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CRC Preprint 2016/19, July 2016

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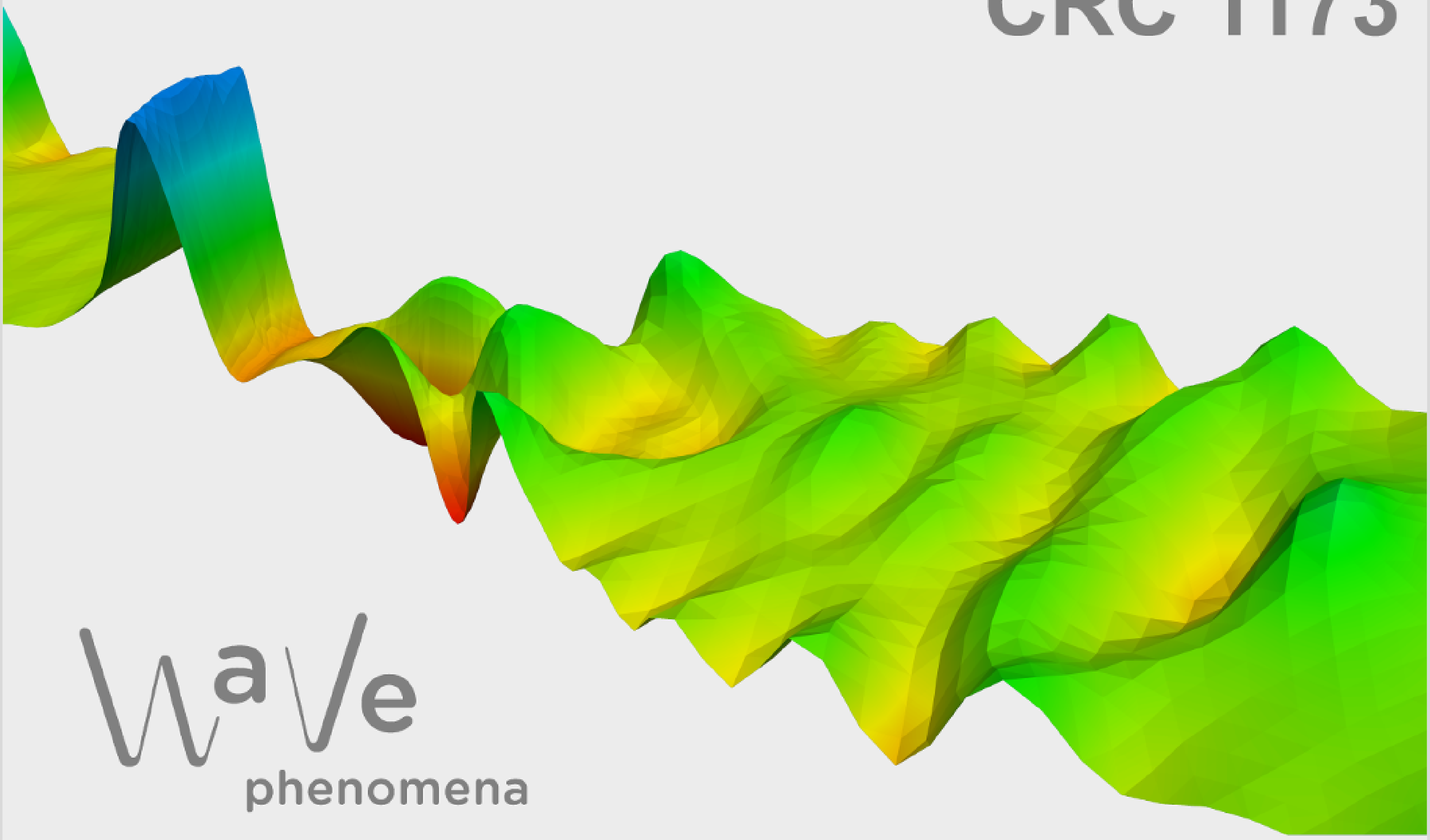
CRC 1173



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Funded by

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ISSN 2365-662X

Efficient time integration of the Maxwell-Klein-Gordon equation in the non-relativistic limit regime

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Abstract

The Maxwell-Klein-Gordon equation describes the interaction of a charged particle with an electromagnetic field. Solving this equation in the non-relativistic limit regime, i.e. the speed of light c formally tending to infinity, is numerically very delicate as the solution becomes highly-oscillatory in time. In order to resolve the oscillations, standard numerical time integration schemes require severe time step restrictions depending on the large parameter c^2.

The idea to overcome this numerical challenge is to filter out the high frequencies explicitly by asymptotically expanding the exact solution with respect to the small parameter c^{-2}. This allows us to reduce the highly-oscillatory problem to its corresponding non-oscillatory Schrödinger-Poisson limit system. On the basis of this expansion we are then able to construct efficient numerical time integration schemes, which do NOT suffer from any c-dependent time step restriction.

Keywords: Maxwell-Klein-Gordon, time integration, highly-oscillatory, wave equation, non-relativistic limit

1. Introduction

The Maxwell-Klein-Gordon (MKG) equation describes the motion of a charged particle in an electromagnetic field and the interactions between the field and the particle. The MKG equation can be derived from the linear Klein-Gordon (KG) equation

$$\left(\frac{\partial_t}{c}\right)^2 z - \nabla^2 z + c^2 z = 0 \tag{1}$$

by coupling the scalar field $z(t, x) \in \mathbb{C}$ to the electromagnetic field via a so-called *minimal substitution* (cf. [17, 24, 25]), i.e.

$$\begin{aligned} \frac{\partial_t}{c} \quad &\to \quad \frac{\partial_t}{c} + i\frac{\Phi}{c} \quad &=: D_0, \\ \nabla \quad &\to \quad \nabla - i\frac{\boldsymbol{\mathcal{A}}}{c} \quad &=: \boldsymbol{D}_\alpha, \end{aligned} \tag{2}$$

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where the electromagnetic field is represented by the real Maxwell potentials $\Phi(t,x) \in \mathbb{R}$ and $\boldsymbol{\mathcal{A}}(t,x) \in \mathbb{R}^d$.

We replace the operators $\frac{\partial_t}{c}$ and ∇ in the KG equation (1) by their minimal substitution (2) such that in the so-called Coulomb gauge (cf. [1]), i.e. under the constraint $\operatorname{div} \boldsymbol{\mathcal{A}} \equiv 0$, we obtain a KG equation coupled to the electromagnetic field as

$$\begin{cases} \left(\frac{\partial_t}{c} + i\frac{\Phi}{c}\right)^2 z - \left(\nabla - i\frac{\boldsymbol{\mathcal{A}}}{c}\right)^2 z + c^2 z = 0, \\ \partial_{tt}\boldsymbol{\mathcal{A}} - c^2\Delta\boldsymbol{\mathcal{A}} = c\mathcal{P}\left[\boldsymbol{J}\right], \\ -\Delta\Phi = \rho, \end{cases} \tag{3}$$

for some charge density $\rho(t,x) \in \mathbb{R}$ and some current density $\boldsymbol{J}(t,x) \in \mathbb{R}^d$, where we define

$$\mathcal{P}\left[\boldsymbol{J}\right] := \boldsymbol{J} - \nabla\Delta^{-1} \operatorname{div} \boldsymbol{J}$$

the projection of $\boldsymbol{J}$ onto its divergence-free part, i.e. $\operatorname{div} \mathcal{P}\left[\boldsymbol{J}\right] \equiv 0$.

Setting

$$\rho = \rho[z] := -\operatorname{Re}\left(i\frac{z}{c}\left(\frac{\partial_t}{c} - i\frac{\Phi}{c}\right)\overline{z}\right), \qquad \boldsymbol{J} = \boldsymbol{J}[z] := \operatorname{Re}\left(iz\left(\nabla + i\frac{\boldsymbol{\mathcal{A}}}{c}\right)\overline{z}\right), \tag{4}$$

where z solves (3), we find that ρ and $\boldsymbol{J}$ satisfy the continuity equation

$$\partial_t\rho + \operatorname{div} \boldsymbol{J} = 0. \tag{5}$$

For notational simplicity in the following we may also write $\rho(t,x)$, $\boldsymbol{J}(t,x)$ instead of $\rho[z(t,x)]$ and $\boldsymbol{J}[z(t,x)]$.

The definition of ρ and $\boldsymbol{J}$ in (4) together with the constraint $\operatorname{div} \boldsymbol{\mathcal{A}}(t,x) \equiv 0$ yields the so-called *Maxwell-Klein-Gordon* equation in the Coulomb gauge

$$\begin{cases} \partial_{tt} z = -c^2(-\Delta + c^2)z + \Phi^2 z - 2i\Phi\partial_t z - iz\partial_t\Phi - 2ic\boldsymbol{\mathcal{A}}\cdot\nabla z - \left|\boldsymbol{\mathcal{A}}\right|^2 z, \\ \partial_{tt}\boldsymbol{\mathcal{A}} = c^2\Delta\boldsymbol{\mathcal{A}} + c\mathcal{P}\left[\boldsymbol{J}\right], \quad \boldsymbol{J} = \operatorname{Re}\left(iz\overline{\boldsymbol{D}_\alpha z}\right), \\ -\Delta\Phi = \rho, \quad \rho = -c^{-1}\operatorname{Re}\left(iz\overline{D_0 z}\right), \qquad (6a) \\ z(0,x) = \varphi(x), \quad D_0 z(0,x) = \sqrt{-\Delta + c^2}\psi(x), \\ \boldsymbol{\mathcal{A}}(0,x) = A(x), \quad \partial_t\boldsymbol{\mathcal{A}}(0,x) = cA'(x), \\ \int_{\mathbb{T}^d} \rho(0,x)dx = 0, \quad \int_{\mathbb{T}^d} \Phi(t,x)dx = 0. \qquad (6b) \end{cases}$$

Note that for practical implementation issues we assume *periodic boundary conditions* (p.b.c.) in space in the above model, i.e. $x \in \mathbb{T}^d$. For simplicity we also assume that the total charge $Q(t) := (2\pi)^{-d}\int_{\mathbb{T}^d} \rho(t,x)dx$ at time $t = 0$ is zero, i.e. $Q(0) = 0$. Also due to the constraint $\operatorname{div} \boldsymbol{\mathcal{A}}(t,x) \equiv 0$ we assume that the initial data A, A' for $\boldsymbol{\mathcal{A}}$ are divergence-free. Finally, the following assumption guarantees strongly well-prepared initial data. However, approximation results also hold true under weaker initial assumptions, see for instance [21].

Assumption 1. *The initial data φ, ψ, A, A' is independent of c.*

Remark 1. *Note that the continuity equation* (5) *together with the initial assumption* $Q(0) = 0$ *implies that for all* t *we have* $\int_{\mathbb{T}^d} \rho(t,x)dx = \int_{\mathbb{T}^d} \rho(0,x)dx = 0$.*This yields the first condition in* (6b).

Remark 2. *Up to minor changes, all the results of this paper remain valid for Dirichlet boundary conditions instead of periodic boundary conditions.*

Remark 3. *Note that the MKG system* (6) *is invariant under the gauge transform* $(z, \Phi, \boldsymbol{\mathcal{A}}) \mapsto (z', \Phi', \boldsymbol{\mathcal{A}}')$, *where for a suitable choice of* $\chi = \chi(t,x)$ *we set*

$$\Phi' := \Phi + \partial_t \chi, \qquad \boldsymbol{\mathcal{A}}' := \boldsymbol{\mathcal{A}} - c\nabla\chi, \qquad z' := z\ \exp(-i\chi),$$

i.e. if $(z, \Phi, \boldsymbol{\mathcal{A}})$ *solves the MKG system* (6) *then also does* $(z', \Phi', \boldsymbol{\mathcal{A}}')$ *without modification of the system (cf. [1, 11, 24, 25]). Henceforth, the second condition in* (6b) *holds without loss of generality: If* $0 \neq (2\pi)^{-d} \int_{\mathbb{T}^d} \Phi(t,x)dx =: M(t) \in \mathbb{R}$, *we choose* χ *as* $\chi(t,x) = \chi(t) = -(M(0) + \int_0^t M(\tau)d\tau)$, *such that* (6b) *is satisfied for* Φ'.

For more physical details on the derivation of the MKG equation, on Maxwell's potentials, gauge theory formalisms and many more related topics we refer to [1, 11, 12, 17, 24, 25] and the references therein.

Here we are interested in the so-called non-relativistic limit regime $c \gg 1$ of the MKG system (6). In this regime the numerical time integration becomes severely challenging due to the highly-oscillatory behaviour of the solution. In order to resolve these high oscillations standard numerical schemes require severe time step restrictions depending on the large parameter c^2, which leads to a huge computational effort. This numerical challenge has lately been extensively studied for the nonlinear Klein-Gordon (KG) equation, see [2, 3, 8, 14]. In particular it was pointed out that a Gautschi-type exponential integrator only allows convergence under the constraint that the time step size is of order $\mathcal{O}(c^{-2})$ (cf. [3]).

In this paper we construct numerical schemes for (6) which do not suffer from any c-dependent time step restriction. Our strategy is thereby similar to [2, 14] where the Klein-Gordon equation is considered: In a first step we expand the exact solution into a formal asymptotic expansion in terms of c^{-2} for z, Φ and in terms of c^{-1} for $\boldsymbol{\mathcal{A}}$. This allows us to filter out the high oscillations in the solution explicitly. Therefore we can break down the numerical task to only solving the corresponding non-oscillatory Schrödinger-Poisson limit system. The latter can be carried out very efficiently without imposing any CFL type condition on c nor the spatial grid size. This construction is based on the *Modulated Fourier Expansion* (MFE) of the exact solution in terms of the small parameter $c^{-l}, l \geq 1$, see for instance [10, 14], [15, Chapter XIII] and the references therein. However, as in [14] we control the expansion by computing the coefficients of the MFE directly and in particular exploit the results in [6, 21] on the asymptotic behaviour of the exact solution of the MKG equation (6). More precisely, formally the following approximations hold

$$\begin{aligned} z(t,x) &= \frac{1}{2}\left(u_0(t,x)\exp(ic^2t) + \overline{v}_0(t,x)\exp(-ic^2t)\right) + \mathcal{O}\left(c^{-2}\right), \\ \boldsymbol{\mathcal{A}}(t,x) &= \cos(c\sqrt{-\Delta}t)A(x) + \sqrt{-\Delta}^{-1}\sin(c\sqrt{-\Delta}t)A'(x) + \mathcal{O}\left(c^{-1}\right), \end{aligned} \tag{7}$$

where u_0 and v_0 solve the Schrödinger-Poisson (SP) system

$$\begin{cases} i\partial_t u_0 = \frac{1}{2}\Delta u_0 + \Phi_0 u_0, & u_0(0) = \varphi - i\psi, \\ i\partial_t v_0 = \dfrac{1}{2}\Delta v_0 - \Phi_0 v_0, & v_0(0) = \overline{\varphi} - i\overline{\psi}, \\ -\Delta\Phi_0 = -\dfrac{1}{4}\big(|u_0|^2 - |v_0|^2\big), & \displaystyle\int_{\mathbb{T}^d} \Phi_0(t,x)dx = 0. \end{cases} \tag{8}$$

Remark 4. *The L^2 conservation of u_0, v_0 together with the choice $Q(0) = 0$ yields that*

$$\int_{\mathbb{T}^d} |u_0(t,x)|^2 - |v_0(t,x)|^2 \, dx = \int_{\mathbb{T}^d} |u_0(0,x)|^2 - |v_0(0,x)|^2 \, dx = 0.$$

Here we point out that in the asymptotic expansion (7) the highly-oscillatory nature of the solution is only contained in the high-frequency terms $\exp(\pm ic^2 t)$ and $\cos(c\sqrt{-\Delta}t)$, $\sin(c\sqrt{-\Delta}t)$, respectively. In particular the SP system (8) does not depend on the large parameter c. Henceforth, the expansion (7) allows us to derive an efficient and fast numerical approximation without any c-dependent time step restriction: We only need to solve the non-oscillatory SP system numerically and multiply the numerical approximations to the SP solution with the highly-oscillatory phases.

After a full discretization using for instance the second-order Strang splitting scheme for the time discretization of the SP system (8) (see [20]) with time step size τ and a Fourier pseudospectral (FP) method for the space discretization with mesh size h, the resulting numerical schemes then approximate the exact solution of the MKG equation up to error terms of order $\mathcal{O}(c^{-2} + \tau^2 + h^s)$ for z, Φ and $\mathcal{O}(c^{-1} + h^s)$ for $\boldsymbol{\mathcal{A}}$ respectively.

The main advantage here is that we can choose τ and h independently of the large parameter c. The value of s depends on the smoothness of the solution. We will discuss the numerical scheme in more detail later on in Section 5.

Remark 5. *Under additional smoothness assumptions on the initial data we can also carry out the asymptotic expansion up to higher order terms in c^{-l}. In particular, every term in this expansion can be easily computed numerically as the high oscillations can be filtered out explicitly.*

If we consider other boundary conditions, such as for example Dirichlet or Neumann boundary conditions it may be favorable to use a finite element (FEM) space discretization or a sine pseudospectral discretization method instead of the FP method. For details on the convergence of a FEM applied to the MKG equation in the so-called temporal gauge, see for instance [9] and references therein.

For further results on the construction of efficient methods on related Klein-Gordon type equations in the non-relativistic limit regime we refer to [2–5, 8].

2. A priori bounds

We follow the strategy presented in [14, 21]: Firstly, we rewrite the MKG equation (6) as a first order system. Therefore, for a given c we introduce the operator

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

which in Fourier space can be written as a diagonal operator $(\langle\nabla\rangle_c)_{k\ell} = \delta_{k\ell}\sqrt{|k|^2+c^2}$, $k,\ell \in \mathbb{Z}^d$, where $\delta_{k\ell}$ denotes the Kronecker symbol. By Taylor series expansion of $\sqrt{1+x}^{-1}$ we can easliy see that for all $k \in \mathbb{Z}^d$ there holds $|(c\langle\nabla\rangle_c^{-1})_{kk}| \leq 1$, i.e. $c\langle\nabla\rangle_c^{-1}$ is uniformly bounded with respect to c. In particular, there holds $\left\|c\langle\nabla\rangle_c^{-1} u\right\|_s \leq \|u\|_s$, where $\|\cdot\|_s$ denotes the standard Sobolev norm corresponding to the function space $H^s := H^s(\mathbb{T}^d, \mathbb{C})$.

In order to rewrite the equation for z in (6) as a first order system we set

$$u = z - i\langle\nabla\rangle_c^{-1} D_0 z, \qquad v = \overline{z} - i\langle\nabla\rangle_c^{-1}\overline{D_0 z}, \tag{9}$$

as proposed in [21]. By the definition of $D_0 z = c^{-1}(\partial_t + i\Phi)z$ and since Φ is real we have that $z = \frac{1}{2}(u+\overline{v})$. We define the abbreviations

$$\begin{aligned}\mathcal{N}_u[u,v,\Phi,\boldsymbol{\mathcal{A}}] :=& -\frac{i}{2}(\Phi + \langle\nabla\rangle_c^{-1}\Phi\langle\nabla\rangle_c)u - \frac{i}{2}(\Phi - \langle\nabla\rangle_c^{-1}\Phi\langle\nabla\rangle_c)\overline{v} \\ &+ ic^{-1}\langle\nabla\rangle_c^{-1}\left(|\boldsymbol{\mathcal{A}}|^2\frac{1}{2}(u+\overline{v})\right) - \langle\nabla\rangle_c^{-1}(\boldsymbol{\mathcal{A}}\cdot\nabla(u+\overline{v}))\end{aligned} \tag{10}$$

and $\mathcal{N}_v[u,v,\Phi,\boldsymbol{\mathcal{A}}] := \mathcal{N}_u[v,u,-\Phi,-\boldsymbol{\mathcal{A}}]$. Differentiating u and v in (9) with respect to t we obtain the system

$$\begin{cases} i\partial_t u = -c\langle\nabla\rangle_c u + i\mathcal{N}_u[u,v,\Phi,\boldsymbol{\mathcal{A}}], \quad u(0) = \varphi - i\psi \\ i\partial_t v = -c\langle\nabla\rangle_c v + i\mathcal{N}_v[u,v,\Phi,\boldsymbol{\mathcal{A}}], \quad v(0) = \overline{\varphi} - i\overline{\psi}, \\ -\Delta\Phi = \rho[u,v], \\ \partial_{tt}\boldsymbol{\mathcal{A}} = c^2\Delta\boldsymbol{\mathcal{A}} + c\mathcal{P}\left[\boldsymbol{J}[u,v,\boldsymbol{\mathcal{A}}]\right], \quad \boldsymbol{\mathcal{A}}(0) = A,\ \partial_t\boldsymbol{\mathcal{A}}(0) = cA' \end{cases} \tag{11}$$

where the definition of $u(0), v(0)$ follows from the ansatz (9) together with the initial data φ, ψ, A, A' in (6). Furthermore since $z = \frac{1}{2}(u+\overline{v})$ we have by (6) that

$$\begin{aligned}\rho[u,v] &= -\frac{1}{4}\operatorname{Re}\left((u+\overline{v})c^{-1}\langle\nabla\rangle_c(\overline{u}-v)\right), \\ \boldsymbol{J}[u,v,\boldsymbol{\mathcal{A}}] &= \frac{1}{4}\operatorname{Re}\left(i(u+\overline{v})\nabla(\overline{u}+v) - \frac{\boldsymbol{\mathcal{A}}}{c}|u+\overline{v}|^2\right).\end{aligned} \tag{12}$$

Setting $T_c(t) = \exp(ic\langle\nabla\rangle_c t)$ we can formulate the mild solutions of (11) as

$$\begin{aligned} u(t) =& T_c(t)u(0) + \int_0^t T_c(t-\tau)\mathcal{N}_u[u,v,\Phi,\boldsymbol{\mathcal{A}}](\tau)d\tau, \\ v(t) =& T_c(t)v(0) + \int_0^t T_c(t-\tau)\mathcal{N}_v[u,v,\Phi,\boldsymbol{\mathcal{A}}](\tau)d\tau, \\ \boldsymbol{\mathcal{A}}(t) =& \cos(c\langle\nabla\rangle_0 t)\boldsymbol{\mathcal{A}}(0) + (c\langle\nabla\rangle_0)^{-1}\sin(c\langle\nabla\rangle_0 t)\partial_t\boldsymbol{\mathcal{A}}(0) \\ &+ \langle\nabla\rangle_0^{-1}\int_0^t \sin(c\langle\nabla\rangle_0(t-\tau))\mathcal{P}\left[\boldsymbol{J}[u,v,\boldsymbol{\mathcal{A}}](\tau)\right]d\tau, \end{aligned} \tag{13}$$

where we define $\exp(ic\langle\nabla\rangle_c t)w$, $\cos(c\langle\nabla\rangle_0 t)w$ and $c^{-1}\langle\nabla\rangle_0^{-1}\sin(c\langle\nabla\rangle_0 t)w$ for $w \in H^s$ in Fourier space as follows: Let $\hat{w}_k = (\mathcal{F}w)_k$ denote the k-th Fourier coefficient of w.

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

$$\begin{aligned}(\mathcal{F}[\exp(ic\langle\nabla\rangle_c t)w])_k &= \exp\left(ict\sqrt{|k|^2+c^2}\right)\hat{w}_k,\\ (\mathcal{F}[\cos(c\langle\nabla\rangle_0 t)w])_k &= \cos(c|k|t)\,\hat{w}_k,\\ (\mathcal{F}[(c\langle\nabla\rangle_0)^{-1}\sin(c\langle\nabla\rangle_0 t)w])_k &= t\,\mathrm{sinc}(c|k|t)\hat{w}_k.\end{aligned}$$

Since the Fourier transform is an isometry in H^s it follows easily, that the operators $\cos(c\langle\nabla\rangle_0 t)$ and $\sin(c\langle\nabla\rangle_0 t)$ are uniformly bounded with respect to c and that $\exp(ic\langle\nabla\rangle_c t)$ is an isometry in H^s, i.e. for all $w \in H^s$ and for all $t \in \mathbb{R}$ we have

$$\|\exp(ic\langle\nabla\rangle_c t)w\|_s = \|w\|_s\,,\ \|\cos(c\langle\nabla\rangle_0 t)w\|_s \le \|w\|_s\,,\ \left\|\frac{\sin(c\langle\nabla\rangle_0 t)}{c\langle\nabla\rangle_0}w\right\|_s \le t\,\|w\|_s\,. \tag{14}$$

As the nonlinearities $\mathcal{N}_u$ and $\mathcal{N}_v$ in the system (11) involve products of $u, v, \Phi, \boldsymbol{\mathcal{A}}$ we will exploit the standard bilinear estimates in H^s: For $s > d/2$ we have

$$\|uv\|_s \le C_s\,\|u\|_s\,\|v\|_s \tag{15}$$

91 for some constant C_s depending only on s and d.

In the following we assume that $s > d/2$. By representation in Fourier space we see that for $w \in H^{s'}$, $s' = \max\{s, s+m\}$, $m \in \mathbb{Z}$ there holds

$$\|\langle\nabla\rangle_1^m w\|_s \le C_{s,m}\,\|w\|_{s+m}\,. \tag{16}$$

Thus, (15) and (16) yield for $w \in H^s, \Phi \in H^{s+2}$

$$\begin{aligned}\left\|\langle\nabla\rangle_c^{-1}(\Phi\langle\nabla\rangle_c w)\right\|_s &\le C_1\left\|\langle\nabla\rangle_c^{-1}(\Phi\langle\nabla\rangle_0 w)\right\|_s + C_2\left\|c\langle\nabla\rangle_c^{-1}(\Phi w)\right\|_s\\ &\le C\,\|\Phi\|_{s+2}\,\|w\|_s\,,\end{aligned} \tag{17}$$

since (16) implies that for all $\tilde{w} \in H^s$ and $c \ge 1$ we find a constant C such that

$$\left\|\langle\nabla\rangle_c^{-1}\tilde{w}\right\|_s \le \left\|\langle\nabla\rangle_1^{-1}\tilde{w}\right\|_s \le C\,\|\tilde{w}\|_{s-1}\,.$$

After a short calculation we find that for $u_j, v_j, \boldsymbol{\mathcal{A}}_j \in H^s, \Phi_j \in H^{s+2}$, $j = 1, 2$ there holds, with $\mathcal{N} = \mathcal{N}_u$ and $\mathcal{N} = \mathcal{N}_v$ respectively, that

$$\begin{aligned}&\|\mathcal{N}[u_1, v_1, \Phi_1, \boldsymbol{\mathcal{A}}_1] - \mathcal{N}[u_2, v_2, \Phi_2, \boldsymbol{\mathcal{A}}_2]\|_s\\ &\le K_{\mathcal{N}}(\|u_1-u_2\|_s + \|v_1-v_2\|_s + \|\Phi_1-\Phi_2\|_{s+2} + \|\boldsymbol{\mathcal{A}}_1-\boldsymbol{\mathcal{A}}_2\|_s)\end{aligned}$$

and

$$\begin{aligned}&\left\|\langle\nabla\rangle_0^{-1}(\boldsymbol{J}[u_1, v_1, \boldsymbol{\mathcal{A}}_1] - \boldsymbol{J}[u_2, v_2, \boldsymbol{\mathcal{A}}_2])\right\|_s\\ &\le K_{\boldsymbol{J}}(\|u_1-u_2\|_s + \|v_1-v_2\|_s + \|\boldsymbol{\mathcal{A}}_1-\boldsymbol{\mathcal{A}}_2\|_s),\end{aligned}$$

92 where the constants $K_{\mathcal{N}}$ and $K_{\boldsymbol{J}}$ only depend on $\|u_j\|_s\,, \|v_j\|_s\,, \|\Phi_j\|_{s+2}\,, \|\boldsymbol{\mathcal{A}}_j\|_s$, $j = 1, 2$.

Together with (14) a standard fix point argument now implies immediately local well-posedness in H^s, $s > d/2$ (see for instance [13, Theorem III.7]), i.e. for initial data $u(0), v(0), \boldsymbol{\mathcal{A}}(0) \in H^s$, $\partial_t\boldsymbol{\mathcal{A}}(0) \in H^{s-1}$ there exists $T_s > 0$ and a constant $B_s > 0$ such that

$$\|u(t)\|_s + \|v(t)\|_s + \|\Phi(t)\|_{s+2} + \|\boldsymbol{\mathcal{A}}(t)\|_s \le B_s, \qquad \forall t \in [0, T_s]. \tag{18}$$

93 For local and global well-posedness results on the MKG equation in other gauges, e.g. in
94 Lorentz gauge, and low regularity spaces we refer to [18, 21, 26] and references therein.

3. Formal asymptotic expansion

In this section we formally derive the Schrödinger-Poisson system (8) as the non-relativistic limit of the MKG equation (6), i.e. we formally motivate the expansion (7). For a detailed rigorous analysis in low regularity spaces we refer to [6, 21] and references therein; results on asymptotics of related systems such as the Maxwell-Dirac system can be found in [7, 21].

On the c-independent finite time interval $[0,T]$ we now look, at first formally, for a solution $(u, v, \Phi, \boldsymbol{\mathcal{A}})$ of (6) in the form of a Modulated Fourier expansion (cf. [15, Chapter XIII]), i.e. we make the ansatz

$$u(t,x) = U(t,\theta,x) = \sum_{n=0}^{\infty} c^{-2n} U_n(t,\theta,x), \qquad v(t,x) = V(t,\theta,x) = \sum_{n=0}^{\infty} c^{-2n} V_n(t,\theta,x),$$
$$\Phi(t,x) = \tilde{\Phi}(t,\theta,x) = \sum_{n=0}^{\infty} c^{-2n} \Phi_n(t,\theta,x), \qquad \boldsymbol{\mathcal{A}}(t,x) = \mathfrak{A}(t,\sigma,x) = \sum_{n=0}^{\infty} c^{-n} \boldsymbol{\mathcal{A}}_n(t,\sigma,x), \tag{19}$$

where $\sigma = ct$, $\theta = c^2 t$ are fast time scales which are used to seperate the high oscillations from the slow time dependency of the solution. Next we apply the so-called method of multiple scales to U, V, $\tilde{\Phi}$ and $\mathfrak{A}$, where the idea is to treat the time scales t, σ and θ as independent variables. This allows us to derive a sequence of equations for the MFE coefficients $U_n, V_n, \Phi_n, \boldsymbol{\mathcal{A}}_n$, $n \geq 0$ and henceforth to determine the asymptotic expansion (19). For more details on the method of multiple scales and perturbation theory we refer to [19, 22, 23].

We start off by plugging the ansatz (19) into (11) and obtain for $W = (U,V)^T$ the equation

$$\partial_t W + c^2 \partial_\theta W = ic \langle \nabla \rangle_c W + \begin{pmatrix} \mathcal{N}_u(U,V,\tilde{\Phi},\mathfrak{A}) \\ \mathcal{N}_v(U,V,\tilde{\Phi},\mathfrak{A}) \end{pmatrix} \tag{20}$$

with initial condition

$$U(0,0,x) = \varphi(x) - i\psi(x), \qquad V(0,0,x) = \overline{\varphi(x)} - i\overline{\psi(x)} \tag{21}$$

and an equation for $\mathfrak{A}$ in terms of t and σ, i.e.

$$\partial_{tt}\mathfrak{A} + 2c\partial_\sigma \partial_t \mathfrak{A} + c^2 \partial_{\sigma\sigma}\mathfrak{A} = c^2 \Delta \mathfrak{A} + c\mathcal{P}\left[\boldsymbol{J}[U,V,\mathfrak{A}]\right] \tag{22}$$

with initial condition

$$(\mathfrak{A}(0,0,x), (\partial_t + c\partial_\sigma)\mathfrak{A}(0,0,x)) = (\boldsymbol{\mathcal{A}}(0,x), \partial_t \boldsymbol{\mathcal{A}}(0,x)).$$

For the potential $\tilde{\Phi}$ we find the equation

$$-\Delta \tilde{\Phi} = -\frac{1}{4} \operatorname{Re}\left((U + \overline{V}) c^{-1} \langle \nabla \rangle_c (\overline{U} - V)\right). \tag{23}$$

In the next step we expand the operators $\langle \nabla \rangle_c$ and $\langle \nabla \rangle_c^{-1}$ into their Taylor series expansion. For w sufficiently smooth we have

$$c \langle \nabla \rangle_c w = (c^2 - \frac{1}{2}\Delta - c^{-2}\frac{1}{8}\Delta^2 + \sum_{n \geq 2} \alpha_{n+1} c^{-2n} (-\Delta)^{n+1}) w. \tag{24}$$

Similarly, we find

$$c\langle\nabla\rangle_c^{-1} w = (1 + c^{-2}\frac{1}{2}\Delta + \sum_{n\geq 2}\beta_n c^{-2n}(-\Delta)^n)w. \tag{25}$$

Now (24) and (25) yield for $\Psi, w \in H^{s+2}$

$$\langle\nabla\rangle_c^{-1}\Psi\langle\nabla\rangle_c w = \Psi w + \mathcal{O}\left(c^{-2}[\Delta,\Psi]w\right) \tag{26}$$

in the sense of the H^s norm and where $[A,B] := AB - BA$ denotes the commutator of the operators A and B, i.e. $[\Delta,\Psi]w = \Delta(\Psi w) - \Psi(\Delta w)$.

Since φ and ψ are independent of c, the ansatz (19) yields by (21) that

$$\begin{aligned} U_0(0,0,x) &= \varphi(x) - i\psi(x), \quad U_n(0,0,x) = 0, n \geq 1,\\ V_0(0,0,x) &= \overline{\varphi(x)} - i\overline{\psi(x)}, \quad V_n(0,0,x) = 0, n \geq 1. \end{aligned} \tag{27}$$

Now the idea is to compare the coefficients of the left- and right-hand side of (20) with respect to equal powers of c by plugging the ansatz (19) and the expansions (24), (25) and (26) into the equation. This finally yields a sequence of partial differential equations at each order of c.

At order c^2 we obtain

$$\begin{cases} (\partial_\theta - i)U_0(t,\theta,x) = 0,\\ (\partial_\theta - i)V_0(t,\theta,x) = 0, \end{cases}$$

which allows solutions of the form

$$U_0(t,\theta,x) = \exp(i\theta)u_0(t,x), \quad V_0(t,\theta,x) = \exp(i\theta)v_0(t,x) \tag{28}$$

where u_0, v_0 will be determined in the next step.

Plugging (28) into (23) we obtain the first term Φ_0 in the expansion (19) of $\tilde{\Phi}$ as the solution of the Poisson equation

$$-\Delta\Phi_0(t,\theta,x) = -\Delta\Phi_0(t,x) = -\frac{1}{4}\left(|u_0(t,x)|^2 - |v_0(t,x)|^2\right). \tag{29}$$

At order c^0 we use (28) and obtain the equations

$$\begin{cases} (\partial_\theta - i)U_1(t,\theta,x) = \exp(i\theta)\left(-\partial_t u_0(t,x) - \frac{i}{2}\Delta u_0(t,x) - i\Phi_0(t,x)u_0(t,x)\right)\\ (\partial_\theta - i)V_1(t,\theta,x) = \exp(i\theta)\left(-\partial_t v_0(t,x) - \frac{i}{2}\Delta v_0(t,x) + i\Phi_0(t,x)v_0(t,x)\right). \end{cases} \tag{30}$$

Since $\exp(i\theta)$ lies in the kernel of the operator $(\partial_\theta - i)$ and since u_0, v_0, Φ_0 are independent of θ, we demand u_0 and v_0 to satisfy

$$\begin{cases} i\partial_t u_0(t,x) = \frac{1}{2}\Delta u_0(t,x) + \Phi_0(t,x)u_0(t,x),\\ i\partial_t v_0(t,x) = \frac{1}{2}\Delta v_0(t,x) - \Phi_0(t,x)v_0(t,x), \end{cases} \tag{31}$$

with initial data $u_0(0,x) = \varphi(x) - i\psi(x)$, and $v_0(0,x) = \overline{\varphi(x)} - i\overline{\psi(x)}$.

As u_0, v_0 satisfy (31), we can proceed as above: (30) allows solutions of the form

$$U_1(t,\theta,x) = \exp(i\theta)u_1(t,x), \quad V_1(t,\theta,x) = \exp(i\theta)v_1(t,x),$$

where we can determine u_1 and v_1 by considering the equation arising at order c^{-2}. In the same way the coefficients $U_n,\ V_n,\ n \geq 2$ can be obtained.

In this paper we will only treat the expansion (19) up to its first term at order c^0. Therefore, in the following we set

$$z_0(t,x) = \frac{1}{2}\big(\exp(ic^2t)u_0(t,x) + \exp(-ic^2t)\overline{v_0}(t,x)\big). \tag{32}$$

Then, by the above procedure we know that at least formally the approximation

$$\|z(t,x) - z_0(t,x)\|_s \leq Kc^{-2}$$

holds for sufficiently smooth data. In Section 4 below we will state the precise regularity assumptions and give the ideas of the convergence proof. For a rigorous analysis we refer to [6, 21] and references therein.

Next we repeat the same procedure with equation (22) for the MFE coefficients of $\boldsymbol{\mathcal{A}}$. As $\boldsymbol{\mathcal{A}}$ is a real vector field we look for real coefficients $\boldsymbol{\mathcal{A}}_n,\ n \geq 0$. At order c^2 we find the homogeneous equation

$$(\partial_{\sigma\sigma} - \Delta)\boldsymbol{\mathcal{A}}_0(t,\sigma,x) = 0, \tag{33}$$

which allows solutions of the form

$$\boldsymbol{\mathcal{A}}_0(t,\sigma,x) = \cos(\sigma\sqrt{-\Delta})a_0(t,x) + \sqrt{-\Delta}^{-1}\sin(\sigma\sqrt{-\Delta})b_0(t,x) \tag{34}$$

with some a_0, b_0 that will be determined in the next step.

The equation arising from the comparison of the terms at order c^1 reads

$$(\partial_{\sigma\sigma} - \Delta)\boldsymbol{\mathcal{A}}_1 = -2\partial_\sigma\partial_t\boldsymbol{\mathcal{A}}_0 + \frac{1}{4}\mathcal{P}\left[\mathrm{Re}\left(i(U_0 + \overline{V_0})\nabla(\overline{U_0} + V_0)\right)\right].$$

As the term

$$\partial_\sigma\partial_t\boldsymbol{\mathcal{A}}_0(t,\sigma,x) = -\sin(\sigma\sqrt{-\Delta})\sqrt{-\Delta}\partial_t a_0(t,x) + \cos(\sigma\sqrt{-\Delta})\partial_t b_0(t,x)$$

lies in the kernel of the operator $(\partial_{\sigma\sigma} - \Delta)$ we demand by the same argumentation as before that $\partial_\sigma\partial_t\boldsymbol{\mathcal{A}}_0(t,\sigma,x) = 0$. This in particular implies that $\partial_t a_0(t,x) = 0$ and $\partial_t b_0(t,x) = 0$. Hence $\partial_t\boldsymbol{\mathcal{A}}_0(t,\sigma,x) \equiv 0$ and we find

$$\boldsymbol{\mathcal{A}}_0(t,\sigma,x) = \boldsymbol{\mathcal{A}}_0(\sigma,x) \quad \text{and} \quad a_0(t,x) = a_0(x),\ b_0(t,x) = b_0(x).$$

At $\sigma = 0$ we find $a_0(x) = \boldsymbol{\mathcal{A}}_0(0,x)$ and by differentiation of $\boldsymbol{\mathcal{A}}_0$ with respect to σ we obtain $b_0(x) = \partial_\sigma\boldsymbol{\mathcal{A}}(0,x)$. The data $\boldsymbol{\mathcal{A}}_0(0,x)$ and $\partial_\sigma\boldsymbol{\mathcal{A}}(0,x)$ are again determined via comparison of coefficients: the initial data of $\boldsymbol{\mathcal{A}}$ in (6) are given as

$$\boldsymbol{\mathcal{A}}(0,x) = A(x), \quad \partial_t\boldsymbol{\mathcal{A}}(0,x) = cA'(x),$$

where A, A' do not depend on c. Hence, the formal asymptotic expansion

$$\boldsymbol{\mathcal{A}}(t=0,x) = \boldsymbol{\mathcal{A}}_0(\sigma=0,x) + \sum_{n\geq 1} c^{-n}\boldsymbol{\mathcal{A}}_n(t=0,\sigma=0,x)$$

yields that

$$a_0(x) = \boldsymbol{\mathcal{A}}_0(0,x) = A(x). \tag{35}$$

Since

$$cA'(x) = \partial_t \boldsymbol{\mathcal{A}}(0,x) \simeq (\partial_t + c\partial_\sigma)\mathfrak{A}(0,0,x) = c\partial_\sigma \boldsymbol{\mathcal{A}}_0(0,x) + \sum_{n\geq 1} c^{-n}(\partial_t + c\partial_\sigma)\boldsymbol{\mathcal{A}}_n(0,0,x)$$

we choose

$$b_0(x) = \partial_\sigma \boldsymbol{\mathcal{A}}_0(0,x) = A'(x). \tag{36}$$

Finally by (34),(35) and (36) we obtain the first term of the expansion as

$$\boldsymbol{\mathcal{A}}_0(t,x) = \cos(ct\sqrt{-\Delta})A(x) + (c\sqrt{-\Delta})^{-1}\sin(ct\sqrt{-\Delta})cA'(t,x). \tag{37}$$

We remark that at this point we can explicitly evaluate the first term $\boldsymbol{\mathcal{A}}_0(t,x)$ of the MFE of $\boldsymbol{\mathcal{A}}$ for all $t \in [0,T]$.

Collecting the results in (29), (31) and (37) yields the non-relativistic limit Schrödinger-Poisson system as in [21], i.e.

$$\begin{cases} i\partial_t \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = \frac{1}{2}\Delta \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + \Phi_0 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix}, & \begin{pmatrix} u_0(0) \\ v_0(0) \end{pmatrix} = \begin{pmatrix} \varphi - i\psi \\ \overline{\varphi} - i\overline{\psi} \end{pmatrix}, \\ -\Delta\Phi_0 = -\frac{1}{4}\left(|u_0|^2 - |v_0|^2 \right), & \int_{\mathbb{T}^d} \Phi_0(t,x)dx = 0. \\ \boldsymbol{\mathcal{A}}_0(t,x) = \cos(ct\sqrt{-\Delta})A(x) + (c\sqrt{-\Delta})^{-1}\sin(ct\sqrt{-\Delta})cA'(x). \end{cases} \tag{38}$$

The numerical advantage of the above approximation lies in the fact that compared to the challenging highly-oscillatory MKG system (6), the SP system (38) can be solved very efficiently (for example by applying a Strang splitting method, see [20]), without imposing any CFL type condition on c nor the spatial discretization parameter h. Details will be given in Section 5 below.

4. Error bounds

In the following, let $(u, v, \boldsymbol{\mathcal{A}}, \Phi)$ denote the solution of the first order MKG system (11) and let $(u_0, v_0, \Phi_0, \boldsymbol{\mathcal{A}}_0)$ denote the solution of the corresponding limit system (8) with initial data φ, ψ, A, A', where the limit vector potential $\boldsymbol{\mathcal{A}}_0$ is given by (37).

The following Theorem states rigorous error bounds on the asymptotic approximations z_0, Φ_0 and $\boldsymbol{\mathcal{A}}_0$ towards z, Φ and $\boldsymbol{\mathcal{A}}$, where z_0 is defined in (32). For a detailed analysis and bounds in low regularity spaces we refer to [6, 21]. Here, we will only outline the ideas of the proof.

Theorem 1 (cf. [6, 21]). *Let $s > d/2$ and let $\varphi, \psi \in H^{s+4}, A \in H^{s+1}, A' \in H^s$. Then there exists a $T > 0$ such that for all $t \in [0,T]$ and $c \geq 1$ there holds*

$$\|z(t) - z_0(t)\|_s + \|\Delta(\Phi(t) - \Phi_0(t))\|_s \leq c^{-2}(1 + K_\Phi^T)b(T)\exp(\lambda(T)))$$
$$\|\boldsymbol{\mathcal{A}}(t) - \boldsymbol{\mathcal{A}}_0(t)\|_s \leq c^{-1}(K_{\boldsymbol{\mathcal{A}}.1}^T + TK_{\boldsymbol{\mathcal{A}}.2}^T),$$

where

$$b(t) = M_0^T + tM_1^T + t^2M_2^T, \qquad \lambda(t) = M_3^T + tM_4^T$$

with constants $K_\Phi^T, K_{\boldsymbol{\mathcal{A}}.1}^T, K_{\boldsymbol{\mathcal{A}}.2}^T, M_0^T, \dots, M_4^T$ only depending on $\|\varphi\|_{s+4}$, $\|\psi\|_{s+4}$, $\|A\|_{s+1}$, $\|A'\|_s$ as well as on

$$K = \sup_{\tau\in[0,T]} \left\{\|\boldsymbol{\mathcal{A}}(\tau)\|_s + \|u(\tau)\|_{s+2} + \|v(\tau)\|_{s+2} + \|u_0(\tau)\|_{s+4} + \|v_0(\tau)\|_{s+4}\right\}.$$

We outline the ideas in the proof in several steps. Note that since

$$z(t) = \frac{1}{2}(u(t) + \overline{v}(t)) \quad \text{and} \quad z_0(t) = \frac{1}{2}(\exp(ic^2t)u_0(t) + \exp(-ic^2t)\overline{v_0}(t))$$

the triangle inequality allows us to break down the problem as follows:

$$\|z(t) - z_0(t)\|_s \leq \left\|u(t) - \exp(ic^2t)u_0(t)\right\|_s + \left\|v(t) - \exp(ic^2t)v_0(t)\right\|_s =: \mathcal{R}(t). \tag{39}$$

We start with the following proposition.

Proposition 1 (cf. [21]). *Under the assumptions of Theorem 1 for all $t \in [0,T]$ there holds that*

$$\|\Delta(\Phi(t) - \Phi_0(t))\|_s \leq c^{-2}K_{\Phi.1}^T + K_{\Phi.2}^T\mathcal{R}(t),$$

where $K_{\Phi.1}^T, K_{\Phi.2}^T$ depend on $\sup_{\tau\in[0,T]}\left\{\|u(\tau)\|_{s+2} + \|v(\tau)\|_{s+2} + \|u_0(\tau)\|_s + \|v_0(\tau)\|_s\right\}$.

Proof. The idea of the proof is to write down the representation of $\Delta\Phi$ and $\Delta\Phi_0$ given in (11) and (38). Using the expansion (25) and adding "zeros" in terms of $\exp(ic^2t)u_0(t)$ and $\exp(ic^2t)v_0(t)$ yields the result. □

Proposition 2 (cf. [21]). *Under the assumptions of Theorem 1 for all $t \in [0,T]$ there holds that*

$$\|\boldsymbol{\mathcal{A}}(t) - \boldsymbol{\mathcal{A}}_0(t)\|_s \leq c^{-1}(K_{\boldsymbol{\mathcal{A}}.1}^T + tK_{\boldsymbol{\mathcal{A}}.2}^T) + M^T\int_0^t \mathcal{R}(\tau)d\tau,$$

where M^T depends on $\sup_{\tau\in[0,T]}\left\{\|u(\tau)\|_s + \|v(\tau)\|_s + \|u_0(\tau)\|_{s+1} + \|v_0(\tau)\|_{s+1}\right\}$ and where the dependency of $K_{\boldsymbol{\mathcal{A}}.1}^T, K_{\boldsymbol{\mathcal{A}}.2}^T$ on the solutions is stated in Theorem 1.

Proof. The idea of the proof is to replace $\boldsymbol{\mathcal{A}}(t)$ by its mild formulation given in (13). The difference $\boldsymbol{\mathcal{A}} - \boldsymbol{\mathcal{A}}_0$ then only involves an integral term over the current density $\mathcal{P}\left[\boldsymbol{J}[u,v,\boldsymbol{\mathcal{A}}]\right]$. We introduce the limit current density as $\boldsymbol{J}_0[u_0,v_0](t) = \operatorname{Re}\left(iz_0\nabla\overline{z_0}\right)$. Now adding "zeros" in terms of $\boldsymbol{J}_0[u_0,v_0]$ gives an integral term involving the difference

$$\|\boldsymbol{J}[u,v,\boldsymbol{\mathcal{A}}](\tau) - \boldsymbol{J}_0[u_0,v_0](\tau)\|_s = \mathcal{O}\left(c^{-1}\right) + K\mathcal{R}(\tau)$$

for some constant K not depending on c, and another integral term involving

$$\langle\nabla\rangle_0^{-1}\sin(c\langle\nabla\rangle_0(t-\tau))\mathcal{P}\left[\boldsymbol{J}_0[z_0](\tau)\right].$$

Integration by parts then yields the assertion. □

The above propositions allow us to prove Theorem 1 as follows:

Proof of Theorem 1. Note that both terms in $\mathcal{R}(t)$ (see (39)) can be estimated in exactly the same way. Thus, we only establish a bound on $\left\|u(t) - \exp(ic^2t)u_0(t)\right\|_s$. The main tool thereby is to exploit that the operators $T_c(t) = \exp(ic\left\langle\nabla\right\rangle_c t)$ and $T_0(t) = \exp(-i\frac{1}{2}\Delta t)$ are isometries in H^s. Expanding $\exp(i(-c\left\langle\nabla\right\rangle_c + c^2 - \frac{1}{2}\Delta)t)$ into its Taylor series yields with the aid of (24) that

$$\left\|T_c(t)w - T_0(t)\exp(ic^2t)\tilde{w}\right\|_s \leq \|w - \tilde{w}\|_s + \mathcal{O}\left(c^{-2}t\,\|\tilde{w}\|_{s+4}\right). \tag{40}$$

Note that the mild solutions of (38) read

$$\begin{aligned} u_0(t) &= T_0(t)u_0(0) - i\int_0^t T_0(t-\tau)\Phi_0(\tau)u_0(\tau)d\tau, \\ v_0(t) &= T_0(t)v_0(0) + i\int_0^t T_0(t-\tau)\Phi_0(\tau)v_0(\tau)d\tau. \end{aligned} \tag{41}$$

As $u(0) = u_0(0)$, the mild formulation of u and u_0 given in (13) and (41) together with (40) thus imply that

$$\begin{aligned} \left\|u(t) - \exp(ic^2t)u_0(t)\right\|_s &\leq c^{-2}tK\,\|u_0(0)\|_{s+4} \\ &+ \left\|\int_0^t T_c(t-\tau)\mathcal{N}_u[u,v,\Phi,\boldsymbol{\mathcal{A}}](\tau) + i\exp(ic^2t)T_0(t-\tau)\Phi_0(\tau)u_0(\tau)d\tau\right\|_s, \end{aligned} \tag{42}$$

where $\mathcal{N}_u[u,v,\Phi,\boldsymbol{\mathcal{A}}]$ is defined in (10).

Our aim is now to express the integral term in (42) as a term of type

$$\mathcal{O}\left(c^{-2}\right) + \int_0^t \mathcal{R}(\tau)d\tau,$$

which will allow us to conclude the assertion by Gronwall's lemma. Therefore we consider each term in $\mathcal{N}_u[u,v,\Phi,\boldsymbol{\mathcal{A}}]$ seperately.

By (25) and (26) we find after a short calculation that

$$\|\mathcal{N}_u[u,v,\Phi,\boldsymbol{\mathcal{A}}] + i\Phi u + \left\langle\nabla\right\rangle_c^{-1}\left(\boldsymbol{\mathcal{A}}\cdot\nabla(u+\overline{v})\right)\|_s \leq Kc^{-2},$$

where $K = K(\|\Phi\|_{s+2}, \|u\|_{s+2}, \|v\|_{s+2}, \|\boldsymbol{\mathcal{A}}\|_s)$. Thus, using (40) we can bound the integral term in (42) as follows:

$$\begin{aligned} &\left\|\int_0^t T_c(t-\tau)\mathcal{N}_u[u,v,\Phi,\boldsymbol{\mathcal{A}}](\tau) + i\exp(ic^2t)T_0(t-\tau)\Phi_0(\tau)u_0(\tau)d\tau\right\|_s \\ \leq& Kc^{-2}t\sup_{\tau\in[0,t]}\|\Phi_0(\tau)u_0(\tau)\|_{s+4} + \int_0^t\left\|\Phi(\tau)u(\tau) - \Phi_0(\tau)\exp(ic^2\tau)u_0(\tau)\right\|_s d\tau \\ &+ \left\|\int_0^t T_c(t-\tau)\left\langle\nabla\right\rangle_c^{-1}\Big(\boldsymbol{\mathcal{A}}(\tau)\cdot\nabla(u(\tau)+\overline{v}(\tau)\Big)d\tau\right\|_s. \end{aligned} \tag{43}$$

The latter term can be bounded up to a term of order $\mathcal{O}\left(c^{-2}\right) + \int_0^t\mathcal{R}(\tau)d\tau$ by inserting "zeros" in terms of $\boldsymbol{\mathcal{A}}_0(\tau)$, $\exp(ic^2\tau)u_0(\tau)$ and $\exp(ic^2\tau)v_0(\tau)$ and then applying integration by parts with respect to τ and applying Proposition 2.

Furthermore we can estimate $\left\|\Phi(\tau)u(\tau) - \Phi_0(\tau)\exp(ic^2\tau)u_0(\tau)\right\|_s$ as

$$\left\|\Phi u - \Phi_0 \exp(ic^2\tau)u_0\right\|_s \le C(\|\Phi - \Phi_0\|_s \|u\|_s + \|\Phi_0\|_s \left\|u - \exp(ic^2\tau)u_0\right\|_s)$$

such that by Proposition 1 we find that

$$\left\|\Phi u - \Phi_0 \exp(ic^2\tau)u_0\right\|_s \le c^{-2}C_1 + C_2\mathcal{R}(\tau),$$

where the constants C_1 and C_2 depend on the same data as the constants in the assertion of Proposition 1.

Plugging the above bounds into (42) yields that

$$\mathcal{R}(t) \le c^{-2}(M_0^T + M_1^T t + M_2^T t^2) + (M_3^T + tM_4^T)\int_0^t \mathcal{R}(\tau)d\tau$$

which by Gronwall's Lemma implies the desired bound

$$\mathcal{R}(t) \le c^{-2}b(T)\exp(\lambda(T)), \qquad \forall t \in [0,T]. \tag{44}$$

The results on $\Phi_0(t)$ and $\boldsymbol{\mathcal{A}}_0(t)$ follow the line of argumentation by using (44) in the results of Proposition 1 and Proposition 2. $\square$

5. Construction of numerical schemes

In this section we construct an efficient and robust numerical scheme for the highly-oscillatory MKG equation (6) in the non-relativistic limit regime, i.e. for $c \gg 1$. In order to overcome any c-dependent time step restriction we exploit the limit approximation (38) derived in Section 3.

5.1. The numerical scheme and its error

We consider the MKG equation (6) in the Coulomb gauge in the non-relativistic limit regime $c \gg 1$

$$\begin{cases} \partial_{tt}z = -c^2\langle\nabla\rangle_c^2 z + \Phi^2 z - 2i\Phi\partial_t z - iz\partial_t\Phi - 2ic\boldsymbol{\mathcal{A}}\nabla z - |\boldsymbol{\mathcal{A}}|^2 z, \\ \partial_{tt}\boldsymbol{\mathcal{A}} = c^2\Delta\boldsymbol{\mathcal{A}} + c\mathcal{P}[\boldsymbol{J}], \quad \boldsymbol{J} = \mathrm{Re}\left(iz\overline{\boldsymbol{D}_\alpha z}\right), \\ -\Delta\Phi = \rho, \qquad\qquad \rho = -c^{-1}\,\mathrm{Re}\left(iz\overline{D_0 z}\right), \qquad (45a) \\ z(0,x) = \varphi(x), \quad D_0 z(0,x) = \sqrt{-\Delta + c^2}\psi(x), \\ \boldsymbol{\mathcal{A}}(0,x) = A(x), \quad \partial_t\boldsymbol{\mathcal{A}}(0,x) = cA'(x), \\ \int_{\mathbb{T}^d}\rho(0,x)dx = 0, \quad \int_{\mathbb{T}^d}\Phi(t,x)dx = 0 \qquad (45b) \end{cases}$$

equipped with periodic boundary conditions, i.e. $x \in \mathbb{T}^d = [-\pi,\pi]^d$. In the previous sections we derived the corresponding SP limit system (cf. (38))

$$\begin{cases} i\partial_t\begin{pmatrix}u_0\\v_0\end{pmatrix} = \frac{1}{2}\Delta\begin{pmatrix}u_0\\v_0\end{pmatrix} + \Phi_0\begin{pmatrix}u_0\\-v_0\end{pmatrix}, \quad \begin{pmatrix}u_0(0)\\v_0(0)\end{pmatrix} = \begin{pmatrix}\varphi - i\psi\\ \overline{\varphi} - i\overline{\psi}\end{pmatrix}, \\ -\Delta\Phi_0 = -\frac{1}{4}\left(|u_0|^2 - |v_0|^2\right), \qquad \int_{\mathbb{T}^d}\Phi_0(t,x)dx = 0, \\ \boldsymbol{\mathcal{A}}_0(t,x) = \cos(ct\sqrt{-\Delta})A(x) + (c\sqrt{-\Delta})^{-1}\sin(ct\sqrt{-\Delta})cA'(x) \end{cases} \tag{46}$$

which will now allow us to derive an efficient numerical time integration scheme: Since the SP system (46) does not depend on the large parameter c we can solve it very efficiently; in particular without any c-depending time step restriction. Multiplying the numerical approximations of the non-oscillatory functions u_0 and v_0 with the high frequency terms $\exp(\pm ic^2t)$ then gives a good approximation to the exact solution, see Theorem 2 below for the detailed description. In particular this approach allows us to overcome any c-dependent time step restriction.

Time discretization: We carry out the numerical time integration of the Schrödinger-Poisson system

$$\begin{cases} i\partial_t \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = \frac{1}{2}\Delta \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} + \Phi_0 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix}, & \begin{pmatrix} u_0(0) \\ v_0(0) \end{pmatrix} = \begin{pmatrix} \varphi - i\psi \\ \overline{\varphi} - i\overline{\psi} \end{pmatrix}, \\ -\Delta\Phi_0 = -\frac{1}{4}\left(|u_0|^2 - |v_0|^2\right), & \displaystyle\int_{\mathbb{T}^d} \Phi_0(t,x)dx = 0. \end{cases} \tag{47}$$

with an exponential Strang splitting method (cf. [20]), where we naturally split the system into the kinetic part

$$i\partial_t \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = \frac{1}{2}\Delta \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \tag{T}$$

with the exact flow $\varphi_T^t(u_0(0), v_0(0))$ and the potential part

$$\begin{cases} i\partial_t \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} = \Phi_0 \begin{pmatrix} u_0 \\ -v_0 \end{pmatrix}, \\ -\Delta\Phi_0 = -\frac{1}{4}\left(|u_0|^2 - |v_0|^2\right), \quad \displaystyle\int_{\mathbb{T}^d} \Phi_0(t,x)dx = 0, \end{cases} \tag{P}$$

with the exact flow $\varphi_P^t(u_0(0), v_0(0))$. The Strang splitting approximation to the exact flow $\varphi^t(u_0(0), v_0(0)) = \varphi_{T+P}^t(u_0(0), v_0(0))$ of the SP system (47) at time $t_n = n\tau, n = 0, 1, 2, \ldots$ with time step size τ is then given by

$$\varphi^{t_n}(u_0(0), v_0(0)) \approx \left(\varphi_T^{\tau/2} \circ \varphi_P^{\tau} \circ \varphi_T^{\tau/2}\right)^n (u_0(0), v_0(0)). \tag{48}$$

We can solve the kinetic subproblem (T) in Fourier space exactly in time. In subproblem (P) we can show that the modulus of u_0 and v_0 are constant in time, i.e. $|u_0(t)|^2 = |u_0(0)|^2$ and $|v_0(t)|^2 = |v_0(0)|^2$, and thence also Φ_0 is constant in time, i.e. $\Phi_0(t) = \Phi_0(0)$. Thus, we can also solve the potential subproblem (P) exactly in time.

Space discretization: For the space discretization we choose a Fourier pseudospectral method with N grid points (or frequencies respectively), i.e. we choose a mesh size $h = 2\pi/N$ and grid points $x_j = -\pi + jh$, $j = 0, \ldots, N-1$. We then denote the discretized spatial operators by Δ_h and ∇_h respectively.

Full discretization: The fully discrete numerical scheme can then be implemented efficiently using the Fast Fourier transform (FFT).

This ansatz allows us to state the following convergence result on the approximation of the MKG system (45) in the non-relativistic limit regime:

Theorem 2. *Consider the MKG (45) on the torus $\mathbb{T}^d$. Fix $s_1', s_2', s > d/2$ and let $\varphi, \psi \in H^{s+r_1}(\mathbb{T}^d)$, $A, A' \in H^{s+r_2}(\mathbb{T}^d)$ with $r_1 = \max\{4, s_1'\}$, $r_2 = \max\{2, s_2'\}$. Then* *there exist $T, C, h_0, \tau_0 > 0$ such that the following holds: Let us define the numerical approximation of the the first-order approximation term $z_0(t)$ at time $t_n = n\tau$ through*

$$z_0^{n,h} := \frac{1}{2}\left(u_0^{n,h}\exp(ic^2 t_n) + \overline{v_0}^{n,h}\exp(-ic^2 t_n)\right),$$

where $u_0^{n,h}, v_0^{n,h}$ denote the numerical approximation to the solutions $u_0(t_n), v_0(t_n)$ of the limit system (46) obtained by the Fourier Pseudospectral Strang splitting scheme (48) with mesh size $h \leq h_0$ and time step $\tau \leq \tau_0$. Furthermore let $\Phi_0^{n,h}$ denote the numerical approximation to $\Phi_0(t_n)$ given through the discrete Poisson equation

$$-\Delta_h \Phi_0^{n,h} := -\frac{1}{4}\left(\left|u_0^{n,h}\right|^2 - \left|v_0^{n,h}\right|^2\right). \tag{49}$$

Also let

$$\boldsymbol{\mathcal{A}}_0^{n,h} = \cos\left(ct_n\sqrt{-\Delta_h}\right)A_h + \left(c\sqrt{-\Delta_h}\right)^{-1}\sin\left(ct_n\sqrt{-\Delta_h}\right)cA_h'$$

denote the numerical approximation to $\boldsymbol{\mathcal{A}}_0(t_n)$, where A_h, A_h' are the evaluations of A and A' on the grid points.

Then, the following convergence towards the exact solution of the MKG equation (45) holds for all $t_n \in [0, T]$ and $c \geq 1$:

$$\left\|z(t_n) - z_0^{n,h}\right\|_s + \left\|\Delta\Phi(t_n) - \Delta_h\Phi_0^{n,h}\right\|_s \leq C\left(\tau^2 + h^{s_1'} + c^{-2}\right),$$
$$\left\|\boldsymbol{\mathcal{A}}(t_n) - \boldsymbol{\mathcal{A}}_0^{n,h}\right\|_s \leq C\left(h^{s_2'} + c^{-1}\right).$$

Proof. The proof follows the same ideas as the proof of [14, Theorem 3]. The triangle inequality yields

$$\begin{aligned}
\left\|z(t_n) - z_0^{n,h}\right\|_s &\leq \|z(t_n) - z_0(t_n)\|_s + \left\|z_0(t_n) - z_0^{n,h}\right\|_s, \\
\left\|\Delta\Phi(t_n) - \Delta_h\Phi_0^{n,h}\right\|_s &\leq \|\Delta(\Phi(t_n) - \Phi_0(t_n))\|_s + \left\|\Delta\Phi_0(t_n) - \Delta_h\Phi_0^{n,h}\right\|_s, \\
\left\|\boldsymbol{\mathcal{A}}(t_n) - \boldsymbol{\mathcal{A}}_0^{n,h}\right\|_s &\leq \|\boldsymbol{\mathcal{A}}(t_n) - \boldsymbol{\mathcal{A}}_0(t_n)\|_s + \left\|\boldsymbol{\mathcal{A}}_0(t_n) - \boldsymbol{\mathcal{A}}_0^{n,h}\right\|_s.
\end{aligned} \tag{50}$$

Theorem 1 allows us to bound the first term in each of the inequalities above in order c^{-2} and c^{-1}, respectively. Henceforth, we only need to derive bounds on the numerical errors of the Fourier Pseudospectral Strang splitting scheme approximating the SP system.

Error in $z_0^{n,h}$: Note that

$$\begin{aligned}
\left\|z_0(t_n) - z_0^{n,h}\right\|_s &\leq \left\|\exp(ic^2 t)(u_0(t_n) - u_0^{n,h})\right\|_s + \left\|\exp(-ic^2 t)(\overline{v_0}(t_n) - \overline{v_0}^{n,h})\right\|_s \\
&\leq \left\|u_0(t_n) - u_0^{n,h}\right\|_s + \left\|v_0(t_n) - v_0^{n,h}\right\|_s \\
&\leq C(\tau^2 + h^{s_1'}).
\end{aligned}$$

The latter follows for sufficiently smooth solutions (i.e. if $u_0, v_0 \in H^r$, $r = s + s_1'$) by the convergence bound on the Strang splitting applied to the Schrödinger-Poisson system derived in [20].

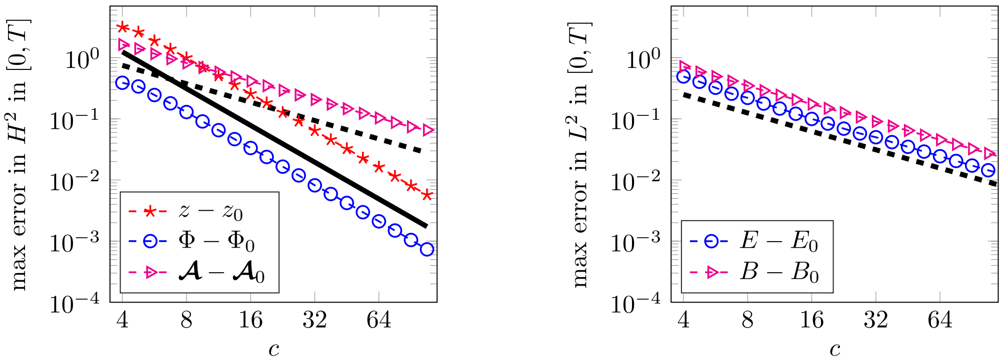

Figure 1: **Left:** H^2 error of the numerical limit approximation $(z_0^{n,h}, \Phi_0^{n,h}, \boldsymbol{\mathcal{A}}_0^{n,h})$ to the exact solution. **Right:** L^2 error of the numerical approximations $E_0^{n,h}, B_0^{n,h}$ to the electromagnetic field. The reference solution $(z, \Phi, \boldsymbol{\mathcal{A}})$ was computed with a Gautschi-type exponential integrator with time step size $\tau = 2^{-22} \approx 10^{-7}$. The black dashed line with slope -1 and the black solid line with slope -2 represent the order $\mathcal{O}\left(c^{-1}\right)$ and $\mathcal{O}\left(c^{-2}\right)$ respectively.

Error in $\Phi_0^{n,h}$***:*** By (46) and (49) we obtain that

$$\left\|\Delta\Phi_0(t_n) - \Delta_h \Phi_0^{n,h}\right\|_s \leq M(\left\|u_0(t_n) - u_0^{n,h}\right\|_s + \left\|v_0(t_n) - v_0^{n,h}\right\|_s) \leq C(\tau^2 + h^{s_1'}).$$

Error in $\boldsymbol{\mathcal{A}}_0^{n,h}$***:*** As $\boldsymbol{\mathcal{A}}_0$ is explicitly given in time we do not have any time discretization error. Only the error by the Fourier pseudospectral method comes into play which yields that

$$\left\|\boldsymbol{\mathcal{A}}_0(t_n) - \boldsymbol{\mathcal{A}}_0^{n,h}\right\|_s \leq C h^{s_2'},$$

if the exact solution is smooth enough, i.e. if $\boldsymbol{\mathcal{A}}_0 \in H^{\tilde{r}}$, $\tilde{r} = s + s_2'$.

Collecting the results yields the assertion. $\square$

5.2. Numerical results

In this section we numerically underline the sharpness of the theoretical results derived in the previous sections.

For the MKG equation (45) on the two-dimensional torus, i.e. $d = 2$, $(x, y)^T \in \mathbb{T}^2 = [-\pi, \pi]^2$, we choose the initial data φ, ψ, A, A' as

$$\begin{aligned}
\tilde{\varphi}(x, y) &= \sin(y) + \cos(x) + i(\cos(2x) + \sin(y)), & \varphi &= \tilde{\varphi} / \left\|\tilde{\varphi}\right\|_{L^2}, \\
\tilde{\psi}(x, y) &= \cos(x) + \sin(2y) + i\cos(2x)\sin(y), & \psi &= \tilde{\psi} / \left\|\tilde{\varphi}\right\|_{L^2}, \\
\tilde{A}(x, y) &= \left(\partial_y V_1(x, y), -\partial_x V_1(x, y)\right)^T, & A &= \tilde{A} / \left\|\tilde{A}\right\|_{L^2}, \\
\tilde{A}'(x, y) &= c\left(\partial_y V_2(x, y), -\partial_x V_2(x, y)\right)^T, & A' &= \tilde{A}' / \left\|\tilde{A}\right\|_{L^2},
\end{aligned}$$

where

$$V_1(x, y) = \sin(x)\cos(y) + \sin(2y) + \cos(x), \qquad V_2(x, y) = \sin(y) + \cos(2x).$$

It is easy to check that $\operatorname{div} A = 0$ and $\operatorname{div} A' = 0$. Furthermore the initial data satisfy Remark 1, i.e. $\int_{\mathbb{T}^d} \rho(0,x)dx = 0$, where $\rho(0) = -\operatorname{Re}\left(i\varphi \left\langle \nabla \right\rangle_c \overline{\psi}\right)$. We simulate the limit solution on the time interval $t \in [0, T = 1]$ with a time step size $\tau = 2^{-10} \approx 10^{-3}$, and a spatial grid with $N = 128$ grid points in both dimensions and measure the maximal error of the limit approximation $(z_0, \Phi_0, \boldsymbol{\mathcal{A}}_0)$ on the time interval $[0, T]$ in the H^2 norm. A reference solution of the MKG equation (45) is obtained with an adapted Gautschi-type exponential integrator, as proposed in [16] for highly-oscillatory ODEs or in [3] for the nonlinear Klein-Gordon equation. Thereby a very small time step size τ_{ref} satisfying the CFL condition $\tau_{\text{ref}} \leq c^{-2}h$ is necessary. Fig. 1 verifies the theoretical convergence bounds stated in Theorem 2. We furthermore observe numerically that also the electric field $E_0^{n,h} := -c^{-1}\partial_t \boldsymbol{\mathcal{A}}_0^{n,h} - \nabla_h \Phi_0^{n,h}$ and the magnetic field $B_0^{n,h} := \nabla_h \times \boldsymbol{\mathcal{A}}_0^{n,h}$ show a c^{-1} convergence towards $E = -c^{-1}\partial_t \boldsymbol{\mathcal{A}} - \nabla\Phi$ and $B = \nabla \times \boldsymbol{\mathcal{A}}$ in L^2, respectively.

6. Conclusion

In order to derive an efficient and accurate numerical method for solving the MKG equation in the non-relativistic limit regime $c \gg 1$ we followed the idea of a formal asymptotic expansion of the exact solution $(z, \Phi, \boldsymbol{\mathcal{A}})$ in terms of c^{-2} and c^{-1}, respectively. This allowed us to reduce the numerical effort of solving the highly-oscillatory MKG system under severe time step restrictions $\tau = \mathcal{O}(c^{-2})$ to solving the corresponding non-oscillatory Schrödinger-Poisson (SP) limit system. The latter can be carried out very efficiently and in particular independently of the large parameter c. We obtained a numerical approximation $(u_0^{n,h}, v_0^{n,h}, \Phi_0^{n,h})$ to the solution (u_0, v_0, Φ_0) of the SP system at time $t_n = n\tau$ by solving the SP system via an exponential Strang splitting method with time step τ in time together with a Fourier pseudospectral method for the space discretization on a grid with mesh size h. In particular τ and h do not depend on the large parameter c. The numerical approximations $z_0^{n,h}, \Phi_0^{n,h}, \boldsymbol{\mathcal{A}}_0^{n,h}$ then satisfy error bounds of order $\mathcal{O}(c^{-2} + \tau^2 + h^{s'})$ and $\mathcal{O}(c^{-1} + h^{s'})$ respectively. We underlined the sharpness of the error bound with numerical experiments. For practical implementation issues we assumed periodic boundary conditions. Up to minor changes all the results of this paper remain valid for Dirichlet boundary conditions and different spatial discretization schemes.

Acknowledgement

We gratefully acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG) through CRC 1173. We furthermore thank Dirk Hundertmark and Claire Scheid for fruitful discussions on this topic.

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