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# Solving the Maxwell-Klein-Gordon equation in the Lattice Gauge Theory formalism

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**Abstract**

In this article we study the discretization of the Maxwell-Klein-Gordon equation from a variational point of view. We first solve the problem with an action corresponding to the Yee scheme for the Maxwell part, which is automatically gauge invariant, and a gauge invariant action for the Klein-Gordon part given by the Lattice Gauge Theory. The action is showed to be consistent with the continuous formulation, and the equations to be solved are derived from a discrete stationary action principle.

Due to the gauge invariance, the local electric charge can be shown to be conserved through Noether's theorem. As this is an essential feature of the continuous model, this conservation can be viewed as the great achievement of this scheme.

Thereafter we compare the above described scheme with a scheme that uses a standard finite difference approximation of the derivatives, and where the coupling between the scalar field and the gauge field is done in the simplest way. This scheme will posess a global gauge symmetry which ensures the conservation of global charge as in the hybrid case, but the scheme has no local symmetry and no locally conserved charge.

At last we present some numerical results in the temporal gauge, shedding light on the theoretical discussion.

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# 1 Introduction

The Standard model of physics describes the fundamental particles and the forces of nature, except gravity. It is a theory described by a Lagrangian formulation, and the fundamental quantities are described by fields. A key property of the theory is that the Lagrangian is invariant under so called continuous local gauge transformations, i.e. rotations in the phase space where the fundamental fields live. The gauge symmetry can be viewed as an analogue to the equivalence principle of general relativity in which each point in spacetime is allowed a choice of local reference (coordinate) frame. Symmetries are regarded as a very important feature of almost every physical theory, and continuous symmetries give rise to conserved quantities through Noether's theorem. The continuous local gauge transformations will for instance lead to a conserved charge, and maybe the most common example is the U(1)-symmetry which ensures the conservation of electric charge.

The Lagrangian in the Standard model gives rise to the evolution equations of the gauge fields, called the Yang-Mills equations (actually the name Yang-Mills is most often used in the context of gauge group SU(2) or SU(3), a generalization of the U(1) case). In physics the primary aim is not to find classical solutions to these equations, but rather to quantize the theory (hence the name quantum mechanics) with the Lagrangian as the starting point, and from there on calculate correlation functions and cross sections in order to describe how the particles and fields in the theory behave. This is done via the (ill-defined) path integral formalism, "integration over every possible path", which especially in Quantum ElectroDynamics (QED), the U(1)$\times$SU(2) part of the Standard model, yields extremely sucessfull perturbation calculations.

In the SU(3) part of the Standard model (Quantum ChromoDynamics, or QCD), the description of the nuclear force, perturbation calculations are more troublesome, and even if it works on some occasions, it breaks down especially in the high energy regime. This fact motivated Kenneth Wilson to develop Lattice Gauge Theory (LGT)[1]. In the continuum formulation, ultraviolet divergences occur, i.e. divergences at high energy/small distances. To remove these divergences Wilson wanted to construct the theory on a space-time lattice, which effectively introduces a cut off, i.e. a smallest length determined by the lattice constant. Since the continuous local gauge symmetry is fundamental in the theory, Wilson wanted the discrete theory to also possess this property, and in an ingenious way he developed what is now called Lattice Gauge Theory. This theory abides the gauge symmetry and is also consistent with the continuum formulation. *P.t.* this is the only theory that gives non-perturbative results in QCD, and calculations using LGT give both asymptotic freedom and confinement[1, 2, 3, 4]. The theory is therefore regarded as a great success.

This gave us the motivation to use this theory in the field of numerical analysis to find classical solutions of the fields. We started out with the simplest gauge group, the U(1) group, which corresponds to pure electromagnetism, and compared the results with the classical Yee-scheme[5]. One peculiar fact in this case is that LGT with gauge group U(1) gives you a set of non-linear equations to solve, while Maxwell's equations describing the electromagnetic field are linear. However, numerical experiments indicate a good agreement between the LGT-scheme and the Yee-scheme.

General Relativity can be viewed as a gauge theory, with the Poincare group as gauge group, and should have wave-like solutions. One would like a geometric discretization of these nonlinear equations. This is exactly what LGT provides for the Yang-Mills equations, so this is an attempt towards creating a good numerical scheme for GR. In view of that, some of the purpose of this article is to bring LGT to the attention of numerical analysts, and as such the paper is partly expository.

In this article we expand the earlier work to also include a complex scalar field, implying that the equations to be solved are the Maxwell-Klein-Gordon equations. Since it may seem a bit too much to use the Lattice Gauge Theory formalism on the Maxwell part of the action, which in any case is gauge invariant, we will instead study a hybrid scheme, consisting of the 2. order Yee action for the Maxwell part and the LGT-action for the Klein-Gordon part. The scheme we then end up with is locally gauge invariant. Because of this symmetry we can use a discrete version of Noether's theorem to extract the conserved quantity. As in the continuous case, we get a locally conserved charge consistent with Maxwell's equations. The conservation of the local charge implies of course the conservation of a global charge as well.

We will also compare this hybrid scheme with a more standard finite difference scheme for solving the Maxwell-Klein-Gordon-equations. This scheme uses the 2. order Yee action for the Maxwell part of the action, as the hybrid scheme does, and a finite difference approximation of the derivatives in the KG action. This scheme does not possess a local U(1) symmetry, hence Noether's theorem can not be used to deduce a locally conserved charge. However, the scheme is invariant with respect to global U(1) transformations, implying a globally conserved charge.

The paper is organized as follows: In §2 we introduce the continuous Maxwell-Klein-Gordon equation from a variational point of view and prove constraint preservation. In §3 we discretize the MKG-action using an LGT inspired action for the Klein-Gordon part and a Yee-action for the Maxwell part, and we show that the resulting discrete action is indeed gauge invariant. In §4 a numerical scheme which uses standard finite difference discretization is discussed. This scheme does not possess the local gauge symmetry, so it does not preserve the constraint. In §5 a discussion of the energy of the schemes is included. Finally in §6 we present some numerical results.

## 2 The continuum equations

The domain we are looking at is $\Sigma = \mathbb{R} \times \mathbb{R}^3$ with coordinates $x = (t, \mathbf{x})$ ($\mathbb{R}^3$, which describes the spatial domain, can in general be interchanged with a Riemannian manifold). The unknowns in the theory are a gauge potential $x \mapsto A_0(x)\mathrm{d}t + \mathbf{A}(x) = A_\mu(x)$, where $A_0$ is a real-valued function and $\mathbf{A}$ is a real-valued one-form, and a complex scalar function $x \mapsto \phi(x)$. Actually, in physics one considers $\phi$ and $\phi^*$ to be independent degrees of freedom, with $\phi$ describing the particle (a boson) and $\phi^*$ its anti-particle. This is equivalent to consider two real fields $\phi_1$ and $\phi_2$ with equal mass, and write $\phi = 1/\sqrt{2}(\phi_1 + i\phi_2)$. However, considering only $\phi$ as an independent degree of freedom provides all information necessary, and this is the point of view we choose here. The action is given by [6, 7] (we are using the Minkowski space-time metric $\eta_{\mu\nu}$ =diag$(-1, 1, 1, 1)$ to raise and lower indices)

$$S[A, \phi] = -\int \mathrm{d}t\mathrm{d}^3x(\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + (D_\mu\phi)(D^\mu\phi)^* + m^2|\phi|^2) = \int \mathrm{d}t\mathrm{d}^3x\mathcal{L}, \tag{1}$$

where Einstein's summation convention is assumed, $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the field strenght and $D_\mu = \partial_\mu - iqA_\mu$ is the covariant derivative where $q$ is the coupling constant between the scalar field and the gauge field. In the limit $q = 0$ we are left with free field theory. We observe that the action is invariant under local transformations of the type

$$\begin{aligned} \phi(x) &\mapsto e^{i\lambda(x)}\phi(x) \\ A_\mu(x) &\mapsto A_\mu(x) + \frac{1}{q}\partial_\mu\lambda(x). \end{aligned} \tag{2}$$

where $i\lambda(x) \in i\mathbb{R}$ is in the Lie-algebra $\mathfrak{u}(1)$ of U(1), so that $e^{i\lambda(x)} \in U(1)$. $A_\mu$ transforms in the adjoint representation of the Lie-algebra.

Introducing the notation $\partial_\mu\psi := \psi_{,\mu} := \frac{\partial\psi}{\partial x^\mu}$, the Euler-Lagrange-equations are given by

$$\partial_\mu \left( \frac{\partial \mathcal{L}}{\partial \psi_\mu} \right) - \frac{\partial \mathcal{L}}{\partial \psi} = 0, \tag{3}$$

for each independent field $\psi$. The independent fields in the Maxwell-Klein-Gordon case are $\phi$ and $A_\mu$, and we get the following partial differential equations

$\underline{\phi}$:

$$\left( D_\mu D^\mu - m^2 \right) \phi = 0, \tag{4}$$

$\underline{A^\mu}$:

$$\partial_\nu F^{\mu\nu} + qJ^\mu = 0, \tag{5}$$

where $J^\mu = i(\phi^* D^\mu \phi - \phi D^{*\mu} \phi^*)$. We also have the Bianchi identity for the field strengt $F^{\mu\nu}$

$$\partial^\lambda F^{\mu\nu} + \partial^\mu F^{\nu\lambda} + \partial^\nu F^{\lambda\mu} = 0, \tag{6}$$

which is satisfied automatically by construction of $F$ from $A$. The above equations, (4)-(6), comprise the complete set of the Maxwell-Klein-Gordon-equations.

Equation (5) can further be divided into two types of equations, one considered as a constraint (no time derivative), i.e. choosing $\mu = 0$ (the temporal component of $A_\mu$) we get

$$\partial_i F^{0i} + qJ^0 = 0, \tag{7}$$

which is, upon defining the electric field as $E^i = F^{0i}$, nothing but the Maxwell equation with source

$$\mathrm{div}\mathbf{E} + qJ^0 = 0. \tag{8}$$

The other type is an evolution equation, i.e. choosing $\mu = j$ we get

$$\partial_0 F^{j0} + \partial_i F^{ji} + qJ^j = 0. \tag{9}$$

Defining the magnetic field as $B_i = \frac{1}{2}\epsilon_{ijk} F^{jk}$, where $\epsilon_{ijk}$ is the antisymmetric Levi-Civita tensor with $\epsilon_{123} = 1$, the above equation is the evolution equation for the electric field

$$\mathrm{curl}\mathbf{B} = \frac{\partial \mathbf{E}}{\partial t} - q\mathbf{J}, \tag{10}$$

where $\mathbf{J} = (J^x, J^y, J^z)$. The Bianchi identity provides the evolution of the magnetic field and a similar constraint as (7), $\mathrm{div}\mathbf{B} = 0$.

An important result regarding the constraint equation, eq. (7), is

**Proposition 1** *Suppose ($\phi, A_\mu$) solves the equations (4, 9) on a time interval [0,T]. Suppose furthermore that the constraint* (7) *is satisfied at $t = 0$. Then the constraint* (7) *is satisfied for all $t \in [0, T]$.*

-*Proof:* Observe first that upon differentiating (9) (a summation over $j$ is assumed)

$$\partial_j \partial_0 F^{j0} + \partial_j \partial_i F^{ji} + q\partial_j J^j = \partial_j \partial_0 F^{j0} + q\partial_j J^j = 0. \tag{11}$$

Furthermore, differentiating eq. (7) with respect to $t$ gives

$$\partial_0 (\partial_i F^{0i} + qJ^0) = -\partial_i \partial_0 F^{i0} + q\partial_0 J^0, \tag{12}$$

which combined with (11) gives

$$\partial_0(\partial_i F^{0i} + qJ^0) = q(\partial_0 J^0 + \partial_i J^i) = q\partial_\mu J^\mu. \tag{13}$$

Since ($\phi$) satisfies (4), we have that

$$\partial_\mu J^\mu = i(\phi^* D_\mu D^\mu \phi - \phi D^*_\mu D^{*\mu}\phi^*) = 0. \tag{14}$$

■

The result above can be seen as a direct consequence of the local gauge invariance. The connection can be made explicit through Noether's theorem, which states that to every continuous symmetry there exists a conserved charge.

### 2.1 Noether's theorem and constraint preservation

Since the Lagrangian is invariant under gauge transformations, given by eq. 2, it is possible to reduce the number of Euler-Lagrange equations by choosing a particular gauge. Physical observables are of course independent of this choice of gauge, so doing this will not alter the physics, it will only simplify the equations to be solved. In other words, physical initial and boundary values determine ($\phi, A$) only up to gauge transformations.

By choosing for instance the temporal gauge, $A_0 = 0$, the Euler-Lagrange equations are reduced to the evolution equation for the electric field, eq. 9. The constraint equation, eq. 7, has in effect been eliminated, i.e. is no longer an Euler-Lagrange equation since variation of $A_0$ is excluded. The temporal gauge is an incomplete gauge, meaning that there is a remaining gauge symmetry in the system, i.e. the reduced Lagrangian with $A_0 = 0$ is still invariant under the gauge transformations, eq. 2, with $\lambda$ a constant in time. Due to this remaining symmetry, Noether's theorem [8, 9, 10] states that the following current is conserved

$$K^\mu = i\lambda\left(\phi^* D^\mu\phi - \phi(D^\mu\phi)^*\right) + \frac{1}{q}F^{i\mu}\partial_i\lambda, \tag{15}$$

i.e. $\partial_\mu K^\mu = 0$, and from the conservative nature of the above quantity, one can give an alternative proof of proposition 1.

**Proposition 2** *Given the Lagrangian from equation 1 in temporal gauge, and suppose that ($\phi, \mathbf{A}$) solves the equations (4, 9) on a time interval [0,T]. Suppose furthermore that the constraint* (7) *is satisfied at $t = 0$. Then the constraint* (7) *is satisfied for all $t \in [0, T]$.*

-*Proof* (By Noether's theorem) Define the charge

$$Q = \int \mathrm{d}^3x K^0. \tag{16}$$

From Noether's theorem, $Q$ is conserved since

$$\partial_0 Q = \int \mathrm{d}^3x \partial_0 K^0 = -\int \mathrm{d}^3x \partial_i K^i = 0 \tag{17}$$

(where we have assumed as always that the fields diminish fast enough when $|x| \to \infty$). From the definition of $K$, we get that

$$Q = \int \mathrm{d}^3x\lambda\left[i\left(\phi^*\partial^0\phi - \phi\partial^0\phi^*\right) - \frac{1}{q}\partial_i F^{i0}\right], \tag{18}$$

and since this should be valid for any choice of $\lambda$ we can conclude that

$$\left[i\left(\phi^*\partial^0\phi-\phi\partial^0\phi^*\right)-\frac{1}{q}\partial_i F^{i0}\right]=\frac{1}{q}\mathrm{div}\mathbf{E}+J^0 \tag{19}$$

is conserved.

■

The same procedure of reducing the Euler-Lagrange equations by choosing the temporal gauge, and then using the remaining symmetry and Noether's theorem to show that the constraint is conserved can be found in [11, 12]

If $\lambda$ is a constant, which is the case when only a global U(1) symmetry is present, the conserved charge is given by

$$Q=\int \mathrm{d}^3x\, i\left(\phi^*\partial^0\phi-\phi\partial^0\phi^*\right). \tag{20}$$

This is the quantity that physicist usually call the total charge of the system.

# 3 Lattice Gauge Theory

We are now going to develop the gauge invariant lattice action for the Maxwell-Klein-Gordon case[1, 13, 14, 15, 16, 2]. One starts out with the continuum action for the complex Klein-Gordon field which reads

$$S[\phi]=-\int \mathrm{d}t\mathrm{d}^3x\,(\partial_\mu\phi)(\partial^\mu\phi^*)+m^2\phi\phi^*=\int \mathrm{d}t\mathrm{d}^3x\mathcal{L}(\phi). \tag{21}$$

We then define this action on a space-time lattice with lattice points $n=(n_t,\mathbf{n})=(n_t,n_x,n_y,n_z)$, convert the integral to a summation and approximate the derivative by $\partial_\mu\phi(x)\approx\frac{1}{a_\mu}(\phi(n+a_\mu)-\phi(n))$, where $a_\mu$ is the lattice spacing in the direction $\mathbf{e}_\mu$. We also write out the summation in the action, $(\partial_\mu\phi)(\partial^\mu\phi^*)=-\partial_t\phi\partial_t\phi^*+\nabla\phi\cdot\nabla\phi^*$ (we use the Minkowski space-time metric $\eta_{\mu\nu}=$diag$(-1,1,1,1)$). The discrete action can therefore be written as

$$S[\phi]=\sum_n\left[h(a)\left|\frac{1}{a_t}(\phi(n+a_t)-\phi(n))\right|^2-\left|\frac{1}{a_i}(\phi(n+a_i)-\phi(n))\right|^2-m^2|\phi(n)|^2\right] \tag{22}$$

where $h(a)=a_ta_xa_ya_z$, and a summation over $i$ is assumed. We now want to impose a continuous local U(1) gauge invariance, i.e. we want the theory to be invariant under the set of transformations

$$\phi(n)\mapsto G(n)\phi(n) \tag{23}$$

where $G(n)=e^{i\lambda(n)}$, $\lambda(n)\in\mathbb{R}$. We clearly see that the above action (22) does not satisfy this, due to non-local terms. Hence we have to modify the action, and we do this by inspiration from the Wilson line.

## 3.1 The Wilson line and loop

In the continuous theory terms that are non-local need to be modified in order to be gauge invariant[7]. The way this is done is by using the transformation property of the Wilson line defined by

$$U(x,y)=e^{iq\int_P A_\alpha(z)\mathrm{d}z^\alpha}, \tag{24}$$

where $P$ is a path between $x$ and $y$. We see that under a local U(1) gauge transformation, where the gauge field transforms in the adjoint representation of the Lie-algebra, i.e. $A_\mu(x) \to A_\mu(x) + \frac{1}{q}\partial_\mu \lambda(x)$, the Wilson line transforms as

$$U(x,y) \mapsto G^{-1}(x)U(x,y)G(y), \qquad G(x) = e^{i\lambda(x)}. \tag{25}$$

This means that expressions like $\phi(x)U(x,y)\phi^*(y)$ will transform as $\phi(x)G(x)G^{-1}(x)U(x,y)G(y)G^{-1}(y)\phi^*(y) = \phi(x)U(x,y)\phi^*(y)$, meaning that they are gauge invariant.

If $x = y$, the path $P$ is a closed loop, $U(x,x)$ is called the Wilson loop, and we see that it transforms as $U(x,x) \mapsto U(x,x)$, so it is gauge invariant.

The above considerations suggest that to arrive at a gauge invariant expression for the Klein-Gordon action on the lattice, we should make the following substitutions in (22)

$$|\phi(n+a_\mu) - \phi(n)| \longmapsto |\phi(n+a_\mu) - U_{n;n+a_\mu}\phi(n)| \tag{26}$$

where $U_{n+a_\mu;n} = U^\dagger_{n;n+a_\mu}$, and $U_{n;n+a_\mu}$ is an element of the U(1) gauge group. Hence it can be written as

$$U_{n;n+a_\mu} = e^{i\psi_\mu(n+\frac{1}{2}a_\mu)}, \tag{27}$$

where $\psi_\mu(n+\frac{1}{2}a_\mu)$ is in the compact domain $[0,2\pi]$. The right hand side of (26) is now invariant under the following set of local transformations

$$\begin{aligned} \phi(n) &\mapsto G(n)\phi(n) \\ U_{n;n+a_\mu} &\mapsto G^{-1}(n)U_{n;n+a_\mu}G(n+a_\mu), \qquad G(n) = e^{i\lambda(n)} \end{aligned} \tag{28}$$

As we see, the group elements $U_{n;n+a_\mu}$ live on the links connecting two neighbouring lattice sites, hence they are often called link variables.

Let us write $\psi_\mu(n+\frac{1}{2}a_\mu) = qa_\mu A_\mu(n+\frac{1}{2}a_\mu)$. This means that $A_0$ is defined at $(n+\frac{1}{2}a_t) = (\mathbf{n}, t+\frac{1}{2}a_t)$, and the spatial part $A_i$ at $(n+\frac{1}{2}a_i) = (\mathbf{n}+\frac{1}{2}a_i, t)$. If we now make the substitution

$$U_{n;n+a_\mu} \to 1 + iqa_\mu A_\mu(n+\frac{1}{2}a_\mu), \tag{29}$$

we see that (22) with the substitution from (26) reduces to a possible discretization of (1) minus the kinetic term of the gauge potential $A_\mu$. Because of this connection between $U_{n,n+a_\mu}$ and $A_\mu(n+\frac{1}{2}a_\mu)$ we write from here on

$$U_\mu(n) \equiv U_{n;n+a_\mu} = e^{iqa_\mu A_\mu(n+\frac{1}{2}a_\mu)}. \tag{30}$$

With this identification it is an easy matter to verify that $U_\mu(n)$ transforms as follows under gauge transformations

$$U_\mu(n) \mapsto G^{-1}(n)U_\mu(n)G(n+a_\mu) = e^{iqa_\mu A^G_\mu(n+\frac{1}{2}a_\mu)}, \tag{31}$$

where $A^G_\mu(n+\frac{1}{2}a_\mu)$ is the discretized version of $A_\mu(x+\frac{1}{2}a_\mu) + \frac{1}{q}\partial_\mu\lambda(x)$. Hence, a gauge invariant action for the complex scalar field can be expressed as

$$\begin{aligned} S_{\text{LGT}}[\phi, A] = h(a)\sum_n \Bigg[ &\left|\frac{1}{a_t}\left(\phi(n+a_t) - e^{iqa_t A_0(n+\frac{1}{2}a_t)}\phi(n)\right)\right|^2 - \\ &\left|\frac{1}{a_i}\left(\phi(n+a_i) - e^{iqa_i A_i(n+\frac{1}{2}a_i)}\phi(n)\right)\right|^2 - m^2|\phi(n)|^2\Bigg]. \end{aligned} \tag{32}$$

To complete the construction of the Maxwell-Klein-Gordon action we need to construct a gauge invariant action for the gauge potential $A_\mu$. One possibility is to use the action from LGT, which is motivated from the fact that the Wilson loop is gauge invariant. We are not going to use this action, and the main reason is that while Maxwell's equations in vacuum are linear, the Maxwell-action from LGT gives a nonlinear evolution equation for the electric field. Instead we will use the gauge invariant 2. order Yee action described in the next section.

### 3.2 A 2. order Yee-type action

In this section a 2. order Yee-type action for the gauge potential will be developed [17, 18]. This action will be motivated by the classical Yee-scheme [5].

Maxwell's equations in vacuum are formulated through a gauge potential $A_\mu = (A_0, \mathbf{A})$ as

$$\begin{aligned} \partial_0^2 \mathbf{A} - \Delta \mathbf{A} + \nabla(\nabla \cdot \mathbf{A}) - \nabla \partial_0 A_0 = 0, &\qquad -\partial_0 F_{i0} + \partial_j F_{ij} = 0 \\ -\Delta A_0 + \partial_0 \nabla \cdot \mathbf{A} = 0, &\qquad \partial_i F_{0i} = 0, \end{aligned} \tag{33}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the field strength, and with the identification

$$\mathbf{E} = \nabla A_0 - \partial_0 \mathbf{A}, \qquad \mathbf{B} = \nabla \times \mathbf{A}. \tag{34}$$

From the above equation we see that in the discretized version:

- $\mathbf{E}$ and $\mathbf{A}$ should have the same spatial dependence.
- $\mathbf{E}$ and $A_0$ should have the same temporal dependence.
- $\mathbf{B}$ and $\mathbf{A}$ should have the same temporal dependence.

Comparing with the classical Yee-scheme, (33) should be discretized as

$$\begin{aligned} -\frac{1}{a_t}\bar{\delta}_t F_{i0}(n) + \frac{1}{a_j}\bar{\delta}_j F_{ij}(n) = 0, &\qquad \frac{1}{a_i}\bar{\delta}_i F_{0i}(n) = 0, \\ F_{\mu\nu}(n) = \frac{1}{a_\mu}\delta_\mu A_\nu(n + \frac{1}{2}a_\nu) - \frac{1}{a_\nu}\delta_\nu A_\mu(n + \frac{1}{2}a_\mu), & \end{aligned} \tag{35}$$

where we have introduced forward and backward difference operators $\bar{\delta}_i f(n) = f(n) - f(n - a_i)$ and $\delta_i f(n) = f(n + a_i) - f(n)$. Observe that the field strength also satisfies a discrete Bianchi identity

$$\frac{1}{a_\lambda}\delta_\lambda F_{\mu\nu}(n) + \frac{1}{a_\mu}\delta_\mu F_{\nu\lambda}(n) + \frac{1}{a_\nu}\delta_\nu F_{\lambda\mu}(n) = 0. \tag{36}$$

The action corresponding to (35) is

$$S_{\text{Yee}}[A] = -\sum_n h(a)\left(\frac{1}{4}F_{\mu\nu}(n)F^{\mu\nu}(n)\right), \tag{37}$$

where $h(a) = a_x a_y a_z a_t$ and summations over repeated indices are assumed. In this article we are going to use this action in combination with the Klein-Gordon action (32), i.e.

$$S_{\text{MKG}}[\phi, A] = S_{\text{LGT}}[\phi, A] + S_{\text{Yee}}[A]. \tag{38}$$

It is easy to verify that this action is locally gauge invariant, i.e. invariant under the following set of transformations

$$
\begin{aligned}
\phi(n) &\mapsto \phi(n)e^{i\lambda(n)} \\
A_\mu(n+\frac{1}{2}a_\mu) &\mapsto A_\mu(n+\frac{1}{2}a_\mu)+\frac{1}{q}\frac{1}{a_\mu}\left(\lambda(n+a_\mu)-\lambda(n)\right).
\end{aligned}
\tag{39}
$$

We also want to make sure that the action we are using is consistent with the continuous action in some sence. That is, making sure that we approximate the right equations. We define consistency through the action as follows[19]

**Definition 1** *Let $S[u]$ be an action describing a set of fields u on a space domain $\Omega$. We say that a discrete action $S_h[\cdot]$, defined on a discretization $\mathcal{T}_h$ of $\Omega$ with lattice spacing $h$, is consistent with $S[\cdot]$ if for any smooth enough u*

$$
\underset{u'\in X_h}{sup}\,\frac{|DS[u]u'-DS_h[\pi_h u]u'|}{||u'||}\underset{h\to 0}{\longrightarrow}0
\tag{40}
$$

*where $\pi_h u$ is some given projection of $u$ on the lattice, and $X_h$ is the element space where we seek solutions. $||\cdot||$ is the natural norm for $S$.*

The appropriate element spaces in the MKG-case are ($\mathcal{T}_h$ is a mesh made of equal cubes $K\in\mathcal{T}_h$ of equal side $h$)

$$
\begin{cases}
U_h=\{\phi_h\in U=H^1(\Omega)\,|\,\forall K\in\mathcal{T}_h,\ \phi_h|_K\in\mathcal{Q}_{1,1,1}\}\\
V_h=\{\mathbf{A}_h\in H(\text{curl},\Omega)\,|\,\forall K\in\mathcal{T}_h,\ \mathbf{A}_h|_K\in\mathcal{Q}_{0,1,1}\times\mathcal{Q}_{1,0,1}\times\mathcal{Q}_{1,1,0}\},
\end{cases}
\tag{41}
$$

where we recall that by definition $\mathcal{Q}_{i_1,i_2,i_3}$ is the set of polynomials of three variables whose degree with respect to the k'th variable is less than or equal to $i_k$. Concerning our MKG-action, the scalar field is projected down on the lattice points (standard nodal interpolation) while the gauge potential is projected as an integral of the tangential component along each edge, i.e.

$$
(\pi_h\phi)(n)=\phi(n)\quad(\pi_h A_i)(n+\frac{1}{2}a_i)=\frac{1}{a_i}\int_n^{n+a_i}A_i(y)dy.
\tag{42}
$$

These projections correspond to the interpolations used in Finite Element theory [18]. With these projections we get

**Theorem 1** *If $(\phi,\mathbf{A})$ defined on $\Omega$ is smooth enough, and $\Omega$ is a bounded domain in $\mathbb{R}^3$ (alternatively, $(\phi,\mathbf{A})$ has compact support in $\mathbb{R}^3$), and if we use the projections from equation 42, then the action from equation 38 is consistent with the continuous MKG-action, equation 1.*

*-Proof:* The differential of the space part of the continuous and discrete action in direction $u'=(\phi',\mathbf{A}')$ are given by ($u=(\phi,\mathbf{A})$, and for simplicity we assume a uniform lattice with periodic boundary conditions and $|a_i|=h\,\forall i$)

$$
\begin{aligned}
DS[u]u'=-\int_\Omega d^3x\Big\{&D_i\phi' D_i^*\phi^*+D_i\phi D_i^*\phi^{*'}+m^2(\phi'\phi^*+\phi\phi^{*'})+\\
&\frac{1}{2}F_{ij}F_{ij}'+iqA_i'(\phi^*D_i\phi-\phi D_i^*\phi^*)\Big\}
\end{aligned}
\tag{43}
$$

$$DS_h[\pi_h u]u' = -\sum_n h^3 \Big\{ \tilde{D}_i\phi(n)^{'} \tilde{D}_i^*\phi(n)^* + \tilde{D}_i\phi(n)\tilde{D}_i^*\phi(n)^{*'} + m^2(\phi(n)^{'}\phi(n)^* + \phi(n)\phi(n)^{*'}) +$$
$$\frac{1}{2}\tilde{F}_{ij}(n)\tilde{F}_{ij}(n)^{'} + iq\Big(\frac{1}{a_i}\int_n^{n+a_i} A_i(y)^{'}dy\Big)(e^{-iq\int_n^{n+a_i}A_i(y)dy}\phi(n)^*\tilde{D}_i\phi(n) - e^{iq\int_n^{n+a_i}A_i(y)dy}\phi(n)\tilde{D}_i^*\phi(n)^*) \Big\} \tag{44}$$

where we have defined

$$\begin{aligned} \tilde{D}_i\phi(n) &= \frac{1}{a_i}\delta_i\phi(n) + \phi(n)\frac{1}{a_i}(1 - e^{iq\int_n^{n+a_i}A_i(y)dy}) \\ \tilde{F}_{ij}(n) &= \frac{1}{a_i}\delta_i\int_n^{n+a_j} A_j(y)dy - \frac{1}{a_j}\delta_j\int_n^{n+a_i} A_i(y)dy. \end{aligned} \tag{45}$$

We observe that due to the definition of the element spaces

$$\frac{1}{a_i}\int_n^{n+a_i} A_i(y)^{'}dy = A_i(n+\frac{1}{2}a_i)^{'}, \quad \frac{1}{a_j}\delta_j A_i(n+\frac{1}{2}a_i)^{'} = \partial_j A_i(n+\frac{1}{2}a_i)^{'} \quad \frac{1}{a_i}\delta_i\phi(n)^{'} = \partial_i\phi(n)^{'}. \tag{46}$$

In addition, because our numerical quadrature scheme is exact for $\mathcal{Q}_{1,1,1}$ the Bramble-Hilbert lemma gives us the estimate[19]

$$|\int_\Omega fv - \sum_n h^3 fv| \leq Ch||f||_{H^{5/2}}|v|_{L^2}, \tag{47}$$

for $v$ of finite element type and $f \in H^{5/2}$. $C$ is a constant independent of $h$. Furthermore since $(\phi, \mathbf{A})$ is assumed smooth enough, we can write

$$\begin{aligned} \tilde{F}_{ij}(n) &= \frac{1}{a_i}\delta_i\int_n^{n+a_j} A_j(y)dy - \frac{1}{a_j}\delta_j\int_n^{n+a_i} A_i(y)dy = F_{ij}(n) + \mathcal{O}(h) \\ e^{-iq\int_n^{n+a_i}A_i(y)dy}\tilde{D}_i\phi(n) &= D_i\phi(n) + \mathcal{O}(h) \\ \tilde{D}_i\phi(n)' &= D_i\phi(n)' + Ch\phi(n)', \end{aligned} \tag{48}$$

where $C$ depends on $A$ but not on $\phi'$.

Now, with $u' = (\phi^{'}, \mathbf{A}' = 0)$

$$\begin{aligned} |DS[u]u' - DS[\pi_h u]u'| \leq \\ &|\int_\Omega d^3x D_i\phi^{'} D_i^*\phi^* - \sum_n h^3 D_i\phi^{'} D_i^*\phi^*| + \\ &|\int_\Omega d^3x D_i\phi D_i^*\phi^{*'} - \sum_n h^3 D_i\phi D_i^*\phi^{*'}| + \\ &|\int_\Omega d^3x m^2(\phi^{'}\phi^* + \phi\phi^{*'}) - m^2\sum_n h^3(\phi^{'}\phi^* + \phi\phi^{*'})| + Ch(|D_i\phi^{'}|_{L^2} + |\phi^{'}|_{L^2}) \\ &\leq Ch(||D_i\phi||_{H^{5/2}} + ||\phi||_{H^{5/2}} + 2)||\phi^{'}||_{H^1}, \end{aligned} \tag{49}$$

and by choosing $u' = (\phi' = 0, \mathbf{A}')$

$$
\begin{aligned}
|DS[u]u' - DS[\pi_h u]u'| \leq \\
& |\int_\Omega d^3x iqA_i'(\phi^* D_i\phi - \phi D_i^*\phi^*) - \sum_n h^3 iqA_i'(\phi^* D_i\phi - \phi D_i^*\phi^*)| + \\
& |\int_\Omega d^3x \frac{1}{2} F_{ij}F_{ij}' - \sum_n h^3 \frac{1}{2} F_{ij}F_{ij}'| + Ch(|A'|_{L^2} + |F'|_{L^2}) \\
& \leq Ch(||\phi^* D_i\phi - \phi D_i^*\phi^*||_{H^{5/2}} + ||F||_{H^{5/2}} + 2)||A'||_{H(curl)}.
\end{aligned} \tag{50}
$$

Equations (49) and (50) imply the desired result.

■

This is not the only way of defining consistency, and one could equally well define it through the finite difference equations approximating the partial differential equations. However, consistency as we have defined it, implies that the finite difference equations to be derived are an approximation of the continuous equations.

### 3.3 The discretized equations

Next we are going to use (38) to find the discrete E-L equations, i.e. we are going to vary the action with respect to the independent fields and demand the variation to be extremal. Variation with respect to the scalar field gives the generalized discrete wave equation

$\underline{\phi :}$

$$
\begin{aligned}
& \frac{1}{a_t^2}\Big(\phi(n+a_t)e^{-iqa_tA_0(n+\frac{1}{2}a_t)} + \phi(n-a_t)e^{iqa_tA_0(n-\frac{1}{2}a_t)} - 2\phi(n)\Big) - \\
& \frac{1}{a_i^2}\Big(\phi(n+a_i)e^{-iqa_iA_i(n+\frac{1}{2}a_i)} + \phi(n-a_i)e^{iqa_iA_i(n-\frac{1}{2}a_i)} - 2\phi(n)\Big) + m^2\phi(n) = 0,
\end{aligned} \tag{51}
$$

where a summation over $i$ is understood.

Variation with respect to $A_0$ gives the constraint equation

$\underline{A_0 :}$

$$
\sum_i \frac{1}{a_i}\bar{\delta}_i F_{0i}(n)) + q\frac{1}{a_t} i\Big(\phi(n+a_t)\phi^*(n)e^{-iqa_tA_0(n+\frac{1}{2}a_t)} - \phi(n)\phi^*(n+a_t)e^{iqa_tA_0(n+\frac{1}{2}a_t)}\Big) = 0, \tag{52}
$$

which is the equivalent of (7).

Finally, variation with respect to $A_i$ gives the evolution equation

$\underline{A_i :}$

$$
\begin{aligned}
& \frac{1}{a_t}\bar{\delta}_t F_{0i}(n) - \sum_j \frac{1}{a_j}\bar{\delta}_j F_{ji}(n) + \\
& \qquad q\frac{1}{a_i} i\left(\phi(n+a_i)\phi^*(n)e^{-iqa_iA_i(n+\frac{1}{2}a_i)} - \phi(n)\phi^*(n+a_i)e^{iqa_iA_i(n+\frac{1}{2}a_i)}\right) = 0,
\end{aligned} \tag{53}
$$

which is the equivalent of (9). Equations (51), (52), (53) and the discrete version of the Bianchi identity comprise the discrete version of the Maxwell-Klein-Gordon equations.

An important result is the following (the equivalent of proposition 1)

**Proposition 3** *Suppose ($\phi, A_\mu$) solves the equations (51, 53) on a time interval [0,T] at the lattice points. Suppose furthermore that the constraint* (52) *is satisfied at $t=0$. Then the constraint* (52) *is satisfied for all $n_t \in [0,T]$ at the lattice points.*

*-Proof:* Define

$$C_\mu(n) = qa_\mu A_\mu(n), \tag{54}$$

$$J_0(n) = i\frac{1}{a_t}\Bigg(\phi(n+a_t)e^{-iC_0(n+\frac{1}{2}a_t)}\phi^*(n) - \phi(n)e^{iC_0(n+\frac{1}{2}a_t)}\phi^*(n+a_t)\Bigg), \tag{55}$$

$$J_i(n) = i\frac{1}{a_i}\Bigg(\phi(n)e^{iC_i(n+\frac{1}{2}a_i)}\phi^*(n+a_i) - \phi(n+a_i)e^{-iC_i(n+\frac{1}{2}a_i)}\phi^*(n)\Bigg), \tag{56}$$

and

$$D(n) = \sum_i \frac{1}{a_i}\bar{\delta}_i F_{0i}(n) + qJ_0(n). \tag{57}$$

We see that (52) is equivalent to $D(n) = 0$. We then calculate the discrete backward time derivative of (57) with the use of (53)

$$\begin{aligned}
\frac{1}{a_t}\bar{\delta}_t D(n) &= \sum_i \frac{1}{a_t a_i}\bar{\delta}_t\bar{\delta}_i F_{0i}(n) + q\frac{1}{a_t}\bar{\delta}_t J_0(n) \\
&= \sum_i \frac{1}{a_i}\bar{\delta}_i\big(\sum_j \frac{1}{a_j}\bar{\delta}_j F_{ji}(n) + qJ_i(n)\big) + q\frac{1}{a_t}\bar{\delta}_t J_0(n) \\
&= q\sum_i \frac{1}{a_i}\bar{\delta}_i J_i(n) + q\frac{1}{a_t}\bar{\delta}_t J_0(n) \quad , \qquad F_{ij} = -F_{ji}.
\end{aligned} \tag{58}$$

Since we have assumed that (51) is satisfied, we have (multiply (51) with $\phi^*(n)$)

$$\begin{aligned}
\frac{1}{a_t}\bar{\delta}_t J_0(n) &= i\frac{1}{a_t^2}\Bigg(\phi(n+a_t)e^{-iC_0(n+\frac{1}{2}a_t)}\phi^*(n) - \phi(n)e^{iC_0(n+\frac{1}{2}a_t)}\phi^*(n+a_t) - \\
&\qquad \phi(n)e^{-iC_0(n-\frac{1}{2}a_t)}\phi^*(n-a_t) + \phi(n-a_t)e^{iC_0(n-\frac{1}{2}a_t)}\phi^*(n)\Bigg) \\
&= i\sum_i\Bigg[\frac{1}{a_i^2}\Big(\phi(n+a_i)e^{-iC_i(n+\frac{1}{2}a_i)}\phi^*(n) - \phi(n)e^{iC_i(n+\frac{1}{2}a_i)}\phi^*(n+a_i)\Big) - \\
&\qquad \frac{1}{a_i^2}\Big(\phi(n)e^{-iC_i(n-\frac{1}{2}a_i)}\phi^*(n-a_i) - \phi(n-a_i)e^{iC_i(n-\frac{1}{2}a_i)}\phi^*(n)\Big)\Bigg] \\
&= -\sum_i \frac{1}{a_i}\bar{\delta}_i J_i(n),
\end{aligned} \tag{59}$$

implying that

$$\frac{1}{a_t}\bar{\delta}_t D(n) = 0. \tag{60}$$

■

Again this can be seen as a consequence of the local gauge invariance, and we will, as in the continuous case, show this connection through Noether's theorem.

### 3.4 Noether's theorem and constraint preservation on the lattice

The discrete Lagrangian, eq. 38, is U(1) gauge invariant, and by choosing the temporal gauge, $A_0 = 0$, the discrete Euler-Lagrange equations are reduced in the same manner as in the continuous case, meaning that the constraint equation has been eliminated. Again, this is an incomplete gauge, and due to the remaining symmetry, i.e. transformations with $\lambda$ a constant of time in eq. 39, a discrete version of Noether's theorem [20] provides the following divergence free current

$$
\begin{aligned}
K_0 &= i\lambda(n)\frac{1}{a_t}\Big(\phi(n)\phi^*(n+a_t) - \phi(n+a_t)\phi^*(n)\Big) + \frac{1}{q}F_{0k}(n)\frac{1}{a_k}\delta_k\lambda(n) \\
K_i &= i\lambda(n+a_i)\frac{1}{a_i}\Big(\phi(n+a_i)e^{-iqa_iA_i(n+\frac{1}{2}a_i)}\phi^*(n) - \phi(n)e^{iqa_iA_i(n+\frac{1}{2}a_i)}\phi^*(n+a_i)\Big) + \\
&\quad + \frac{1}{q}F_{ki}(n)\frac{1}{a_k}\delta_k\lambda(n+a_i),
\end{aligned}
\tag{61}
$$

i.e. $\frac{1}{a_t}\bar{\delta}_0 K_0 + \frac{1}{a_i}\bar{\delta}_i K_i = 0$.

This conserved current can be used to give an alternative proof of proposition 3.

**Proposition 4** *Given the Lagrangian from equation 38 in temporal gauge, and suppose that ($\phi, \mathbf{A}$) solves the equations (51, 53) at the lattice points on a time interval [0,T]. Suppose furthermore that the constraint* (52) *is satisfied at $t = 0$. Then the constraint* (52) *is satisfied at the lattice points for all $n_t \in [0, T]$.*

-*Proof*(By Noether's theorem) The proof has the same structure as in the continuous case. We start out by defining the charge

$$
Q = a_{x_i}^3 \sum_{\mathbf{n}} K_0, \tag{62}
$$

which is conserved due to Noether's theorem and the fact that we consider a lattice with periodic boundary conditions;

$$
\frac{1}{a_t}\bar{\delta}_0 Q = a_{x_i}^3 \sum_{\mathbf{n}} \frac{1}{a_t}\bar{\delta}_0 K_0 = -a_{x_i}^3 \sum_{\mathbf{n},i} \frac{1}{a_i}\bar{\delta}_i K_i = 0. \tag{63}
$$

From the definition of K and a partial integration on the lattice, the charge can be rewritten as

$$
Q = a_{x_i}^3 \sum_{\mathbf{n}} \lambda(n)\left[i\frac{1}{a_t}\Big(\phi(n)\phi^*(n+a_t) - \phi(n+a_t)\phi^*(n)\Big) - \frac{1}{q}\frac{1}{a_k}\bar{\delta}_k F_{0k}(n)\right], \tag{64}
$$

and since this should be valid for any choice of $\lambda$ we can conclude that the constraint, (52), is conserved.

■

If $\lambda$ is a constant, the conserved charge is given by

$$
Q = a_{x_i}^3 \sum_{\mathbf{n}} i\frac{1}{a_t}\Big(\phi(n)\phi^*(n+a_t) - \phi(n+a_t)\phi^*(n)\Big), \tag{65}
$$

and this is again the quantity that physicist call the total charge of the system. We will see later on that this charge is also conserved for the standard scheme, as can be seen from the global U(1) invariance.

# 4 Standard finite difference discretization

In this section we are going to present the more standard scheme for dealing with the Maxwell-Klein-Gordon-equations, which we will compare with our hybrid scheme. The standard scheme consists of the 2. order Yee action for the Maxwell part, as for the hybrid scheme, and a standard finite difference discretization of the Klein-Gordon part.

To find the discrete action for the Klein-Gordon part, we start out with the continuous action

$$S_{\text{KG}}[\phi, A] = -\int \mathrm{d}t\mathrm{d}^3x \left((D_\mu\phi)(D^\mu\phi)^* + m^2|\phi|^2\right) = \int \mathrm{d}t\mathrm{d}^3x \left(|D_0\phi|^2 - |D_i\phi|^2 - m^2|\phi|^2\right). \tag{66}$$

This action is then defined on a space-time lattice. The integral is converted to a summation and the derivatives are approximated by $\delta_\mu\phi(x) \approx \frac{1}{a_\mu}(\phi(n+a_\mu) - \phi(n))$, where $a_\mu$ is the lattice spacing in the direction $\mathbf{e}_\mu$. The fields are of course defined at the same points as for the hybrid scheme. The discrete Klein-Gordon action is therefore given by

$$\begin{aligned} S_{\text{KG}}[\phi, A] = h(a)\sum_n \Bigg[ &\left|\frac{1}{a_t}\Big(\phi(n+a_t) - \phi(n)\Big) - iqA_0(n+\frac{1}{2}a_t)\phi(n)\right|^2 - \\ &- \left|\frac{1}{a_i}\Big(\phi(n+a_i) - \phi(n)\Big) - iqA_i(n+\frac{1}{2}a_i)\phi(n)\right|^2 - m^2|\phi(n)|^2\Bigg]. \end{aligned} \tag{67}$$

Hence, the total action is

$$S_{\text{MKG}}[\phi, A] = S_{\text{KG}}[\phi, A] + S_{\text{Yee}}[A], \tag{68}$$

where $S_{\text{Yee}}[A]$ is given by equation (37). It is an easy matter to verify that

**Theorem 2** *If $(\phi, \mathbf{A})$ defined on $\Omega$ is smooth enough, and $\Omega$ is a bounded domain in $\mathbb{R}^3$ (alternatively, $(\phi, \mathbf{A})$ has compact support in $\mathbb{R}^3$), and if we use the projections from equation 42, then the action from equation 68 is consistent with the continuous MKG-action, equation 1.*

## 4.1 The discretized equations

This action, equation 68, implies the following discrete Euler-Lagrange equations:

$\underline{\phi:}$

$$\begin{aligned} &\frac{1}{a_t^2}\bar{\delta}_t\delta_t\phi(n) - \frac{1}{a_i^2}\bar{\delta}_i\delta_i\phi(n) - iqA_0(n+\frac{1}{2}a_t)\frac{1}{a_t}\delta_t\phi(n) - \\ &iq\frac{1}{a_t}\left(\phi(n)\bar{\delta}_tA_0(n+\frac{1}{2}a_t) + A_0(n)\bar{\delta}_t\phi(n)\right) - \\ &q^2A_0^2(n+\frac{1}{2}a_t)\phi(n) + iqA_i(n+\frac{1}{2}a_i)\frac{1}{a_i}\delta_i\phi(n) + \\ &iq\frac{1}{a_i}\left(\phi(n)\bar{\delta}_iA_i(n+\frac{1}{2}a_i) + A_i(n-\frac{1}{2}a_i)\bar{\delta}_i\phi(n)\right) + \\ &q^2A_i^2(n+\frac{1}{2}a_i)\phi(n) + m^2\phi(n) = 0 \end{aligned} \tag{69}$$

$\underline{A_0:}$

$$\sum_i \frac{1}{a_i}\bar{\delta}_iF_{0i}(n) + iq\frac{1}{a_t}\Big(\phi^*(n)\delta_t\phi(n) - \phi(n)\delta_t\phi^*(n)\Big) + 2q^2A_0(n+\frac{1}{2}a_t)|\phi(n)|^2 = 0. \tag{70}$$

$\underline{A_i :}$

$$\frac{1}{a_t}\bar{\delta}_t F_{0i}(n) - \sum_j \frac{1}{a_j}\bar{\delta}_j F_{ji}(n) + iq\frac{1}{a_i}\left(\phi^*(n)\delta_i\phi(n) - \phi(n)\delta_i\phi^*(n)\right) + \\ + 2q^2 A_i(n+\frac{1}{2}a_i)|\phi(n)|^2 = 0. \tag{71}$$

The important difference between this scheme and the hybrid scheme is concerning the constraint, eq. (52) and eq. (70). For the hybrid scheme we showed that the constraint is preserved, both through a direct calculation, proposition 3, and through Noether's theorem, proposition 4. The more standard scheme, presented in this section, does not possess this property, as can be related to the lack of a continuous local gauge symmetry.

**Proposition 5** *The constraint, equation* (70), *is not conserved for the standard scheme.*

*-Proof:* Define

$$D(n) = \sum_i \frac{1}{a_i}\bar{\delta}_i F_{0i}(n)) + iq\frac{1}{a_t}\left(\phi^*(n)\delta_t\phi(n) - \phi(n)\delta_t\phi^*(n)\right) + 2q^2 A_0(n+\frac{1}{2}a_t)|\phi(n)|^2. \tag{72}$$

A direct calculation shows that

$$\begin{aligned} &\frac{1}{a_t}\bar{\delta}_t D(n) = q^2\left(-a_t I_t + a_i I_i\right) \neq 0 \\ &I_t = \frac{1}{a_t}\bar{\delta}_t\Big\{A_0(n+\frac{1}{2}a_t)\frac{1}{a_t}\left(\phi^*(n)\delta_t\phi(n) + \phi(n)\delta_t\phi^*(n)\right)\Big\} \\ &I_i = \frac{1}{a_i}\bar{\delta}_i\Big\{A_i(n+\frac{1}{2}a_i)\frac{1}{a_i}\left(\phi^*(n)\delta_i\phi(n) + \phi(n)\delta_i\phi^*(n)\right)\Big\} \end{aligned} \tag{73}$$

■

Although this scheme is lacking a continuous local gauge symmetry, it admits global U(1) transformations, which implies a conserved global charge. This can be seen directly from Noether's theorem with $\lambda$ equal a constant in equation (39). With $\lambda$ a constant, Noether's theorem predicts the following divergence free current

$$\begin{aligned} K_0 &= i\Bigg[\frac{1}{a_t}\Big(\phi(n)\phi^*(n+a_t) - \phi(n+a_t)\phi^*(n)\Big) + \\ &\qquad iqA_0(n+\frac{1}{2}a_t)(\phi(n+a_t)\phi^*(n) + \phi(n)\phi^*(n+a_t))\Bigg] \\ K_i &= i\Bigg[\frac{1}{a_i}\Big(\phi(n+a_i)\phi^*(n) - \phi(n)\phi^*(n+a_i)\Big) - \\ &\qquad iqA_i(n+\frac{1}{2}a_i)(\phi(n+a_i)\phi^*(n) + \phi(n)\phi^*(n+a_i))\Bigg]. \end{aligned} \tag{74}$$

In the same way as in the continuous theory and for the hybrid scheme, this conserved current leads to a conserved global charge given by

$$Q = a_{x_i}^3 \sum_{\mathbf{n}} K_0. \tag{75}$$

This means that although the local charge may fluctuate, the total charge in the system is a constant of motion, meaning that there is no dissipation of charge from the system.

## 5 Energy

Results concerning the energy of the system are of course of interest. In the continuous case the energy is conserved, as a direct consequence of Noether's theorem and the fact that the system admits continuous time translation symmetry and a continuous gauge symmetry, i.e. $t \mapsto t + s\ s \geq 0$ and $A_\mu \mapsto A_\mu + \frac{1}{q}\partial_\mu A_0$. The conserved energy in the Maxwell-Klein-Gordon case is

$$H = \int \mathrm{dx}\, \mathcal{H} = \int \mathrm{dx}\ \left( \frac{1}{2}F_{0i}^2 + \frac{1}{4}F_{ij}^2 + (D_0\phi)(D_0\phi)^* + (D_i\phi)(D_i\phi)^* + m^2\phi\phi^* \right). \tag{76}$$

On the lattice we don't have a continuous time translation symmetry, and for that reason one cannot use Noether's theorem to find a conserved energy. In spite of this, we have for both the hybrid scheme and the standard scheme calculated a discrete energy. The energy which we calculated for the hybrid scheme was found in a similar manner as the discrete Lagrangian was found. I.e. we discretized the Hamiltonian for a complex scalar field, and then made it gauge invariant through the link variables $U_\mu$. In addition we added the Maxwell energy from the Yee-scheme, which in the free Maxwell theory actually is conserved. Concerning the standard scheme, we just discretized the continuous Hamiltonian, and used that for the energy.

Both of these energies are not conserved as can be seen from a direct calculation, but both their values and their fluctuations are comparable. It should also be said that in continuous time the energies are conserved.

## 6 Numerical results

We have implemented both of these schemes in the temporal gauge, $A_0 = 0$, on a space-time lattice with periodic boundary conditions in space. One may be tempted to ask wether a gauge condition can be introduced for the standard scheme since it isn't gauge invariant, but since the starting point of our calculations concerning the standard scheme is the continuous equations, a discretization with an imposed gauge condition can be justified. The reason for this choice of gauge is that the Finite Difference Equations we need to solve are considerably simplified. For instance, one does not have to think about the time evolution of $A_0$ which is somewhat problematic, because there isn't an evolution equation for $A_0$. If another gauge is chosen, the evolution of $A_0$ has to be calculated either through the gauge condition, or through the constraint equation. We see that this is problematic for the standard scheme, since the constraint is not conserved.

For both the schemes the vector potential, $\mathbf{A}$, and the complex scalar field, $\phi$, were initialized as plane waves with the right periodicity. We used a lattice restricted to the spatial domain $[0,1] \times [0,1] \times [0,1]$ and solved the equations in the time domain $t \in [0,1]$. $N = 30$ lattice points in the spatial directions and $N_t = 100$ lattice points in the temporal direction were used

The quantities we calculated were

- The local charge, i.e. the constraint equation div$\mathbf{E}$ + q$J^0$, equations (52) and (70) as a function of both space and time and the $\mathrm{L}^2$-norm of the same quantity. For comparison we also calculated the $\mathrm{L}^2$-norm of the divergence of the electric field, $\|\mathrm{div}\mathbf{E}\|_{\mathrm{L}^2}$.

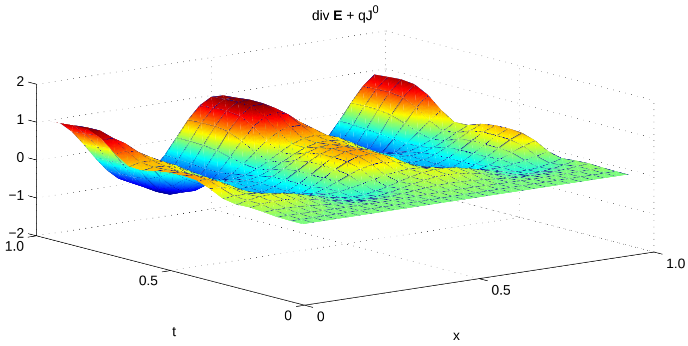


Figure 1: div$\mathbf{E} + qJ^0$ for the standard MKG-scheme.

- The global charge, equations (65) and (75).
- The discrete energy of the system.

The constraint equation is shown in Fig. (1) and (2) at constant $y$ and $z$, while the L$^2$-norm of the same quantity is depicted in Fig. (3) and (4). The L$^2$-norm of the constraint together with the L$^2$-norm of the divergence of the electric field are shown in Fig. (5) and (6). The global charge is shown in Fig. (7) and (8). Last, but not least the energy as function of time is shown in Fig. (9) and (10).

We observe that the constraint is preserved for the hybrid scheme as predicted, Fig. (2) (the fluctuations are due to numerical errors). As we see, this is not the case for the standard scheme Fig. (1), and the deviation from zero is actually quite large.

Concerning the L$^2$-norm of the constraint, we again see from Fig. (4) that it is conserved for the hybrid scheme while it is becoming substantially different from zero for the standard scheme, Fig. (3). Comparing Fig. (5) and (6) we see that the L$^2$-norm of the divergence of the electric field is comparable for the two schemes.

From Fig. (7) and (8) we see that the total charge is conserved for both schemes, as predicted by the theory. The value is also equal for the two schemes, since they have the same initial condition.

The energy of the two schemes is also comparable, and as wee see from Fig. (9) and (10) it fluctuates with the same period and amplitude. However, the fluctuations are in the order of 10%, hence our approximation of the energy is certainly not the optimal one. On the other hand, the similarity indicates that the schemes are correctly implemented.

The conservation of the divergence of the magnetic field div$\mathbf{B} = 0$, which also can be viewed as a constraint is ommited because it is satisfied by the construction of the field strenght $F_{\mu\nu}$.

# 7 Conclusion

We have in this article examined two possible discretizations of the Maxwell-Klein-Gordon equations. First we looked at a hybrid scheme, based on a 2. order Yee-type action for the Maxwell part, which is gauge invariant, and a gauge invariant action for the Klein-Gordon part, inspired by Lattice Gauge Theory. Symmetries will give rise to conserved quantities through Noether's theorem, and we showed that the local electric charge, i.e. the constraint equation, is conserved for this scheme as a consequence of the local gauge invariance.

We carried on by investigating a more standard scheme for this type of equations. This ”standard” scheme uses a standard finite difference approximation of the derivatives, and for that reason it does

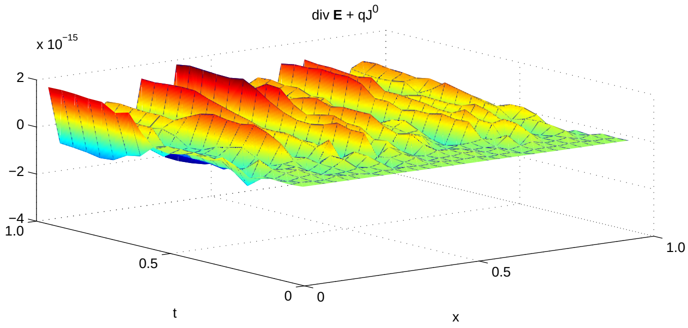


Figure 2: div$\mathbf{E} + qJ^0$ for the hybrid MKG-scheme. Note the scale on the z-axis which indicates that div$\mathbf{E} + qJ^0 = 0$. The fluctuations are due to numerical errors.

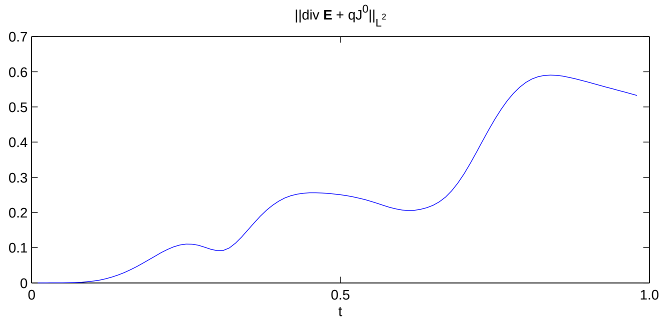


Figure 3: $\|\text{div}\mathbf{E} + qJ^0\|_{L^2}$ as a function of time for the standard MKG-scheme.

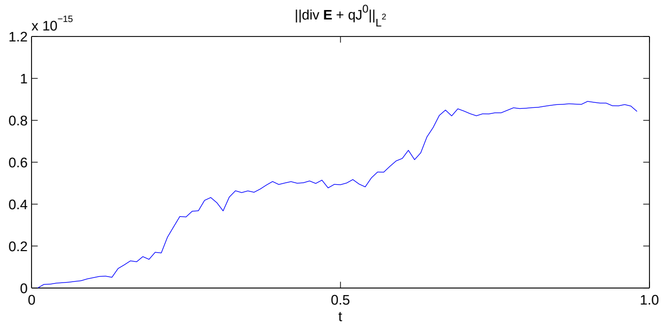


Figure 4: $\|\text{div}\mathbf{E} + qJ^0\|_{L^2}$ as a function of time for the hybrid MKG-scheme. Again, note the scale on the y-axis

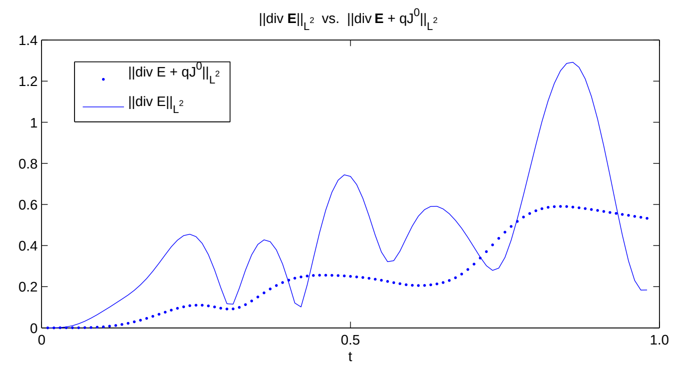


Figure 5: $\|\mathrm{div}\mathbf{E} + qJ^0\|_{L^2}$ and $\|\mathrm{div}\mathbf{E}\|_{L^2}$ as a function of time for the standard MKG-scheme.

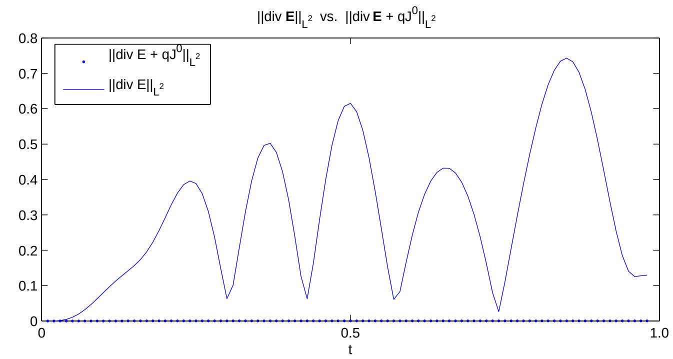


Figure 6: $\|\mathrm{div}\mathbf{E} + qJ^0\|_{L^2}$ and $\|\mathrm{div}\mathbf{E}\|_{L^2}$ as a function of time for the hybrid MKG-scheme.

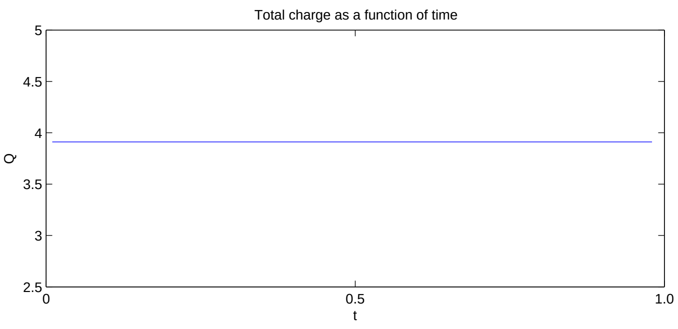


Figure 7: The total charge $Q$ as a function of time for the standard MKG-scheme.

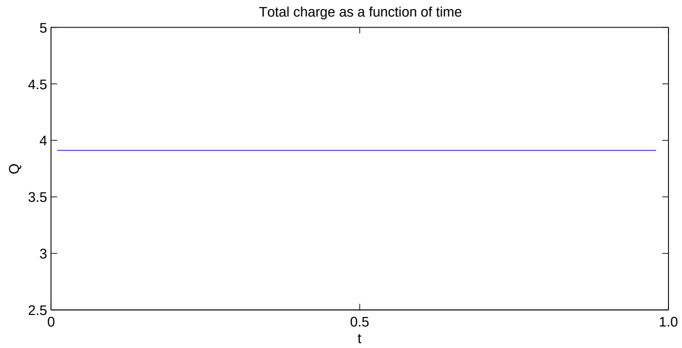


Figure 8: The total charge $Q$ as a function of time for the hybrid MKG-scheme.

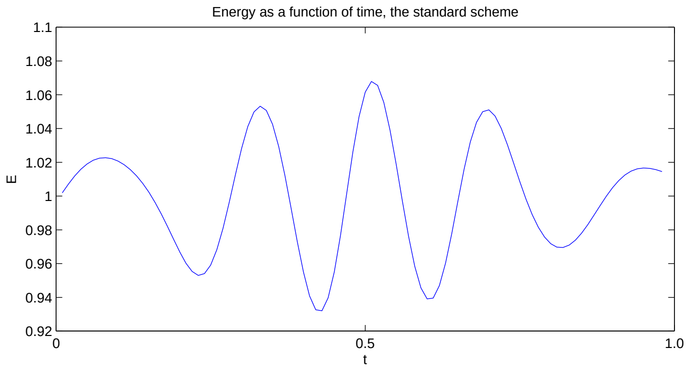


Figure 9: The energy as a function of time for the standard MKG-scheme. The fluctuations are roughly $10\%$.

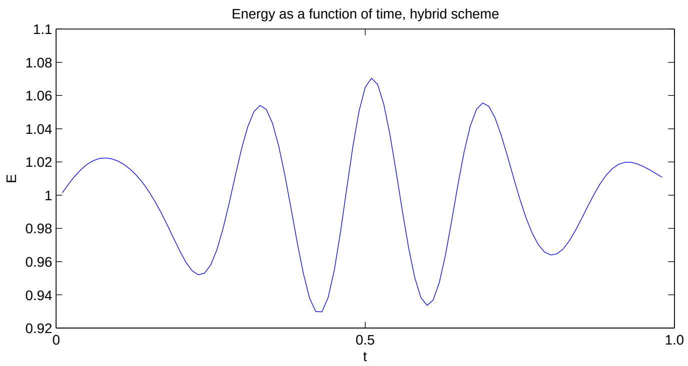


Figure 10: The energy as a function of time for the hybrid MKG-scheme. The fluctuations are roughly $10\%$.

not possess the local gauge symmetry as the hybrid scheme does. As a consequence of this the local charge is not conserved. However, this scheme possesses a global symmetry so the global charge is conserved.

The conservation of the constraint for the hybrid scheme and the lack of the same for the standard scheme were shown through figures. The global charge was also pictured, showing the conservation property of both schemes.

The great advantage of the hybrid scheme is hence that the constraint, which is one of Maxwell's equations, is conserved through the propagation of the solution. Actually, it shows off that the conservation of this constraint is somewhat problematic on the discrete level for other types of schemes, and this concerns not only the standard Finite Difference scheme, but also Finite Element type of schemes [21].

The key to the success of the hybrid scheme is the approximation of the derivatives through the link variables $U_\mu$. This method, inspired by how one makes nonlocal terms gauge invariant in the continuous theory, is a general procedure, and hence should be applicable to other types of equations with gauge symmetry, e.g. the Schrödinger equation or the Dirac equation.

As with every other scheme, the hybrid scheme has an improvement potential, and maybe the biggest one is to formulate Lattice Gauge Theory on a general Riemannian manifold. Stability of the scheme has not been proved either though conservation of energy (in continuous time) and constraint are good indicators of stability. These are questions which are naturally to proceed with. It is also tempting to use the procedure on the more general Yang-Mills-Higgs equations, but these equations are fare more complicated than the Maxwell-Klein-Gordon equations due to nonabelian gauge groups.

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