes for oscillatory Klein–Gordon and wave equations

$$\partial_{tt}\psi + c^2 \left\langle\nabla\right\rangle_c^2 \psi = c^2 \ f[\psi] \quad \text{and} \quad \partial_{tt}\boldsymbol{\mathcal{A}} - c^2\Delta\boldsymbol{\mathcal{A}} = \ c\ h[\boldsymbol{\mathcal{A}}] \quad \text{of type (5.3a) and (5.3b)}, \tag{5.1}$$

and time-splitting (TSFP, [10, 15, 16]) reference integrators for oscillatory Dirac equations

$$i\partial_t\psi = \left(-ic\sum_{j=1}^{d}\boldsymbol{\alpha}_j\partial_j + c^2\boldsymbol{\beta}\right)\psi + \left(\phi - \sum_{j=1}^{d}\boldsymbol{\alpha}_j A_j\right)\psi \quad \text{of type (5.4a)}$$

which we adapt to our MKG and MD system. Note that from the analysis in the latter papers, we deduce severe time step restrictions for these reference schemes of order

$$\tau_{\text{ref}} \leq Kc^{-2} \qquad \text{with a constant } K \text{ independent of } c \text{ and } \tau_{\text{ref}}. \tag{5.2}$$

Recall that the MKG system (2.20) with solutions $\psi(t,x) \in \mathbb{C}$ and $(\phi(t,x), \boldsymbol{\mathcal{A}}(t,x))^\top \in \mathbb{R}^{1+d}$ reads

$$\begin{cases} \partial_{tt}\psi + c^2 \langle\nabla\rangle_c^2 \psi = \left(\phi^2\psi - 2i\phi\partial_t\psi - i(\partial_t\phi)\psi\right) - |\boldsymbol{\mathcal{A}}|^2\psi - 2ic\boldsymbol{\mathcal{A}}\cdot\nabla\psi, & (5.3\text{a})\\ \partial_{tt}\boldsymbol{\mathcal{A}} + c^2\langle\nabla\rangle_0^2\boldsymbol{\mathcal{A}} = c\mathcal{P}_{\text{df}}\left[\operatorname{Re}\left(i\psi\overline{\nabla\psi}\right) - \frac{\boldsymbol{\mathcal{A}}}{c}|\psi|^2\right], \qquad \operatorname{div}\boldsymbol{\mathcal{A}} = 0, & (5.3\text{b})\\ -\Delta\phi = -\operatorname{Re}\left(i\frac{\psi}{c}\cdot\overline{\partial_t^{[\phi]}\psi}\right), & (5.3\text{c})\\ \left(\psi(0,x), \partial_t^{[\phi(0,x)]}\psi(0,x)\right) = \left(\psi_I(x), \langle\nabla\rangle_c\psi_I'(x)\right), & (5.3\text{d})\\ \left(\boldsymbol{\mathcal{A}}(0), \partial_t\boldsymbol{\mathcal{A}}(0)\right) = \left(A_I(x), cA_I'(x)\right). & (5.3\text{e}) \end{cases}$$

For sake of simplicity, we consider the MD system (2.36) in its reduced version (cf. Remark 2.5)

for the case of lower dimensions $d_{\text{low}} :=\in \{1, 2\}$ (see Remark 2.5)

with solutions $\Psi(t,x) = (\psi_1(t,x), \psi_4(t,x))^\top \in \mathbb{C}^2$ and $(\phi(t,x), \boldsymbol{\mathcal{A}}(t,x))^\top \in \mathbb{R}^{1+d_{\text{low}}}$, which reads

$$\begin{cases} i\partial_t\Psi = \left(-ic\sum_{j=1}^{d_{\text{low}}}\boldsymbol{\sigma}_j\partial_j + c^2\boldsymbol{\sigma}_3\right)\Psi + \left(\phi - \sum_{j=1}^{d_{\text{low}}}\boldsymbol{\sigma}_j A_j\right)\Psi & (5.4\text{a})\\ \partial_{tt}\boldsymbol{\mathcal{A}} + c^2\langle\nabla\rangle_0^2\boldsymbol{\mathcal{A}} = c\mathcal{P}_{\text{df}}\left[c\Psi\cdot\overline{\boldsymbol{\sigma}\Psi}\right] = c\mathcal{P}_{\text{df}}\left[\boldsymbol{J}[\Psi]\right], \qquad \operatorname{div}\boldsymbol{\mathcal{A}} = 0 & (5.4\text{b})\\ -\Delta\phi = |\Psi|^2, & (5.4\text{c})\\ \Psi(0,x) = \Psi_I(x), \quad \left(\boldsymbol{\mathcal{A}}(0,x), \partial_t\boldsymbol{\mathcal{A}}(0,x)\right) = \left(A_I(x), cA_I'(x)\right). & (5.4\text{d}) \end{cases}$$

Throughout this chapter, the $(H^r(\mathbb{T}^d))^m$ norm of a m-component function $z : \mathbb{T}^d \to \mathbb{C}^m$ with $z(x) = (z_1(x), \ldots, z_m(x))^\top$ shall be given through

$$\|z\|_r^2 = \|z_1\|_r^2 + \cdots + \|z_m\|_r^2.$$

Before we discuss our numerical experiments, we shall firstly construct reference time integration schemes for the MKG system (5.3) in Section 5.1 and for the MD system (5.4) in Section 5.2, based on the papers [9, 51, 54, 55] and [10, 15, 16].

Later on, Sections 5.3 and 5.4 are dedicated to testing our numerical schemes applied to the MKG and MD system respectively. Finally in Section 5.5, we numerically investigate energy and norm conservation properties of our methods.

Note that for all experiments and time integration schemes presented within this chapter we follow the method of lines, i.e. first we carry out the spatial discretization with the Fourier pseudo-spectral space discretization techniques which we presented in Section 3.5.3 (see also [44, 48, 66]). Afterwards, we perform the numerical time integration. For the rest of this thesis, talking about numerical approximations, we shall always refer to the full discretization in time and space. More precisely, according to Section 3.5.4 we denote

$$\text{an approximation to} \qquad \Delta z(t_n, x) \qquad \text{by} \qquad \Delta_M z^{n,M}$$

at a point $t_n \in [0, T]$ in time and on a discrete spatial grid with M grid points in each direction (see Section 3.5.3 and also [44]). For sake of easier notation we might leave out the sub-/superscript M (which indicates a discretization in space, see Section 3.5.3).

We proceed with the construction of a reference scheme for the MKG system (5.3).

5.1 Reference Solution for MKG

Based on [9, 51, 52, 54, 55], we derive exponential Gautschi-type time integration schemes which shall be used to compute reference solutions for the MKG system (5.3). We give a short description of these schemes in the subsequent subsections.

5.1.1 Description of Exponential Gautschi-type Solvers

In this section, we briefly discuss Gautschi-type exponential integrators for Klein–Gordon and wave type equations. The section is mainly based on [51, 52, 54]. Discretizing equations of type (5.1) in space with the Fourier techniques of Section 3.5.3, we obtain the system of ordinary differential equations

$$\begin{aligned} \partial_{tt}\psi^M(t) + c^2 \langle\nabla\rangle_{c,M}^2 \psi(t) &= c^2 \; f[\psi^M(t)] \quad \text{and} \\ \partial_{tt}\boldsymbol{\mathcal{A}}^M(t) + c^2 \langle\nabla\rangle_{0,M}^2 \boldsymbol{\mathcal{A}}^M(t) &= c \; h[\boldsymbol{\mathcal{A}}^M(t)], \end{aligned} \tag{5.5}$$

where

$$\psi^M(t) \approx (\psi(t, x_j))_{j\in\mathcal{Z}_M^d} \in \mathbb{C}^M \quad \text{and} \quad \boldsymbol{\mathcal{A}}^M(t) \approx (\boldsymbol{\mathcal{A}}(t, x_j))_{j\in\mathcal{Z}_M^d} \in \mathbb{R}^{d\cdot M}$$

are vectors in $\mathbb{C}^M$ and $\mathbb{R}^{d\cdot M}$, respectively. Furthermore, note that the discrete operators $c^2 \langle\nabla\rangle_{c,M}^2$ and $c^2 \langle\nabla\rangle_{0,M}^2$ can be identified with diagonal positive semi-definite matrices in $\mathbb{R}^{M\times M}$ due to their Fourier representation

$$\left(\widehat{\langle\nabla\rangle_{c,M}}\right)_k = \sqrt{|k|^2 + c^2}, \quad \text{for all } k \in \mathcal{Z}_M^d.$$

These matrices are of increasing norm as $M \to \infty$ and/or $c \to \infty$, since

$$\left\| c^2 \langle\nabla\rangle_{c,M}^2 \right\| \le K \cdot (c^2M^2 + c^4) \quad \text{and} \quad \left\| c^2 \langle\nabla\rangle_{0,M}^2 \right\| \le K \cdot (c^2M^2) \tag{5.6}$$

with a constant K independent of M or c, respectively.

Both systems in (5.5) can be written as the following second order differential equation in time (cf. [51, 54])

$$\ddot{y}(t) = -Ay(t) + g[y(t)], \quad y(0) = y_0, \quad \dot{y}(0) = y_0' \qquad \text{for } t \in [0, T] \tag{5.7}$$

with a positive semi-definite, symmetric matrix

$$A = \Omega^2 \in \mathbb{R}^{M\times M} \quad \text{of arbitrary large norm}$$

and where

$$\text{the function } g : \mathbb{C}^M \to \mathbb{C}^M \text{ is smooth.}$$

In [51], the authors proposed the following time integration scheme for (5.7)

$$\begin{pmatrix} y_{n+1} \\ y'_{n+1} \end{pmatrix} = \begin{pmatrix} \cos(\tau_{\text{ref}}\Omega) & \Omega^{-1}\sin(\tau_{\text{ref}}\Omega) \\ -\Omega\sin(\tau_{\text{ref}}\Omega) & \cos(\tau_{\text{ref}}\Omega) \end{pmatrix} \begin{pmatrix} y_n \\ y'_n \end{pmatrix} + \begin{pmatrix} \frac{1}{2}\tau_{\text{ref}}^2 \tilde{\Psi} g(\tilde{\Phi} y_n) \\ \frac{1}{2}\tau_{\text{ref}}\left(\tilde{\Psi}_0 g(\tilde{\Phi} y_n) + \tilde{\Psi}_1 g(\tilde{\Phi} y_{n+1})\right) \end{pmatrix}, \tag{5.8a}$$

where for even analytic filter functions $\tilde{\phi},\ \tilde{\psi},\ \tilde{\psi}_0,\ \tilde{\psi}_1$, we define

$$\tilde{\Psi} = \tilde{\psi}(\tau_{\text{ref}}\Omega), \quad \tilde{\Psi}_0 = \tilde{\psi}_0(\tau_{\text{ref}}\Omega), \quad \tilde{\Psi}_1 = \tilde{\psi}_1(\tau_{\text{ref}}\Omega), \quad \text{and} \quad \tilde{\Phi} = \tilde{\phi}(\tau_{\text{ref}}\Omega). \tag{5.8b}$$

The functions $\tilde{\phi},\ \tilde{\psi},\ \tilde{\psi}_0,\ \tilde{\psi}_1$ must satisfy $\tilde{\phi}(0) = \tilde{\psi}(0) = \tilde{\psi}_0(0) = \tilde{\psi}_1(0) = 1$ and must be bounded for $\operatorname{Re}(\xi) \geq 0, \xi \in \mathbb{C}$. Furthermore, they must satisfy the relations

$$\tilde{\psi}(\xi) = \operatorname{sinc}(\xi)\tilde{\psi}_1(\xi), \quad \tilde{\psi}_0(\xi) = \cos(\xi)\tilde{\psi}_1(\xi),$$

where $\operatorname{sinc}(\xi) = \sin(\xi)/\xi$. In [51, Section 4] several possible choices for $\tilde{\psi}$ and $\tilde{\phi}$ (and thus for $\tilde{\psi}_0, \tilde{\psi}_1$) are discussed, amongst which the functions

$$\tilde{\psi}(\xi) = \operatorname{sinc}^3(\xi), \quad \tilde{\psi}_0(\xi) = \cos(\xi)\operatorname{sinc}^2(\xi), \quad \tilde{\psi}_1(\xi) = \operatorname{sinc}^2(\xi), \quad \tilde{\phi}(\xi) = \operatorname{sinc}(\xi) \tag{5.8c}$$

were performing best. The authors proved in [51, Theorem 1] that the choice (5.8c) allows second order convergence bounds in time of the scheme (5.8), independent of the norm of A under the finite energy condition

$$\frac{1}{2}\|\dot{y}(t)\|^2 + \frac{1}{2}\|\Omega y(t)\|^2 \leq \frac{1}{2}\kappa^2 \qquad \text{for all } t \in [0, T]. \tag{5.9}$$

More precisely, if the exact solution y of (5.7) satisfies the latter condition, then

$$\begin{aligned} \|y(t_n) - y^n\| &\leq \tau_{\text{ref}}^2 K_1(\kappa, \|g\|, \|\partial_y g\|, \|\partial_{yy} g\|) \\ \|\dot{y}(t_n) - \dot{y}^n\| &\leq \tau_{\text{ref}} K_2(\kappa, \|g\|, \|\partial_y g\|, \|\partial_{yy} g\|) \end{aligned} \qquad \text{for all } t_n = n\tau_{\text{ref}},\ n = 0, 1, \ldots, T/\tau_{\text{ref}}, \tag{5.10}$$

where the constants K_1, K_2 explicitly depend on κ, $\|g\|$, $\|\partial_y g\|$, and $\|\partial_{yy} g\|$, but are independent of $\|\Omega\|$ and n. In particular, the bounds on $\Omega_0^2 := c^2 \langle\nabla\rangle_{0,M}^2$ and $\Omega_c^2 := c^2 \langle\nabla\rangle_{c,M}^2$ from (5.6) imply that

$$\left\|\Omega_c^2 \psi^M(t)\right\|^2 = \mathcal{O}\left(c^4\right) \quad \text{and} \quad \left\|\Omega_0^2 \boldsymbol{\mathcal{A}}^M(t)\right\|^2 = \mathcal{O}\left(c^2\right) \quad \text{for all } t \in [0, T],$$

which means that in (5.9) $\kappa = \kappa(c)$ can not be chosen independently of c. Considering the Klein–Gordon or wave type equations (5.5) and replacing in (5.7)

$$g[\cdot] = c^2 f[\cdot] \qquad \text{and} \qquad g[\cdot] = ch[\cdot],$$

this observation leads to an explicit dependence of the error bounds (5.10) on the large parameter c . More precisely, applying the method (5.8) to the Klein–Gordon and wave type equations (5.5) with step size τ_{ref} we obtain the convergence bounds

$$\begin{aligned} \left\|\psi^M(t_n) - \psi^{n,M}\right\| &\leq \tau_{\text{ref}}^2 c^4 K_\psi, \quad \text{(see ([9]))} \\ \left\|\boldsymbol{\mathcal{A}}^M(t_n) - \boldsymbol{\mathcal{A}}^{n,M}\right\| &\leq \tau_{\text{ref}}^2 c^2 K_{\boldsymbol{\mathcal{A}}}, \end{aligned} \tag{5.11}$$

with constants $K_{\boldsymbol{\mathcal{A}}}, K_\psi$ independent of c, M, n. In order to achieve numerical convergence of the method (5.8) applied to (5.5), we thus need step sizes $\tau_{\text{ref}} = \mathcal{O}\left(c^{-2}\right)$.

In the subsequent section, we adapt the Gautschi-type method (5.8) with the filter functions (5.8c) for the MKG system (5.3).

5.1.2 Exponential Gautschi-type Reference Scheme for MKG

We rewrite the MKG system (5.3) such that

$$\begin{cases} \partial_{tt}\psi + c^2 \langle\nabla\rangle_c^2 \psi = F_\psi[\phi,\psi,\partial_t\psi,\boldsymbol{\mathcal{A}}], & (5.12a)\\ \partial_{tt}\boldsymbol{\mathcal{A}} + c^2 \langle\nabla\rangle_0^2 \boldsymbol{\mathcal{A}} = F_{\boldsymbol{\mathcal{A}}}[\psi,\boldsymbol{\mathcal{A}}], & (5.12b)\\ \Delta\partial_t\phi = F_\rho[\psi,\boldsymbol{\mathcal{A}}], & (5.12c)\\ \big(\psi(0,x),\partial_t^{[\phi(0,x)]}\psi(0,x)\big) = \big(\psi_I(x),\langle\nabla\rangle_c\psi_I'(x)\big), & (5.12d)\\ \big(\boldsymbol{\mathcal{A}}(0),\partial_t\boldsymbol{\mathcal{A}}(0)\big) = \big(A_I(x),cA_I'(x)\big), & (5.12e) \end{cases}$$

with

$$\begin{aligned} F_\psi[\phi,\psi,\partial_t\psi,\boldsymbol{\mathcal{A}}] &= \Big(\phi^2\psi - 2i\phi\partial_t\psi - i(\partial_t\phi)\psi\Big) - |\boldsymbol{\mathcal{A}}|^2\psi - 2ic\boldsymbol{\mathcal{A}}\cdot\nabla\psi\\ F_{\boldsymbol{\mathcal{A}}}[\psi,\boldsymbol{\mathcal{A}}] &= c\mathcal{P}_{\mathrm{df}}\left[\mathrm{Re}\left(i\psi\overline{\nabla\psi}\right) - \frac{\boldsymbol{\mathcal{A}}}{c}|\psi|^2\right], \\ F_\rho[\psi,\boldsymbol{\mathcal{A}}] &= \mathrm{Re}\left(i\psi\overline{\Delta\psi} - \frac{2}{c}\psi\cdot\boldsymbol{\mathcal{A}}\cdot\overline{\nabla\psi}\right) \end{aligned} \qquad (5.12f)$$

exploiting the following observation. The structure of the Poisson equation (5.3c)

$$-\Delta\phi = -\mathrm{Re}\left(i\frac{\psi}{c}\cdot\overline{\partial_t^{[\phi]}\psi}\right) = -\frac{1}{c^2}\left(\mathrm{Re}\left(i\psi\overline{\partial_t\psi}\right) + \phi|\psi|^2\right) = \rho$$

does not allow us to simply apply the solution operator $\dot{\Delta}^{-1}$ as defined in (3.130). The reason is found in the presence of the nonlinearity $\phi|\psi|^2$ on the right hand side, which in Fourier space destroys the diagonal structure. Fortunately, we observe that we can transform this Poisson equation into an evolution equation by taking the first time derivative. Substituting the second time derivative $\overline{\partial_{tt}\psi}$ with the Klein–Gordon part (5.12a), we obtain a different Poisson equation for the time derivative $\partial_t\phi$, i.e.

$$\Delta\partial_t\phi = \mathrm{Re}\left(i\psi\overline{\Delta\psi} - \frac{2}{c}\psi\cdot\boldsymbol{\mathcal{A}}\cdot\overline{\nabla\psi}\right) =: F_\rho[\psi,\boldsymbol{\mathcal{A}}].$$

The findings of the previous section now allow us to construct a second order accurate in time reference method for the MKG system (5.12), based on [9, Theorem 9] and [51] as follows. Respecting the time step restriction $\tau_{\mathrm{ref}} \le Kc^{-2}$ from (5.2), we apply the exponential Gautschi-type integrator given in (5.8) together with the choice of the filter functions as in (5.8c) to the Klein–Gordon part (5.12a) and to the wave part (5.12b) of our MKG system. For the time integration of the Poisson evolution equation (5.12c), we choose the trapezoidal rule (also called Crank-Nicolson method, see for instance [33, Chapter 10.2 and 12.7]).

Description of the Reference Method for MKG

Considering the initial data in (5.12)

$$\begin{aligned} \psi(0) &= \psi_I, & \partial_t^{[\phi(0)]}\psi(0) &= c^{-1}(\partial_t\psi(0) + i\phi(0)\psi_I) = \langle\nabla\rangle_c\psi_I',\\ \boldsymbol{\mathcal{A}}(0) &= A_I, & \partial_t\boldsymbol{\mathcal{A}}(0) &= cA_I', \end{aligned}$$

and initially solving the Poisson equation for $\phi(0)$ at time $t = 0$

$$-\Delta\phi(0) = -\mathrm{Re}\left(i\frac{\psi_I}{c}\cdot\overline{\partial_t^{[\phi(0)]}\psi(0)}\right) = -\mathrm{Re}\left(i\frac{\psi_I}{c}\cdot\overline{\langle\nabla\rangle_c\psi_I'}\right),$$

we find the initial data

$$\begin{aligned} \psi(0) =&\psi_I =: \psi^0, \quad \partial_t\psi(0) = c\left\langle\nabla\right\rangle_c \psi_I' - i\phi(0)\psi_I =: \psi^{\prime,0}, \quad \phi(0) = \phi^0, \\ \boldsymbol{\mathcal{A}}(0) =&A_I =: \boldsymbol{\mathcal{A}}^0, \qquad \partial_t\boldsymbol{\mathcal{A}}(0) = cA_I' =: \boldsymbol{\mathcal{A}}^{\prime,0}. \end{aligned}$$

We define the filter functions in (5.8c) for $\chi \in \mathbb{R}$

$$\tilde{\Psi}^\chi = \operatorname{sinc}^3(c\left\langle\nabla\right\rangle_\chi), \quad \tilde{\Psi}_0^\chi = \cos(c\left\langle\nabla\right\rangle_\chi)\operatorname{sinc}^2(c\left\langle\nabla\right\rangle_\chi), \quad \tilde{\Psi}_1^\chi = \operatorname{sinc}^2(c\left\langle\nabla\right\rangle_\chi)$$

and $\tilde{\Phi}^\chi = \operatorname{sinc}(c\left\langle\nabla\right\rangle_\chi)$. Then, the reference scheme for solving the MKG system (5.12) with a small time step size τ_{ref} is given through

$$\begin{aligned} \psi^{n+1} =& \cos(\tau_{\text{ref}}c\left\langle\nabla\right\rangle_c)\psi^n + \tau_{\text{ref}}\operatorname{sinc}(\tau_{\text{ref}}c\left\langle\nabla\right\rangle_c)\psi^{\prime,n} + \tfrac{\tau_{\text{ref}}^2}{2}\tilde{\Psi}^c F_\psi[\phi^n, \tilde{\Phi}^c\psi^n, \tilde{\Phi}^c\psi^{\prime,n}, \boldsymbol{\mathcal{A}}^n] \\ \boldsymbol{\mathcal{A}}^{n+1} =& \cos(\tau_{\text{ref}}c\left\langle\nabla\right\rangle_0)\boldsymbol{\mathcal{A}}^n + \tau_{\text{ref}}\operatorname{sinc}(\tau_{\text{ref}}c\left\langle\nabla\right\rangle_0)\boldsymbol{\mathcal{A}}^{\prime,n} + \tfrac{\tau_{\text{ref}}^2}{2}\tilde{\Psi}^0 F_{\boldsymbol{\mathcal{A}}}[\psi^n, \tilde{\Phi}^0\boldsymbol{\mathcal{A}}^n] \\ \boldsymbol{\mathcal{A}}^{\prime,n+1} =& -c\left\langle\nabla\right\rangle_0\sin(\tau_{\text{ref}}c\left\langle\nabla\right\rangle_0)\boldsymbol{\mathcal{A}}^n + \cos(\tau_{\text{ref}}c\left\langle\nabla\right\rangle_0)\boldsymbol{\mathcal{A}}^{\prime,n} \\ &+ \tfrac{\tau_{\text{ref}}}{2}\Big(\tilde{\Psi}_0^0 F_{\boldsymbol{\mathcal{A}}}[\psi^n, \tilde{\Phi}^0\boldsymbol{\mathcal{A}}^n] + \tilde{\Psi}_1^0 F_{\boldsymbol{\mathcal{A}}}[\psi^{n+1}, \tilde{\Phi}^0\boldsymbol{\mathcal{A}}^{n+1}]\Big) \\ \phi^{n+1} =& \phi^n + \tfrac{\tau_{\text{ref}}}{2}\dot{\Delta}^{-1}\Big(F_\rho[\tilde{\Phi}^c\psi^n, \boldsymbol{\mathcal{A}}^n] + F_\rho[\tilde{\Phi}^c\psi^{n+1}, \boldsymbol{\mathcal{A}}^{n+1}]\Big) \\ \psi^{\prime,n+1/2} =& -c\left\langle\nabla\right\rangle_c\sin(\tau_{\text{ref}}c\left\langle\nabla\right\rangle_c)\psi^n + \cos(\tau_{\text{ref}}c\left\langle\nabla\right\rangle_c)\psi^{\prime,n} \\ \psi^{\prime,n+1} =& -c\left\langle\nabla\right\rangle_c\sin(\tau_{\text{ref}}c\left\langle\nabla\right\rangle_c)\psi^n + \cos(\tau_{\text{ref}}c\left\langle\nabla\right\rangle_c)\psi^{\prime,n} \\ &+ \tfrac{\tau_{\text{ref}}}{2}\Big(\tilde{\Psi}_0^c F_\psi[\phi^n, \tilde{\Phi}^c\psi^n, \tilde{\Phi}^c\psi^{\prime,n}, \boldsymbol{\mathcal{A}}^n] + \tilde{\Psi}_1^c F_\psi[\phi^{n+1}, \tilde{\Phi}^c\psi^{n+1}, \tilde{\Phi}^c\psi^{\prime,n+1/2}, \boldsymbol{\mathcal{A}}^{n+1}]\Big). \end{aligned} \tag{5.13a}$$

where we shortly write

$$\Big(\psi^{n+1}, \psi^{\prime,n+1}, \phi^{n+1}, \boldsymbol{\mathcal{A}}^{n+1}, \boldsymbol{\mathcal{A}}^{\prime,n+1}\Big)^\top := \Phi_{\text{ref,MKG}}^{\tau_{\text{ref}}}\big[\psi^n, \psi^{\prime,n}, \phi^n, \boldsymbol{\mathcal{A}}^n, \boldsymbol{\mathcal{A}}^{\prime,n}\big]. \tag{5.13b}$$

Note that this method is fully explicit.

In the subsequent section, we discuss reference schemes for the numerical solution of the reduced MD system (5.4).

5.2 Reference Solution for MD in Lower Dimensions

Based on [10, 14, 16, 51, 87], we now propose a method for computing a numerical reference solution for the Maxwell–Dirac system (2.36). Note that in [10] the authors proposed and analysed a similar scheme for the time integration of the MD system in the Lorenz gauge.

We consider the MD system in

$$\text{space dimensions} \quad d = d_{\text{low}} := 1, 2.$$

Remark 2.5 then allows us to reduce the MD system (2.36) with the four-spinor Dirac solution $\psi(t,x) \in \mathbb{C}^4$ to the MD system (5.14) below with the two-spinor Dirac solution $\mathit{\Psi}(t,x) = (\psi_1(t,x), \psi_4(t,x))^\top \in \mathbb{C}^2$

and potentials $(\phi(t,x), \boldsymbol{\mathcal{A}}(t,x))^\top \in \mathbb{R}^{1+d_{\text{low}}}$, i.e.

$$\begin{cases} i\partial_t \Psi = \left(-ic\sum_{j=1}^{d_{\text{low}}} \boldsymbol{\sigma}_j \partial_j + c^2\boldsymbol{\sigma}_3\right)\Psi + \left(\phi - \sum_{j=1}^{d_{\text{low}}} \boldsymbol{\sigma}_j A_j\right)\Psi & \text{(5.14a)} \\ \partial_{tt}\boldsymbol{\mathcal{A}} + c^2 \langle\nabla\rangle_0^2 \boldsymbol{\mathcal{A}} = c\mathcal{P}_{\text{df}}\left[c\Psi\cdot\overline{\boldsymbol{\sigma}\Psi}\right] = c\mathcal{P}_{\text{df}}\left[\boldsymbol{J}[\Psi]\right], & \text{(5.14b)} \\ -\Delta\phi = |\Psi|^2, & \text{(5.14c)} \\ \Psi(0,x) = \Psi_I(x), \quad \big(\boldsymbol{\mathcal{A}}(0,x), \partial_t\boldsymbol{\mathcal{A}}(0,x)\big) = \big(A_I(x), cA_I'(x)\big), & \text{(5.14d)} \end{cases}$$

on the finite time interval $t \in [0,T]$ and equipped with periodic boundary conditions on the torus $x \in \mathbb{T}^{d_{\text{low}}}$. Note that the ideas for the construction of the reference method for MD, which shall be described within this chapter, easily transfer to the higher dimensional case ([10, 14–16]).

The basis for the numerical time integration of (5.14) lies in approximately solving the Dirac part (5.14a) with solution $\Psi(t,x) \in \mathbb{C}^2$ with a Time-Splitting Fourier Pseudo-spectral (TSFP) method ([10, 15, 16]) which is described in Section 5.2.1 below. The wave equation (5.14b) with solution $\boldsymbol{\mathcal{A}}$ is solved with an exponential Gautschi-type time integration scheme ([9, 10, 51], see also Section 5.1.1) and for the numerical solution of the Poisson equation (5.14c), we may exploit standard Fourier techniques from Section 3.5.3, using the solution operator $\dot{\Delta}^{-1}$ given in Appendix A.3.

In [15, 16] the authors have given rigorous convergence bounds for the TSFP scheme (see (5.24) below) applied to (5.14a) with a step size τ_{ref}. According to [16, Section 4]

$$\text{the TSFP scheme satifies error bounds of order} \quad \mathcal{O}\left(\tau_{\text{ref}}^2 c^4\right), \tag{5.15}$$

which is verified later by numerical experiments (see Experiment 5.3 and Fig. 5.7c).

Due to these error bounds, we require very small step sizes satisfying

$$\tau_{\text{ref}} \le Kc^{-2} \qquad \text{with a constant } K \text{ independent of } c \text{ and } \tau_{\text{ref}}. \tag{5.16}$$

in order to obtain a feasible reference solution of the MD system (5.14).

In the subsequent Section 5.2.1 we describe the TSFP Dirac solver in more detail. Afterwards, in Section 5.2.2, we formulate a reference time integration scheme for the numerical solution of the MD system (5.14).

5.2.1 Description of the TSFP Dirac Solver

Based on [10, 15, 16, 87], we now describe a Time-Splitting Fourier Pseudo-spectral (TSFP) time integration scheme for a Dirac equation of type (5.14a) together with the Poisson equation (5.14c)

$$\begin{cases} i\partial_t \Psi = \left(-ic\sum_{j=1}^{d_{\text{low}}} \boldsymbol{\sigma}_j \partial_j + c^2\boldsymbol{\sigma}_3\right)\Psi + \left(\phi - \sum_{j=1}^{d_{\text{low}}} \boldsymbol{\sigma}_j A_j\right)\Psi \\ -\Delta\phi = |\Psi|^2, \qquad \Psi(0,x) = \Psi_I(x). \end{cases}$$

We naturally split the system (cf. Section 3.5.1) into the linear subproblem

$$i\partial_t \Psi = \left(-ic\sum_{j=1}^{d_{\text{low}}} \boldsymbol{\sigma}_j \partial_j + c^2\boldsymbol{\sigma}_3\right)\Psi =: H_{0,\text{low}}\Psi, \quad \Psi(0) = \Psi_I \tag{5.17a}$$

with exact flow $\varphi^{\tau_{\text{ref}}}_{H_{0,\text{low}}}(\Psi_I)$, and the potential subproblem

$$\begin{cases} i\partial_t \Psi = \left(\phi - \sum_{j=1}^{d_{\text{low}}} \boldsymbol{\sigma}_j A_j\right)\Psi, \quad \Psi(0) = \Psi_I \\ -\Delta\phi = |\Psi|^2 = |\Psi_I|^2 = \text{const.} \end{cases} \tag{5.17b}$$

with exact flow $\varphi^{\tau_{\text{ref}}}_P(\Psi_I)$ and observe that in the latter subproblem (5.17b) the potential $\phi(t) = \phi(0)$ is constant. This observation is verified using that by (1.19) $\sigma_j^\top = \overline{\sigma_j}$ for all $j = 1, \ldots, d_{\text{low}}$ and that $\big(\phi(t,x), \boldsymbol{\mathcal{A}}(t,x)\big) \in \mathbb{R}^{1+d_{\text{low}}}$ are real potentials and plugging these identities into

$$\partial_t |\Psi| = \partial_t\Psi \cdot \overline{\Psi} + \Psi \cdot \overline{\partial_t \Psi} = -i\Psi^\top \left(\phi - \sum_{j=1}^{d_{\text{low}}} \boldsymbol{\sigma}_j A_j\right)^\top \overline{\Psi} + i\Psi^\top \overline{\left(\phi - \sum_{j=1}^{d_{\text{low}}} \boldsymbol{\sigma}_j A_j\right)}\,\overline{\Psi} = 0. \tag{5.17c}$$

In the following we discuss the (numerical) solution of the subproblems (5.17a) and (5.17b), respectively.

Solution of the Linear Subproblem (5.17a)

This section is mainly based on [10, 15, 16, 87]. According to [87, Chapter 1.2.2], the exact solution of the linear subproblem (5.17a) is given through

$$\varphi^{\tau_{\text{ref}}}_{H_{0,\text{low}}}(\Psi_I) = e^{-i\tau_{\text{ref}} H_{0,\text{low}}}\Psi_I. \tag{5.18}$$

Our aim is now to derive a scheme, which efficiently computes the operator $e^{-i\tau_{\text{ref}} H_{0,\text{low}}}$ exactly in time. The latter can be carried out efficiently using a diagonalisation of $H_{0,\text{low}}$ in Fourier space (see [10, 15, 16, 87]). Recall that the operator $H_{0,\text{low}}$ belongs to the reduced Dirac equation (5.17a). Considering the full (unreduced) Dirac equation (2.35) we have that

$$i\partial_t \psi = \left(-ic\sum_{j=1}^{d} \boldsymbol{\alpha}_j \partial_j + c^2\boldsymbol{\beta}\right)\psi =: H_0\psi, \quad \psi(0) = \psi_I,$$

where in particular the operator H_0 and its corresponding Fourier symbol $\widehat{H_0}(k)$ for $k \in \mathbb{Z}^d$ are given through ([87, Chapter 1.4],[10, 15, 16])

$$H_0 = \begin{pmatrix} c^2\mathcal{I}_2 & c\sum_{j=1}^d \boldsymbol{\sigma}_j(-i\partial_j) \\ c\sum_{j=1}^d \boldsymbol{\sigma}_j(-i\partial_j) & -c^2\mathcal{I}_2 \end{pmatrix}, \quad \widehat{H_0}(k) = \begin{pmatrix} c^2\mathcal{I}_2 & c\sum_{j=1}^d \boldsymbol{\sigma}_j k^j \\ c\sum_{j=1}^d \boldsymbol{\sigma}_j k^j & -c^2\mathcal{I}_2 \end{pmatrix}. \tag{5.19}$$

Exploiting that by (1.19) $\boldsymbol{\sigma}_j^\top = \overline{\boldsymbol{\sigma}_j}$, $j = 1, \ldots, d$, the latter can by diagonalised by a diagonal matrix $\widehat{D}(k)$ and unitary matrices $\widehat{S}^{\pm}(k)$ with $\widehat{S}^{+}(k) = \overline{\widehat{S}^{-}}^\top(k)$ and $\widehat{S}^{+}(k) \cdot \widehat{S}^{-}(k) = \mathcal{I}_4$ for $k = (k^1, \ldots, k^d)^\top \in \mathbb{Z}^d$, where

$$\widehat{D}(k) := \operatorname{diag}(+c\langle k\rangle_c \mathcal{I}_2, -c\langle k\rangle_c \mathcal{I}_2), \qquad \langle k\rangle_c = \sqrt{|k|^2 + c^2}$$

$$\widehat{S}^{\pm}(k) := \frac{1}{\sqrt{2}}\begin{pmatrix} a(k)\mathcal{I}_2 & \mp\sum_{j=1}^d \frac{\boldsymbol{\sigma}_j k^j}{\langle k\rangle_c a(k)} \\ \pm\sum_{j=1}^d \frac{\boldsymbol{\sigma}_j k^j}{\langle k\rangle_c a(k)} & a(k)\mathcal{I}_2 \end{pmatrix}, \quad a(k) := \sqrt{1 + c\langle k\rangle_c^{-1}}.$$

Then we find from [87, Chapter 1.4] and [15, 16]

$$\widehat{H_0}(k) = \widehat{S}^{+}(k) \cdot \widehat{D}(k) \cdot \widehat{S}^{-}(k) \qquad \text{for all } k \in \mathbb{Z}^d.$$

Recall that by (1.21) the Pauli matrices $\boldsymbol{\sigma}_j, j = 1, 2, 3$ read

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Due to the anti-diagonal structure of the matrices $\boldsymbol{\sigma}_j,\ j = 1, \ldots, d_{\text{low}}$ with $d_{\text{low}} = 1, 2$ given in (1.21), the operator $\widehat{H_0}(k)$ in (5.19) can be written as the sum of a 4×4 diagonal and a 4×4 anti-diagonal matrix, respectively. Thus, we retain $H_{0,\text{low}}$ from H_0 by crossing out each the second and third row and column in H_0 and $\widehat{H_0}(k)$ respectively. Then also crossing out the second and third row and column in $\widehat{S}^{\pm}(k)$ and $\widehat{D}(k)$ allows us to simply write down the diagonalisation of $H_{0,\text{low}}$ as ([10, 15, 16, 87])

$$\widehat{H_{0,\text{low}}}(k) = \widehat{S_{\text{low}}}^{+}(k) \cdot \widehat{D_{\text{low}}}(k) \cdot \widehat{S_{\text{low}}}^{-}(k), \qquad \text{for all } k = (k^1, \ldots, k^{d_{\text{low}}})^\top \in \mathbb{Z}^{d_{\text{low}}} \tag{5.21a}$$

with matrices $\widehat{D_{\text{low}}}(k) = \operatorname{diag}(c\,\langle k \rangle_c, -c\,\langle k \rangle_c)$ and

$$\widehat{S_{\text{low}}}^{\pm}(k) = \frac{1}{\sqrt{2}} \begin{pmatrix} a(k) & \mp \dfrac{k^1 - ik^2}{\langle k \rangle_c\, a(k)} \\ \pm \dfrac{k^1 + ik^2}{\langle k \rangle_c\, a(k)} & a(k) \end{pmatrix}, \quad a(k) := \sqrt{1 + c\,\langle k \rangle_c^{-1}}. \tag{5.21b}$$

In case of $d_{\text{low}} = 1$, we set $k^2 = 0$ in the latter relation (5.21).

The diagonalisation (5.21) now allows us to compute the exact flow $\varphi_{H_{0,\text{low}}}^{\tau_{\text{ref}}}$ (5.18) of the linear subproblem (5.17a) in its Fourier representation, via the diagonalisation (5.21), i.e. for $k \in \mathbb{Z}^d$

$$\left(\varphi_{H_{0,\text{low}}}^{\tau_{\text{ref}}}(\Psi_I)\right)_k = \widehat{\left(e^{-itH_{0,\text{low}}}\Psi_I\right)}_k = \widehat{S_{\text{low}}}^{+}(k) \cdot e^{-it\widehat{D_{\text{low}}}(k)} \cdot \widehat{S_{\text{low}}}^{-}(k) \left(\widehat{\Psi_I}\right)_k.$$

Note that this diagonalisation coincides with that from [10, 15, 16]. Applying the inverse Fourier transform to the latter relation finally yields the exact solution in time of the linear subproblem (5.17a).

Next we discuss the solution of the potential subproblem (5.17b).

Solution of the Potential Subproblem (5.17b)

This section is based on [10, 15, 16]. The second subproblem (5.17b) is solved exactly by the flow

$$\varphi_P^{\tau_{\text{ref}}}(\Psi(t_n)) = e^{-i(\int_0^{\tau_{\text{ref}}} \phi(t_n+s) - \sum_{j=1}^{d_{\text{low}}} \boldsymbol{\sigma}_j A_j(t_n+s) ds)} \Psi(t_n). \tag{5.22}$$

Recall that by (5.17c) within this subproblem (5.17b) the scalar potential ϕ is constant, i.e.

$$\phi(t) = \phi(0) \qquad \text{is constant for all times } t.$$

Furthermore, we use the second order accurate trapezoidal rule[①] (also called Crank-Nicolson method, see for instance [33, Chapter 10.2 and 12.7]) in order to approximate the integrals $\int_0^{\tau_{\text{ref}}} A_j(t_n + s)ds$ for $j = 1, \ldots, d_{\text{low}}$, i.e. we have

$$\begin{aligned} \int_0^{\tau_{\text{ref}}} \phi(t_n + s)ds &= \tau_{\text{ref}}\phi(t_n) =: I_\phi^n, \\ \int_0^{\tau_{\text{ref}}} A_j(t_n + s)ds &\approx \frac{\tau_{\text{ref}}}{2}(A_j(t_n) + A_j(t_n + \tau_{\text{ref}})) =: I_{A_j}^n, \quad j = 1, \ldots, d_{\text{low}}. \end{aligned}$$

[①] Note that in [16] the authors suggest to use the fourth order Simpson quadrature rule (see for instance [33, Chapter 10.2]) for the approximation of the integrals. For our purpose of constructing a second order TSFP method [10, 15, 16] for the integration of the MD system (5.14), the second order accuracy of the trapezoidal rule is sufficient.

This allows us to write (in lower dimensions $d_{\text{low}} = 1, 2$)

$$\int_0^{\tau_{\text{ref}}} \phi(t_n + s) - \sum_{j=1}^{d_{\text{low}}} \boldsymbol{\sigma}_j A_j(t_n + s) ds \approx \begin{pmatrix} I_\phi^n & -(I_{A_1}^n - iI_{A_2}^n) \\ -(I_{A_1}^n + iI_{A_2}^n) & I_\phi^n \end{pmatrix},$$

where for the case $d_{\text{low}} = 1$ we set $I_{A_2} = 0$. One may check the following diagonalisation of the latter matrix (see for instance [16, Appendix 3])

$$\begin{pmatrix} I_\phi^n & -(I_{A_1}^n - iI_{A_2}^n) \\ -(I_{A_1}^n + iI_{A_2}^n) & I_\phi^n \end{pmatrix} = P_n \cdot \Lambda_n \cdot \overline{P_n}^\top$$

with matrices

$$P_n := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \frac{(I_{A_1}^n - iI_{A_2}^n)}{|I_A^n|} \\ \frac{-(I_{A_1}^n + iI_{A_2}^n)}{|I_A^n|} & 1 \end{pmatrix} \quad \text{and} \quad \Lambda_n = \begin{pmatrix} I_\phi^n + |I_A^n| & \\ & I_\phi^n - |I_A^n| \end{pmatrix},$$

where $|I_A^n| = \sqrt{|I_{A_1}^n|^2 + |I_{A_2}^n|^2}$.

This diagonalisation allows us to approximate the flow $\varphi_P^{\tau_{\text{ref}}}(\Psi(t_n))$ given in (5.22) above by

$$\Phi_P^{\tau_{\text{ref}}}[\Psi(t_n), \phi(t_n), \boldsymbol{\mathcal{A}}(t_n), \boldsymbol{\mathcal{A}}(t_{n+1})] := P_n \cdot e^{-i\Lambda_n} \overline{P_n}^\top \Psi(t_n) \approx \varphi_P^{\tau_{\text{ref}}}(\Psi(t_n)), \tag{5.23}$$

which has been proposed before in [10, 15, 16].

Gathering the exact flow $\varphi_{H_{0,\text{low}}}^{\tau_{\text{ref}}}$ of the linear subproblem (5.17a) given in (5.18) and the numerical flow $\Phi_P^{\tau_{\text{ref}}}$ of subproblem (5.17b) given in (5.23), we finally obtain the following Time-Splitting Fourier Pseudo-spectral (TSFP) method ([10, 15, 16]) for the numerical time integration of the Dirac equation (5.14a)

$$\Psi^{n+1} = \Phi_{\text{TSFP}}^{\tau_{\text{ref}}}[\Psi^n, \phi^n, \boldsymbol{\mathcal{A}}^n, \boldsymbol{\mathcal{A}}^{n+1}] =: \varphi_{H_{0,\text{low}}}^{\tau_{\text{ref}}/2} \circ \Phi_P^{\tau_{\text{ref}}} \circ \varphi_{H_{0,\text{low}}}^{\tau_{\text{ref}}/2}[\Psi^n, \phi^n, \boldsymbol{\mathcal{A}}^n, \boldsymbol{\mathcal{A}}^{n+1}]. \tag{5.24}$$

Note that the latter (TSFP) method is an exponential Strang splitting method for which the analysis in [16] provided error bounds of order $\mathcal{O}(\tau^2 c^4)$. These results suggest that we need very small time step sizes $\tau_{\text{ref}} \leq Kc^{-2}$ in order to retain a feasible reference solution.

We are now ready to formulate a numerical reference method for the numerical solution of the MD system (5.14). We proceed in the subsequent section.

5.2.2 TSFP-Gautschi Reference Scheme for MD

Based on [9, 10, 15, 16, 51, 87] and exploiting the results of the previous sections, we formulate a reference method for the numerical solution of the reduced Maxwell–Dirac system (5.14) in Coulomb gauge. Note that in [10] the authors proposed and analysed a similar scheme for the time integration of the MD system in Lorenz gauge.

We consider the initial data given in (5.14)

$$\begin{aligned} \Psi(0) &= \Psi_I =: \Psi^0, \quad \phi(0) = -\dot{\Delta}^{-1} |\Psi^0|^2 =: \phi^0, \\ \boldsymbol{\mathcal{A}}(0) &= A_I =: \boldsymbol{\mathcal{A}}^0, \quad \partial_t \boldsymbol{\mathcal{A}}(0) = cA_I' =: \boldsymbol{\mathcal{A}}'^{,0}. \end{aligned}$$

For the definition of the solution operator $\dot{\Delta}^{-1}$ see (A.4) in Appendix A.3.

The idea is now to use the TSFP scheme described in the previous section for the numerical time integration of the Dirac part (5.4a) of the reduced MD system. We furthermore numerically solve the wave equation (5.4b) for the vector potential $\boldsymbol{\mathcal{A}}$ by the exponential Gautschi-type method (5.8) with the filter functions in (5.8c)

$$\Psi^0 = \operatorname{sinc}^3(c\,\langle\nabla\rangle_0), \quad \Psi_0^0 = \cos(c\,\langle\nabla\rangle_0)\operatorname{sinc}^2(c\,\langle\nabla\rangle_0), \quad \Psi_1^0 = \operatorname{sinc}^2(c\,\langle\nabla\rangle_0)$$

and $\tilde{\Phi}^0 = \operatorname{sinc}(c\,\langle\nabla\rangle_0)$.

Then the TSFP-Gautschi reference scheme for solving the reduced MD system (5.14) is given through

$$\begin{aligned}
\boldsymbol{\mathcal{A}}^{n+1} &= \cos(\tau_{\text{ref}} c\,\langle\nabla\rangle_0)\boldsymbol{\mathcal{A}}^n + \tau_{\text{ref}}\operatorname{sinc}(\tau_{\text{ref}} c\,\langle\nabla\rangle_0)\boldsymbol{\mathcal{A}}^{\prime,n} + c\frac{\tau_{\text{ref}}^2}{2}\Psi^0\mathcal{P}_{\text{df}}\left[\boldsymbol{J}[\tilde{\Phi}^0\mathit{\Psi}^n]\right] \\
\mathit{\Psi}^{n+1} &= \Phi_{\text{TSFP}}^{\tau_{\text{ref}}}[\mathit{\Psi}^n, \phi^n, \boldsymbol{\mathcal{A}}^n, \boldsymbol{\mathcal{A}}^{n+1}] \\
\boldsymbol{\mathcal{A}}^{\prime,n+1} &= -c\,\langle\nabla\rangle_0\sin(\tau_{\text{ref}} c\,\langle\nabla\rangle_0)\boldsymbol{\mathcal{A}}^n + \cos(\tau_{\text{ref}} c\,\langle\nabla\rangle_0)\boldsymbol{\mathcal{A}}^{\prime,n} \\
&\qquad + c\frac{\tau_{\text{ref}}}{2}\left(\Psi_0^0\mathcal{P}_{\text{df}}\left[\boldsymbol{J}[\tilde{\Phi}^0\mathit{\Psi}^n]\right] + \Psi_1^0\mathcal{P}_{\text{df}}\left[\boldsymbol{J}[\tilde{\Phi}^0\mathit{\Psi}^{n+1}]\right]\right) \\
\phi^{n+1} &= -\dot{\Delta}^{-1}\left|\mathit{\Psi}^{n+1}\right|^2
\end{aligned} \tag{5.25a}$$

where we may shortly write

$$\left(\mathit{\Psi}^{n+1}, \phi^{n+1}, \boldsymbol{\mathcal{A}}^{n+1}, \boldsymbol{\mathcal{A}}^{\prime,n+1}\right)^\top := \Phi_{\text{ref,MD}}^{\tau_{\text{ref}}}\left[\mathit{\Psi}^n, \phi^n, \boldsymbol{\mathcal{A}}^n, \boldsymbol{\mathcal{A}}^{\prime,n}\right]. \tag{5.25b}$$

Note that the method $\Phi_{\text{ref,MD}}^{\tau_{\text{ref}}}$ given in (5.25) is fully explicit.

In the subsequent Sections 5.3 and 5.4, we underline by numerical experiments the theoretical results of the previous chapters for the asymptotic nonrelativistic limit approximation (see Theorem 3.15) and for the uniformly accurate time integration scheme (see Theorem 4.7 for MKG and Theorem 4.8 for MD respectively). We start off with experiments for the MKG system.

5.3 Maxwell–Klein–Gordon Experiments

In this section we consider the Maxwell–Klein–Gordon system (2.20) with exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ corresponding to the initial data

$$(\boldsymbol{\mathcal{A}}(0), \partial_t\boldsymbol{\mathcal{A}}(0))^\top = (A_I, cA_I')^\top \qquad \text{and} \qquad (\psi(0), \partial_t^{[\phi(0)]}\psi(0))^\top = (\psi_I, \langle\nabla\rangle_c\,\psi_I')^\top,$$

where the initial data $\psi_I, \psi_I', A_I, A_I'$ can be expanded such that (cf. (3.9b))

$$\begin{aligned}
\psi_I &= \psi_{I,0} + c^{-1}\psi_{I,1} + \sum_{n=2}^{\infty} c^{-n}\psi_{I,n}, &\qquad \psi_I' &= \psi_{I,0}' + c^{-1}\psi_{I,1}' + \sum_{n=2}^{\infty} c^{-n}\psi_{I,n}', \\
A_I &= A_{I,0} + c^{-1}A_{I,1} + \sum_{n=2}^{\infty} c^{-n}A_{I,n}, &\qquad A_I' &= A_{I,0}' + c^{-1}A_{I,1}' + \sum_{n=2}^{\infty} c^{-n}A_{I,n}'.
\end{aligned}$$

Our aim is now to numerically confirm the convergence results $\mathcal{O}\left(\tau^2 + c^{-N}\right)$ for $N \in \mathbb{N}$ of the asymptotic nonrelativistic limit approximation for $c \gg 1$ from Theorem 3.15 and the convergence result $\mathcal{O}(\tau)$ uniformly in $c \geq 1$ from Theorem 4.7 of the numerical approximation obtained with the uniformly accurate time integration scheme (the "twisted scheme"). Additionally, we test the exponential Gautschi-type reference time integration scheme ([9, 51, 54]) which we discussed in Section 5.1.2.

In the subsequent subsections, we give s short recap of the nonrelativistic limit time integration scheme from Section 3.5 and the uniformly accurate time integration scheme from Section 4.2.

Repetition of the Nonrelativistic Limit Time Integration Scheme for MKG

We consider the numerical approximation in the nonrelativistic limit regime $c \gg 1$ to $\psi(t_n)$, i.e. (cf. (3.33))

$$\begin{aligned}\psi_\infty^{(0),n} &= \psi_0^n, \\ \psi_\infty^{(1),n} &= \psi_0^n + c^{-1}\psi_1^n,\end{aligned} \qquad \text{where} \qquad \psi_j^n = \frac{1}{2}\left(e^{ic^2t_n}u_j^n + e^{-ic^2t_n}\overline{v_j^n}\right) \qquad \text{for } j = 0, 1.$$

Recall that we obtain the numerical approximations

$$w_0^n = (u_0^n, v_0^n)^\top \quad \text{and} \quad w_1^n = (u_1^n, v_1^n)^\top \quad \text{with the schemes } \Phi^\tau_{w_0,\mathrm{Strang}} \text{ and } \Phi^\tau_{w_1,\mathrm{Strang}},$$

to the solutions $w_0(t_n)$ and $w_1(t_n)$ of the limit systems (3.109) and (3.111). These schemes were given in (3.110) and (3.117), respectively, with

$$\begin{aligned} w_0^n &= \left(\Phi^\tau_{w_0,\mathrm{Strang}}\right)^n (w_{I,0}) \quad \text{with} \quad w_{I,0} = \begin{pmatrix} \psi_{I,0} - i\psi'_{I,0} \\ \overline{\psi_{I,0} - i\psi'_{I,0}} \end{pmatrix} \qquad \text{and} \\ w_1^n &= \left(\Phi^\tau_{w_1,\mathrm{Strang}}\right)^n (w_{I,1}) \quad \text{with} \quad w_{I,1} = \begin{pmatrix} \psi_{I,1} - i\psi'_{I,1} \\ \overline{\psi_{I,1} - i\psi'_{I,1}} \end{pmatrix}. \end{aligned}$$

Moreover, we obtain approximations to $\phi(t_n)$ in the nonrelativistic limit regime $c \gg 1$ via (cf. (3.33))

$$\phi_\infty^{(0),n} = \phi_0^n, \qquad \phi_\infty^{(1),n} = \phi_0^n + c^{-1}\phi_1^n,$$

where ϕ_0^n and ϕ_1^n solve the Poisson equations (see Theorem 3.15 and cf. (3.111), (3.112))

$$-\Delta\phi_0^n = -\frac{1}{4}(|u_0^n|^2 - |v_0^n|^2) \qquad \text{and} \qquad -\Delta\phi_1^n = \frac{1}{2}\,\mathrm{Re}\left(-u_0^n \cdot \overline{u_1^n} + v_0^n \cdot \overline{v_1^n}\right).$$

Approximations to $\boldsymbol{\mathcal{A}}(t_n)$ and $\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n)$ are given through (see Theorem 3.15)

$$\begin{aligned} \boldsymbol{\mathcal{A}}_\infty^{(0),n} = \boldsymbol{\mathcal{A}}_0^n &= \cos(ct_n \langle\nabla\rangle_0)A_{I,0} + t_n \operatorname{sinc}(ct_n\langle\nabla\rangle_0)cA_{I,0} \quad \text{and} \\ \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_\infty^{(0),n} = \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_0^n &= -c\langle\nabla\rangle_0 \sin(ct_n\langle\nabla\rangle_0)A_{I,0} + \cos(ct_n\langle\nabla\rangle_0)cA_{I,0}. \end{aligned} \tag{5.26}$$

Next, we recall the uniformly accurate time integration scheme from Section 4.2 based on the "twisted variables" (see also [18] for the case of the nonlinear Klein–Gordon equation).

Repetition of the Uniformly Accurate "Twisted" Time Integration Scheme for MKG

Recall that by Theorem 4.7 the numerical solutions

$$\begin{aligned} \psi_*^n &= \frac{1}{2}(e^{ic^2t_n}u_*^n + e^{-ic^2t_n}\overline{v_*^n}), \qquad\qquad \boldsymbol{\mathcal{A}}_*^n = \frac{1}{2}(\mathfrak{a}_*^{\gamma,n} + \overline{\mathfrak{a}_*^{\gamma,n}}) \\ \phi_*^{\mathrm{tot},n} &= \phi_*^{0,n} + e^{2ic^2t_n}\phi_*^{2,n} + e^{-2ic^2t_n}\overline{\phi_*^{2,n}} \end{aligned}$$

are uniformly accurate in $c \geq 1$ approximations to the exact solution $(\psi(t_n), \phi(t_n), \boldsymbol{\mathcal{A}}(t_n))^\top$ of the MKG system (2.20). Thereby, gathering

$$w_*^n = (u_*^n, v_*^n)^\top, \quad \mathfrak{a}_*^{\gamma,n} \qquad \text{obtained with the “twisted scheme” } \Psi_*^\tau \text{ given in (4.39)}$$

and $\phi_*^{0,n}$ and $\phi_*^{2,n}$ being the solution of the Poisson equations (see (4.40a))

$$\begin{aligned} -\Delta\phi_*^{0,n} &= -\frac{1}{4c}\operatorname{Re}\left(u_*^n \langle\nabla\rangle_c \overline{u_*^n} - \overline{v_*^n}\langle\nabla\rangle_c v_*^n\right), \\ -\Delta\phi_*^{2,n} &= -\frac{1}{8c}\left(-u_*^n \langle\nabla\rangle_c v_*^n + v_*^n \langle\nabla\rangle_c u_*^n\right), \end{aligned}$$

we have uniformly accurate in $c \geq 1$ numerical approximations to the “twisted variables” (see Chapter 4) $w_*(t_n) = e^{-ic^2 t_n} w(t_n)$ and to $\phi(t_n) = \phi_*^{\text{tot}}(t_n)$ and $\mathfrak{a}_*^\gamma(t_n)$. Note that

$$(w_*, \phi_*^{\text{tot}}, \mathfrak{a}_*^\gamma)^\top \qquad \text{solve the “twisted system” (4.15).}$$

Recall that in case of MKG the nonlinearities $G_*^m \equiv 0$, $m = -4, -2, 0, 2$ vanish. Moreover, note that in case of MKG we choose

$$\gamma = 0 \qquad \text{which is involved in the scheme } \Psi_*^\tau \text{ (see (4.39)).} \tag{5.27}$$

In the subsequent subsection we discuss the numerical convergence results in two experiments.

5.3.1 Numerical Convergence in case of MKG

In this section we discuss the numerical tests described in Experiment 5.1 and Experiment 5.2 below. In both experiments we consider the MKG system on the two-dimensional torus $\mathbb{T}^2 = [-\pi, \pi]^2$, i.e. $d = 2$, and on the finite time interval $[0, T = 1]$, and we choose

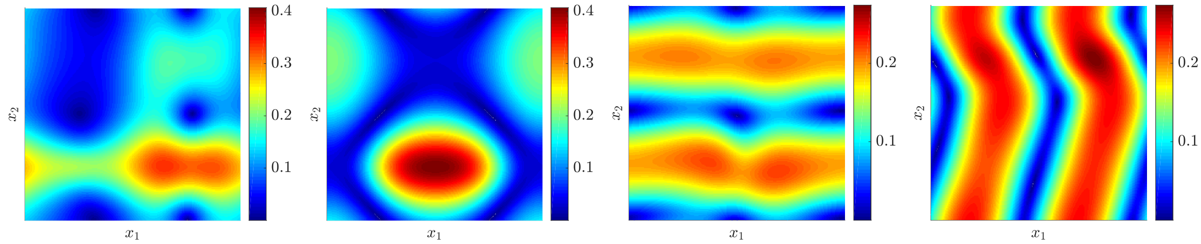
$$\begin{aligned} \text{the reference time step} \qquad & \tau_{\text{ref}} = 1/756000 \approx 1.59 \cdot 10^{-6}, \\ \text{the number of grid points in both directions} \qquad & M = 128 \quad (\text{mesh size } h = 2\pi/M \approx 0.049). \end{aligned}$$

We set $r = 2$ the index corresponding to the Sobolev norms from Theorems 3.15 and 4.7 on the convergence of our schemes. Note that in particular $r > d/2$. We furthermore fix the following coefficients of the initial data

$$\psi_{I,j} = \frac{\widetilde{\psi_{I,j}}}{\left\|\widetilde{\psi_{I,j}}\right\|_{L^2}}, \quad \psi'_{I,j} = \frac{\widetilde{\psi'_{I,j}}}{\left\|\widetilde{\psi'_{I,j}}\right\|_{L^2}}, \quad A_{I,j} = \frac{\mathcal{P}_{\text{df}}\left[\widetilde{A_{I,j}}\right]}{\left\|\mathcal{P}_{\text{df}}\left[\widetilde{A_{I,j}}\right]\right\|_{L^2}}, \quad A'_{I,j} = \frac{\mathcal{P}_{\text{df}}\left[\widetilde{A'_{I,j}}\right]}{\left\|\mathcal{P}_{\text{df}}\left[\widetilde{A'_{I,j}}\right]\right\|_{L^2}},$$

for $j = 0, 1$ and $x = (x_1, x_2) \in \mathbb{T}^2$ with

$$\begin{aligned} \widetilde{\psi_{I,0}}(x) &= \exp\left(\sin(x_1)\right) \cdot \frac{(\cos(x_1) + i\sin(x_2))}{2.5 + \sin(x_1) + \sin(x_2)}, & \widetilde{\psi_{I,1}}(x) &= \sin(x_1) + \cos(x_2), \\ \widetilde{\psi'_{I,0}}(x) &= \frac{\sin(x_2) - \cos(x_1)}{2.5 - i\cos(x_1) + \sin(x_2)}, & \widetilde{\psi'_{I,1}}(x) &= i(\cos(x_1) + \sin(x_2)), \\ \widetilde{A_{I,0}}(x) &= \begin{pmatrix} -\sin(x_2) \\ \dfrac{\sin(x_1) + \sin(x_2)}{3 - \cos(x_1) + \sin(x_2)} \end{pmatrix}, & \widetilde{A_{I,1}}(x) &= \begin{pmatrix} \exp\left(\sin(x_1)\right) + \sin(x_2) \\ \cos(x_1) + \sin(x_2) \end{pmatrix}, \\ \widetilde{A'_{I,0}}(x) &= \begin{pmatrix} \sin(x_1) \cdot \exp\left(\sin(x_2)\right) \\ -\sin(x_1) - \sin(x_2) \end{pmatrix}, & \widetilde{A'_{I,1}}(x) &= \begin{pmatrix} \cos(x_1) + \sin(x_2) \\ -\sin(x_1) \end{pmatrix}. \end{aligned}$$



(a) $|\psi_I(x_1,x_2)|$ (b) $\left|\psi_I'(x_1,x_2)\right|$ (c) $|A_I(x_1,x_2)|$ (d) $\left|A_I'(x_1,x_2)\right|$

Figure 5.1: (MKG initial data): Absolute values of the initial data ψ_I, ψ_I', A_I, A_I' of the MKG system (2.20) corresponding to Experiment 5.1 on the torus $\mathbb{T}^2$, i.e. $x=(x_1,x_2)\in[-\pi,\pi]^2$.

We investigate the following numerical errors

$$\begin{aligned}
\mathfrak{E}^{(0),n}_{\boldsymbol{\mathcal{A}}_\infty} &= \left\|\boldsymbol{\mathcal{A}}(t_n)-\boldsymbol{\mathcal{A}}^{(0),n}_\infty\right\|_{2,0}+\left\|\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n)-\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}^{(0),n}_\infty\right\|_{1,0}\\
\mathfrak{E}^{(0),n}_{\infty} &= \left\|\psi(t_n)-\psi^{(0),n}_\infty\right\|_{2}+\left\|\phi(t_n)-\phi^{(0),n}_\infty\right\|_{4,0}\\
\mathfrak{E}^{(1),n}_{\infty} &= \left\|\psi(t_n)-\psi^{(1),n}_\infty\right\|_{2}+\left\|\phi(t_n)-\phi^{(1),n}_\infty\right\|_{4,0}\\
\mathfrak{E}^{n}_{*} &= \|\psi(t_n)-\psi^{n}_*\|_2+\|\phi(t_n)-\phi^{\mathrm{tot},n}_*\|_{3,0}+\|\boldsymbol{\mathcal{A}}(t_n)-\boldsymbol{\mathcal{A}}^n_*\|_{2,0}+\left\|\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n)-\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}^n_*\right\|_{1,0}\\
\mathfrak{E}^{n}_{\mathrm{ref}} &= \|\psi(t_n)-\psi^{n}_{\mathrm{ref}}\|_2+\|\phi(t_n)-\phi^{n}_{\mathrm{ref}}\|_{3,0}+\|\boldsymbol{\mathcal{A}}(t_n)-\boldsymbol{\mathcal{A}}^n_{\mathrm{ref}}\|_{2,0}+\left\|\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n)-\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}^n_{\mathrm{ref}}\right\|_{1,0}
\end{aligned}\tag{5.28}$$

where we denote by $(\psi^n_{\mathrm{ref}},\phi^n_{\mathrm{ref}},\boldsymbol{\mathcal{A}}^n_{\mathrm{ref}})^\top$ the numerical solution obtained with the exponential Gautschi-type reference scheme $\Phi^\tau_{\mathrm{ref,MKG}}$ (see (5.13)). Note that here, the chosen Sobolev norms match the theory from Theorems 3.15 and 4.7 for $r=2$. Furthermore, note that in the terms $\mathfrak{E}^{(0),n}_\infty$, $\mathfrak{E}^{(1),n}_\infty$ and $\mathfrak{E}^n_*$ the "exact solution" $(\psi(t_n),\phi(t_n),\boldsymbol{\mathcal{A}}(t_n))^\top$ of the MKG system (2.20) is actually replaced by the reference solution, obtained with the exponential Gautschi-type ([9, 51]) time integration scheme (5.13)

$$\Phi^{\tau_{\mathrm{ref}}}_{\mathrm{ref,MKG}}\quad\text{with the very small time step}\quad\tau_{\mathrm{ref}}\approx 1.59\cdot 10^{-6}.$$

The reference solution for the term $\mathfrak{E}^n_{\mathrm{ref}}$ is computed with our first order uniformly accurate "twisted scheme" $\Psi^{\tau_{\mathrm{ref}}}_*$ given in (4.39) with $\gamma=0$ and $\tau_{\mathrm{ref}}\approx 1.59\cdot 10^{-6}$. This allows us to test the scheme $\Phi^\tau_{\mathrm{ref,MKG}}$.

Experiment 5.1 (General MKG Initial Data)**.** *In the first numerical MKG experiment, we consider the initial data (cf. Fig. 5.1)*

$$\psi_I=\psi_{I,0}+c^{-1}\psi_{I,1},\quad \psi_I'=\psi_{I,0}'+c^{-1}\psi_{I,1}',\quad A_I=A_{I,0}+c^{-1}A_{I,1},\quad A_I'=A_{I,0}'+c^{-1}A_{I,1}'.$$

According to Theorem 3.15 and (3.133), the error of the numerical first order limit approximation $(\psi^{(0),n}_\infty,\phi^{(0),n}_\infty,\boldsymbol{\mathcal{A}}^{(0),n}_\infty)^\top$ satisfies

$$\mathfrak{E}^{(0),n}_\infty+\mathfrak{E}^{(0),n}_{\boldsymbol{\mathcal{A}}_\infty}=\mathcal{O}\left(\tau^2+c^{-1}\right)\quad \textit{for all } t_n\in[0,1].$$

The results of our numerical tests confirm these convergence rates (cf. Fig. 5.2a). Moreover, Fig. 5.2a shows that the numerical second order limit approximation $(\psi^{(1),n}_\infty,\phi^{(1),n}_\infty)^\top$ satisfies

$$\mathfrak{E}^{(1),n}_\infty=\mathcal{O}\left(\tau^2+c^{-2}\right),\quad \textit{for all } t_n\in[0,1],$$

which underlines Remark 3.16.

Fig. 5.2b confirms the first order in time uniformly accurate in $c \geq 1$ convergence (see Theorem 4.7) of the numerical approximation $(\psi_*^n, \phi_*^{\text{tot},n}, \boldsymbol{\mathcal{A}}_*^n, \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_*^n)^\top$ obtained with the "twisted scheme" Ψ_*^τ given in (4.39) (note that we choose $\gamma = 0$ (see (5.27)), i.e.

$$\mathfrak{E}_*^n = \mathcal{O}(\tau) \quad \text{uniformly in } c \geq 1 \text{ for all } t_n \in [0,1].$$

Fig. 5.2c shows that in our numerical experiments the numerical solution obtained with the method $\Phi_{\text{ref,MD}}^{\tau_{\text{ref}}}$ (5.13) has an error behaviour

$$\mathfrak{E}_{\text{ref}}^n = \mathcal{O}\left(\tau c^4\right) \quad \text{for all } t_n \in [0,1]$$

which is even worse than expected (instead of $\mathcal{O}\left(\tau^2 c^4\right)$, see [9, 51, 54] and also (5.11)). Recall that for the investigation of $\mathfrak{E}_{\text{ref}}^n$, we use our first order accurate scheme $\Psi_*^{\tau_{\text{ref}}}$ given in (4.39) with $\gamma = 0$ as a reference method with very small time step $\tau_{\text{ref}} \approx 1.59 \cdot 10^{-6}$. The order reduction observed in Fig. 5.2c below from the expected order $\mathcal{O}\left(\tau^2 c^4\right)$ (see [9, 51, 54] and also (5.11)) to the order $\mathcal{O}\left(\tau c^4\right)$ can be explained by the explicit dependency of the right hand side of the MKG system (2.20) on the time derivatives $\partial_t \psi$ and $\partial_t \phi$ of the solutions ψ and ϕ. Because the reference scheme $\Phi_{\text{ref,MKG}}^\tau$ approximates $\partial_t \psi$ only up to $\mathcal{O}\left(\tau c^2\right)$ bounds (cf. [51, 54] and (5.10) and also (5.11)), we retain global bounds for the scheme $\Phi_{\text{ref,MKG}}^\tau$ of order $\mathcal{O}\left(\tau c^4\right)$.

Additionally, in Fig. 5.3a, we study the second order in time error bounds of the Strang splitting schemes $\Phi_{w_0,\text{Strang}}^\tau$ (see [44, 65] and also Corollary 3.10) and $\Phi_{w_1,\text{Strang}}^\tau$. We measure the error of the corresponding numerical solutions

$$\mathfrak{E}_j^n := \left\|\psi_j(t_n) - \psi_j^n\right\|_2 + \left\|\phi_j(t_n) - \phi_j^n\right\|_{4,0} = \mathcal{O}\left(\tau^2\right) \quad \text{for all } t_n \in [0,1], \text{ see Fig. 5.3a} \tag{5.29}$$

for $j = 0, 1$. Note that the same methods $\Phi_{w_0,\text{Strang}}^{\tau_{\text{ref}}}$ and $\Phi_{w_1,\text{Strang}}^{\tau_{\text{ref}}}$ with the very small step size $\tau_{\text{ref}} \approx 1.59 \cdot 10^{-6}$ provide numerical reference solutions for measuring the numerical error.

In Fig. 5.4, we compare the efficiency of the above schemes for several values of c by plotting the resulting error of each scheme against the corresponding consumed CPU time. Fig. 5.4 underlines, that

in slowly oscillatory regimes $c \lesssim 10$ *the exponential Gautschi-type scheme $\Phi_{\text{ref,MKG}}^\tau$ performs well,*

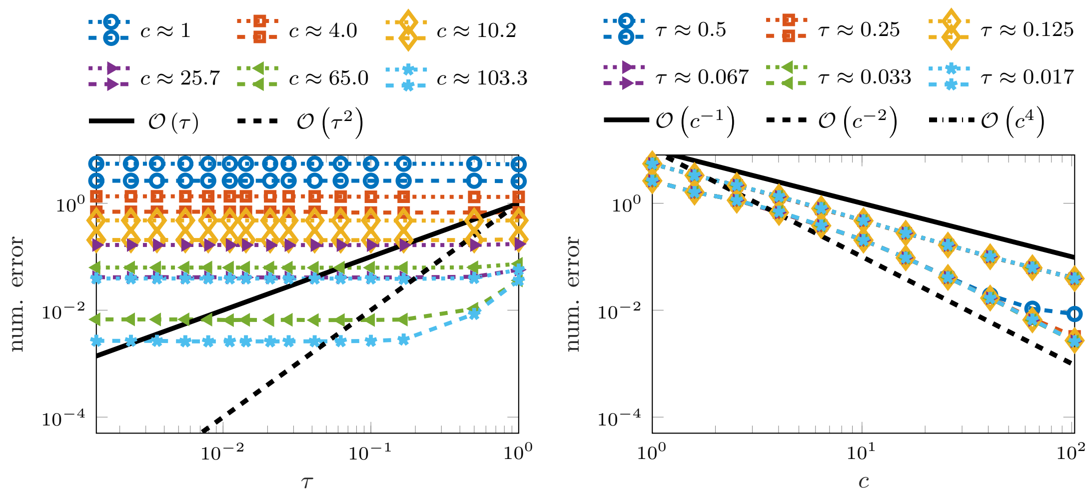
in intermediate regimes $10 \lesssim c \lesssim 150$ *the uniformly accurate scheme Ψ_*^τ (with $\gamma = 0$) is most efficient and*

in highly oscillatory regimes $c \gtrsim 150$ *the asymptotic limit approximation schemes $\Phi_{w_j,\text{Strang}}^\tau$ for $j = 0, 1$ outperform the "twisted scheme" Ψ_*^τ.*

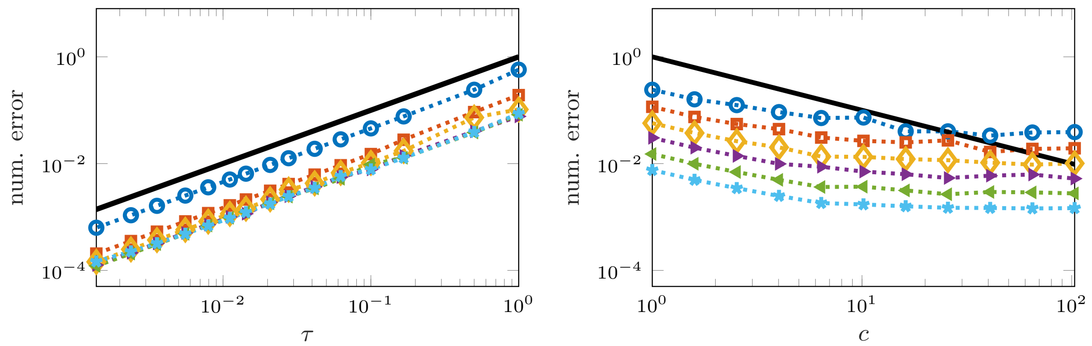
In the subsequent experiment, we see that we can improve the convergence of the limit approximation $(\psi_\infty^{(0),n}, \phi_\infty^{(0),n})^\top$ to $\mathcal{O}\left(\tau^2 + c^{-2}\right)$ if we choose the initial data for the MKG system (2.20) in a suitable way (cf. Theorem 3.15).

Experiment 5.2 (Particular MKG Initial Data)**.** *In the second numerical MKG experiment, we consider the initial data*

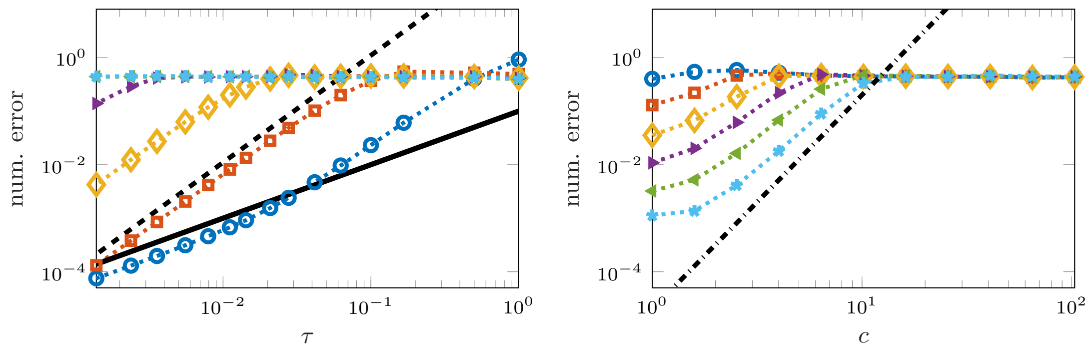
$$\psi_I = \psi_{I,0}, \quad \psi_I' = \psi_{I,0}', \quad A_I = A_{I,0} + c^{-1} A_{I,1}, \quad A_I' = A_{I,0}' + c^{-1} A_{I,1}'.$$



(a) Experiment 5.1 (asymptotic $\Phi^{\tau}_{w_j,\mathrm{Strang}}$): Dotted (⋅⋅ʘ⋅): $\sup_{t_n\in[0,1]} \mathfrak{E}^{(0),n}_{\infty} + \mathfrak{E}^{(0),n}_{\boldsymbol{\mathcal{A}}_\infty}$
Dashed (- ʘ -): $\sup_{t_n\in[0,1]} \mathfrak{E}^{(1),n}_{\infty}$

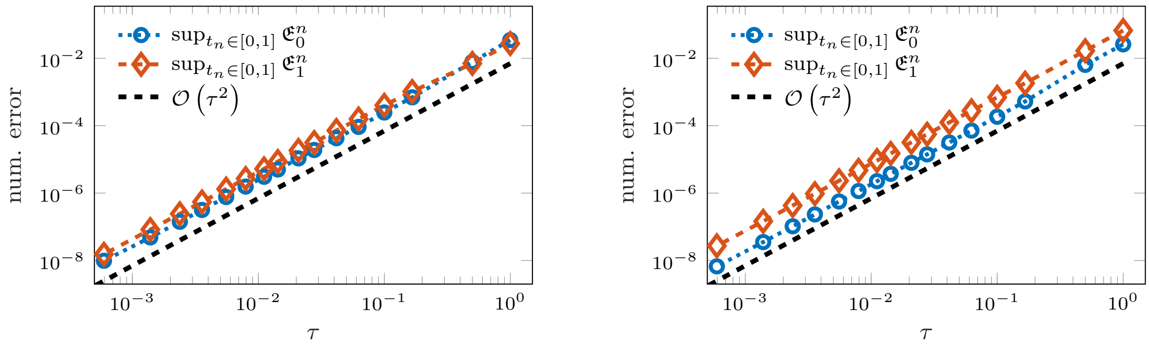


(b) Experiment 5.1 (uniformly Ψ^{τ}_{*}): Dotted (⋅⋅ʘ⋅): $\sup_{t_n\in[0,1]} \mathfrak{E}^{n}_{*}$



(c) Experiment 5.1 (exp. Gautschi type $\Phi^{\tau}_{\mathrm{ref,MKG}}$): Dotted (⋅⋅ʘ⋅): $\sup_{t_n\in[0,1]} \mathfrak{E}^{n}_{\mathrm{ref}}$

Figure 5.2: (MKG, Convergence, Experiment 5.1): **Left:** Convergence in τ, **Right:** Convergence in c. Fig. 5.2a underlines the $\mathcal{O}\left(\tau^2 + c^{-1}\right)$ bound from Theorem 3.15 and the $\mathcal{O}\left(\tau^2 + c^{-2}\right)$ bound from Remark 3.16 for the error terms $\mathfrak{E}^{(0),n}_{\infty} + \mathfrak{E}^{(0),n}_{\boldsymbol{\mathcal{A}}_\infty}$ and $\mathfrak{E}^{(1),n}_{\infty}$, respectively. In Fig. 5.2b we observe the uniformly in c first order in time error bound $\mathcal{O}(\tau)$ for $\mathfrak{E}^{n}_{*}$ from Theorem 4.7. Fig. 5.2c shows that the numerical bounds for the error term $\mathfrak{E}^{n}_{\mathrm{ref}}$ corresponding to the reference scheme $\Phi^{\tau}_{\mathrm{ref,MKG}}$ are even worse than expected, namely $\mathcal{O}\left(\tau c^4\right)$ instead of the expected bound of order $\mathcal{O}\left(\tau^2 c^4\right)$ (see [9, 51, 54] and also (5.11)).
The error terms $\mathfrak{E}^{(0),n}_{\boldsymbol{\mathcal{A}}_\infty}, \mathfrak{E}^{(0),n}_{\infty}, \mathfrak{E}^{(1),n}_{\infty}, \mathfrak{E}^{n}_{*}, \mathfrak{E}^{n}_{\mathrm{ref}}$ are given explicitly in (5.28).



(a) MKG Experiment 5.1, $\tau_{\text{ref}} \approx 1.59 \cdot 10^{-6}$

(b) MD Experiment 5.4, $\tau_{\text{ref}} \approx 3.31 \cdot 10^{-6}$

Figure 5.3: (Convergence Order of the Limit Splitting Schemes $\Phi^{\tau}_{w0,\text{Strang}}$ and $\Phi^{\tau}_{w1,\text{Strang}}$ for MKG and MD): Convergence order $\mathcal{O}\left(\tau^2\right)$ at fixed $c \approx 10.2$ of the schemes $\Phi^{\tau}_{w0,\text{Strang}}$ and $\Phi^{\tau}_{w1,\text{Strang}}$. The corresponding initial data to the MKG case (Fig. 5.3a) are given in Experiment 5.1, the ones for the MD case (Fig. 5.3b) in Experiment 5.4. The same methods $\Phi^{\tau_{\text{ref}}}_{w0,\text{Strang}}$ and $\Phi^{\tau_{\text{ref}}}_{w1,\text{Strang}}$ with very small step sizes τ_{ref} provide a reference solution. The error terms $\mathfrak{E}_j^n$ for $j = 0, 1$ are given in (5.29) and (5.35), respectively.

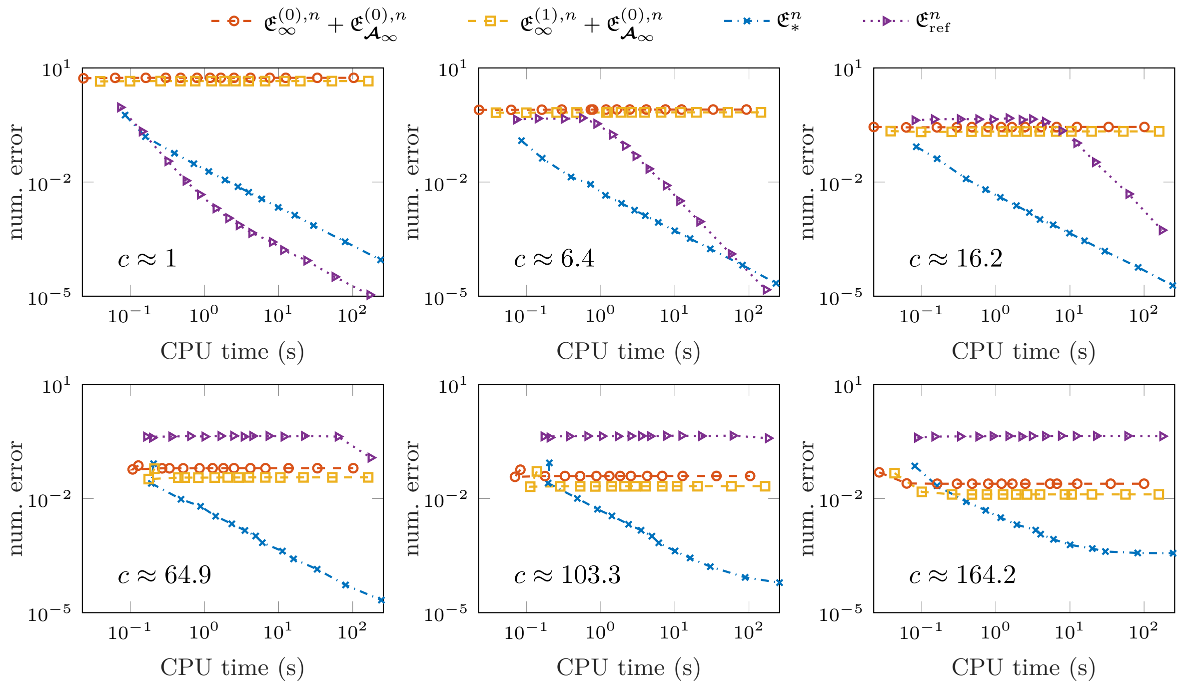


Figure 5.4: (MKG, Efficiency of the Numerical Time Integration Schemes, Experiment 5.1): Efficiency plot of the methods $\Phi^{\tau}_{w0,\text{Strang}}$ (-⊖-), $\Phi^{\tau}_{w1,\text{Strang}}$ (-⊟-), Ψ^{τ}_{*} (-·×·-), $\Phi^{\tau}_{\text{ref,MKG}}$ (···▷···) for several values of c. The corresponding errors are plotted against the consumed CPU time for computing the respective numerical solution. Values in the lower left corner of each plot are desired. We observe that already for small values $c \approx 6.4$ (upper middle) and for all higher values $c \gtrsim 6.4$ our uniformly accurate in $c \geq 1$ scheme Ψ^{τ}_{*} shows a (much) smaller error than the reference scheme $\Phi^{\tau}_{\text{ref,MKG}}$ at the same CPU time. Additionally, the lower plots underline that for $c \gtrsim 100$ at small CPU times the usage of the asymptotic limit schemes $\Phi^{\tau}_{w0,\text{Strang}}$ and $\Phi^{\tau}_{w1,\text{Strang}}$ pays off. We furthermore observe that the efficiency of the scheme Ψ^{τ}_{*} is more or less constant for increasing $c \gtrsim 16.2$ (see upper right to lower right). Because the numerical schemes $\Phi^{\tau}_{w0,\text{Strang}}$ and $\Phi^{\tau}_{w1,\text{Strang}}$ are independent of c and because of the $\mathcal{O}\left(\tau^2 + c^{-1}\right)$ convergence (see Fig. 5.2a) we deduce that for $c \gtrsim 150$ these limit schemes become more efficient than the other schemes. Note that in the lower middle and lower right plot, the plateaus in the lines corresponding to $\mathfrak{e}_{*}^{n}$ for large CPU times can be explained by a bad quality of the respective reference solution.

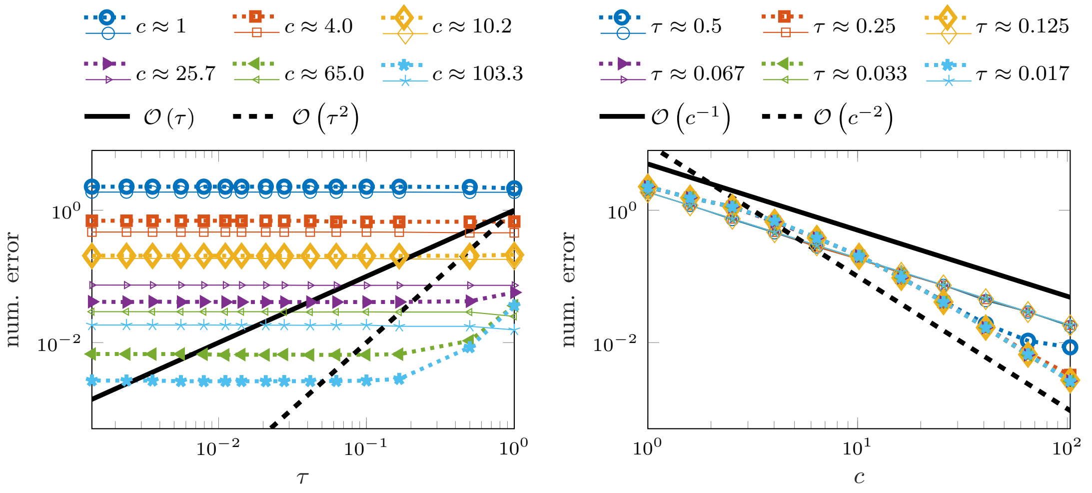


Figure 5.5: (MKG, Asymptotic Limit Approximation, Experiment 5.2): Dotted (··⊙·): $\sup_{t_n\in[0,1]} \mathfrak{E}_\infty^{(0),n}$, Thin solid (—⊖—): $\sup_{t_n\in[0,1]} \mathfrak{E}_{\boldsymbol{\mathcal{A}}_\infty}^{(0),n}$. **Left:** Convergence in τ, **Right:** Convergence in c. We observe that a suitable choice of the initial data for MKG the convergence of $\mathfrak{E}_\infty^{(0),n}$ improves from $\mathcal{O}\left(\tau^2 + c^{-1}\right)$ (cf. Fig. 5.2a) to $\mathcal{O}\left(\tau^2 + c^{-2}\right)$ which underlines Theorem 3.15.

Especially note that

$$\|\psi_I - \psi_{I,0}\|_{2+4} + \left\|\psi_I' - \psi_{I,0}'\right\|_{2+4} = 0 \leq Kc^{-2}.$$

The errors of the first order limit approximation $(\psi_\infty^{(0),n}, \phi_\infty^{(0),n}, \boldsymbol{\mathcal{A}}_\infty^{(0),n})^\top$ *satisfy according to Theorem 3.15 (respecting (3.133))* $\mathfrak{E}_{\boldsymbol{\mathcal{A}}_\infty}^{(0),n} = \mathcal{O}\left(c^{-1}\right)$ *and in particular*

$$\mathfrak{E}_\infty^{(0),n} = \mathcal{O}\left(\tau^2 + c^{-2}\right) \quad \textit{for all } t_n \in [0,1].$$

These bounds are confirmed in Fig. 5.5.

Note that in [45] the authors observed this convergence for numerical experiments with the nonlinear Klein–Gordon equation for a similar choice of the initial data.

In the subsequent subsection we discuss energy and norm conservation properties of our schemes.

5.4 Maxwell–Dirac Experiments

In this section, we consider the reduced[②] Maxwell–Dirac system (2.37) with its exact solution $(\Psi, \phi, \boldsymbol{\mathcal{A}})^\top$ corresponding to the initial data

$$(\boldsymbol{\mathcal{A}}(0), \partial_t \boldsymbol{\mathcal{A}}(0))^\top = (A_I, cA_I')^\top \qquad \text{and} \qquad \Psi(0) = \Psi_I = (\Psi_I^+, \Psi_I^-)^\top,$$

[②]Recall that according to [10, 14–16, 87] (see also Remark 2.5) the full MD system (2.36) with solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ can be reduced in the case of $d = d_{\text{low}} = 1, 2$ dimensions to the system (2.37) with solution $(\Psi, \phi, \boldsymbol{\mathcal{A}})^\top$, where $\Psi = (\psi_1, \psi_4)^\top$.

where the initial data $\Psi_I^+, \Psi_I^-, A_I, A_I'$ can be expanded such that (cf. (3.9b))

$$\Psi_I^+ = \Psi_{I,0}^+ + c^{-1}\Psi_{I,1}^+ + \sum_{n=2}^{\infty} c^{-n}\Psi_{I,n}^+, \qquad \Psi_I^- = \Psi_{I,0}^- + c^{-1}\Psi_{I,1}^- + \sum_{n=2}^{\infty} c^{-n}\Psi_{I,n}^-,$$
$$A_I = A_{I,0} + c^{-1}A_{I,1} + \sum_{n=2}^{\infty} c^{-n}A_{I,n}, \qquad A_I' = A_{I,0}' + c^{-1}A_{I,1}' + \sum_{n=2}^{\infty} c^{-n}A_{I,n}'.$$

Our aim is now to numerically underline the convergence results $\mathcal{O}\left(\tau^2 + c^{-N}\right)$ for $N \in \mathbb{N}$ of the asymptotic nonrelativistic limit approximation for $c \gg 1$ from Theorem 3.15 and the convergence result $\mathcal{O}(\tau)$ uniformly in $c \geq 1$ of the numerical approximation obtained with the uniformly accurate time integration scheme from Section 4.2 (see Theorem 4.7) which we may call in the following "twisted scheme". Additionally, we test the TSFP-Gautschi reference time integration scheme ([9, 10, 15, 16, 51]) which we discussed in Section 5.2.2

Next, we give a short recap of the nonrelativistic limit time integration scheme from Section 3.5 and the uniformly accurate time integration scheme from Section 4.2 .

Repetition of the Nonrelativistic Limit Time Integration Scheme for MD

We consider the numerical approximation in the nonrelativistic limit regime $c \gg 1$ to $\psi(t_n)$, i.e. (cf. (3.61))

$$\Psi_\infty^{(0),n} = \frac{1}{2}\left(e^{ic^2 t_n} u_0^n + e^{-ic^2 t_n}\overline{v_0^n}\right) \qquad \text{and}$$
$$\Psi_\infty^{(1),n} = \frac{1}{2}\left(e^{ic^2 t_n}(u_0^n + c^{-1}u_1^n) + e^{-ic^2 t_n}(\overline{v_0^n} + c^{-1}\overline{v_1^n})\right).$$

Recall that we obtain the numerical approximations

$$w_0^n = (u_0^n, v_0^n)^\top \quad \text{and} \quad w_1^n = (u_1^n, v_1^n)^\top \quad \text{with the schemes } \Phi^\tau_{w_0,\text{Strang}} \text{ and } \Phi^\tau_{w_1,\text{Strang}},$$

to the solution $w_0(t_n)$ and $w_1(t_n)$ of the limit systems (3.109) and (3.111). These schemes[3] were given in (3.110) and (3.117), respectively, with

$$w_0^n = \left(\Phi^\tau_{w_0,\text{Strang}}\right)^n (w_{I,0}) \quad \text{with} \quad w_{I,0} = \begin{pmatrix} u_{I,0} \\ v_{I,0} \end{pmatrix}, \quad u_{I,0} = \begin{pmatrix} 0 \\ 2\Psi_{I,0}^- \end{pmatrix}, \quad v_{I,0} = \begin{pmatrix} 2\overline{\Psi_{I,0}^+} \\ 0 \end{pmatrix} \quad \text{and}$$
$$w_1^n = \left(\Phi^\tau_{w_1,\text{Strang}}\right)^n (w_{I,1}) \quad \text{with} \quad w_{I,1} = \begin{pmatrix} (\mathcal{I}_2 - \boldsymbol{\sigma}_3)\Psi_{I,1} \\ (\mathcal{I}_2 + \boldsymbol{\sigma}_3)\overline{\Psi_{I,1}} \end{pmatrix} + \sum_{j=1}^{d_\text{low}} \begin{pmatrix} i\boldsymbol{\sigma}_j \partial_j \Psi_{I,0} \\ i\overline{\boldsymbol{\sigma}_j \partial_j \Psi_{I,0}} \end{pmatrix}.$$

Moreover, we obtain approximations to $\phi(t_n)$ in the nonrelativistic limit regime $c \gg 1$ via (cf. (3.33) and (3.112))

$$\phi_\infty^{(0),n} = \phi_0^n, \qquad \phi_\infty^{(1),n} = \phi_0^n + c^{-1}\phi_1^n, \quad \text{with} \quad \phi_1^n = \tilde{\phi}_1^n + e^{2ic^2 t_n}\phi_1^{(2,0),n} + e^{-2ic^2 t_n}\overline{\phi_1^{(2,0),n}},$$

where ϕ_0^n and $\tilde{\phi}_1^n$, $\phi_1^{(2,0),n}$ solve the Poisson equations (see Theorem 3.15 and cf. (3.111), (3.112))

$$-\Delta\phi_0^n = \frac{1}{4}(|u_0^n|^2 + |v_0^n|^2) \qquad \text{and} \qquad \begin{aligned} -\Delta\tilde{\phi}_1^n &= \frac{1}{2}\,\mathrm{Re}\left(u_0^n \cdot \overline{u_1^n} + v_0^n \cdot \overline{v_1^n}\right) \\ -\Delta\phi_1^{(2,0),n} &= \frac{1}{4}(u_0^n \cdot v_1^n + u_1^n \cdot v_0^n). \end{aligned}$$

[3] Note that we need to replace the matrices $\boldsymbol{\alpha}_j$ by $\boldsymbol{\sigma}_j$ for $j = 1, 2$ and $\boldsymbol{\beta}$ by $\boldsymbol{\sigma}_3$, see Remark 2.5.

Approximations to $\boldsymbol{\mathcal{A}}(t_n)$ and $\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n)$ are given through (see Theorem 3.15)

$$\begin{aligned}\boldsymbol{\mathcal{A}}_\infty^{(0),n} = \boldsymbol{\mathcal{A}}_0^n &= \cos(ct_n \langle\nabla\rangle_0)A_{I,0} + t_n \operatorname{sinc}(ct_n \langle\nabla\rangle_0)cA_{I,0} \quad \text{and} \\ \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_\infty^{(0),n} = \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_0^n &= -c\langle\nabla\rangle_0 \sin(ct_n \langle\nabla\rangle_0)A_{I,0} + \cos(ct_n \langle\nabla\rangle_0)cA_{I,0}.\end{aligned}$$

In the subsequent subsection„ we recall the uniformly accurate time integration scheme from Section 4.2 based on the “twisted variables”.

Repetition of the Uniformly Accurate “Twisted” Time Integration Scheme for MD

Recall that by Theorem 4.7 the numerical solutions

$$\begin{aligned}\Psi_*^n &= \frac{1}{2}(e^{ic^2t_n}u_*^n + e^{-ic^2t_n}\overline{v_*^n}), \qquad \boldsymbol{\mathcal{A}}_*^n = \frac{1}{2}(\mathfrak{a}_*^{\gamma,n} + \overline{\mathfrak{a}_*^{\gamma,n}}) \\ \phi_*^{\text{tot},n} &= \phi_*^{0,n} + e^{2ic^2t_n}\phi_*^{2,n} + e^{-2ic^2t_n}\overline{\phi_*^{2,n}}\end{aligned}$$

are uniformly accurate in $c \geq 1$ approximations to the exact solution $(\Psi(t_n), \phi(t_n), \boldsymbol{\mathcal{A}}(t_n))^\top$ of the reduced MD system (2.37). Thereby, gathering

$$w_*^n = (u_*^n, v_*^n)^\top, \quad \mathfrak{a}_*^{\gamma,n} \qquad \text{obtained with the “twisted scheme” } \Psi_*^\tau \text{ given in (4.39)}$$

and $\phi_*^{0,n}$ and $\phi_*^{2,n}$ being the solution of the Poisson equations (see (4.40b))

$$\begin{aligned}-\Delta\phi_*^{0,n} &= \frac{1}{4}\left(|u_*^n|^2 + |v_*^n|^2\right), \\ -\Delta\phi_*^{2,n} &= \frac{1}{4}u_*^n \cdot v_*^n,\end{aligned}$$

we have uniformly accurate in $c \geq 1$ numerical approximations to the “twisted variables” (see Chapter 4) $w_*(t_n) = e^{-ic^2t_n}w(t_n)$ and to $\phi(t_n) = \phi_*^{\text{tot}}(t_n)$ and $\mathfrak{a}_*^\gamma(t_n)$. Note that

$$(w_*, \phi_*^{\text{tot}}, \mathfrak{a}_*^\gamma)^\top \qquad \text{solve the “twisted system” (4.15)}$$

in which we replace in the nonlinearities G_*^m for $m = -4, -2, 0, 2$ the matrices $\boldsymbol{\alpha}_j$ by $\boldsymbol{\sigma}_j$ for $j = 1, 2$ (see Remark 2.5). Furthermore, note that in case of MD we choose

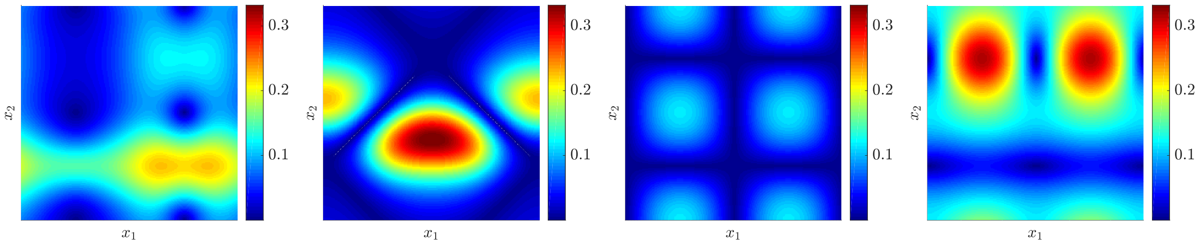
$$\gamma = 1 \qquad \text{which is involved in the scheme } \Psi_*^\tau \text{ (see (4.39)).} \tag{5.30}$$

In the subsequent subsection, we discuss the numerical convergence results for the MD case in two experiments.

5.4.1 Numerical Convergence in case of MD

The subject of this section is the discussion of the numerical tests described in Experiment 5.3 and Experiment 5.4 below. In the latter experiments, we consider the reduced MD system on the two-dimensional torus $\mathbb{T}^2 = [-\pi, \pi]^2$, i.e. $d = 2$, and on the finite time interval $[0, T = 1]$, and we choose

$$\begin{aligned}\text{the reference time step} \qquad & \tau_{\text{ref}} = 1/302400 \approx 3.31 \cdot 10^{-6}, \\ \text{the number of grid points in both directions} \qquad & M = 128 \quad (\text{mesh size } h = 2\pi/M \approx 0.049).\end{aligned}$$



(a) $\left|\Psi^+_{I,0}(x_1,x_2)\right|$ (b) $\left|\Psi^-_{I,0}(x_1,x_2)\right|$ (c) $\left|\Psi^+_{I,1}(x_1,x_2)\right|$ (d) $\left|\Psi^-_{I,1}(x_1,x_2)\right|$

Figure 5.6: (MD initial data): Absolute values of the initial data $\Psi_{I,0} = (\Psi^+_{I,0}, \Psi^-_{I,0})^\top$, $\Psi_{I,1} = (\Psi^+_{I,1}, \Psi^-_{I,1})^\top$ given in (5.31) of the reduced MD system (2.37) on the torus $\mathbb{T}^2$, i.e. $x = (x_1, x_2) \in [-\pi, \pi]^2$.

We set $r = 2$ the index corresponding to the Sobolev norms from Theorems 3.15 and 4.8 on the convergence of our schemes. Note that in particular $r > d/2$.

We furthermore fix the following coefficients of the initial data (cf. Figs. 5.1c, 5.1d and 5.6)

$$\Psi^\pm_{I,j} = \frac{\widetilde{\Psi^\pm_{I,j}}}{\sqrt{\left\|\widetilde{\Psi^+_{I,j}}\right\|^2_{L^2} + \left\|\widetilde{\Psi^-_{I,j}}\right\|^2_{L^2}}}, \quad A_{I,j} = \frac{\mathcal{P}_{\mathrm{df}}\left[\widetilde{A_{I,j}}\right]}{\left\|\mathcal{P}_{\mathrm{df}}\left[\widetilde{A_{I,j}}\right]\right\|_{L^2}}, \quad A'_{I,j} = \frac{\mathcal{P}_{\mathrm{df}}\left[\widetilde{A'_{I,j}}\right]}{\left\|\mathcal{P}_{\mathrm{df}}\left[\widetilde{A'_{I,j}}\right]\right\|_{L^2}}, \tag{5.31}$$

for $j = 0, 1$ and $x = (x_1, x_2) \in \mathbb{T}^2$

$$\begin{aligned}
\widetilde{\Psi^+_{I,0}}(x) &= \exp\big(\sin(x_1)\big) \cdot \frac{(\cos(x_1) + i\sin(x_2))}{2.5 + \sin(x_1) + \sin(x_2)}, & \widetilde{\Psi^+_{I,1}}(x) &= \sin(x_1)\cdot\cos(x_2),\\
\widetilde{\Psi^-_{I,0}}(x) &= \exp\big(\cos(x_2)\big) \cdot \frac{\sin(x_2) - \cos(x_1)}{2.5 - i\cos(x_1) + \sin(x_2)}, & \widetilde{\Psi^-_{I,1}}(x) &= \sin(x_1)\cdot\exp\big(\sin(x_2)\big) + i\cos(x_2),\\
\widetilde{A_{I,0}}(x) &= \begin{pmatrix} -\sin(x_2) \\ \dfrac{\sin(x_1)+\sin(x_2)}{3-\cos(x_1)+\sin(x_2)} \end{pmatrix}, & \widetilde{A_{I,1}}(x) &= \begin{pmatrix} \exp\big(\sin(x_1)\big) + \sin(x_2) \\ \cos(x_1) + \sin(x_2) \end{pmatrix},\\
\widetilde{A'_{I,0}}(x) &= \begin{pmatrix} \sin(x_1)\cdot\exp\big(\sin(x_2)\big) \\ -\sin(x_1) - \sin(x_2) \end{pmatrix}, & \widetilde{A'_{I,1}}(x) &= \begin{pmatrix} \cos(x_1) + \sin(x_2) \\ -\sin(x_1) \end{pmatrix}.
\end{aligned}$$

We investigate the following numerical errors

$$\begin{aligned}
\mathfrak{E}^{(0),n}_{\boldsymbol{\mathcal{A}}_\infty} &= \left\|\boldsymbol{\mathcal{A}}(t_n) - \boldsymbol{\mathcal{A}}^{(0),n}_\infty\right\|_{2,0} + \left\|\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n) - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}^{(0),n}_\infty\right\|_{1,0}\\
\mathfrak{E}^{(0),n}_\infty &= \left\|\psi(t_n) - \psi^{(0),n}_\infty\right\|_2 + \left\|\phi(t_n) - \phi^{(0),n}_\infty\right\|_{4,0}\\
\mathfrak{E}^{(1),n}_\infty &= \left\|\psi(t_n) - \psi^{(1),n}_\infty\right\|_2 + \left\|\phi(t_n) - \phi^{(1),n}_\infty\right\|_{4,0}\\
\mathfrak{E}^n_* &= \|\psi(t_n) - \psi^n_*\|_2 + \|\phi(t_n) - \phi^{\mathrm{tot},n}_*\|_{4,0} + \|\boldsymbol{\mathcal{A}}(t_n) - \boldsymbol{\mathcal{A}}^n_*\|_{2,0} + \left\|\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n) - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}^n_*\right\|_{1,0}\\
\mathfrak{E}^n_{\mathrm{ref}} &= \|\psi(t_n) - \psi^n_{\mathrm{ref}}\|_2 + \|\phi(t_n) - \phi^n_{\mathrm{ref}}\|_{4,0} + \|\boldsymbol{\mathcal{A}}(t_n) - \boldsymbol{\mathcal{A}}^n_{\mathrm{ref}}\|_{2,0} + \left\|\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t_n) - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}^n_{\mathrm{ref}}\right\|_{1,0}
\end{aligned} \tag{5.32}$$

where we denote by $(\psi^n_{\mathrm{ref}}, \phi^n_{\mathrm{ref}}, \boldsymbol{\mathcal{A}}^n_{\mathrm{ref}})^\top$ the numerical solution obtained with the TSFP-Gautschi reference scheme $\Phi^{\tau_{\mathrm{ref}}}_{\mathrm{ref,MD}}$ (see (5.25)). Note that here, the chosen Sobolev norms match the theory from Theorems 3.15 and 4.8 for $r = 2$. Furthermore, note that in the terms $\mathfrak{E}^{(0),n}_\infty$, $\mathfrak{E}^{(1),n}_\infty$ and $\mathfrak{E}^n_*$ the "exact solution" $(\psi(t_n), \phi(t_n), \boldsymbol{\mathcal{A}}(t_n))^\top$ of the reduced MD system (2.37) is actually replaced by the reference solution obtained by the TSFP-Gautschi ([9, 10, 15, 16, 51]) time integration scheme (5.25)

$$\Phi_{\text{ref,MD}}^{\tau_{\text{ref}}} \quad \text{with the very small time step} \quad \tau_{\text{ref}} \approx 3.31 \cdot 10^{-6}.$$

The reference solution for the term $\mathfrak{E}_{\text{ref}}^n$ is computed with our first order uniformly accurate "twisted scheme" $\Psi_*^{\tau_{\text{ref}}}$ given in (4.39) with $\gamma = 1$ and $\tau_{\text{ref}} \approx 3.31 \cdot 10^{-6}$. This allows us to test the scheme $\Phi_{\text{ref,MD}}^{\tau_{\text{ref}}}$.

In the first MD Experiment 5.3 we choose our initial data according to Assumption 4.5 such that

$$\Psi_I^- \overline{\boldsymbol{\sigma}_j \Psi_I^+} \qquad \text{for } j = 1, \dots, d.$$

In lower dimensions $d = d_{\text{low}} = 1, 2$ (cf. Remark 2.5) the Assumption 4.5 reduces to

$$\Psi_I^- \cdot \overline{\Psi_I^+} = \mathcal{O}\left(c^{-1}\right) \qquad \text{in the sense of the } H^2 \text{ norm} \tag{5.33}$$

which can be seen easily by replacing the matrices $\boldsymbol{\alpha}_j$ by $\boldsymbol{\sigma}_j$, $j = 1, \dots, d$ in the current densities $\boldsymbol{J}_*^{P,0}$ and $\boldsymbol{J}_*^{P,2}$, respectively, given in (4.18) and following the considerations of Remark 4.4.

According to Theorem 4.8, under these assumptions, our method Ψ_*^τ applied to the reduced MD system is stable and uniformly in $c \geq 1$ first order in time convergent.

Fortunately, the subsequent Experiment 5.4, treating general initial data for MD, strengthens the hypothesis that Assumption 4.5 might not be necessary in order to guarantee the uniform convergence of Ψ_*^τ. A proof of the uniformly accurate convergence of Ψ_*^τ in the case of initial data, which do not satisfy Assumption 4.5 might be an interesting topic of future research.

Experiment 5.3 (Particular MD Initial Data)**.** *In the first numerical MD experiment, we consider initial data satisfying* (5.33) *(which is an adaption of Assumption 4.5 to the reduced MD system* (2.37)*), i.e.*

$$\Psi_I = \begin{pmatrix} \Psi_I^+ \\ \Psi_I^- \end{pmatrix} = \begin{pmatrix} \Psi_{I,0}^+ \\ c^{-1}\Psi_{I,1}^- \end{pmatrix} \qquad A_I = A_{I,0} + c^{-1}A_{I,1}, \quad A_I' = A_{I,0}' + c^{-1}A_{I,1}'.$$

According to Theorem 3.15 and (3.133) *the error of the numerical first order limit approximations* $(\psi_\infty^{(0),n}, \phi_\infty^{(0),n}, \boldsymbol{\mathcal{A}}_\infty^{(0),n})^\top$ *satisfies*

$$\mathfrak{E}_\infty^{(0),n} + \mathfrak{E}_{\boldsymbol{\mathcal{A}}_\infty}^{(0),n} = \mathcal{O}\left(\tau^2 + c^{-1}\right) \quad \text{for all } t_n \in [0,1].$$

The results of our numerical tests confirm these convergence rates (cf. Fig. 5.7a). Moreover, Fig. 5.7a shows that the numerical second order limit approximation $(\psi_\infty^{(1),n}, \phi_\infty^{(1),n})^\top$ *satisfies*

$$\mathfrak{E}_\infty^{(1),n} = \mathcal{O}\left(\tau^2 + c^{-2}\right) \quad \text{for all } t_n \in [0,1],$$

which underlines Remark 3.16.

Fig. 5.7b confirms the first order in time uniformly accurate in $c \geq 1$ *convergence (see Theorem 4.8) of the numerical approximation* $(\Psi_*^n, \phi_*^{tot,n}, \boldsymbol{\mathcal{A}}_*^n, \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_*^n)^\top$ *obtained with the scheme* Ψ_*^τ *given in* (4.39) *(note that we choose* $\gamma = 1$ *(see* (5.30)*), i.e.*

$$\mathfrak{E}_*^n = \mathcal{O}(\tau) \quad \text{uniformly in } c \geq 1 \text{ for all } t_n \in [0,1].$$

Fig. 5.7c shows that the numerical solution obtained with the TSFP-Gautschi method $\Phi^{\tau_{\text{ref}}}_{\text{ref,MD}}$ *(see [9, 10, 15, 16, 51] and also (5.25)) has an error behaviour*

$$\mathfrak{E}^n_{\text{ref}} = \mathcal{O}\left(\tau^2 c^4\right) \quad \text{for all } t_n \in [0,1], \text{ see Fig. 5.7c},$$

This confirms the explicit dependence of the error bounds for the TSFP-Gautschi method $\Phi^{\tau_{\text{ref}}}_{\text{ref,MD}}$ *on the large parameter* c^4*, as expected (see [9, 10, 15, 16, 51] and also (5.25), (5.11) and (5.15)) and underlines*

$$\text{the severe time step restrictions} \quad \tau = \mathcal{O}\left(c^{-2}\right).$$

Recall that for the investigation of $\mathfrak{E}^n_{\text{ref}}$*, we use our first order uniformly accurate scheme* $\Psi^{\tau_{\text{ref}}}_*$ *given in (4.39) with* $\gamma = 1$ *as a reference method with very small time step* $\tau_{\text{ref}} \approx 3.31 \cdot 10^{-6}$*.*

In Fig. 5.8, we compare the efficiency of the above schemes for several values of c by plotting the resulting error of each scheme against the corresponding consumed CPU time. Fig. 5.8 underlines, that

in slowly oscillatory regimes $c \lesssim 16$ *the TSFP-Gautschi scheme* $\Phi^{\tau_{\text{ref}}}_{\text{ref,MD}}$ *performs well,*

in intermediate regimes $16 \lesssim c \lesssim 100$ *the uniformly accurate scheme* Ψ^{τ}_* *(with* $\gamma = 1$*) is most efficient and*

in highly oscillatory regimes $c \gtrsim 100$ *the asymptotic limit approximation schemes* $\Phi^{\tau}_{w_j,\text{Strang}}$ *for* $j = 0, 1$ *outperform the scheme* Ψ^{τ}_**.*

The subsequent Experiment 5.4 strengthens our hypothesis that the Assumption 4.5 (or (5.33), respectively) on the Maxwell–Dirac initial data might not be necessary in order to retain stability and a uniformly first order convergence of our "twisted scheme" Ψ^{τ}_* given in (4.39) (cf. Theorem 4.8).

Experiment 5.4 (General MD Initial Data)**.** *In the second numerical MD experiment, we consider the initial data*

$$\Psi_I = \begin{pmatrix} \Psi_I^+ \\ \Psi_I^- \end{pmatrix} = \begin{pmatrix} \Psi_{I,0}^+ \\ \Psi_{I,0}^- \end{pmatrix} + c^{-1} \begin{pmatrix} \Psi_{I,1}^+ \\ \Psi_{I,1}^- \end{pmatrix} \qquad A_I = A_{I,0} + c^{-1} A_{I,1}, \quad A_I' = A_{I,0}' + c^{-1} A_{I,1}'. \tag{5.34}$$

Recall that in order to show the uniformly in $c \geq 1$ *first order in time convergence of our "twisted scheme"* Ψ^{τ}_* *given in (4.39), we needed to set up the Assumption 4.5 on the initial data of the MD system (2.37) (cf. Theorem 4.8).*

Fig. 5.9 strengthens the hypothesis that for general initial data (5.34) violating Assumption 4.5 (or more precisely (5.33)), we still numerically retain the uniformly first order convergence of the scheme $\Psi^{\tau_{\text{ref}}}_*$ *given in (4.39) with the choice* $\gamma = 1$*. This topic is interesting future research. In Fig. 5.9 we observe the same convergence rates*

$$\mathfrak{E}^n_* = \mathcal{O}(\tau) \quad \text{uniformly in } c \geq 1 \text{ for all } t_n \in [0,1]$$

as proven in Theorem 4.8.

In particular, we observe that the corresponding numerical errors in comparison to the errors from Experiment 5.3 only differ by a very small constant, i.e. for both choices of initial data, we retain almost the same errors.

Additionally, in Fig. 5.3b, we test the second order in time error bounds of the Strang splitting schemes $\Phi^{\tau}_{w_0,\text{Strang}}$ *(see [44, 65] and also Corollary 3.10) and* $\Phi^{\tau}_{w_1,\text{Strang}}$*. We measure the error of the corresponding numerical solutions*

$$\mathfrak{E}_j^n := \left\|\psi_j(t_n) - \psi_j^n\right\|_2 + \left\|\phi_j(t_n) - \phi_j^n\right\|_{4,0} = \mathcal{O}\left(\tau^2\right) \quad \text{for all } t_n \in [0,1], \text{ see Fig. 5.3b} \tag{5.35}$$

for $j = 0, 1$*. Note that the same methods* $\Phi^{\tau_{ref}}_{w_0,\text{Strang}}$ *and* $\Phi^{\tau_{ref}}_{w_1,\text{Strang}}$ *with the very small step size* $\tau_{ref} \approx 3.31 \cdot 10^{-6}$ *provide numerical reference solutions for measuring the numerical error.*

5.5 Numerical Energy and Norm Conservation

In this section, we discuss the numerical energy conservation properties of our uniformly accurate "twisted scheme" Ψ^{τ}_{*} given in (4.39) and of the asymptotic limit scheme $\Phi^{\tau}_{w_0,\text{Strang}}$ given in (3.110).

Recall that by (2.12) the electromagnetic field $(\boldsymbol{E}, \boldsymbol{B})^{\top}$ corresponding to the MKG and MD systems (2.20) and (2.36), respectively, is given through

$$\begin{aligned} \boldsymbol{E}(t,x) &= -\nabla\phi(t,x) - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t,x), \\ \boldsymbol{B}(t,x) &= \nabla \times \boldsymbol{\mathcal{A}}(t,x) \end{aligned} \tag{5.36}$$

where in dimension $d = 2$ we consider electromagnetic fields of type (cf. Section 2.1.1)

$$\boldsymbol{E}(t,x) = (E_1(t,x), E_2(t,x),\ 0\ )^{\top} \qquad \text{and} \qquad \boldsymbol{B} = (\ 0\ ,\ 0\ , B_3(t,x))^{\top}.$$

In particular, $B_3 = \partial_1 A_2 - \partial_2 A_1$ (see (1.3)).

Furthermore, recall that in the MKG system (2.20), we carried out the coupling of its Klein–Gordon part (2.20a) with solution ψ to the Maxwell's potentials $(\phi, \boldsymbol{\mathcal{A}})^{\top}$ via the minimal coupling operators (see Section 2.1.2 and Definition A.23)

$$\partial_t^{[\phi]}\psi := \left(\frac{\partial_t}{c} + i\frac{\phi}{c}\right)\psi \qquad \text{and} \qquad \nabla^{[\boldsymbol{\mathcal{A}}]}\psi := \left(\nabla - i\frac{\boldsymbol{\mathcal{A}}}{c}\right)\psi.$$

Similarly, in the MD system (2.36), we carried out the coupling of the Dirac equation (2.36a) to $(\phi, \boldsymbol{\mathcal{A}})^{\top}$.

Firstly, we discuss the energy conservation in case of the MKG system.

5.5.1 Total Energy of the MKG System

Based on [21, 70, 80], we define the energy of the MKG system (2.20) by

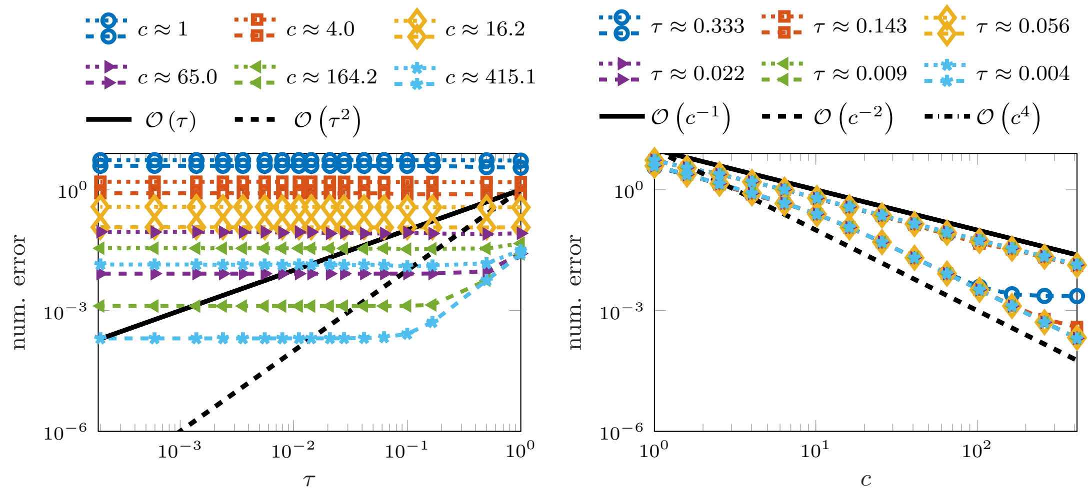
$$\mathcal{E}_{\text{MKG}}(t) = \|\boldsymbol{E}(t)\|_{L^2}^2 + \|\boldsymbol{B}(t)\|_{L^2}^2 + \left\|\nabla^{[\boldsymbol{\mathcal{A}}(t)]}\psi(t)\right\|_{L^2}^2 + \left\|\partial_t^{[\phi(t)]}\psi(t)\right\|_{L^2}^2 + c^2\|\psi(t)\|_{L^2}^2\,, \tag{5.37}$$

which is conserved over all times $t \geq 0$ ([21, 70]), i.e.

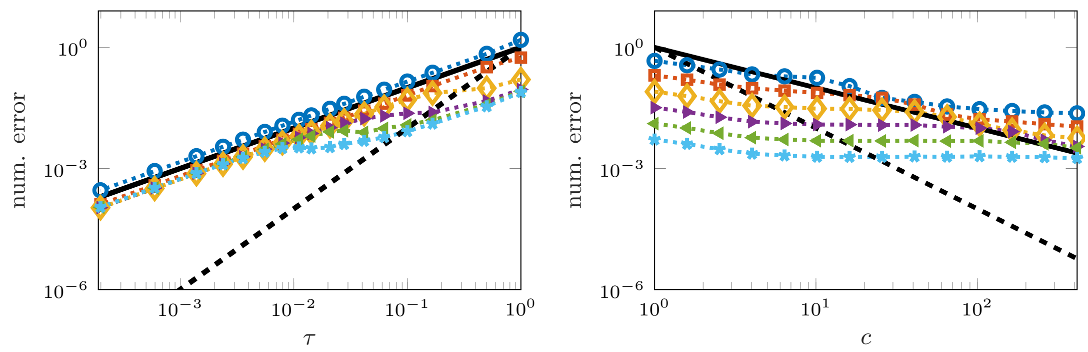
$$\mathcal{E}_{\text{MKG}}(t) = \mathcal{E}_{\text{MKG}}(0) \qquad \text{for all times } t \geq 0 \text{ ([70])}. \tag{5.38}$$

In ([70]) the authors have proven that

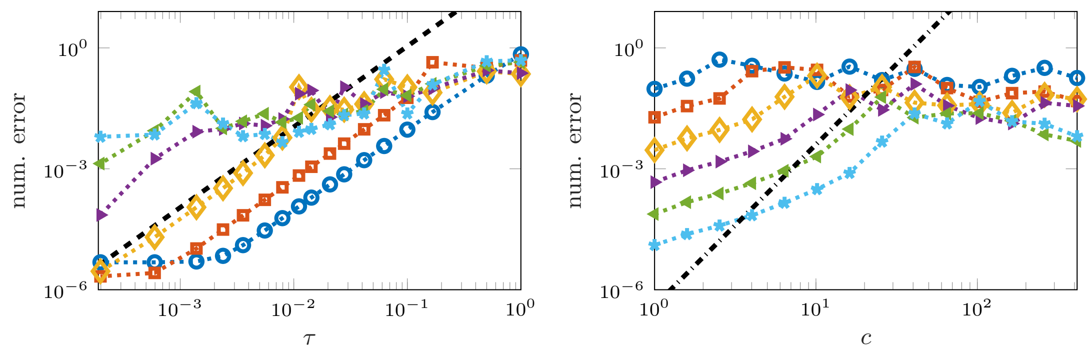
$$\mathcal{E}_{\text{MKG}}(t) - \mathcal{E}_{0,\text{MKG}}(t) \leq K \quad \text{for all } t \in [0,T] \text{ uniformly in } c \tag{5.39}$$



(a) Experiment 5.3 (asymptotic limit): Dotted: $\sup_{t_n\in[0,1]} \mathfrak{E}_{\infty}^{(0),n} + \mathfrak{E}_{\mathcal{A}_\infty}^{(0),n}$
Dashed: $\sup_{t_n\in[0,1]} \mathfrak{E}_{\infty}^{(1),n}$



(b) Experiment 5.3 (uniformly Ψ_*^τ): Dotted: $\sup_{t_n\in[0,1]} \mathfrak{E}_{*}^{n}$



(c) Experiment 5.3 (TSFP-Gautschi $\Phi^{\tau_{\mathrm{ref}}}_{\mathrm{ref,MD}}$): Dotted: $\sup_{t_n\in[0,1]} \mathfrak{E}_{\mathrm{ref}}^{n}$

Figure 5.7: (MD, Convergence, Experiment 5.3): **Left:** Convergence in τ, **Right:** Convergence in c. Fig. 5.7a underlines the $\mathcal{O}\left(\tau^2 + c^{-1}\right)$ bound from Theorem 3.15 and the $\mathcal{O}\left(\tau^2 + c^{-2}\right)$ bound from Remark 3.16 for the error terms $\mathfrak{E}_{\infty}^{(0),n} + \mathfrak{E}_{\mathcal{A}_\infty}^{(0),n}$ and $\mathfrak{E}_{\infty}^{(1),n}$, respectively. In Fig. 5.7b we observe the uniformly in c first order in time error bound $\mathcal{O}(\tau)$ for $\mathfrak{E}_{*}^{n}$ from Theorem 4.7. Fig. 5.7c underlines the $\mathcal{O}\left(\tau^2 c^4\right)$ error bound of the TSFP-Gautschi scheme $\Phi^{\tau_{\mathrm{ref}}}_{\mathrm{ref,MD}}$ (see [9, 10, 15, 16, 51] and also (5.11) and (5.15)), which leads to severe time step restrictions $\tau \leq Kc^{-2}$ for $\Phi^{\tau_{\mathrm{ref}}}_{\mathrm{ref,MD}}$ (cf. (5.16)). The error terms $\mathfrak{E}_{\mathcal{A}_\infty}^{(0),n}, \mathfrak{E}_{\infty}^{(0),n}, \mathfrak{E}_{\infty}^{(1),n}, \mathfrak{E}_{*}^{n}, \mathfrak{E}_{\mathrm{ref}}^{n}$ are given explicitly in (5.32).

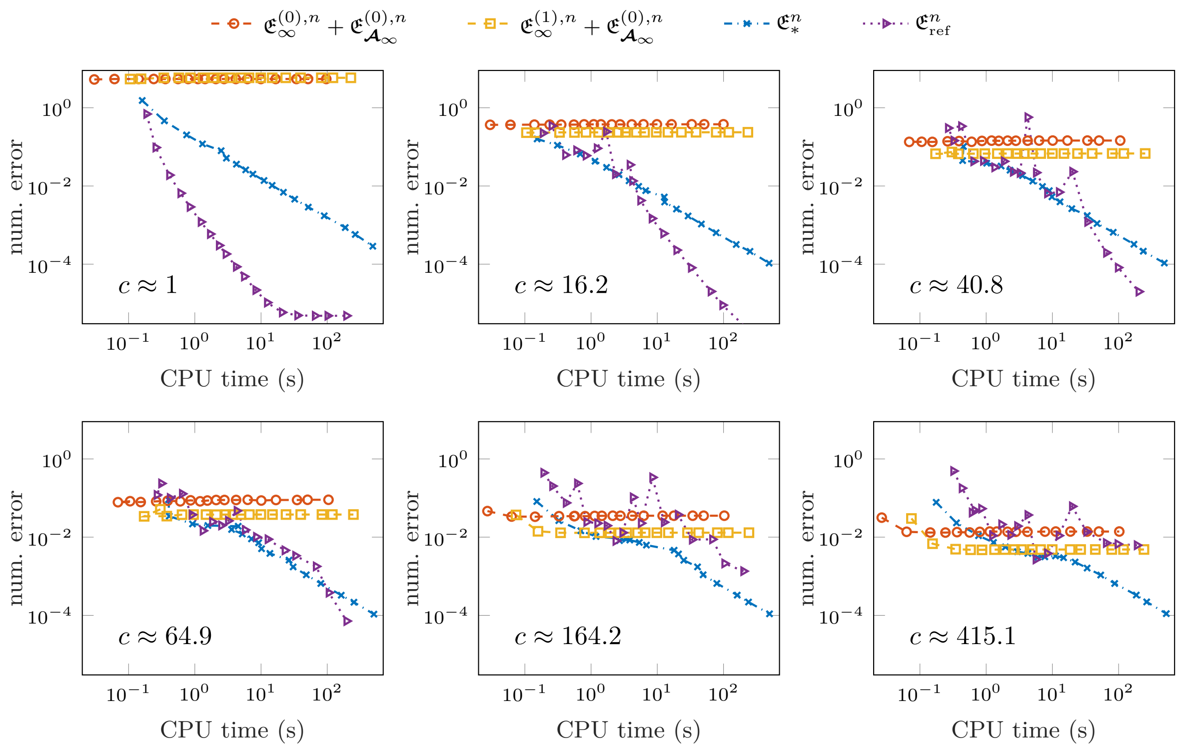


Figure 5.8: (MD, Efficiency of the Numerical Time Integration Schemes, Experiment 5.3): Efficiency plot of the methods $\Phi^{\tau}_{w0,\text{Strang}}$ (–⊖–), $\Phi^{\tau}_{w1,\text{Strang}}$ (–⊟–), Ψ^{τ}_{*} (-·×·-), $\Phi^{\tau}_{\text{ref,MKG}}$ (···▷···) for several values of c. The corresponding errors are plotted against the consumed CPU time for computing the respective numerical solution. Values in the lower left corner of each plot are desired. We observe that the reference scheme $\Phi^{\tau}_{\text{ref,MKG}}$ seems to be reliable only for small values $c \lesssim 16$ (upper left and upper middle). For larger values it behaves more and more chaotic as c increases. In the intermediate regime $16 \lesssim c \lesssim 100$ our uniformly accurate scheme Ψ^{τ}_{*} shows a smaller and more reliable error compared to the reference scheme at the same CPU time (upper right, lower left). In the highly oscillatory regime $c \gtrsim 100$ our asymptotic limit schemes $\Phi^{\tau}_{w0,\text{Strang}}$ and $\Phi^{\tau}_{w1,\text{Strang}}$ become more efficient than the other schemes the larger c gets.

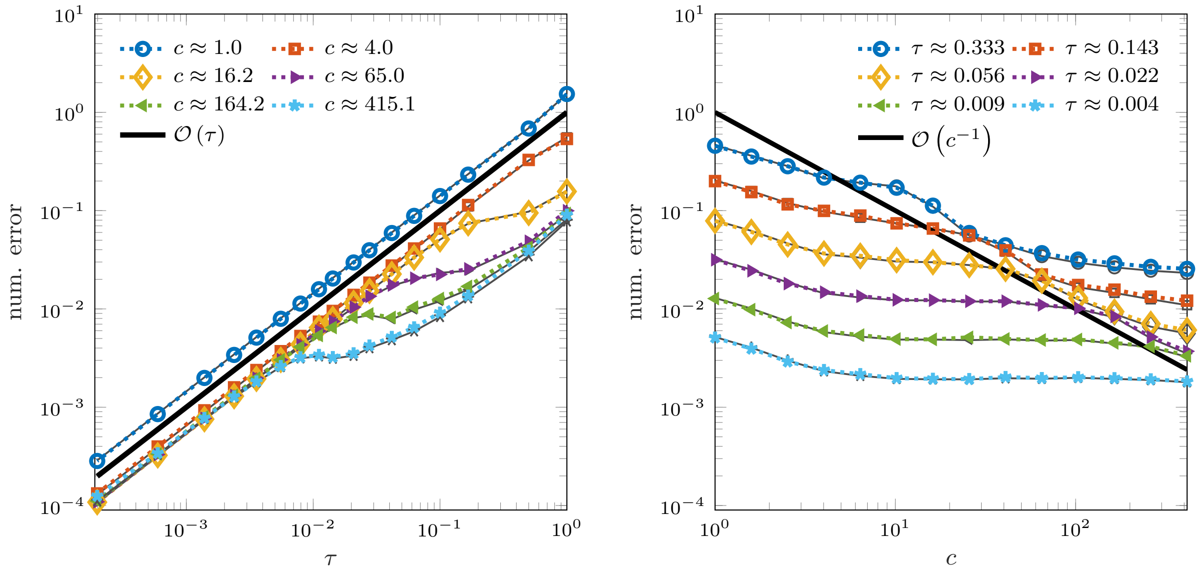


Figure 5.9: (MD, Convergence of the "Twisted Scheme" Ψ_*^τ for General Initial Data, Experiment 5.4): **Left:** Convergence in τ, **Right:** Convergence in c. The coloured lines in the figure suggest that the error $\sup_{t_n \in [0,1]} \mathfrak{E}_*^n$ of the scheme Ψ_*^τ (with $\gamma = 1$) satisfies first order in time uniform in $c \geq 1$ error bounds $\mathcal{O}(\tau)$ also for **initial data violating Assumption 4.5** (or (5.33), respectively), see Experiment 5.4 and cf. Theorem 4.8. The thin solid lines in grey (behind the coloured lines) allow us to directly compare the respective errors for the initial data from Experiment 5.3, which satisfy Assumption 4.5 (or (5.33), respectively). We observe that the numerical error of our scheme for more general initial data (coloured lines) has the same behaviour as for the restricted initial data (thin solid grey lines, cf. Theorem 4.8).

with a constant K independent of c, where $\mathcal{E}_{0,\text{MKG}}$ denotes the rest energy (german: Ruheenergie,[78]) which is given by ([69])

$$\mathcal{E}_{0,\text{MKG}}(t) := \left(\left\| \partial_t^{[\phi(t)]} \psi(t) \right\|_{L^2}^2 + c^2 \left\| \psi(t) \right\|_{L^2}^2 \right). \tag{5.40}$$

Note that $\partial_t \psi = \mathcal{O}(c^2)$ (see for instance [45, 69]) and thus

$$\mathcal{E}_{0,\text{MKG}}(t) = \mathcal{O}(c^2) \quad \text{and also (see (5.38))} \quad \mathcal{E}_{\text{MKG}}(t) = \mathcal{O}(c^2) \qquad \text{for all } t \in [0,T].$$

Therefore small errors corresponding to approximations to the exact solution $(\psi, \phi, \boldsymbol{\mathcal{A}})^\top$ of the MKG system (2.20) might lead to severe energy errors of order $\mathcal{O}(c^2)$ in the total energy $\mathcal{E}_{\text{MKG}}$. Instead, in the following we exploit the uniform bound (5.39) on the total energy $\mathcal{E}_{\text{MKG}}$ reduced by the rest energy $\mathcal{E}_{0,\text{MKG}}$.

Our aim is now to numerically investigate the conservation properties of our methods for the energy (cf. (5.39))

$$\tilde{\mathcal{E}}_{\text{MKG}}(t) = \mathcal{E}_{\text{MKG}}(t) - \mathcal{E}_{0,\text{MKG}}(0) = \mathcal{E}_{\text{MKG}}(t) - \left(\| \langle \nabla \rangle_c \psi_I' \|_{L^2}^2 + c^2 \| \psi_I \|_{L^2}^2 \right), \tag{5.41}$$

where similar to [45, 69] we plug the initial data of the MKG system (2.20)

$$\psi(0) = \psi_I \quad \text{and} \quad \partial_t^{[\phi(0)]} \psi(0) = \langle \nabla \rangle_c \psi_I'.$$

into $\mathcal{E}_{0,\text{MKG}}(0)$ (see (5.40)).

Note that using the identities (2.22) and (4.5), i.e.

$$w(t) = e^{ic^2 t} w_*(t) = e^{ic^2 t}(u_*(t), v_*(t))^\top, \quad \text{and} \quad \psi(t) = \psi_*(t) = \frac{1}{2}(e^{ic^2 t} u_*(t) + e^{-ic^2 t} \overline{v_*}(t)),$$

and with the aid of (2.24) we can write

$$\partial_t^{[\phi(t)]}\psi_*(t) = i\left\langle\nabla\right\rangle_c \left(e^{ic^2t}u_*(t) - \psi_*(t)\right). \tag{5.42}$$

Thus the discrete energy in case of MKG for our uniformly accurate scheme Ψ_*^τ with $\gamma = 0$ (see (4.39)) with numerical solution $(w_*^n, \phi_*^{\mathrm{tot},n}, \mathfrak{a}_*^{\gamma,n})^\top$ (or $(\psi_*^n, \phi_*^{\mathrm{tot},n}, \boldsymbol{\mathcal{A}}_*^n)^\top$, respectively) is given by (cf. (5.37))

$$\begin{aligned}\mathcal{E}_{\mathrm{MKG}}^{*,n} =& \left\|\boldsymbol{E}_*^n\right\|_{L^2}^2 + \left\|\boldsymbol{B}_*^n\right\|_{L^2}^2 + \left\|\nabla^{[\boldsymbol{\mathcal{A}}_*^n]}\psi_*^n\right\|_{L^2}^2 + \left\|\left\langle\nabla\right\rangle_c\left(e^{ic^2t_n}u_*^n - \psi_*^n\right)\right\|_{L^2}^2 + c^2\left\|\psi_*^n\right\|_{L^2}^2\\ \approx&\mathcal{E}_{\mathrm{MKG}}(t_n)\end{aligned}$$

where according to (5.36)

$$\boldsymbol{E}_*^n = -\nabla\phi_*^{\mathrm{tot},n} - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_*^n \qquad \text{and} \qquad \boldsymbol{B}_*^n = \nabla\times\boldsymbol{\mathcal{A}}_*^n.$$

In Fig. 5.10a we numerically underline the conservation of $\tilde{\mathcal{E}}_{\mathrm{MKG}}^{*,n}$ reduced by the rest energy at time $t = 0$ (cf. (5.41))

$$\tilde{\mathcal{E}}_{\mathrm{MKG}}^{*,n} := \mathcal{E}_{\mathrm{MKG}}^{*,n} - \left(\left\|\left\langle\nabla\right\rangle_c\psi_I'\right\|_{L^2}^2 + c^2\left\|\psi_I\right\|_{L^2}^2\right) \approx \tilde{\mathcal{E}}_{\mathrm{MKG}}^{*,0} \qquad \text{for all } t_n\in[0,10].$$

A rigorous analysis of the energy conservation properties of our scheme Ψ_*^τ given in (4.39) might be an interesting topic in future research.

Moreover, in Fig. 5.10 we observe a convergence of the energy level $\tilde{\mathcal{E}}_{\mathrm{MKG}}^{*,n}$ towards the limit energy level $\mathcal{E}_{\mathrm{MKG}}^{\infty,n}$ (see (5.43) below) as c increases.

In [45, 69] for the case of the nonlinear Klein–Gordon equation, the authors discussed the convergence of a Klein–Gordon (KG) energy of type (5.41) towards the corresponding limit energy of type (5.43). The authors use a formal asymptotic expansion (cf. Chapter 3) of the total KG energy in order to derive the limit energy.

The MKG energy in the nonrelativistic limit regime $c\to\infty$ is subject of the next section.

5.5.2 Nonrelativistic Limit Energy of the MKG System

Based on [45, 69, 70], we now discuss the energy conservation properties of our asymptotic limit time integration scheme $\Phi_{w_0,\mathrm{Strang}}^\tau$ given in (3.110). According to [70], the conserved energy, corresponding to the Schrödinger–Poisson limit system (3.30b) with solution $(w_0, \phi_0, \boldsymbol{\mathcal{A}}_0)^\top$ (combined with the energy of the corresponding electromagnetic field), is given by

$$\mathcal{E}_{\mathrm{MKG}}^{\infty}(t) := \left\|\boldsymbol{E}_0(t)\right\|_{L^2}^2 + \left\|\boldsymbol{B}_0(t)\right\|_{L^2}^2 + \frac{1}{4}\left\|\nabla u_0(t)\right\|_{L^2}^2 + \frac{1}{4}\left\|\nabla v_0(t)\right\|_{L^2}^2,$$

where (cf. (5.36))

$$\boldsymbol{E}_0(t) = -\nabla\phi_0(t) - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}_0(t) \quad \text{and} \quad \boldsymbol{B}_0(t) = \nabla\times\boldsymbol{\mathcal{A}}_0(t).$$

Note, that the identity (cf. [69, 70] and also (3.30a))

$$\psi_0(t) = \frac{1}{2}\left(e^{ic^2t}u_0(t) + e^{-ic^2t}\overline{v_0}(t)\right)$$

allows the interpretation of $\mathcal{E}^{\infty}_{\text{MKG}}(t)$ as an energy where the rest energy ([78]) has been already subtracted via the multiplication with the phases $e^{\pm ic^2 t}$ (see [69, 70]). Fig. 5.10b underlines the numerical conservation of the discrete energy $\mathcal{E}^{\infty,n}_{\text{MKG}} \approx \mathcal{E}^{\infty}_{\text{MKG}}(t_n)$ where

$$\mathcal{E}^{\infty,n}_{\text{MKG}} := \|\boldsymbol{E}^n_0\|^2_{L^2} + \|\boldsymbol{B}^n_0\|^2_{L^2} + \frac{1}{4}\|\nabla u^n_0\|^2_{L^2} + \frac{1}{4}\|\nabla v^n_0\|^2_{L^2} \qquad \text{for all } t_n \in [0,10] \tag{5.43}$$

corresponds to the numerical approximation $(w^n_0, \phi^n_0, \boldsymbol{\mathcal{A}}^n_0)^\top$ obtained with the scheme $\Phi^\tau_{w_0,\text{Strang}}$ given in (3.110). Despite the explicit dependence of $\mathcal{E}^{\infty,n}_{\text{MKG}}$ on $\boldsymbol{E}_0$ and $\boldsymbol{B}_0$ and thus on the c-dependent phases $\cos(ct\langle\nabla\rangle_0)$ and $\sin(ct)$ in $\boldsymbol{\mathcal{A}}_0$ (cf. (5.26)) Fig. 5.10b also shows that $\mathcal{E}^{\infty,n}_{\text{MKG}}$ is independent of c. In Fig. 5.10, we observe that the discrete energy levels of the MKG system converge towards the discrete limit energy level as c increases, i.e.

$$\tilde{\mathcal{E}}^{*,n}_{\text{MKG}} \to \mathcal{E}^{\infty,n}_{\text{MKG}} \qquad \text{as } c \to \infty \text{ for all } t_n \in [0,10].$$

Next, we discuss the energy conservation of our uniformly accurate scheme for the Maxwell–Dirac system.

5.5.3 Total Energy of the MD System

Similar to Section 5.5.1 we now discuss the energy conservation properties of our twisted scheme Ψ^τ_* given in (4.39) in case of the MD system (2.36). Based on [70] and [87, Chapter 6] we define the energy of the MD system by

$$\mathcal{E}_{\text{MD}}(t) = \|\boldsymbol{E}(t)\|^2_{L^2} + \|\boldsymbol{B}(t)\|^2_{L^2} + \operatorname{Re}\left(\left\langle ic\partial_t^{[\phi(t)]}\psi(t), \psi(t)\right\rangle_{L^2}\right), \tag{5.44}$$

where $\langle f, g\rangle_{L^2} := (2\pi)^{-d}\int_{\mathbb{T}^d} f(x)\cdot\overline{g(x)}dx$ denotes the L^2 inner product on $\mathbb{T}^d$. In view of the Dirac equation (2.36a)

$$i\partial_t^{[\phi(t)]}\psi(t) = -i\sum_{j=1}^{d}\boldsymbol{\alpha}_j(\partial_j - \frac{i}{c}A_j(t))\psi(t) + c\boldsymbol{\beta}\psi(t), \qquad \psi(0) = \psi_I,$$

and in view of the decomposition $\psi = (\psi^+, \psi^-)^\top$ (see (2.42)) we deduce that the MD rest energy reads ([70], [87, Chapter 6.1.1, Remark 1])

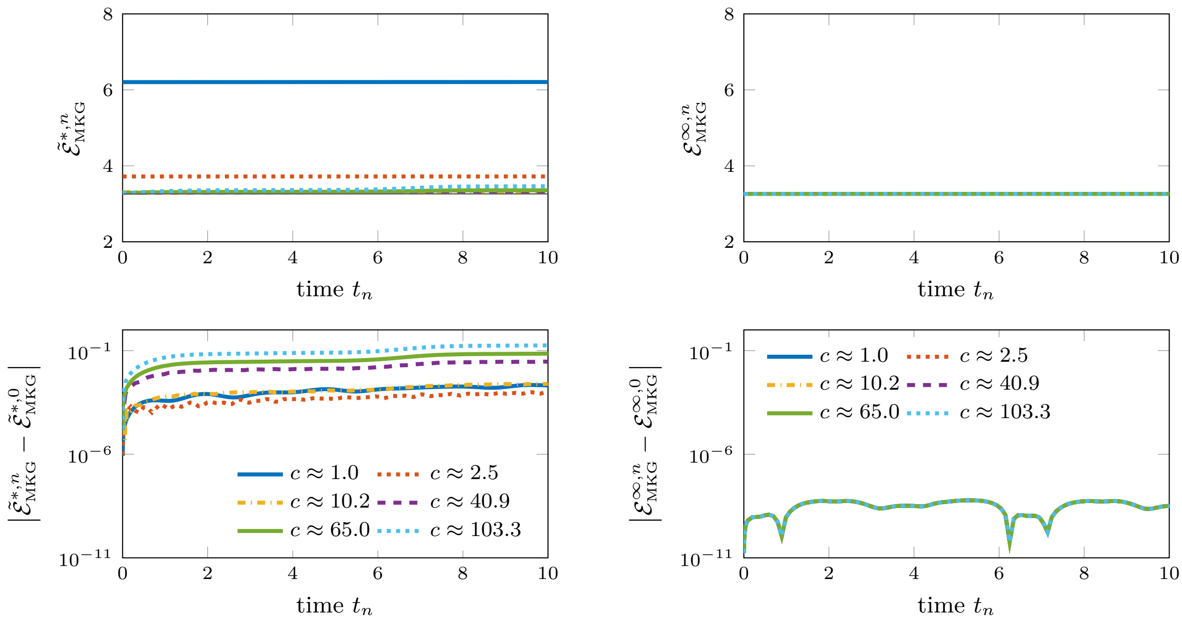
$$\mathcal{E}_{0,\text{MD}}(t) := \operatorname{Re}\left(\langle c^2\boldsymbol{\beta}\psi(t), \psi(t)\rangle_{L^2}\right) = c^2\left(\left\|\psi^+(t)\right\|^2_{L^2} - \left\|\psi^-(t)\right\|^2_{L^2}\right).$$

The last equality is due to the identity $\boldsymbol{\beta} = \operatorname{diag}(\mathcal{I}_2, -\mathcal{I}_2)$ from (1.21).

Recall that in our numerical experiments (see Section 5.4), we considered the reduced MD system (2.37) with solution $(\Psi, \phi, \boldsymbol{\mathcal{A}})^\top$ in dimension $d = d_{\text{low}} = 2$. We obtain the corresponding conserved energy by replacing in (5.44) the Dirac solution ψ with Ψ and the matrices $\boldsymbol{\alpha}_j$ with $\boldsymbol{\sigma}_j$ for $j = 1, 2$ and $\boldsymbol{\beta}$ with σ_3 (see (1.21)).

Our aim is now to numerically underline the numerical conservation of the discrete MD energy $\mathcal{E}^{*,n}_{\text{MD}}$ corresponding to the numerical solution $(w^n_*, \phi^{\text{tot},n}_*, \mathfrak{a}^{\gamma,n}_*)^\top$ (or $(\Psi^n_*, \phi^{\text{tot},n}_*, \boldsymbol{\mathcal{A}}^n_*)^\top$, respectively) obtained with the uniformly accurate "twisted scheme" Ψ^τ_* with $\gamma = 1$ given in (4.39) reduced by its initial rest energy $\mathcal{E}^{*,0}_{0,\text{MD}}$, i.e. we underline the conservation of

$$\tilde{\mathcal{E}}^{*,n}_{\text{MD}} = \mathcal{E}^{*,n}_{\text{MD}} - c^2\left(\left\|\psi^+_I\right\|^2_{L^2} - \left\|\psi^-_I\right\|^2_{L^2}\right) \qquad \text{for all } t_n \in [0, T].$$



(a) (MKG Energy for Ψ^τ_*, Experiment 5.1): Reduced discrete energy (upper) and energy error (lower) for Ψ^τ_* (with $\gamma = 0$).

(b) (MKG Energy for $\Phi^\tau_{w_0,\mathrm{Strang}}$, Experiment 5.1): Discrete energy (upper) and energy error (lower) for $\Phi^\tau_{w_0,\mathrm{Strang}}$.

Figure 5.10: (MKG Energy): Simulation of the reduced energy $\tilde{\mathcal{E}}_{\mathrm{MKG}}$ and of the limit energy $\mathcal{E}^\infty_{\mathrm{MKG}}$ corresponding to Experiment 5.1 with time step $\tau \approx 0.002$. We observe that our uniformly accurate "twisted scheme" Ψ^τ_* conserves the corresponding energy for all times $t_n \in [0, 10]$ up to small numerical errors (see lower left for the energy error $\left|\tilde{\mathcal{E}}^{*,n}_{\mathrm{MKG}} - \tilde{\mathcal{E}}^{*,0}_{\mathrm{MKG}}\right|$). The limit approximation scheme $\Phi^\tau_{w_0,\mathrm{Strang}}$ conserves the limit energy $\mathcal{E}^\infty_{\mathrm{MKG}}$ almost perfectly (see lower right for the energy error $\left|\mathcal{E}^{\infty,n}_{\mathrm{MKG}} - \mathcal{E}^{\infty,0}_{\mathrm{MKG}}\right|$). We observe that the limit energy $\mathcal{E}^\infty_{\mathrm{MKG}}$ (upper right) and its error (lower right) is independent of c and that for increasing c, the energy level of $\tilde{\mathcal{E}}^{*,n}_{\mathrm{MKG}}$ (see upper left) converges towards the limit energy level of $\mathcal{E}^{\infty,n}_{\mathrm{MKG}}$ (thin solid grey line).

Thereby, in view of the identity

$$\partial_t^{[\phi(t)]}\Psi(t) = i\,\langle\nabla\rangle_c\left(e^{ic^2t}u_*(t) - \Psi(t)\right) \qquad \text{(see (2.40) and also (5.42))}$$

we set similar as in the previous sections

$$\begin{aligned}\tilde{\mathcal{E}}^{*,n}_{\mathrm{MD}} &= \|\boldsymbol{E}^n_*\|^2_{L^2} + \|\boldsymbol{B}^n_*\|^2_{L^2} + \mathrm{Re}\left(\left\langle -c\,\langle\nabla\rangle_c\left(e^{ic^2t_n}u^n_* - \Psi^n_*\right), \Psi^n_*\right\rangle_{L^2}\right)\\ &\approx \mathcal{E}_{\mathrm{MD}}(t_n)\end{aligned}$$

where according to (5.36)

$$\boldsymbol{E}^n_* = -\nabla\phi^{\mathrm{tot},n}_* - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}^n_* \qquad \text{and} \qquad \boldsymbol{B}^n_* = \nabla\times\boldsymbol{\mathcal{A}}^n_*.$$

In Fig. 5.11 we observe that our scheme Ψ^τ_* conserves the reduced energy $\tilde{\mathcal{E}}^{*,n}_{\mathrm{MD}}$ for all times $t_n \in [0, 10]$.

In the subsequent section we discuss the norm conservation properties of our twisted scheme Ψ^τ_* given in (4.39) applied to both the MKG and the reduced MD system (2.20)/(2.37).

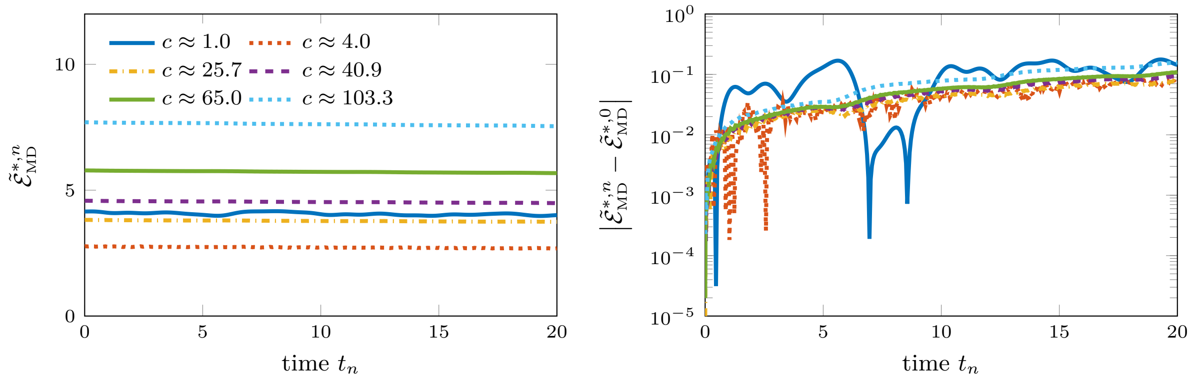
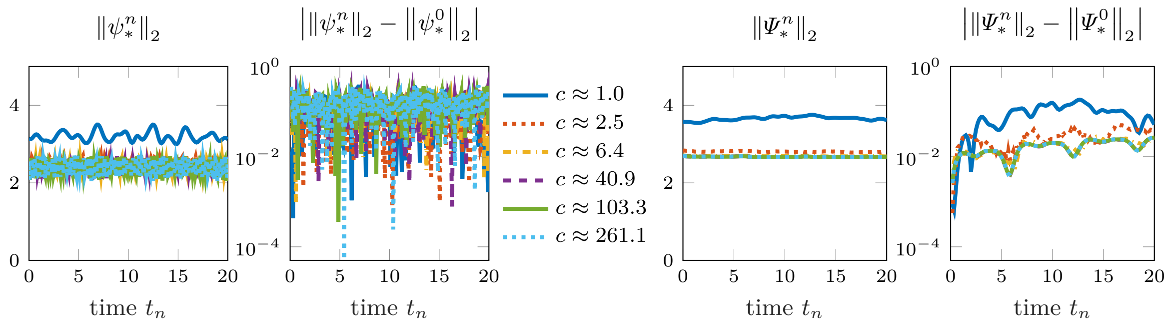


Figure 5.11: (MD Energy): Simulation of the reduced energy $\tilde{\mathcal{E}}_{\mathrm{MD}}$ corresponding to Experiment 5.4 with time step $\tau \approx 0.004$. We observe that our uniformly accurate "twisted scheme" Ψ^τ_* (with $\gamma = 1$) conserves the corresponding energy for all times $t_n \in [0, 20]$ up to small numerical errors (see right figure for the energy error $\left|\tilde{\mathcal{E}}^{*,n}_{\mathrm{MD}} - \tilde{\mathcal{E}}^{*,0}_{\mathrm{MD}}\right|$). Note that here we do not observe a convergence behaviour in the energy $\tilde{\mathcal{E}}^{*,n}_{\mathrm{MD}}$ as $c \to \infty$ in contrast to the MKG case (cf. Fig. 5.10).



(a) MKG H^2 Norm. (b) Reduced MD H^2 Norm.

Figure 5.12: (H^2 Norm Conservation): In Fig. 5.12a, we observe that our "twisted scheme" Ψ^τ_* (with $\gamma = 0$) given in (4.39) applied to the MKG system (2.20) with $\tau \approx 0.024$ for initial data corresponding to Experiment 5.1 conserves $\|\psi^n_*\|_2 \approx \left\|\psi^0_*\right\|_2 = \|\psi_*(0)\|_2$ for all times $t_n \in [0, 20]$ up to small numerical errors, i.e. $\left|\|\psi^n_*\|_2 - \left\|\psi^0_*\right\|_2\right|$ is small. In Fig. 5.12b, we make a similar observation for the application of Ψ^τ_* (with $\gamma = 1$) to the reduced MD system (2.37) for initial data corresponding to Experiment 5.4.

5.5.4 Conservation of the H^2 Norm for the "Twisted Scheme"

Motivated by the analytical norm conservation properties ([21, 22, 34, 70]) of the solution ψ of the MKG/MD system (2.20)/(2.36), we now numerically investigate the norm conservation properties of our uniformly accurate in $c \geq 1$ first order in time "twisted scheme" Ψ^τ_* given in (4.39) applied to the MKG system (2.20) and to the reduced MD system (2.37). In our numerical experiments, we observe that our scheme for both the MKG case (with $\gamma = 0$) and for the MD case (with $\gamma = 1$) conserves the H^2 norm of ψ over all times $t_n \in [0, 20]$ (see Fig. 5.12), i.e. $\|\psi^n_*\|_2 \approx \left\|\psi^0_*\right\|_2 = \|\psi_*(0)\|_2$ for all $t_n \in [0, 20]$.

CHAPTER

SIX

CONCLUSION AND OUTLOOK

This thesis addressed the construction of efficient numerical time integration schemes for Maxwell–Klein–Gordon and Maxwell–Dirac systems in the highly oscillatory nonrelativistic limit regime, the intermediate regime and the slowly oscillatory relativistic regime.

We covered the integration in the nonrelativistic limit regime $c \gg 1$ efficiently with standard Strang splitting schemes applied to non-oscillatory Schrödinger–Poisson systems exploiting the asymptotic behaviour of the exact solution. The construction was based on analytical results from [20–22, 70] and on the ideas presented in [45, 63]. For the latter schemes with time step τ, we rigorously proved numerical error bounds of order $\mathcal{O}\left(\tau^2 + c^{-1}\right)$ and $\mathcal{O}\left(\tau^2 + c^{-2}\right)$, respectively. These results also provide a rigorous proof of the purely numerically investigated error bounds from [57] for MD. The explicit derivation and analysis of higher order limit approximations at order $\mathcal{O}\left(c^{-N}\right)$ is interesting future research.

In slowly oscillatory, intermediate and highly oscillatory regimes, we proposed and analysed efficient uniformly accurate schemes for Maxwell–Klein–Gordon and Maxwell–Dirac systems following the ideas from [18]. Due to error bounds of order $\mathcal{O}\left(\tau\right)$ independent of c, they provide good numerical approximations for all $c \geq 1$. Despite that our error analysis for the case of the Maxwell–Dirac system required additional assumptions on the initial data of the solution, promising numerical experiments (see Experiment 5.4) suggest that the latter assumptions might not be necessary. In future work we shall use different techniques in proving the uniform error bounds for MKG and MD systems under weaker assumptions. The construction of higher order methods in time for both systems as well as a rigorous investigation of the energy conservation properties of our schemes is ongoing research.

Moreover, the results in [18] motivate to study the convergence behaviour of our uniformly accurate schemes towards the corresponding limit schemes as $c \to \infty$ for the MKG and MD systems.

We furthermore plan to incorporate finite element space discretization techniques into our schemes. This will allow us to consider different boundary conditions for MKG and MD systems in more general spatial domains.

APPENDIX

A

APPENDIX

In the Appendix, we provide further details on selected topics which have been addressed within this thesis. Definitions and results corresponding to Sobolev spaces and related topics are given in Appendix A.1. Appendix A.2 deals with asymptotic properties of the operator $\langle \nabla \rangle_c$. In Appendix A.3 we discuss the solution operator to Poisson's equation. A definition and some properties for the projection operator $\mathcal{P}_{\mathrm{df}}$ onto divergence-free vector fields can be found in Appendix A.4. Important tools for the numerical time integration of differential equations are collected in Appendix A.5. Appendix A.6 provides auxiliary results for the derivation of the MKG and MD systems from Chapter 2. Appendix A.7 comprises additional material such as for instance the Cauchy-Schwarz inequality.

A.1 Sobolev Spaces

Definition A.1 ([3, Paragraphs 7.58 & 7.62], [35, 45, 85], Sobolev Spaces on $\mathbb{T}^d$)**.** *For $r \geq 0$ we define the space $H^r(\mathbb{T}^d)$ as the space of all functions u satisfying $\|u\|_{H^r(\mathbb{T}^d)} < \infty$, where the norm $\|\cdot\|_{H^r(\mathbb{T}^d)}$ is defined as*

$$\|u\|^2_{H^r(\mathbb{T}^d)} = \sum_{k \in \mathbb{Z}^d} \left|\langle k \rangle_1^r \, \widehat{u}_k\right|^2 = \sum_{k \in \mathbb{Z}^d} (1 + |k|^2)^r \left|\widehat{u}_k\right|^2 .$$

Here, for $c \in \mathbb{R}$ we define the symbol $\langle k \rangle_c = \sqrt{c^2 + |k|^2}$ with $|k|^2 = (k^1)^2 + \cdots + (k^d)^2$. Furthermore,

$$\widehat{u}_k = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} u(x) e^{-ik\cdot x} dx$$

denotes the (continuous) Fourier transform on $\mathbb{T}^d$ of u corresponding to the Fourier number $k \in \mathbb{Z}^d$. In particular, we associate with $H^0(\mathbb{T}^d)$ the usual L^2 space on the torus $\mathbb{T}^d$ which is an immediate consequence of Parseval's identity (see [5, Corollary 7.16] for $d = 1$), i.e.

$$\|w\|_{L^2(\mathbb{T}^d)} = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} |w(x)|^2 \, dx \overset{\text{(Parseval)}}{=} \sum_{k \in \mathbb{Z}^d} \left|\widehat{w}_k\right|^2 = \|w\|_{H^0(\mathbb{T}^d)} .$$

For vector valued functions $w = (w_1, w_2, \ldots, w_m)^\top \in \left(H^r(\mathbb{T}^d)\right)^m$, $m \in \mathbb{N}$ *we define the norm*

$$\|w\|_{\left(H^r(\mathbb{T}^d)\right)^m} = \sum_{j=1}^{m} \|w_j\|_{H^r}.$$

In the following we may also write $\langle k \rangle = \langle k \rangle_1$ for $c = 1$.

Definition A.2 ([45, 63, 69, 70, 79], The Operator $\langle \nabla \rangle_c$)**.** *Let* $\Omega = \mathbb{T}^d$ *and let* $w \in H^{r+1}(\Omega)$*. For* $c \in \mathbb{R}$ *fixed, we define the operator*

$$\langle \nabla \rangle_c : H^{r+1}(\Omega) \to H^r(\Omega), \quad \langle \nabla \rangle_c w := \sqrt{-\Delta + c^2} w$$

via its Fourier symbol $(\widehat{\langle \nabla \rangle_c})_k := \langle k \rangle_c = \sqrt{|k|^2 + c^2}$*, such that*

$$\langle \nabla \rangle_c w(x) := \sum_{k \in \mathbb{Z}^d} \sqrt{|k|^2 + c^2}\, \widehat{w}_k e^{ik\cdot x} \qquad \text{in case of } \Omega = \mathbb{T}^d.$$

We furthermore define $\langle \nabla \rangle_c^m$ *for* $c \neq 0$ *and* $m \in \mathbb{R}$ *through the Fourier symbol*

$$(\widehat{\langle \nabla \rangle_c^m})_k := \langle k \rangle_c^m = \left(|k|^2 + c^2\right)^{m/2}, \qquad \text{for all } k \in \mathbb{Z}^d.$$

Similarly we define for $c = 0$ *the operator* $\langle \nabla \rangle_0^m$ *through*

$$(\widehat{\langle \nabla \rangle_0^m})_k := \langle k \rangle_0^m = \begin{cases} \left(|k|^2\right)^{m/2} & \text{for all } k \in \mathbb{Z}^d, \text{ if } m \geq 0, \\ \left(|k|^2\right)^{m/2} & \text{for all } k \in \mathbb{Z}^d \setminus \{0\}, \text{ if } m < 0, \\ 0 & \text{for } k = 0, \text{ if } m < 0. \end{cases}$$

In this thesis we focus on the case of the torus $\Omega = \mathbb{T}^d$, whereas some auxiliary results, on which we might refer to, are originally stated on $\mathbb{R}^d$ but can also be transferred to the $\mathbb{T}^d$ case. Next we introduce the Sobolev space $\dot{H}^r(\mathbb{T}^d)$ for functions with vanishing mean.

Definition A.3 ([85, Appendix A] and [64, 79], Homogeneous Sobolev Spaces on T^d)**.** *Let* $r \in \mathbb{N}_0$*. We define the homogeneous Sobolev space* $\dot{H}^r$ *on the torus* $\mathbb{T}^d$ *for its equivalence on* $\mathbb{R}^d$*) by*

$$\dot{H}^r(\mathbb{T}^d) = \left\{ u \in H^r(\mathbb{T}^d) | \int_{\mathbb{T}^d} u(x)dx = 0 \right\}$$

equipped with the norm

$$\begin{cases} \|u\|_{r,0} = \|\langle \nabla \rangle_0 u\|_{r-1} & \text{for } r \geq 1, \\ \|u\|_{0,0} = \sum_{k \in \mathbb{Z}^d \setminus \{0\}} |\widehat{u}_k|^2 & \text{for } r = 0. \end{cases}$$

With the aid of the following Proposition A.4, we show in lemma Lemma A.5 below that $\|\cdot\|_{r,0}$ indeed defines a norm on $\dot{H}^r(\mathbb{T}^d)$.

Proposition A.4 ([83, Section 2.1])**.** *Let* $u \in \dot{H}^r(\mathbb{T}^d)$ *be a periodic function on the torus* $\mathbb{T}^d$*. Then* u *has a vanishing mean, i.e.*

$$\widehat{u}_0 = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} u(x)dx = 0.$$

Proof: Let $u(x) = \sum_{k\in\mathbb{Z}^d} \widehat{u}_k e^{ik\cdot x}$ be the Fourier series expansion of u. Since for $k = (k^1, \dots, k^d)^\top \in \mathbb{Z}^d$ we have

$$\int_{\mathbb{T}^d} \widehat{u}_k e^{ik\cdot x} dx = \widehat{u}_k \int_{\mathbb{T}^d} e^{ik^1 x^1} dx^1 \cdots \int_{\mathbb{T}^d} e^{ik^d x^d} dx^d = \begin{cases} 0, & k \neq 0, \\ (2\pi)^d \widehat{u}_0, & k = 0. \end{cases}$$

Hence if

$$\int_{\mathbb{T}^d} u(x) dx = \int_{\mathbb{T}^d} \sum_{k\in\mathbb{Z}^d} \widehat{u}_k e^{ik\cdot x} dx = 0,$$

then $\widehat{u}_0 = 0$. □

From the definition of the Sobolev spaces H^r and $\dot{H}^r$ above, we see that the definition of the operator $\langle\nabla\rangle_c$ in Definition A.2 is very related to the Fourier multipliers $\langle k\rangle_1$ which we used to define the norm $\|\cdot\|_r$ in Definition A.1. Furthermore, applying the operator $\langle\nabla\rangle_c^m$ to a function w we see in the following Lemma A.5 that for $m > 0$ we lose and for $m < 0$ we gain regularity.

Lemma A.5 ([85, Appendix A])**.** *Let $r \geq 0$ and $m \in \mathbb{R}$ such that $r + m \geq 0$. Furthermore let $r' = \max\{r, r+m\}$. Then for $0 \neq c \in \mathbb{R}$ fixed and $u \in H^{r'}$ we have*

$$\|\langle\nabla\rangle_c^m u\|_r \leq K_{c,m} \|u\|_{r+m}, \quad K_{c,m} = \max\{1, c^m\}.$$

For $c = 0$ and $u \in \dot{H}^{r'}$ respectively we find

$$\|\langle\nabla\rangle_0^m u\|_r \leq K_{0,m} \|u\|_{r+m,0}, \quad K_{0,m} = \max\{\sqrt{2}^{1-m}, 1\}.$$

In particular this implies that

$$\|u\|_r \leq \sqrt{2}\, \|u\|_{r,0} \leq \sqrt{2}\, \|u\|_r,$$

which means that $\|\cdot\|_{r,0}$ defines a norm on $\dot{H}^r$.

Proof (see also [83, Section 2.1])*:* First let $m \geq 0$. It is obvious that for $k \in \mathbb{Z}^d$

$$\begin{aligned} c^2 = 0 \quad &\text{we have that} \quad (\langle k\rangle_0^m)^2 = (|k|^2)^m \leq |k|^2 (1 + |k|^2)^{m-1}, \\ 0 < c^2 \leq 1 \quad &\text{we have that} \quad (\langle k\rangle_c^m)^2 = (c^2 + |k|^2)^m \leq (1 + |k|^2)^m, \\ c^2 > 1 \quad &\text{we have that} \quad (\langle k\rangle_c^m)^2 = c^{2m}(1 + |k|^2 / c^2)^m \leq c^{2m}(1 + |k|^2)^m. \end{aligned}$$

Now let $-\alpha = m < 0$ with $\alpha > 0$. Then

$$\begin{aligned} 0 < c^2 \leq 1 \quad &\text{we have that} \quad (\langle k\rangle_c^m)^2 = c^{-2\alpha}(1 + |k|^2 / c^2)^{-\alpha} \leq c^{2m}(1 + |k|^2)^m, \\ c^2 > 1 \quad &\text{we have that} \quad (\langle k\rangle_c^m)^2 = (c^2 + |k|^2)^{-\alpha} \leq (1 + |k|^2)^m, \end{aligned}$$

where $k \in \mathbb{Z}^d$ for $c \neq 0$. In case of $c = 0$ and $-\alpha = m < 0$ we consider $k \in \mathbb{Z}^d \setminus \{0\}$ and find that

$$(\langle k\rangle_0^m)^2 = \frac{|k|^2}{(|k|^2)^{\alpha+1}} = \frac{2^{\alpha+1} |k|^2}{(2\,|k|^2)^{\alpha+1}} \leq \frac{2^{\alpha+1} |k|^2}{(1 + |k|^2)^{\alpha+1}} = 2^{-m+1} |k|^2 (1 + |k|^2)^{m-1}.$$

Definitions A.1 and A.3 conclude the proof. □

Next we introduce the ℓ_r^p spaces ([44]) which coincide with the $H^r(\mathbb{T}^d)$ Sobolev space for $p = 2$.

Definition A.6 ([44, Chapter III.2], ℓ^p_r spaces)**.** *We define the space* $\ell^p_r := \{z \in \mathbb{C}^{\mathbb{Z}^d} \mid \|z\|_{\ell^p_r} < \infty\}$ *with norm*

$$\|z\|_{\ell^p_r} := \left(\sum_{k\in\mathbb{Z}^d} |\langle k\rangle^r z_k|^p \right)^{1/p}, \quad \langle k\rangle = \sqrt{1+|k|^2}.$$

In particular we define $\ell^p := \ell^p_0$. *Moreover, the norm* $\|z\|^2_{\ell^2} = \langle z, z\rangle_{\ell^2}$ *is induced by the inner product* $\langle z, w\rangle_{\ell^2} := \sum_{k\in\mathbb{Z}^d} z_k \overline{w_k}$.

In particular, setting $\widehat{u} := (\widehat{u}_k)_{k\in\mathbb{Z}^d}$ *for* $u \in H^r(\mathbb{T}^d)$ *we have that by definition of* $\|\cdot\|_r$ *in Definition A.1 the* $\|\widehat{u}\|_{\ell^2_r} = \|u\|_r$, *i.e.* $H^r(\mathbb{T}^d)$ *can be identified with the space* ℓ^2_r *(see also [44, Chapter III.2]).*

Proposition A.7 ([44], Embedding of the ℓ^p_r Spaces)**.** *Let* $s, s' \in \mathbb{R}$ *such that* $s' - s > d/2$. *Then we have*

$$\ell^2_{s'} \subset \ell^1_s \subset \ell^2_s$$

and there exists a constant K *such that for all* z

$$\|z\|_{\ell^2_s} \le \|z\|_{\ell^1_s} \le K \|z\|_{\ell^2_{s'}} .$$

Proof: Let $z \in \ell^2_{s'}$. From Cauchy-Schwartz inequality Proposition A.31 we deduce

$$\begin{aligned}\|z\|_{\ell^1_s} &= \sum_{k\in\mathbb{Z}^d} \langle k\rangle^s |z_k| = \sum_{k\in\mathbb{Z}^d} \langle k\rangle^{s-s'} \cdot \langle k\rangle^{s'} |z_k| \\ &\le \left(\sum_{k\in\mathbb{Z}^d} \langle k\rangle^{2(s-s')}\right)^{1/2} \left(\sum_{k\in\mathbb{Z}^d} \langle k\rangle^{2s'} |z_k|^2\right)^{1/2} \le K(d) \|z\|_{\ell^2_{s'}} ,\end{aligned}$$

where the last inequality follows from the condition $s' - s > d/2$ and Lemma A.30.

Now let $z \in \ell^1_s$. Then from $\langle k\rangle^s |z_k| \le \|z\|_{\ell^1_s}$ for all $k \in \mathbb{Z}^d$, it follows that

$$\|z\|^2_{\ell^2_s} = \sum_{k\in\mathbb{Z}^d} \langle k\rangle^{2s} |z_k|^2 \le \|z\|_{\ell^1_s} \sum_{k\in\mathbb{Z}^d} \langle k\rangle^s |z_k| = \|z\|^2_{\ell^1_s} .$$

This finishes the proof. □

Within this thesis, we repeatedly make use the following bilinear Sobolev product estimates.

Lemma A.8 ([3, Theorem 4.39] and [56, Theorem 8.3.1], Bilinear Sobolev Product Estimates)**.** *Let* $s, s_1, s_2 \in \mathbb{R}$ *satisfying*

$$s \le s_j, j = 1, 2, \qquad s_1 + s_2 - s > d/2.$$

Furthermore for $k = (k^1, \dots, k^d)^\top \in \mathbb{Z}^d$ *let* $\langle k\rangle^2 = (1 + |k|^2)$ *with* $|k|^2 = (k^1)^2 + \dots + (k^d)^2$.

Then, we obtain the following results

(a) For arbitrary $k \in \mathbb{Z}^d$ *we have*

$$\sum_{\ell\in\mathbb{Z}^d} \frac{\langle k\rangle^{2s}}{\langle k-\ell\rangle^{2s_1} \langle \ell\rangle^{2s_2}} \le K(s, d)$$

with a constant $K(s, d)$ *depending on* s *and* d *but not on* $k \in \mathbb{Z}^d$.

(b) *If $u_j \in H^{s_j}(\mathbb{T}^d)$, $j = 1, 2$, then $u_1 u_2 \in H^s(\mathbb{T}^d)$, i.e. $\|u_1 u_2\|_s \le K \|u_1\|_{s_1} \|u_2\|_{s_2}$.*

In particular for $r > d/2$ we thus obtain the following bilinear estimates

(a) $\|u_1u_2\|_r \le K(r,d)\,\|u_1\|_r\,\|u_2\|_r$ *for $s = s_1 = s_2 = r$.*

(b) $\|u_1u_2\|_{r-1} \le K(r,d)\,\|u_1\|_{r-1}\,\|u_2\|_r$ *for $s = s_1 = r-1$ and $s_2 = r$.*

(c) $\|u_1u_2\|_{r-2} \le K(r,d)\,\|u_1\|_{r-1}\,\|u_2\|_{r-1}$ *for $s = r-2$ and $s_1 = s_2 = r-1$.*

(d) $\|u_1u_2\|_{r-2} \le K(r,d)\,\|u_1\|_{r-2}\,\|u_2\|_r$ *for $s = s_1 = r-2$ and $s_2 = r$.*

Remark A.9. *The bilinear estimates of the previous Lemma A.8 are given for periodic functions u_j, $j = 1, 2$ on the torus $\mathbb{T}^d$. Results for the whole space $\mathbb{R}^d$ can be found for example in [3, Theorem 4.39] and [56, Theorem 8.3.1].*

Proof (of Lemma A.8, see also [3, Theorem 4.39] and [56, Theorem 8.3.1])*:* Let $k \in \mathbb{Z}^d$ be arbitrary. We observe that for all $\ell \in \mathbb{Z}^d$

$$\langle k\rangle^2 \le 1 + |k-\ell|^2 + 2\,|k-\ell|\,|\ell| + 1 + |\ell|^2 \le (\langle k-\ell\rangle + \langle \ell\rangle)^2$$

and thus $\langle k\rangle \le 2\max(\langle k-\ell\rangle, \langle \ell\rangle)$. Let us first consider the case $\langle k-\ell\rangle \ge \langle \ell\rangle$. Then

$$\frac{\langle k\rangle^{2s}}{\langle k-\ell\rangle^{2s_1}\langle \ell\rangle^{2s_2}} \le 2^{2s}\frac{\langle k-\ell\rangle^{2s}}{\langle k-\ell\rangle^{2s_1}\langle \ell\rangle^{2s_2}} = 2^{2s}\frac{1}{\langle k-\ell\rangle^{2(s_1-s)}\langle \ell\rangle^{2s_2}} \le 2^{2s}\frac{1}{\langle \ell\rangle^{2(s_1+s_2-s)}},$$

where the last inequality follows from $s_1 - s \ge 0$. Analogously using that $s_2 - s \ge 0$ we find for the case $\langle k-\ell\rangle < \langle \ell\rangle$ that the term on the very left is $\le 2^{2s}\langle k-\ell\rangle^{-2(s_1+s_2-s)}$. Combining these results and exploiting that for $a, b > 0$ we have $\frac{1}{\min(a,b)^2} \le \frac{1}{a^2} + \frac{1}{b^2}$ yields

$$\begin{aligned}\sum_{\ell\in\mathbb{Z}^d}\left(\frac{\langle k\rangle^{2s}}{\langle k-\ell\rangle^{2s_1}\langle \ell\rangle^{2s_2}}\right) &\le 2^{2s}\sum_{\ell\in\mathbb{Z}^d}\frac{1}{\min(\langle k-\ell\rangle, \langle \ell\rangle)^{2(s_1+s_2-s)}}\\ &\le 2^{2s+1}\sum_{\ell\in\mathbb{Z}^d}\langle \ell\rangle^{-2(s_1+s_2-s)} \le K(s,d)\end{aligned}$$

where according to Lemma A.30 the last sum is convergent for $s_1 + s_2 - s > d/2$ and bounded by a constant $K(s,d)$ depending only on s and d but not on k. This proves part (a).

For part (b) we have according to Definition A.6

$$\|uv\|_s^2 = \sum_{k\in\mathbb{Z}^d}\left|\langle k\rangle^s\sum_{\ell\in\mathbb{Z}^d}\frac{1}{\langle k-\ell\rangle^{s_1}\langle \ell\rangle^{s_2}}\langle k-\ell\rangle^{s_1}\hat{u}_{k-\ell}\langle \ell\rangle^{s_2}\hat{v}_\ell\right|^2.$$

Because the second sum is an ℓ^2 inner product (see Definition A.6) we can apply the Cauchy-Schwartz inequality Proposition A.31 and obtain

$$\begin{aligned}&\left|\langle k\rangle^s\sum_{\ell\in\mathbb{Z}^d}\frac{1}{\langle k-\ell\rangle^{s_1}\langle \ell\rangle^{s_2}}\langle k-\ell\rangle^{s_1}\hat{u}_{k-\ell}\langle \ell\rangle^{s_2}\hat{v}_\ell\right|^2\\ &\le\left(\sum_{\ell\in\mathbb{Z}^d}\left(\frac{\langle k\rangle^s}{\langle k-\ell\rangle^{s_1}\langle \ell\rangle^{s_2}}\right)^2\right)\sum_{\ell\in\mathbb{Z}^d}\left(\langle k-\ell\rangle^{2s_1}|\hat{u}_{k-\ell}|^2\langle \ell\rangle^{2s_2}|\hat{v}_\ell|^2\right).\end{aligned}$$

Using part (a) we thus obtain under the given assumptions on s_1, s_2 and s that

$$\|uv\|_s^2 \leq K(s,d) \sum_{k\in\mathbb{Z}^d}\sum_{\ell\in\mathbb{Z}^d} \langle k-\ell\rangle^{2s_1} |\widehat{u}_{k-\ell}|^2 \langle \ell\rangle^{2s_2} |\widehat{v}_\ell|^2 \leq K(s,d)\, \|\widehat{u}\|_{\ell^2_{s_1}} \|\widehat{v}\|_{\ell^2_{s_2}},$$

where $\widehat{u} = (\widehat{u}_\ell)_{\ell\in\mathbb{Z}^d}$ and similarly for $\widehat{v}$. The identity $\|\widehat{u}\|_{\ell^2_r} = \|u\|_r$ finishes the proof. □

Lemma A.10 ([44, 45, 63, 65], Properties of Schrödinger-type (Semi-)Groups)**.** *Let $c \in \mathbb{R}$ and $r \geq 0$ be fixed and consider the Schrödinger-type equation for the operator $\Omega_c \in \{c\langle\nabla\rangle_c, -\frac{1}{2}\Delta, c^2, c\langle\nabla\rangle_0\}$*

$$i\partial_t w = -\Omega_c w \quad \text{with given initial data} \quad w(0) = w_I \in H^r(\mathbb{T}^d)$$

with solution w on the torus $\mathbb{T}^d$ and for times $t \in \mathbb{R}$. From [65], we know that $w(t) = e^{it\Omega_c}w_I$ solves the latter system, where in Fourier space we denote the symbol of the operator $e^{it\Omega_c}$ as

$$\left(\widehat{e^{it\Omega_c}}\right)_k = e^{it\omega_c(k)} \qquad \text{for } k \in \mathbb{Z}^d,$$

where $\omega_c : \mathbb{Z}^d \to \mathbb{R}$ is the corresponding symbol of Ω_c.

Then we have the following properties for the operators $\mathcal{T}^t_{[\Omega_c]} := e^{it\Omega_c}$ for all $t \in \mathbb{R}$.

(a) For all $t \in \mathbb{R}$ the operators $\mathcal{T}^t_{[\Omega_c]}$, with $\Omega_c \in \{c\langle\nabla\rangle_c, -\frac{1}{2}\Delta, c^2, c\langle\nabla\rangle_0\}$ being a Schrödinger-type differential operator, are isometries in $H^r(\mathbb{T}^d)$, i.e. for $w \in H^r(\mathbb{T}^d)$ and for all $t \in \mathbb{R}$ we have

$$\|w\|_r = \left\|\mathcal{T}^t_{[c\langle\nabla\rangle_c]}w\right\|_r = \left\|\mathcal{T}^t_{[-\frac{1}{2}\Delta]}w\right\|_r = \left\|\mathcal{T}^t_{[c^2]}w\right\|_r = \left\|\mathcal{T}^t_{[c\langle\nabla\rangle_0]}w\right\|_r.$$

(b) For $r > d/2$ assume that $w \in H^r, w_0 \in H^{r+4}$. Then

$$\left\|\mathcal{T}^t_{[c\langle\nabla\rangle_c]}w - \mathcal{T}^t_{[c^2-\frac{1}{2}\Delta]}w_0\right\|_r \leq \|w - w_0\|_r + c^{-2}\,|t|\,\|w_0\|_{r+4}.$$

Proof (see also [44, 45, 63, 65])*:* (a) We provide a proof of part (a) for the choice $\Omega_c = c\langle\nabla\rangle_c$. The remaining operators are treated analogously. By Definition A.2 the Fourier symbol of $c\langle\nabla\rangle_c$ reads $\omega_c(k) = \langle k\rangle_c = (|k|^2 + c^2)^{1/2}$. Then we have by Definition A.1 of the Sobolev spaces $H^r(\mathbb{T}^d)$ for $t \in \mathbb{R}$ and $w_I \in H^r(\mathbb{T}^d)$

$$\left\|\mathcal{T}^t_{[c\langle\nabla\rangle_c]}w_I\right\|_r^2 = \sum_{k\in\mathbb{Z}^d} \langle k\rangle_1^{2r} \left|e^{it\omega_c(k)}(\widehat{w_I})_k\right|^2 \overset{(*)}{=} \sum_{k\in\mathbb{Z}^d} \langle k\rangle_1^{2r} |(\widehat{w_I})_k|^2 = \|w_I\|_r^2,$$

where the equality $(*)$ follows from the fact that $\left|e^{ix}\right| = 1$ for all $x \in \mathbb{R}$ and from $\omega_c(k) = \langle k\rangle_c \in \mathbb{R}$ for all $k \in \mathbb{Z}^d$.

(b) First exploit that by part (a) the operator $\mathcal{T}^t_{[c\langle\nabla\rangle_c]}$ is an isometry in H^r and that $c\langle\nabla\rangle_c$ and $(c^2 - \frac{1}{2}\Delta)$ are commuting operators by definition. Then we have

$$\begin{aligned}
\left\|\mathcal{T}^t_{[c\langle\nabla\rangle_c]}w - \mathcal{T}^t_{[c^2-\frac{1}{2}\Delta]}w_0\right\|_r &= \left\|w - \mathcal{T}^t_{[-c\langle\nabla\rangle_c+c^2-\frac{1}{2}\Delta]}w_0\right\|_r \\
&\leq \|w - w_0\|_r + \left\|(1 - \mathcal{T}^t_{[-c\langle\nabla\rangle_c+c^2-\frac{1}{2}\Delta]})w_0\right\|_r \\
&\leq \|w - w_0\|_r + |t|\left\|(-c\langle\nabla\rangle_c + c^2 - \frac{1}{2}\Delta)w_0\right\|_r,
\end{aligned}$$

where the last inequality follows from $\left|1-e^{ix}\right| \leq |x|$ for all $x \in \mathbb{R}$ if we replace the operator $(-c\langle\nabla\rangle_c + c^2 - \frac{1}{2}\Delta)$ by its corresponding representation in Fourier space. An application of Lemma A.11 then finishes the proof □

A.2 Properties of the Operator $\langle\nabla\rangle_c$

This section is based on [45, 69, 70]. In the following let $u : \mathbb{T}^d \to \mathbb{C}^m$ be some smooth function. Moreover let

$$u(x) = \sum_{k\in\mathbb{Z}^d} \widehat{u}_k e^{ik\cdot x}$$

denote the Fourier series expansion of u. The following Lemma provides the Taylor series expansion and some error bounds on the operator $\langle\nabla\rangle_c$ and its inverse. In the literature, $\langle\nabla\rangle_c$ is often called *Japanese bracket* (see for instance [85, Preface].

Lemma A.11 ([45, Section 3],[63, Section 2], Estimates on the Operator $c\langle\nabla\rangle_c$)**.** *For sufficiently smooth z and for $c \in \mathbb{R}$, we expand the operator $c\langle\nabla\rangle_c$ and its inverse $c\langle\nabla\rangle_c^{-1}$ into their Taylor series expansions as*

(a) $c\langle\nabla\rangle_c z = c^2 z - \frac{1}{2}\Delta z + \sum_{n\geq 2} \tilde{\alpha}_n c^{2-2n}(-\Delta)^n z, \quad \text{where} \quad \tilde{\alpha}_n = \frac{1}{n!}\prod_{j=0}^{n-1}(\frac{1}{2}-j),\ n \geq 0$

(b) $c\langle\nabla\rangle_c^{-1} z = z + c^{-2}\frac{1}{2}\Delta z + \sum_{n\geq 2} \tilde{\beta}_n c^{-2n}(-\Delta)^n z, \quad \text{where} \quad \tilde{\beta}_n = \frac{1}{n!}\prod_{j=0}^{n-1}(-\frac{1}{2}-j),\ n \geq 0.$

Let $r \geq 0$. Then for all $c \in \mathbb{R}$ and for $u \in H^r$, $\chi \in H^{r+1}$, $v \in H^{r+2}$ and $w \in H^{r+4}$ respectively satisfies the following error bounds with $K > 0$ only depending on r and d

(c) $\left\|(c\langle\nabla\rangle_c - c^2)v\right\|_r \leq \frac{1}{2}\left\|\Delta v\right\|_r$,

(d) $\left\|(c\langle\nabla\rangle_c - (c^2 - \frac{1}{2}\Delta))w\right\|_r \leq Kc^{-2}\left\|\Delta^2 w\right\|_r$,

(e) $\left\|c\langle\nabla\rangle_c^{-1} u\right\|_r \leq \left\|u\right\|_r$,

(f) $\left\|(1 - c\langle\nabla\rangle_c^{-1})v\right\|_r \leq c^{-2}\frac{1}{2}\left\|v\right\|_{r+2}$,

(g) $\left\|c^{-1}\langle\nabla\rangle_c \chi\right\|_r \leq \left\|\chi\right\|_{r+1}$.

If $r > d/2$, then $V, u \in H^r$ and $\tilde{V}, \tilde{u} \in H^{r+2}$ respectively satisfy

(h) $\left\|\tilde{V}\tilde{u} - \langle\nabla\rangle_c^{-1}(\tilde{V}\langle\nabla\rangle_c \tilde{u})\right\|_r \leq Kc^{-2}\left\|\tilde{V}\right\|_{r+2}\left\|\tilde{u}\right\|_{r+2}$,

(i) $\left\|Vu - \langle\nabla\rangle_c^{-1}(V\langle\nabla\rangle_c u)\right\|_r \leq K\left\|V\right\|_r\left\|u\right\|_r$,

(j) $\left\|\langle\nabla\rangle_c^{-1}(V\langle\nabla\rangle_c u)\right\|_r \leq K\left\|V\right\|_r\left\|u\right\|_r$.

Proof: In order to show the identities of (a) and (b) it is enough to consider the Fourier representation of $\langle \nabla \rangle_c w$ and $\langle \nabla \rangle_c^{-1} w$ which is

$$c \langle \nabla \rangle_c w(x) = \sum_{k \in \mathbb{Z}^d} c\sqrt{|k|^2 + c^2} \widehat{w}_k e^{ik \cdot x},$$
$$c \langle \nabla \rangle_c^{-1} w(x) = \sum_{k \in \mathbb{Z}^d} \frac{c}{\sqrt{|k|^2 + c^2}} \widehat{w}_k . e^{ik \cdot x}$$

(a): We have that $c\sqrt{|k|^2 + c^2} = c^2 \sqrt{1 + \frac{|k|^2}{c^2}}$. Therefore setting $k_c := \frac{|k|^2}{c^2}$, consider the Taylor series expansion of $f(k_c) = \sqrt{1 + k_c} = (1 + k_c)^{1/2}$, i.e.

$$f(0 + k_c) = f(0) + k_c f'(0) + \sum_{n \geq 2} \frac{f^{(n)}(0)}{n!} k_c^n. \tag{A.1}$$

By induction we find that $f^{(n)}(x) = (1 + x)^{\frac{1}{2} - n} \cdot \prod_{j=0}^{n-1} (\frac{1}{2} - j)$, and thus

$$\frac{f^{(n)}(0)}{n!} = \frac{1}{n!} \prod_{j=0}^{n-1} (\frac{1}{2} - j) = \tilde{\alpha}_n.$$

Hence, identifying the operator $-\Delta$ with $|k|^2$ in (A.1) we have the desired assertion.

(b): Similarly to part (a) we obtain the assertion by considering $g(k_c) = (1 + k_c)^{-1/2}$, since $\frac{c}{\sqrt{|k|^2 + c^2}} = (1 + \frac{|k|^2}{c^2})^{-1/2}$. As before $\tilde{\beta}_n = \frac{g^{(n)}(0)}{n!}, n \geq 0$ are the coefficients of the Taylor series expansion of g. □

(c)&(d): For the estimates in parts (c)&(d) we use that for $x \in \mathbb{R}$ and for all $\lambda \geq 0$ we have

$$\sqrt{1 + x^2} \leq 1 + \frac{x^2}{2} + \lambda x^4.$$

Setting $x = |k|/c$ and $\lambda = 0$ this immediately shows (c) in Fourier space. We similarly show (d), setting $\lambda > 0$ arbitrary.

(e)&(f): In order to show (e) we use that

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

Moreover because $\sqrt{|k|^2 + c^2} - c \geq 0$, we have that

$$(1 - \frac{c}{\sqrt{|k|^2 + c^2}} = \frac{\sqrt{|k|^2 + c^2} - c}{\sqrt{|k|^2 + c^2}} \leq \left(\sqrt{1 + \frac{|k|^2}{c^2}} - 1\right) \leq \frac{1}{2} \frac{|k|^2}{c^2}.$$

(g): Follows immediately from

$$\frac{\sqrt{|k|^2 + c^2}}{c} = \sqrt{\frac{|k|^2}{c^2} + 1} \leq \sqrt{|k|^2 + 1} \quad \text{for all } k \in \mathbb{Z}^d \text{ and for all } c \geq 1$$

and the Definition A.1 of the Sobolev spaces $H^r(\mathbb{T}^d)$.

(h): We have that

$$Vu - \langle\nabla\rangle_c^{-1}(V\langle\nabla\rangle_c u) = [1 - c\langle\nabla\rangle_c^{-1}]Vu + c\langle\nabla\rangle_c^{-1}\Big(V\cdot\frac{1}{c^2}[c^2 - c\langle\nabla\rangle_c]u\Big).$$

Then applying (f) to the first term we have that

$$\left\|[1 - c\langle\nabla\rangle_c^{-1}]Vu\right\|_r \le \frac{1}{2}c^{-2}\|Vu\|_{r+2},$$

and applying (e) to the second term, we find

$$\left\|c\langle\nabla\rangle_c^{-1}\Big(V\cdot\frac{1}{c^2}[c^2 - c\langle\nabla\rangle_c]u\Big)\right\|_r \le c^{-2}\left\|V\cdot[c^2 - c\langle\nabla\rangle_c]u\right\|_r.$$

Now the bilinear estimate $\|wu\|_r \le K\|w\|_r\|u\|_r$ for $r > d/2$ from Lemma A.8 together with (c) gives the desired result.

(i): We follow the idea of [70, Section 4.1] and rewrite

$$Vu - \langle\nabla\rangle_c^{-1}(V\langle\nabla\rangle_c u) = \langle\nabla\rangle_c^{-1}\big(\langle\nabla\rangle_c(Vu) - V\langle\nabla\rangle_c u\big).$$

Then we apply the proof of [48, Proposition 3.1]:

By definition of $\|\cdot\|_r$ in Definition A.1 we have

$$\left\|\langle\nabla\rangle_c^{-1}\big(\langle\nabla\rangle_c(Vu) - V\langle\nabla\rangle_c u\big)\right\|_r^2 = \sum_{k\in\mathbb{Z}^d}\langle k\rangle^{2r}\left|\langle k\rangle_c^{-1}\sum_{\ell\in\mathbb{Z}^d}\frac{\langle k\rangle_c^2 - \langle\ell\rangle_c^2}{\langle k\rangle_c + \langle\ell\rangle_c}\widehat{V}_{k-\ell}\widehat{u}_\ell\right|^2$$

$$= \sum_{k\in\mathbb{Z}^d}\left|\sum_{\ell\in\mathbb{Z}^d}\left(\frac{\langle k\rangle}{\langle k-\ell\rangle\langle\ell\rangle}\right)^r\langle k\rangle_c^{-1}\frac{\langle k\rangle_c^2 - \langle\ell\rangle_c^2}{\langle k\rangle_c + \langle\ell\rangle_c}\langle k-\ell\rangle^r\widehat{V}_{k-\ell}\langle\ell\rangle^r\widehat{u}_\ell\right|^2$$

where $\langle k\rangle_c^2 = c^2 + |k|^2$. The second sum is an inner product in the space ℓ^2 according to Definition A.6 such that the application of the Cauchy-Schwarz inequality Proposition A.31 gives

$$\begin{aligned}&\left|\sum_{\ell\in\mathbb{Z}^d}\left(\frac{\langle k\rangle}{\langle k-\ell\rangle\langle\ell\rangle}\right)^r\langle k\rangle_c^{-1}\frac{\langle k\rangle_c^2 - \langle\ell\rangle_c^2}{\langle k\rangle_c + \langle\ell\rangle_c}\langle k-\ell\rangle^r\widehat{V}_{k-\ell}\langle\ell\rangle^r\widehat{u}_\ell\right|^2\\ &\le\left(\sum_{\ell\in\mathbb{Z}^d}\left(\frac{\langle k\rangle^r}{\langle k-\ell\rangle^r\langle\ell\rangle^r\langle k\rangle_c}\cdot\frac{\left|\langle k\rangle_c^2 - \langle\ell\rangle_c^2\right|}{\langle k\rangle_c + \langle\ell\rangle_c}\right)^2\right)\left(\sum_{\ell\in\mathbb{Z}^d}\langle k-\ell\rangle^{2r}\left|\widehat{V}_{k-\ell}\right|^2\langle\ell\rangle^{2r}|\widehat{u}_\ell|^2\right).\end{aligned}\tag{A.2}$$

If we can show that the first sum is convergent for all $k\in\mathbb{Z}^d$ and bounded independent of $k\in\mathbb{Z}^d$, we are done since

$$\sum_{k\in\mathbb{Z}^d}\sum_{\ell\in\mathbb{Z}^d}\langle k-\ell\rangle^{2r}\left|\widehat{V}_{k-\ell}\right|^2\langle\ell\rangle^{2r}|\widehat{u}_\ell|^2 \le K\left\|\widehat{V}\right\|_{\ell_r^2}\cdot\|\widehat{u}\|_{\ell_r^2} = K\|V\|_r\|u\|_r.$$

Exploiting that $|k-\ell| \le \langle k-\ell\rangle$ by definition and that by the Cauchy-Schwartz inequality Proposition A.31 for $c \ge 1$

$$|k+\ell|^2 \le \langle k+\ell\rangle^2 \le 1 + |k|^2 + 2|k||\ell| + 1 + |\ell|^2 \le (\langle k\rangle + \langle\ell\rangle)^2 \le (\langle k\rangle_c + \langle\ell\rangle_c)^2$$

we find

$$\frac{\left|\langle k\rangle_c^2 - \langle\ell\rangle_c^2\right|}{\langle k\rangle_c + \langle\ell\rangle_c} \le \frac{\left||k|^2 - |\ell|^2\right|}{\langle k\rangle_c + \langle\ell\rangle_c} = \frac{\left|(k+\ell)^\top(k-\ell)\right|}{\langle k\rangle_c + \langle\ell\rangle_c} \le \frac{\langle k\rangle + \langle\ell\rangle}{\langle k\rangle_c + \langle\ell\rangle_c}\langle k-\ell\rangle \le \langle k-\ell\rangle.$$

Therefore we obtain that

$$\sum_{\ell\in\mathbb{Z}^d}\left(\frac{\langle k\rangle^r}{\langle k-\ell\rangle^r\langle \ell\rangle^r\langle k\rangle_c}\cdot\frac{\left|\langle k\rangle_c^2-\langle \ell\rangle_c^2\right|}{\langle k\rangle_c+\langle \ell\rangle_c}\right)^2\le\sum_{\ell\in\mathbb{Z}^d}\left(\frac{\langle k\rangle^{r-1}}{\langle k-\ell\rangle^{r-1}\langle \ell\rangle^r}\right)^2\le K(r-1,d)$$

which is bounded under application of Lemma A.8 with $s:=r-1$, $s_1:=r-1$ and $s_2:=r$ since $s\le s_j$, $j=1,2$ and $s_1+s_2-s>d/2$ if $r>d/2$. Thus, the first sum in the inequality (A.2) is bounded which finally shows (h).

(j): We observe that

$$\langle\nabla\rangle_c^{-1}\left(V\langle\nabla\rangle_c u\right)=Vu-\big(Vu-\langle\nabla\rangle_c^{-1}\left(V\langle\nabla\rangle_c u\right)\big).$$

The result then follows by triangle inequality and application of (h). □

Proposition A.12 ([45, 70], Formal Expansion of $c\langle\nabla\rangle_c$)**.** *Let $c\ge 0$ and consider for smooth functions $\mathbb{W},\mathbb{F},\Phi$ the following (formal) asymptotic expansion*

$$\mathbb{W}=\sum_{n=0}^{\infty}c^{-n}\mathbb{W}_n,\quad \mathbb{F}=\sum_{n=0}^{\infty}c^{-n}\mathbb{F}_n,\quad \Phi=\sum_{n=0}^{\infty}c^{-n}\Phi_n.$$

Let $\tilde\alpha_m,\tilde\beta_m,m\ge 0$ be the coefficients from Lemma A.11. Then, with $\tilde\alpha_0=1,\tilde\alpha_1=\frac{1}{2}$, we have

$$\begin{aligned}c\langle\nabla\rangle_c\mathbb{W}&=c^2\mathbb{W}_0+c\mathbb{W}_1+\sum_{n=0}^{\infty}c^{-n}\Bigg(\mathbb{W}_{n+2}-\frac{1}{2}\Delta\mathbb{W}_n+\sum_{\substack{m,\ell\in\mathbb{N}_0\\2m+\ell=n+2\\m\ge2}}\tilde\alpha_m(-\Delta)^m\mathbb{W}_\ell\Bigg)\\&=c^2\mathbb{W}_0+c\mathbb{W}_1+\sum_{n=0}^{\infty}c^{-n}\big(\mathbb{W}_{n+2}-\frac{1}{2}\Delta\mathbb{W}_n\big)+\sum_{n=2}^{\infty}c^{-n}\sum_{\substack{m,\ell\in\mathbb{N}_0\\2m+\ell=n+2\\m\ge2}}\tilde\alpha_m(-\Delta)^m\mathbb{W}_\ell\Bigg).\end{aligned}$$

Moreover, with $\tilde\beta_0=1,\tilde\beta_1=-\frac{1}{2}$, we obtain for $M\in\mathbb{N}_0$

$$\begin{aligned}c^{-M}c\langle\nabla\rangle_c^{-1}\mathbb{F}&=\sum_{n=0}^{\infty}c^{-(n+M)}\sum_{\substack{m,\ell\in\mathbb{N}_0\\2m+\ell=n}}\tilde\beta_m(-\Delta)^m\mathbb{F}_\ell\\&=\sum_{n=M}^{\infty}c^{-n}\mathbb{F}_{n-M}+\sum_{n=2+M}^{\infty}c^{-n}\sum_{\substack{m,\ell\in\mathbb{N}_0\\2m+\ell=n-M\\m\ge1}}\tilde\beta_m(-\Delta)^m\mathbb{F}_\ell\end{aligned}$$

and

$$\begin{aligned}\langle\nabla\rangle_c^{-1}\Phi\langle\nabla\rangle_c\mathbb{W}&=\Phi_0\mathbb{W}_0+c^{-1}\big(\Phi_0\mathbb{W}_1+\Phi_1\mathbb{W}_0\big)\\&\quad+\sum_{n\ge2}c^{-n}\sum_{\substack{k,\ell,m\in\mathbb{N}_0\\2(m+k)+\ell=n}}\sum_{j=0}^{\ell}\tilde\beta_k(-\Delta)^k\Big(\Phi_j\cdot\tilde\alpha_m(-\Delta)^m\mathbb{W}_{\ell-j}\Big).\end{aligned}$$

Proof: For the proof note that we operate on a formal level only. No regularity assumption on $\mathbb{W}$ are made. By Lemma A.11 we have that

$$
\begin{aligned}
c\langle\nabla\rangle_c \mathbb{W} =& \sum_{\ell=0}^{\infty} c^{-\ell} c\langle\nabla\rangle_c \mathbb{W}_\ell = c^2 \sum_{\ell=0}^{\infty} c^{-\ell} \sum_{m=0}^{\infty} \tilde{\alpha}_m c^{-2m}(-\Delta)^m \mathbb{W}_\ell \\
=& c^2 \sum_{m,\ell=0}^{\infty} c^{-2m-\ell} \tilde{\alpha}_m (-\Delta)^m \mathbb{W}_\ell \\
=& \sum_{n=-2}^{\infty} c^{-n} \sum_{\substack{m,\ell\in\mathbb{N}_0 \\ 2m+\ell=n+2}} \tilde{\alpha}_m (-\Delta)^m \mathbb{W}_\ell \\
=& c^2\mathbb{W}_0 + c\mathbb{W}_1 + \sum_{n=0}^{\infty} c^{-n} \Big(\mathbb{W}_{n+2} - \frac{1}{2}\Delta \mathbb{W}_n + \sum_{\substack{m,\ell\in\mathbb{N}_0 \\ 2m+\ell=n+2 \\ m\geq 2}} \tilde{\alpha}_m (-\Delta)^m \mathbb{W}_\ell \Big) \\
=& c^2\mathbb{W}_0 + c\mathbb{W}_1 + \sum_{n=0}^{\infty} c^{-n} \big(\mathbb{W}_{n+2} - \frac{1}{2}\Delta \mathbb{W}_n \big) \\
&+ \sum_{n=2}^{\infty} c^{-n} \sum_{\substack{m,\ell\in\mathbb{N}_0 \\ 2m+\ell=n+2 \\ m\geq 2}} \tilde{\alpha}_m (-\Delta)^m \mathbb{W}_\ell \Big),
\end{aligned}
$$

where the last equality is due to the fact that

$$
\sum_{\substack{m,\ell\in\mathbb{N}_0 \\ 2m+\ell=n+2 \\ m\geq 2}} \tilde{\alpha}_m (-\Delta)^m \mathbb{W}_\ell = 0, \qquad n = 0, 1.
$$

Analogously we find the result for $c\langle\nabla\rangle_c^{-1}\mathbb{F}$, since

$$
\sum_{\substack{m,\ell\in\mathbb{N}_0 \\ 2m+\ell=n}} \tilde{\beta}_m (-\Delta)^m \mathbb{F}_\ell = \mathbb{F}_n + \sum_{\substack{m,\ell\in\mathbb{N}_0 \\ 2m+\ell=n \\ m\geq 1}} \tilde{\beta}_m (-\Delta)^m \mathbb{F}_\ell
$$

and since

$$
\sum_{\substack{m,\ell\in\mathbb{N}_0 \\ 2m+\ell=n \\ m\geq 1}} \tilde{\beta}_m (-\Delta)^m \mathbb{F}_\ell = 0, \qquad n = 0, 1.
$$

Multiplying $c\langle\nabla\rangle_c^{-1}\mathbb{F}$ by c^{-M} then causes an index shift n to $n-M$. Furthermore,

$$
\begin{aligned}
&\langle\nabla\rangle_c^{-1} \Phi \langle\nabla\rangle_c \mathbb{W} \\
&= \sum_{\ell=0}^{\infty} c^{-\ell} \sum_{j=0}^{\ell} c\langle\nabla\rangle_c^{-1} \big(\Phi_j \frac{\langle\nabla\rangle_c}{c} \mathbb{W}_{\ell-j} \big) \\
&= \sum_{\ell=0}^{\infty} c^{-\ell} \sum_{j=0}^{\ell} \sum_{k=0}^{\infty} c^{-2k} \tilde{\beta}_k (-\Delta)^k \Big(\Phi_j \cdot \sum_{m=0}^{\infty} c^{-2m} \tilde{\alpha}_m (-\Delta)^m \mathbb{W}_{\ell-j} \Big) \\
&= \sum_{\ell=0}^{\infty} \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} \sum_{j=0}^{\ell} c^{-2k-2m-\ell} \tilde{\beta}_k (-\Delta)^k \Big(\Phi_j \cdot \tilde{\alpha}_m (-\Delta)^m \mathbb{W}_{\ell-j} \Big) \\
&= \sum_{n=0}^{\infty} c^{-n} \sum_{\substack{k,\ell,m\in\mathbb{N}_0 \\ 2(m+k)+\ell=n}} \sum_{j=0}^{\ell} \tilde{\beta}_k (-\Delta)^k \Big(\Phi_j \cdot \tilde{\alpha}_m (-\Delta)^m \mathbb{W}_{\ell-j} \Big).
\end{aligned}
$$

This finishes the proof. □

A.3 Solution Operator to Poisson's Equation in Fourier Space

This section is based on [44, 65]. Within this thesis, the Poisson's equation plays an important role in almost all systems which we consider. Having the Poisson problem

$$-\Delta\phi(x) = \rho(x) \quad \text{on the torus} \quad x \in \mathbb{T}^d \tag{A.3}$$

it becomes clear that regarding its Fourier representation

$$\sum_{k\in\mathbb{Z}^d} |k|^2 \,\widehat{\phi}_k e^{ik\cdot x} = \sum_{k\in\mathbb{Z}^d} \widehat{\rho}_k e^{ik\cdot x}$$

the solution is uniquely determined via $\widehat{\phi}_k := \frac{1}{|k|^2}\widehat{\rho}_k$ for all $k \in \mathbb{Z}^d \setminus \{0\}$ up to the constant term corresponding to $k = 0$. Therefore, if the right hand side ρ is in H^r we look for solutions $\phi \in \dot{H}^r$ according to Definition A.3, where we assume that the constant term $\widehat{\phi}_0 = 0$ vanishes. This motivates us to define the solution operator to Poisson's problem (A.3) as

$$\dot{\Delta}^{-1} : H^r \to \dot{H}^{r+2} \quad \text{with} \quad \phi = -\dot{\Delta}^{-1}\rho =: \sum_{k\in\mathbb{Z}^d\setminus\{0\}} \frac{1}{|k|^2}\widehat{\rho}_k e^{ik\cdot x} \tag{A.4a}$$

with its representation in Fourier space

$$(\widehat{\dot{\Delta}^{-1}})_k = -\,|k|^{-2} \quad \text{for } k \in \mathbb{Z}^d \setminus \{0\} \quad \text{and} \quad (\widehat{\dot{\Delta}^{-1}})_0 = 0. \tag{A.4b}$$

A.4 Projection Operator onto Divergence-Free Vector Fields

This section is based on [21, 22, 35, 60, 70, 76, 79], [37, Section 0] and [85, Exercise A.23]. Our aim in this section is to define the projection operator $\mathcal{P}_{\text{df}}$ of a vector field onto its divergence-free part as a mapping from H^r to $\dot{H}^r$ (see Definitions A.1 and A.3). In the derivation of the Maxwell–Klein–Gordon system (2.20) and the Maxwell–Dirac system (2.36) in the Coulomb gauge (see Section 2.1.1) we encountered the projection operator $\mathcal{P}_{\text{df}}$. This projection maps a function $\boldsymbol{J} : \mathbb{T}^d \to \mathbb{C}^d$ onto its divergence-free part $\boldsymbol{J}^{\text{df}}$ up to a constant vector field $\tilde{\boldsymbol{J}}_0 \in \mathbb{C}^d$, i.e. according to (2.10)

$$\mathcal{P}_{\text{df}}[J] = \boldsymbol{J}^{\text{df}} - \tilde{\boldsymbol{J}}_0 \quad \text{and} \quad \operatorname{div} \mathcal{P}_{\text{df}}[J] = 0 \quad \text{for arbitrary } \tilde{\boldsymbol{J}}_0 \in \mathbb{C}^d.$$

Choosing $\tilde{\boldsymbol{J}}_0 := (\widehat{\boldsymbol{J}})_0$ to be the Fourier coefficient of $\boldsymbol{J}$ corresponding to $k = 0$, this projection is uniquely defined. Therefore exploiting the definition of $\dot{\Delta}^{-1}$ in (A.4) we define the projection $\mathcal{P}_{\text{df}}$ by

$$\mathcal{P}_{\text{df}} : H^r \to \dot{H}^r \quad \text{and} \quad \mathcal{P}_{\text{df}}[\boldsymbol{J}] := \big(\boldsymbol{J} - (\widehat{\boldsymbol{J}})_0\big) - \nabla\dot{\Delta}^{-1} \operatorname{div} \boldsymbol{J}. \tag{A.5a}$$

This definition allows us to shortly write

$$\mathcal{P}_{\text{df}} := \dot{\mathcal{I}} - \nabla\dot{\Delta}^{-1} \operatorname{div} \quad \text{with} \quad \dot{\mathcal{I}}\boldsymbol{J}(x) = \boldsymbol{J}(x) - (\widehat{\boldsymbol{J}})_0 = \sum_{k\in\mathbb{Z}^d\setminus\{0\}} (\widehat{\boldsymbol{J}})_k e^{ik\cdot x}. \tag{A.5b}$$

Here $\dot{\mathcal{I}}$ is the identity mapping from H^r to $\dot{H}^r$. In Fourier space, we thus define the projection $\mathcal{P}_{\text{df}}$ via

$$(\widehat{\mathcal{P}_{\text{df}}[\boldsymbol{J}]})_k = (\widehat{\boldsymbol{J}})_k - \begin{pmatrix} ik^1 \\ \vdots \\ ik^d \end{pmatrix} \cdot \sum_{j=1}^{d} \frac{ik^j}{-|k|^2} (\widehat{\boldsymbol{J}_j})_k \quad \text{for } k \in \mathbb{Z}^d \setminus \{0\} \quad \text{and} \quad (\widehat{\mathcal{P}_{\text{df}}[\boldsymbol{J}]})_0 = 0. \tag{A.5c}$$

This particular definition of $\mathcal{P}_{\text{df}}$ is also motivated by [70].

In the latter paper, the authors Masmoudi and Nakanishi use Sobolev spaces related to $\dot{H}^r(\mathbb{R}^d)$ for the analysis of the MKG/MD systems. Therefore, it makes sense to look for solutions $\boldsymbol{\mathcal{A}} \in \dot{H}^r$ and $c^{-1}\partial_t\boldsymbol{\mathcal{A}} \in \dot{H}^{r-1}$ of the wave equations (2.20b) and (2.38b) respectively in the Coulomb gauge (see Section 2.1.1), i.e.

$$\partial_{tt}\boldsymbol{\mathcal{A}} - c^2\Delta\boldsymbol{\mathcal{A}} = c\mathcal{P}_{\text{df}}[\boldsymbol{J}], \qquad \boldsymbol{\mathcal{A}}(0) = A_I, \quad \partial_t\boldsymbol{\mathcal{A}}(0) = cA_I', \quad \operatorname{div}\boldsymbol{\mathcal{A}} \equiv 0, \tag{A.6}$$

if the initial data satisfy $A_I = \mathcal{P}_{\text{df}}\left[\tilde{A}_I\right] \in \dot{H}^r$ and $A_I' = \mathcal{P}_{\text{df}}\left[\tilde{A}_I'\right] \in \dot{H}^{r-1}$ with $r > d/2$. It is easy to see that the solution then satisfies the Coulomb gauge condition $\operatorname{div}\boldsymbol{\mathcal{A}} \equiv 0$.

Using the projection operator (A.5) allows us to define the spaces $\mathcal{P}_{\text{df}}H^r$ of functions with vanishing mean and vanishing divergence as follows.

Definition A.13 (Based on [22], Spaces of Vanishing Mean and Vanishing Divergence)**.** *Let $r > 0$ and let $\mathcal{P}_{\text{df}} : H^r(\mathbb{T}^d) \to \dot{H}^r(\mathbb{T}^d)$ be the projection onto divergence-free vector fields as defined in (A.5). Then we define the spaces*

$$\mathcal{P}_{\text{df}}H^r(\mathbb{T}^d) := \{A \in \dot{H}^r(\mathbb{T}^d) \quad \textit{with} \quad \operatorname{div} A = 0\}.$$

We observe from the following Proposition A.14 that the operator $\mathcal{P}_{\text{df}}$ is bounded in $\dot{H}^r$.

Proposition A.14 (See also [70], Bound on the Projection Operator)**.** *The projection $\mathcal{P}_{\text{df}} : (H^r)^d \to (\dot{H}^r)^d$ defined in (A.5) is bounded in H^r by 1, i.e. for $\boldsymbol{J} \in H^r$ we have*

$$\|\mathcal{P}_{\text{df}}[\boldsymbol{J}]\|_{r,0} = \|\mathcal{P}_{\text{df}}[\boldsymbol{J}]\|_r \le K(d)\,\|\boldsymbol{J}\|_{r,0} \le K(d)\,\|\boldsymbol{J}\|_r\,,$$

where the constant $K(d)$ only depends on d.

Proof: The first equality and the last inequality is clear from $(\widehat{\mathcal{P}_{\text{df}}[\boldsymbol{J}]})_0 = 0$ and the definition of $\dot{H}^r$ in Definition A.3. The rest of the assertion follows from the Fourier coefficients of the ℓ-th component of $\mathcal{P}_{\text{df}}[\boldsymbol{J}]$:

Let $k \in \mathbb{Z}^d \setminus \{0\}$ and let $\ell = 1, \dots, d$. Then

$$\left|(\widehat{\mathcal{P}_{\text{df}}[\boldsymbol{J}]_\ell})_k\right| = \left|(\widehat{\boldsymbol{J}}_\ell)_k - \sum_{j=1}^d \frac{-k^\ell k^j}{-|k|^2}(\widehat{\boldsymbol{J}}_j)_k\right| \le \left|(\widehat{\boldsymbol{J}}_\ell)_k\right| + \frac{\left|k^\ell\right|}{|k|^2}\left|\sum_{j=1}^d k^j(\widehat{\boldsymbol{J}}_j)_k\right|.$$

From the Cauchy-Schwartz inequality in $\mathbb{C}^d$ (see Proposition A.31) and from $\left|k^\ell\right| \le |k|$ we thus conclude that

$$\left|(\widehat{\mathcal{P}_{\text{df}}[\boldsymbol{J}]_\ell})_k\right|^2 \le \left(\left|(\widehat{\boldsymbol{J}}_\ell)_k\right| + \sqrt{\sum_{j=1}^d\left|(\widehat{\boldsymbol{J}}_j)_k\right|^2}\right)^2 \le 2\sum_{j=1}^d\left|(\widehat{\boldsymbol{J}}_j)_k\right|^2.$$

Therefore

$$\sum_{\ell=1}^d \|\mathcal{P}_{\text{df}}[\boldsymbol{J}]_\ell\|_{r,0} \le K(d)\sum_{\ell=1}^d\|\boldsymbol{J}_\ell\|_{r,0} = K(d)\,\|\boldsymbol{J}\|_{r,0}\,.$$

This finishes the proof. □

In the literature, the projection $\mathcal{P}_{\text{df}}$ onto divergence-free vector fields is often called Leray projection, see for example [37, Section 0]. In [85, Exercise A.23], the author Tao introduces a related projection operator in the context of a "Hodge decomposition".

Note that due to the definition of $\mathcal{P}_{\text{df}}$ in (A.5), we observe in particular that

$$\text{for all } \boldsymbol{J} \in H^r \text{ the projection } \mathcal{P}_{\text{df}}[\boldsymbol{J}] \in \dot{H}^r \text{ and } \left(\widehat{\mathcal{P}_{\text{df}}[\boldsymbol{J}]}\right)_0 = 0.$$

This observation allows us to formulate the Corollary A.15, on the zero mode of the solution to the following equations (A.7) and (A.8), respectively. We now consider a wave equation of type (A.6) with solution $\tilde{\boldsymbol{\mathcal{A}}}(t,x) \in \mathbb{R}^d$, i.e.

$$\partial_{tt}\tilde{\boldsymbol{\mathcal{A}}} - c^2\Delta\tilde{\boldsymbol{\mathcal{A}}} = c\mathcal{P}_{\text{df}}[\boldsymbol{J}], \qquad \tilde{\boldsymbol{\mathcal{A}}}(0), \partial_t\tilde{\boldsymbol{\mathcal{A}}}(0) \quad \text{given} \tag{A.7}$$

on $\mathbb{T}^d$ and on a finite time interval $[0,T]$ with a smooth function $\boldsymbol{J}(t,x) \in \mathbb{R}^d$. Furthermore, we consider a system of type (4.9) with solution $\tilde{\mathbf{a}}(t,x) \in \mathbb{C}^d$, i.e.

$$i\partial_t\tilde{\mathbf{a}} = -c\langle\nabla\rangle_{\gamma/c}\tilde{\mathbf{a}} + \langle\nabla\rangle_{\gamma/c}^{-1}\left(\frac{\gamma^2}{2c}(\tilde{\mathbf{a}} + \overline{\tilde{\mathbf{a}}}) + \mathcal{P}_{\text{df}}[\boldsymbol{J}]\right), \qquad \tilde{\mathbf{a}}(0) \quad \text{given}, \qquad \gamma \in [0,1], \tag{A.8}$$

on $\mathbb{T}^d$ and on a finite time interval $[0,T]$ with a smooth function $\boldsymbol{J}(t,x) \in \mathbb{R}^d$. According to Definition A.2 we define $\langle\nabla\rangle_{\gamma/c} := \left(-\Delta + \frac{\gamma^2}{c^2}\right)^{1/2}$.

Corollary A.15 (See also [44, 66], Zero Mode of Solutions to Wave Equations)**.** *Let $r \geq 0$ and let the initial data of (A.7) satisfy*

$$\tilde{\boldsymbol{\mathcal{A}}}(0) \in \mathcal{P}_{\text{df}}H^r, \quad \frac{\partial_t}{c}\tilde{\boldsymbol{\mathcal{A}}}(0) \in \mathcal{P}_{\text{df}}H^{r-1}$$

and let $\boldsymbol{J} \in H^r$ be smooth, then for all times $t \in [0,T]$ we have that

$$\left(\widehat{\tilde{\boldsymbol{\mathcal{A}}}(t)}\right)_0 = 0 = \left(\widehat{\partial_t\tilde{\boldsymbol{\mathcal{A}}}(t)}\right)_0. \tag{A.9}$$

Furthermore, let the initial data of (A.8) satisfy $\tilde{\mathbf{a}}(0) \in \mathcal{P}_{\text{df}}H^r$ and let $\boldsymbol{J} \in H^r$ be smooth, then for all times $t \in [0,T]$ we have that

$$\left(\widehat{\tilde{\mathbf{a}}(t)}\right)_0 = 0. \tag{A.10}$$

Proof: We carry out the proof by considering the equations (A.7) and (A.8), respectively, in Fourier space. Then we obtain for each $k \in \mathbb{Z}^d$ the following equations

$$\left(\widehat{\partial_{tt}\tilde{\boldsymbol{\mathcal{A}}}}\right)_k + c^2|k|^2\left(\widehat{\tilde{\boldsymbol{\mathcal{A}}}}\right)_k = c\left(\widehat{\mathcal{P}_{\text{df}}[\boldsymbol{J}]}\right)_k$$

and

$$i\left(\widehat{\partial_t\tilde{\mathbf{a}}}\right)_k = -c\sqrt{|k|^2 + \frac{\gamma^2}{c^2}}\left(\widehat{\tilde{\mathbf{a}}}\right)_k + \frac{1}{\sqrt{|k|^2 + \frac{\gamma^2}{c^2}}}\left(\frac{\gamma^2}{2c}\left(\widehat{\tilde{\mathbf{a}} + \overline{\tilde{\mathbf{a}}}}\right)_k + \left(\widehat{\mathcal{P}_{\text{df}}[\boldsymbol{J}]}\right)_k\right).$$

In particular, for $k = 0$ this yields using $\left(\widehat{\mathcal{P}_{\text{df}}[\boldsymbol{J}]}\right)_0 = 0$ (see (A.5)) that

$$\left(\widehat{\partial_{tt}\tilde{\boldsymbol{\mathcal{A}}}}\right)_0 = 0 \qquad \text{and} \qquad i\left(\widehat{\partial_t\tilde{\mathbf{a}}}\right)_0 = -\gamma\left(\widehat{\tilde{\mathbf{a}}}\right)_0 + \frac{\gamma}{2}\left(\widehat{\tilde{\mathbf{a}} + \overline{\tilde{\mathbf{a}}}}\right)_0. \tag{A.11}$$

Note that since $\mathcal{P}_{\mathrm{df}}H^r \subset \dot{H}^r$ by Definition A.13 and because $\left(\widehat{A}\right)_0 = 0$ for all $A \in \dot{H}^r$ and all $r \in \mathbb{R}$ (see Definition A.3), the initial data $\tilde{\boldsymbol{\mathcal{A}}}(0)$, $\partial_t\tilde{\boldsymbol{\mathcal{A}}}(0)$ and $\tilde{\mathbf{a}}(0)$ satisfy the assertions (A.9) and (A.10), respectively, initially at time $t = 0$. From (A.11) we therefore deduce the assertion for all times $t \in [0, T]$. This finishes the proof. □

A.5 Tools in the Numerical Time Integration of Differential Equations

This section is based on [44, 52, 85]. Our aim is now to recap some basic concepts which play a major role in the numerical analysis of time integration schemes for differential equations. For sake of simplicity, we focus on the case of ordinary differential equations. Note that the contents of this section can be extended also to partial differential equations, see for instance [44, 85].

We consider the following model problem

$$\dot{y}(t) = Ly + f(y), \quad y(0) = y_0 \qquad \text{for all } t \in [0, T] \tag{A.12}$$

with a matrix $L \in \mathbb{R}^{m\times m}$ and with a smooth nonlinearity $f : \mathbb{C}^m \to \mathbb{C}^m$. Furthermore, we consider the discretization

$$t_n = n\tau \le T \qquad \text{of the interval } [0, T] \text{ with time step } \tau \in (0, 1]$$

and a numerical method Φ^τ for solving (A.12) defined by the recursion

$$y_{n+1} = \Phi^\tau(y_n) \quad \text{such that } y_{n+1} \approx y(t_{n+1}) \text{ for all } t_{n+1} \in [0, T].$$

In Definition A.16 below we introduce the concept of

the flow φ^t of the differential equation (A.12) (see [52, Chapter I.1.1]),

which maps a given initial value y_0 to the corresponding solution $y(t)$ at time $t \in [0, T]$. Afterwards in Definitions A.17 and A.18, we define

the local error and stability of the method Φ^τ (see [44, Definition II.7])

which alow us to discuss

the global error of Φ^τ (see [44, Proposition II.8] and also Lemma A.19 below).

Later in Proposition A.20 and Lemma A.21, we give some details on Duhamel's formula ([85, Proposition 1.35]) and Gronwall's Lemma ([85, Theorem 1.10]) which are important tools in the numerical analysis of methods Φ^τ for nonlinear problems of type (A.12). We furthermore provide Definition A.22 of the φ_j functions ([55]) which have been originally introduced in the context of exponential time integration schemes in [55].

Definition A.16 ([52, Chapter I.1.1], see also [44], Flow of a Differential Equation)**.** *We define the flow φ^t of the differential equation* (A.12) *by*

$$\varphi^t(y_0) = y(t) \qquad \text{for } y_0 \in \mathbb{C}^m,$$

which maps any initial value $y(0) = y_0 \in \mathbb{C}^m$ to the corresponding solution $y(t)$ of (A.12) at time t.

Definition A.17 ([44, Definition II.7], Local Error and Order of Consistency of a Numerical Time Integration Scheme)**.** *A numerical method Φ^τ for solving (A.12) with step size τ is (consistent) of order p if the local error satisfies for $t_n = n\tau \le T$, $n = 0, 1, 2, \dots, \lfloor T/\tau \rfloor$*

$$\|y(t_{n+1}) - \Phi^\tau(y(t_n))\| \le K\tau^{p+1},$$

where the constant $K > 0$ depends on $\sup_{0\le s\le\tau} \left\|\partial_y^p f(y(t_n + s))\right\|$.

Definition A.18 ([44, Definition II.7], Stability of a Numerical Time Integration Scheme)**.** *A numerical method Φ^τ for solving (A.12) with step size τ is called stable if for $w^0, z^0 \in \mathbb{R}^d$ there exists a constant L independent of τ such that*

$$\left\|\Phi^\tau(w^0) - \Phi^\tau(z^0)\right\| \le e^{L\tau} \left\|w^0 - z^0\right\|.$$

Lemma A.19 ([44, Proposition II.8], Global Error of a Numerical Time Integration Scheme)**.** *Let Φ^τ be a stable numerical method of order p for solving (A.12) according to Definitions A.17 and A.18. Then the global error at time $t_n = n\tau$ for some $n \in \mathbb{N}$ is bounded by*

$$\|y(t_{n+1}) - \Phi^\tau(y^n)\| \le \tau^p e^{Lt_{n+1}} K,$$

where the constant $K > 0$ depends on $\sup_{0\le s\le t_{n+1}} \left\|\partial_y^p f(y(s))\right\|$.

Proof (see also [44, Proposition II.8])*:* We have

$$\|y(t_{n+1}) - \Phi^\tau(y^n)\| \le \|y(t_{n+1}) - \Phi^\tau(y(t_n))\| + \|\Phi^\tau(y(t_n)) - \Phi^\tau(y^n)\|.$$

From the local error bound and the stability estimate in Definitions A.17 and A.18 we deduce for $n \ge 1$.

$$\|y(t_{n+1}) - \Phi^\tau(y^n)\| \le K\tau^{p+1} + e^{L\tau} \left\|y(t_n) - \Phi^\tau(y^{n-1})\right\|.$$

Inductively we obtain

$$\begin{aligned}\|y(t_{n+1}) - \Phi^\tau(y^n)\| \le & \sum_{j=0}^{n} e^{Lj\tau} K\tau^{p+1} \le \tau^p((n+1)\tau)Ke^{Ln\tau} \\ \le & \tau^p(Kt_{n+1}e^{Lt_n}).\end{aligned}$$

This finishes the proof. □

Note that we can interpret the nonlinear equation (A.12) as a perturbation of the linear equation (see [85, Chapter 1.6])

$$\dot{y} = Ly \qquad \text{for } y(0) = y_0 \in \mathbb{C}^m \text{ with solution} \quad y(t) = e^{tL}y_0 \quad \text{for all } t \in [0, T].$$

This interpretation gives rise to "Duhamel's perturbation formula" ([85, Proposition 1.35]) which is subject of the following Proposition A.20.

Proposition A.20 ([85, Proposition 1.35] and subsequent paragraphs, Duhamel's Formula)**.** *If in (A.12) the function $f : \mathbb{C}^m \to \mathbb{C}^m$ is continuous and if we assume $y : [0, T] \to \mathbb{C}^m$ to be continuous, then y solves (A.12) for all $t \in [0, T]$ if and only if it satisfies the following "Duhamel's (perturbation) formula"*

$$y(t_0 + \tau) = e^{\tau L} y(t_0) + \int_0^{\tau} e^{(\tau - s)L} f(y(t_0 + s))ds \quad \text{for all } t_0, \tau \in [0, T] \text{ with } t_0 + \tau \in [0, T]. \tag{A.13}$$

Proof: For the proof, see [85, Proposition 1.35] and subsequent paragraphs. The proof is a variant of the proof of the well-known variation-of-constants formula. □

We encounter the latter Duhamel's formula (A.13) very often in the construction and analysis of numerical methods applied to nonlinear differential equations of type (A.12) (see for instance [18, Remark 2] and also (3.69), (4.26)). The error analysis of such methods then very often leads to inequalities of type

$$\mathrm{err}(t) \le K + \int_{t_0}^{t} \lambda(s) \cdot \mathrm{err}(s)ds \qquad \text{for } t \in [t_0, t_1], \tag{A.14}$$

where $\mathrm{err}, \lambda : [t_0, t_1] \to [0, \infty)$ are continuous and non-negative and where $K \ge 0$. The following Lemma A.21 (also referred to by "Gronwall's Lemma") (see [85, Theorem 1.10]) yields "Gronwall's inequality" (A.15), which allows us to resolve the integral inequality (A.14).

Lemma A.21 ([85, Theorem 1.10], Gronwall's Lemma)**.** *Let $err : [t_0, t_1] \to [0, \infty)$ be continuous and non-negative and suppose that $err(t)$ satisfies (A.14) with $\lambda : [t_0, t_1] \to [0, \infty)$ being continuous and non-negative and let $K \ge 0$ be a constant. Then,*

$$err(t) \le K e^{\Lambda(t)} \qquad \text{for all } t \in [t_0, t_1], \text{ where}, \qquad \Lambda(t) := \int_{t_0}^{t} \lambda(s)ds. \tag{A.15}$$

Proof: For the proof see for instance [85, Proof of Theorem 1.10]. □

In the construction of exponential time integration schemes ([55]), we encounter the following φ functions.

Definition A.22 ([55], φ functions)**.** *We define the φ functions as*

$$\varphi_0(z) := e^z, \qquad \varphi_k(z) := \int_0^1 e^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!} d\theta, k \ge 1.$$

In particular $\varphi_1(z) = \frac{e^z - 1}{z}$.

A.6 Auxiliary Results for the Derivation of the MKG/MD Systems

The content of this section is mostly based on [21, 22, 70, 79, 80, 87]. Most of the results in this section are given for $x \in \mathbb{R}^d$. They remain valid for the case $x \in \mathbb{T}^d$.

Definition A.23 ([78, Chapter 5.3.5.4],[70, 71, 80, 87], Minimal Coupling Operators)**.** *Let*

$$\phi : \mathbb{R}^d \to \mathbb{R} \quad \text{and} \quad \boldsymbol{\mathcal{A}} : \mathbb{R}^d \to \mathbb{R}^d$$

be sufficiently smooth Maxwell potentials, satisfying (2.12)*. We define the minimal coupling operators* $\partial_t^{[\phi]}, \nabla^{[\boldsymbol{\mathcal{A}}]}$ *by*

$$\partial_t^{[\phi]}\psi := \big(\frac{\partial_t}{c} + i\frac{\phi}{c}\big)\psi \qquad \text{and} \qquad \nabla^{[\boldsymbol{\mathcal{A}}]}\psi := \big(\nabla - i\frac{\boldsymbol{\mathcal{A}}}{c}\big)\psi.$$

Corollary A.24 ([70])**.** *By Definition A.23 we obtain for sufficiently smooth* $\psi, \phi, \boldsymbol{\mathcal{A}}$ *that*

$$\begin{aligned}
(\partial_t^{[\phi]})^2\psi =& \frac{1}{c^2}\big(\partial_t + i\phi\big)^2\ \psi &&= \frac{1}{c^2}\Big(\partial_{tt}\psi - \phi^2\psi + 2i\phi\partial_t\psi + i(\partial_t\phi)\psi\Big)\\
(\nabla^{[\boldsymbol{\mathcal{A}}]})^2\psi =& \ \big(\nabla - i\frac{\boldsymbol{\mathcal{A}}}{c}\big)^2\ \psi &&= \ \nabla^2\psi - \frac{|\boldsymbol{\mathcal{A}}|^2}{c^2}\psi - 2i\frac{\boldsymbol{\mathcal{A}}}{c}\nabla\psi - i(\operatorname{div}\boldsymbol{\mathcal{A}})\psi.
\end{aligned}$$

Proof (see also [70])*:* The proof is a straight forward calculation, respecting the product formula of differentiation. □

Proposition A.25 ([70], Gauge Invariance of the MKG system)**.** *Let* $\phi : \mathbb{R}^d \to \mathbb{R}$ *and* $\boldsymbol{\mathcal{A}} : \mathbb{R}^d \to \mathbb{R}^d$ *be sufficiently smooth Maxwell's potentials according to [42, 58, 59] such that*

$$\begin{aligned}
\boldsymbol{E}(t,x) =& -\nabla\phi(t,x) - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}(t,x),\\
\boldsymbol{B}(t,x) =& \nabla \times \boldsymbol{\mathcal{A}}(t,x).
\end{aligned}$$

Furthermore let $\chi : [0,T] \times \mathbb{R}^d \to \mathbb{R}$ *be a sufficiently smooth gauge function.*

Then the electric and magnetic fields $\boldsymbol{E}, \boldsymbol{B}$ *are invariant under the gauge transform (cf. Section 2.1.1)*

$$\begin{aligned}
\boldsymbol{\mathcal{A}}'(t,x) =& \boldsymbol{\mathcal{A}}(t,x) + c\nabla\chi(t,x),\\
\phi'(t,x) =& \phi(t,x) - \partial_t\chi(t,x).
\end{aligned}$$

Furthermore, if ψ *solves the coupled KG equation* (2.16) *with nonlinearity* f *satisfying* (2.14)*, then* $\psi' := e^{i\chi}\psi$ *solves*

$$\begin{aligned}
&(\partial_t^{[\phi']})^2\psi' - (\nabla^{[\boldsymbol{\mathcal{A}}']})^2\psi' + c^2\psi' = f[\psi'],\\
&\psi'(0) = e^{i\chi(0,x)}\psi(0),\ \ \partial_t^{[\phi']}\psi'(0) = e^{i\chi(0,x)}\partial_t^{[\phi]}\psi(0),
\end{aligned}$$

where $\partial_t^{[\phi']} = \big(\frac{\partial_t}{c} + i\frac{\phi'}{c}\big)$, $\nabla^{[\boldsymbol{\mathcal{A}}']} = \big(\nabla - i\frac{\boldsymbol{\mathcal{A}}'}{c}\big)$*. In particular*

$$\begin{aligned}
\partial_t^{[\phi']}\psi' =&\ e^{i\chi}\partial_t^{[\phi]}\psi, &\quad (\partial_t^{[\phi']})^2\psi' =&\ e^{i\chi}(\partial_t^{[\phi]})^2\psi\\
\nabla^{[\boldsymbol{\mathcal{A}}']}\psi' =&\ e^{i\chi}\nabla^{[\boldsymbol{\mathcal{A}}]}\psi, &\quad (\nabla^{[\boldsymbol{\mathcal{A}}']})^2\psi' =&\ e^{i\chi}(\nabla^{[\boldsymbol{\mathcal{A}}]})^2\psi.
\end{aligned}$$

Proof: Exploiting that $\nabla\partial_t\chi - \partial_t\nabla\chi = 0$, since χ is smooth, and $\operatorname{curl}(\nabla\chi) = 0$ (see (1.2)), we immediately obtain the invariance of the electric and magnetic field

$$\begin{aligned}
\boldsymbol{E}' =& -\nabla\phi' - \frac{\partial_t}{c}\boldsymbol{\mathcal{A}}' = \boldsymbol{E}\\
\boldsymbol{B}' =& \nabla \times \boldsymbol{\mathcal{A}}' = \boldsymbol{B}.
\end{aligned}$$

Moreover, the gauge transform (cf. Section 2.1.1)

$$\boldsymbol{\mathcal{A}} \mapsto \boldsymbol{\mathcal{A}}', \quad \phi \mapsto \phi', \quad \psi \mapsto e^{i\chi}\psi =: \psi'$$

implies that

$$\begin{aligned}
\partial_t^{[\phi']}\psi' =& c^{-1}(\partial_t + i\phi')\psi' = c^{-1}\big(i(\partial_t\chi)e^{i\chi}\psi + e^{i\chi}\partial_t\psi + i(\phi - \partial_t\chi)e^{i\chi}\psi\big) \\
=& c^{-1}e^{i\chi}(\partial_t + i\phi)\psi = e^{i\chi}\partial_t^{[\phi]}\psi, \\
\nabla^{[\boldsymbol{\mathcal{A}}']}\psi' =& (\nabla - i\frac{\boldsymbol{\mathcal{A}}'}{c})\psi' = \big(i(\nabla\chi)e^{i\chi}\psi + e^{i\chi}\nabla\psi - \frac{i}{c}(\boldsymbol{\mathcal{A}} + c\nabla\chi)e^{i\chi}\psi\big) \\
=& e^{i\chi}(\nabla + i\frac{\boldsymbol{\mathcal{A}}}{c})\psi = e^{i\chi}\nabla^{[\boldsymbol{\mathcal{A}}]}\psi,
\end{aligned}$$

and similar

$$\begin{aligned}
(\partial_t^{[\phi']})^2\psi' =& \partial_t^{[\phi']}(e^{i\chi}\partial_t^{[\phi]}\psi) = e^{i\chi}(\partial_t^{[\phi]})^2\psi \\
(\nabla^{[\boldsymbol{\mathcal{A}}']})^2\psi' =& \nabla^{[\boldsymbol{\mathcal{A}}']}(e^{i\chi}\nabla^{[\boldsymbol{\mathcal{A}}]}\psi) = e^{i\chi}(\nabla^{[\boldsymbol{\mathcal{A}}]})^2\psi.
\end{aligned}$$

The assumption (2.14) on f yields that $f[\psi'] = f[e^{i\chi}\psi] = e^{i\chi}f[\psi]$. This finishes the proof. □

Proposition A.26 ([70, Section 5], Klein–Gordon Reformulation of Dirac's Equation)**.** *Applying* $-i\partial_t^{[\phi]}$ *to the Dirac equation coupled to* ϕ *and* $\boldsymbol{\mathcal{A}}$ *via the minimal coupling operators*

$$\partial_t^{[\phi]} = \frac{\partial_t}{c} + i\frac{\phi}{c} \quad \text{and} \quad \nabla^{[\boldsymbol{\mathcal{A}}]} = \nabla - i\frac{\boldsymbol{\mathcal{A}}}{c} \quad \text{given in Definition A.23},$$

i.e. applying $-i\partial_t^{[\phi]}$ *to*

$$i\partial_t^{[\phi]}\psi = -i\sum_{j=1}^{d}\boldsymbol{\alpha}_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_j\psi + c\boldsymbol{\beta}\psi, \quad \psi(0,x) = \psi_I(x), \tag{A.16}$$

we obtain the following Klein–Gordon type system

$$\begin{aligned}
&(\partial_t^{[\phi]})^2\psi - (\nabla^{[\boldsymbol{\mathcal{A}}]})^2\psi + c^2\psi = \frac{i}{c}\mathfrak{D}^{\boldsymbol{\alpha}}[\phi, \boldsymbol{\mathcal{A}}]\psi, \\
&\psi(0) = \psi_I, \quad \partial_t^{[\phi(0)]}\psi(0) = \langle\nabla\rangle_c\,\psi_I',
\end{aligned}$$

where we define

$$\psi_I' := -i\boldsymbol{\beta}c\,\langle\nabla\rangle_c^{-1}\,\psi_I - \langle\nabla\rangle_c^{-1}\sum_{j=1}^{d}\boldsymbol{\alpha}_j(\nabla^{[\boldsymbol{\mathcal{A}}(0)]})_j\psi_I$$

and where $\mathfrak{D}^{\boldsymbol{\alpha}}[\phi, \boldsymbol{\mathcal{A}}] := \mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{div}}[\phi] + \mathfrak{D}^{\boldsymbol{\alpha}}_0[\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}] + \mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{curl}}[\boldsymbol{\mathcal{A}}]$ *with (cf. Definition 2.6)*

$$\begin{aligned}
&\mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{curl}}[\boldsymbol{\mathcal{A}}] := -\frac{1}{2}\sum_{\substack{j,k=1\\ j\neq k}}^{d}\boldsymbol{\alpha}_j\boldsymbol{\alpha}_k[(\partial_j(A_k)) - (\partial_k(A_j))], \quad \mathfrak{D}^{\boldsymbol{\alpha}}_{\mathrm{div}}[\phi] := \sum_{j=1}^{d}\boldsymbol{\alpha}_j(\partial_j\phi), \\
&\mathfrak{D}^{\boldsymbol{\alpha}}_0[\frac{\partial_t}{c}\boldsymbol{\mathcal{A}}] := \sum_{j=1}^{d}\boldsymbol{\alpha}_j(\frac{\partial_t}{c}A_j).
\end{aligned}$$

Proof (see also [70])*:* Applying $-i\partial_t^{[\phi]}$ to (A.16), we have

$$\partial_t^{[\phi]^2}\psi = i\sum_{j=1}^{d}\boldsymbol{\alpha}_j\;(i\partial_t^{[\phi]})(\nabla^{[\boldsymbol{\mathcal{A}}]})_j\psi - c\boldsymbol{\beta}(i\partial_t^{[\phi]}\psi). \tag{A.17}$$

Because

$$\begin{aligned}(i\partial_t^{[\phi]})(\nabla^{[\boldsymbol{\mathcal{A}}]})_j\psi =& i\frac{1}{c}(\partial_t + i\phi)(\partial_j - i\frac{A_j}{c})\psi \\ =& i\frac{1}{c}\left(\partial_t\partial_j\psi + i\phi\partial_j\psi + \phi\frac{A_j}{c}\psi - i\frac{A_j}{c}\partial_t\psi - i\frac{(\partial_t A_j)}{c}\psi\right)\end{aligned}$$

we have that

$$\begin{aligned}(\nabla^{[\boldsymbol{\mathcal{A}}]})_j(i\partial_t^{[\phi]})\psi =& i\frac{1}{c}(\partial_j - i\frac{A_j}{c})(\partial_t + i\phi)\psi \\ =& i\frac{1}{c}\left(\partial_j\partial_t\psi + i\phi\partial_j\psi + i(\partial_j\phi)\psi - i\frac{A_j}{c}\partial_t\psi + \frac{A_j}{c}\phi\psi\right) \\ =& i\frac{1}{c}\Bigg(\partial_t\partial_j\psi + i\phi\partial_j\psi + \phi\frac{A_j}{c}\psi - i\frac{A_j}{c}\partial_t\psi - i\frac{(\partial_t A_j)}{c}\psi \\ & + i\frac{(\partial_t A_j)}{c}\psi + i(\partial_j\phi)\psi\Bigg) \\ =& (i\partial_t^{[\phi]})(\nabla^{[\boldsymbol{\mathcal{A}}]})_j\psi - \frac{1}{c}\big(\frac{\partial_t A_j}{c} + \partial_j\phi\big)\psi.\end{aligned}$$

Employing this identity into (A.17), we obtain

$$\begin{aligned}{\partial_t^{[\phi]}}^2\psi =& i\sum_{j=1}^d \boldsymbol{\alpha}_j\ (i\partial_t^{[\phi]})(\nabla^{[\boldsymbol{\mathcal{A}}]})_j\psi - c\boldsymbol{\beta}(i\partial_t^{[\phi]}\psi) \\ =& \left(i\sum_{j=1}^d \boldsymbol{\alpha}_j\ (\nabla^{[\boldsymbol{\mathcal{A}}]})_j - c\boldsymbol{\beta}\right)(i\partial_t^{[\phi]}\psi) \\ & + i\frac{1}{c}\sum_{j=1}^d \boldsymbol{\alpha}_j\big(\frac{\partial_t A_j}{c} + \partial_j\phi\big).\end{aligned}$$

Now inserting (A.16), i.e.

$$i\partial_t^{[\phi]}\psi = -i\sum_{j=1}^d \boldsymbol{\alpha}_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_j\psi + c\boldsymbol{\beta}\psi$$

into the latter, yields that

$$\begin{aligned}&\left(i\sum_{j=1}^d \boldsymbol{\alpha}_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_j - c\boldsymbol{\beta}\right)(i\partial_t^{[\phi]}\psi) \\ =& \left(i\sum_{j=1}^d \boldsymbol{\alpha}_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_j - c\boldsymbol{\beta}\right)\left(-i\sum_{j=1}^d \boldsymbol{\alpha}_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_j\psi + c\boldsymbol{\beta}\psi\right) \\ =& \sum_{j=1}^d\sum_{k=1}^d \boldsymbol{\alpha}_j\boldsymbol{\alpha}_k(\nabla^{[\boldsymbol{\mathcal{A}}]})_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_k\psi + ic\sum_{j=1}^d\big(\boldsymbol{\alpha}_j\boldsymbol{\beta} + \boldsymbol{\beta}\boldsymbol{\alpha}_j\big)(\nabla^{[\boldsymbol{\mathcal{A}}]})_j\psi - c^2\beta^2\psi.\end{aligned}$$

Exploiting the relations (1.24) of the matrices $\boldsymbol{\alpha}_j, \boldsymbol{\beta}, j = 1, \ldots, d$ then gives

$${\partial_t^{[\phi]}}^2\psi = (\nabla^{[\boldsymbol{\mathcal{A}}]})^2\psi - c^2\psi \quad + \sum_{\substack{j,k=1 \\ j\neq k}}^d \boldsymbol{\alpha}_j\boldsymbol{\alpha}_k(\nabla^{[\boldsymbol{\mathcal{A}}]})_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_k\psi + i\frac{1}{c}\sum_{j=1}^d \boldsymbol{\alpha}_j\big(\frac{\partial_t A_j}{c} + \partial_j\phi\big)\psi.$$

Furthermore, since $\boldsymbol{\alpha}_k\boldsymbol{\alpha}_j = -\boldsymbol{\alpha}_j\boldsymbol{\alpha}_k, j \neq k$ by (1.24), and due to

$$(\nabla^{[\boldsymbol{\mathcal{A}}]})_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_k\psi = \partial_j\partial_k\psi - \frac{i}{c}(\partial_j A_k)\psi - \frac{i}{c}A_k\partial_j\psi - \frac{i}{c}A_j\partial_k\psi - \frac{1}{c^2}A_jA_k\psi,$$

the double sum reduces to

$$\begin{aligned}
&\sum_{\substack{j,k=1\\ j\neq k}}^{d} \boldsymbol{\alpha}_j\boldsymbol{\alpha}_k(\nabla^{[\boldsymbol{\mathcal{A}}]})_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_k\psi\\
=&\frac{1}{2}\sum_{\substack{j,k=1\\ j\neq k}}^{d}\Big(\boldsymbol{\alpha}_j\boldsymbol{\alpha}_k(\nabla^{[\boldsymbol{\mathcal{A}}]})_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_k\psi+\boldsymbol{\alpha}_k\boldsymbol{\alpha}_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_k(\nabla^{[\boldsymbol{\mathcal{A}}]})_j\psi\Big)\\
=&\frac{1}{2}\sum_{\substack{j,k=1\\ j\neq k}}^{d}\boldsymbol{\alpha}_j\boldsymbol{\alpha}_k\Big(\big(\nabla^{[\boldsymbol{\mathcal{A}}]})_j(\nabla^{[\boldsymbol{\mathcal{A}}]})_k\psi-(\nabla^{[\boldsymbol{\mathcal{A}}]})_k(\nabla^{[\boldsymbol{\mathcal{A}}]})_j\psi\Big)\Big)\\
=&-\frac{i}{c}\frac{1}{2}\sum_{\substack{j,k=1\\ j\neq k}}^{d}\boldsymbol{\alpha}_j\boldsymbol{\alpha}_k\big((\partial_jA_k)-(\partial_kA_j)\big)\psi.
\end{aligned}$$

Then, we deduce

$$\begin{aligned}
{\partial_t^{[\phi]}}^2\psi =&(\nabla^{[\boldsymbol{\mathcal{A}}]})^2\psi-c^2\psi\\
&+\frac{i}{c}\Big(-\frac{1}{2}\sum_{\substack{j,k=1\\ j\neq k}}^{d}\boldsymbol{\alpha}_j\boldsymbol{\alpha}_k\big((\partial_jA_k)-(\partial_kA_j)\big)+\sum_{j=1}^{d}\boldsymbol{\alpha}_j\big(\frac{\partial_tA_j}{c}+\partial_j\phi\big)\Big)\psi.
\end{aligned}$$

Additionally, the way we define ψ_I' is an immediate consequence of plugging the initial data ψ_I together with $\phi(0)$ and $\boldsymbol{\mathcal{A}}(0)$ into the Dirac equation (A.16). This finishes the proof. □

A.7 Miscellaneous

Corollary A.27 ([45, Section 3], Orthogonality Condition for MFE)**.** *Let $m\in\mathbb{Z}$ and let $G:\mathbb{R}\times\mathbb{T}\to\mathbb{C}$ and $g^{(a)}:\mathbb{R}\to\mathbb{C}$ for $a\in\mathbb{Z}$ with*

$$G(t,\theta)=\sum_{a=-\infty}^{\infty}e^{ia\theta}g^{(a)}(t).$$

Consider the differential equation

$$(i\partial_\theta+m)W(t,\theta)=G(t,\theta),\qquad W(0,0)\quad \text{given,} \tag{A.18}$$

and look for solutions $W:\mathbb{R}\times\mathbb{T}\to\mathbb{C}$ of type

$$W(t,\theta)=\sum_{a=-\infty}^{\infty}e^{ia\theta}w^{(a)}(t).$$

Then (A.18) will be solvable if the right hand side is orthogonal to $e^{-im\theta}$ i.e. if

$$\sum_{a=-\infty}^{\infty}\int_{\mathbb{T}}e^{-im\theta}e^{ia\theta}g^{(a)}(t)d\theta=\int_{\mathbb{T}}e^{-im\theta}e^{im\theta}d\theta g^{(m)}(t)=2\pi g^{(m)}(t)\overset{!}{=}0.$$

Note that because

$$(i\partial_\theta+m)\big(e^{im\theta}z(t)\big)=0,$$

for $z : \mathbb{R} \to \mathbb{C}$, the latter is equivalent to demanding that the terms, lying in the kernel of $(i\partial_\theta + m)$, namely $e^{im\theta} g^{(m)}(t)$ must vanish.

The solution is then given by

$$W(t,\theta) = e^{im\theta} w(t) + \sum_{\substack{a=-\infty \\ m\neq a}}^{\infty} \frac{1}{m-a} e^{ia\theta} g^{(a)}(t)$$

for an arbitrary function $w : \mathbb{R} \to \mathbb{C}$.

Proof: See [45]. □

Proposition A.28 ([6, Chapter 18.4 and 18.5], Trace of Matrices)**.** *Let $m \in \mathbb{N}$ and let $A, B \in \mathbb{C}^{m\times m}$ be two matrices. Let $\operatorname{tr} M := \sum_{\ell=1}^{m} M_{\ell\ell}$ be the trace of a matrix $M \in \mathbb{C}^{m\times m}$. Furthermore let $A = SDS^{-1}$ be a diagonalisation of A with a diagonal matrix $D = \operatorname{diag}(\lambda_1, \dots, \lambda_m)$, where $\lambda_1, \dots, \lambda_m$ are the eigenvalues of A, and a regular matrix $S \in \mathbb{C}^{m\times m}$. Then*

(a) $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ *and*

(b) $\operatorname{tr}(A) = \operatorname{tr}(SDS^{-1}) = \operatorname{tr}(SS^{-1}D) = \operatorname{tr}(D) = \lambda_1 + \dots + \lambda_m$*.*

Proof (see also [6, Chapter 18.4 and 18.5])*:* For a proof of (a), see [6, Chapter 18.4]. Part (b) is an immediate consequence of (a). □

Proposition A.29 ([4, II.8.11 Theorem], Cauchy Product Formula)**.** *Let the series $\sum_{j=0}^{\infty} U_j$, $\sum_{k=0}^{\infty} V_k$ and $\sum_{\ell=0}^{\infty} W_\ell$ converge absolutely. Then we have*

$$\left(\sum_{k=0}^{\infty} V_k\right) \cdot \left(\sum_{\ell=0}^{\infty} W_\ell\right) = \sum_{n=0}^{\infty} \sum_{\ell=0}^{n} V_\ell\, W_{n-\ell} = \sum_{n=0}^{\infty} Z_n, \quad Z_n := \sum_{\ell=0}^{n} V_\ell\, W_{n-\ell}$$

and thus

$$\left(\sum_{j=0}^{\infty} U_j\right) \cdot \left(\sum_{k=0}^{\infty} V_k\right) \cdot \left(\sum_{\ell=0}^{\infty} W_\ell\right) = \sum_{n=0}^{\infty} \sum_{j=0}^{n} U_j Z_{n-j} = \sum_{n=0}^{\infty} \sum_{j=0}^{n} U_j \sum_{\ell=0}^{n-j} V_\ell W_{n-j-\ell}.$$

Lemma A.30 ([47, Proof of Lemma (german: Hilfssatz) VI.1.5])**.** *Let $d \in \mathbb{N}$ and let $\langle k\rangle$ be defined as in Definition A.6. Furthermore let $r > d/2$. Then the series*

$$\sum_{k\in\mathbb{Z}^d} \langle k\rangle^{-2r} \le K(d)$$

converges and is bounded with a constant $K(d)$ only depending on d.

Proof: We have that

$$\sum_{k\in\mathbb{Z}^d} \langle k\rangle^{-2r} \le 1 + \sum_{k\in\mathbb{Z}^d\setminus\{0\}} |k|^{-2r}.$$

According to [47, Beweis von Hilfssatz VI.1.5] the second sum is dominated by

$$\sum_{k\in\mathbb{Z}^d\setminus\{0\}} |k|^{-2r} \leq \int_{\substack{x\in\mathbb{R}^d\\ |x|^2\geq 1}} \frac{1}{|x|^{2r}}dx.$$

Switching to polar coordinates, the integral becomes

$$\int_1^\infty \int_{\mathcal{S}^{d-1}} d\hat{s}\frac{R^{d-1}}{R^{2r}}dR = K(d)\int_1^\infty R^{-(1+(2r-d))}dR$$

which converges if and only if $r > d/2$, where $\mathcal{S}^{d-1}$ is the d dimensional unit sphere (see [5, VII.9.5 Examples (b)]). □

Proposition A.31 ([6, Chapter 31.1], Cauchy-Schwarz Inequality)**.** *Let X be a Hilbert space with inner product $\langle\cdot,\cdot\rangle_X$ and let $\|\cdot\|_X$ be the norm induced by $\langle\cdot,\cdot\rangle_X$, i.e. $\|a\|_X^2 = \langle a,a\rangle$ for $a\in X$. Then we have $|\langle a,b\rangle_X| \leq \|a\|_X\,\|b\|_X$.*

Proof: For a proof see [6, Chapter 31.1] and references therein. □

Proposition A.32 ([18, Proof of Lemma 4])**.** *For all $x\in\mathbb{R}$ we have the following auxiliary result:*

$$\left|e^{ix}-1\right| \leq |x| \quad \text{and thus also} \quad \left|\frac{e^{ix}-1}{x}\right| \leq 1 \quad \text{for all } x\in\mathbb{R}.$$

In particular we can globally bound this term by 2, i.e.

$$\left|e^{ix}-1\right| \leq 2 \quad \text{for all } x\in\mathbb{R}.$$

Proof (see also [18, Proof of Lemma 4])*:* We structure the proof in three parts. Firstly, we consider the case $|x| > 2$, then the case $x\in[0,2]$ and afterwards the case $x\in[-2,0)$.

Consider $f(x) := \left|e^{ix}-1\right|^2 = (\cos(x)-1)^2 + (\sin(x))^2 = 2(1-\cos(x))$. It is obvious that $0\leq f(x)\leq 4$ for all $x\in\mathbb{R}$ which immediately proves that $\left|e^{ix}-1\right|\leq 2$ for all $x\in\mathbb{R}$.

In particular this also implies that

$$\left|e^{ix}-1\right| \leq |x|\,, \quad \text{for all } |x| > 2.$$

We observe that $f\in C^\infty(\mathbb{R})$. Its first two derivatives are given by $f'(\xi) = 2\sin(\xi)$ and $f''(\xi) = 2\cos(\xi)$. Now assume that $0\leq x\leq 2$.

From Taylor's theorem in [53, Kapitel 3.13, Korollar 1] we deduce that

$$f(x) = f(0) + xf'(0) + \int_0^x (x-t)f''(t)dt = \int_0^x (x-t)f''(t)dt,$$

where we used that $f(0) = f'(0) = 0$.

Therefore applying triangle inequality to the integral remainder and taking the supremum of f'' we obtain

$$f(x) = |f(x)| \leq \int_0^x (x-t)dt\cdot 2\sup_{0\leq t\leq x}|\cos(t)| \leq 2\cdot\left((x-0)x - \tfrac{1}{2}x^2\right) = x^2,$$

Similarly we show that for $-2 \leq x < 0$

$$f(x) = \int_0^x (x-t)f''(t)dt = \int_x^0 (t-x)f''(t)dt$$

such that by the same arguments

$$f(x) = |f(x)| \leq 2\int_x^0 (t-x)dt = 2\cdot\left(-\frac{1}{2}x^2 - (0-x)x\right) = x^2$$

Therefore, we conclude by taking the square root of the inequality

$$f(x) = \left|e^{ix} - 1\right|^2 \leq |x|^2 \,. \tag{A.19}$$

Applying the square root to (A.19) immediately gives the assertion. □

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