ARTICLE IN PRESS

Journal of Computational and Applied Mathematics ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

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

Patrick Krämer *, Katharina Schratz

Karlsruhe Institute of Technology, Faculty of Mathematics, Englerstr. 2, 76131 Karlsruhe, Germany

ARTICLE INFO

Article history:
Received 3 December 2015

Keywords:
Maxwell–Klein–Gordon
Time integration
Highly-oscillatory
Wave equation
Non-relativistic limit

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.

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. [1–3]), i.e.

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

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

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. [4]), i.e. under the constraint $\operatorname{div} \mathcal{A} \equiv 0$, we obtain a KG equation coupled to the electromagnetic

* Corresponding author.
E-mail addresses: patrick.kraemer3@kit.edu (P. Krämer), katharina.schratz@kit.edu (K. Schratz).

http://dx.doi.org/10.1016/j.cam.2016.07.007

field as

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

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

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

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

Setting

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

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 $\operatorname{div}\mathcal{A}(t,x) \equiv 0$ yields the so-called *Maxwell–Klein–Gordon* equation in the Coulomb gauge

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

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 $\operatorname{div}\mathcal{A}(t,x) \equiv 0$ we assume that the initial data A, A' for $\mathcal{A}$ 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 [5].

Assumption 1. The initial data φ, ψ, A, A' are 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 $(z,\Phi,\mathcal{A}) \mapsto (z',\Phi',\mathcal{A}')$, where for a suitable choice of $\chi = \chi(t,x)$ we set

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

i.e. if $(z,\Phi,\mathcal{A})$ solves the MKG system (6) then also does $(z',\Phi',\mathcal{A}')$ without modification of the system (cf. [4,2,3,6]). 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 [4,7,1–3,6] 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 [8–11]. 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. [9]).

Please cite this article in press as: P. Krämer, K. Schratz, Efficient time integration of the Maxwell–Klein–Gordon equation in the non-relativistic limit regime, Journal of Computational and Applied Mathematics (2016), http://dx.doi.org/10.1016/j.cam.2016.07.007