

Convergence of a discretization of the Maxwell–Klein–Gordon equation based on finite element methods and lattice gauge theory

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Funding information

FP7 Ideas: European Research Council, FP7-IDEAS-ERC Starting Grant scheme, Grant/Award Number: 27801

Abstract

The Maxwell–Klein–Gordon equations are a set of coupled nonlinear time-dependent wave equations, used to model the interaction of an electromagnetic field with a particle. The solutions, expressed with a magnetic vector potential, are invariant under gauge transformations. This characteristic implies a constraint on the solution fields that might be broken at the discrete level. In this article, we propose and study a constraint preserving numerical scheme for this set of equations in dimension 2. At the semidiscrete level, we combine conforming Finite Element discretizations with the so-called Lattice Gauge Theory to design a compatible gauge invariant discretization, leading to preservation of a discrete constraint. Relying on energy techniques and compactness arguments, we establish the convergence of this semidiscrete scheme, without a priori knowledge of the solution. Finally, at the fully discrete level, we propose a compatible explicit time-integration strategy of leapfrog type. We implement the resulting fully discrete scheme and provide assessment on academic scenarios.

KEYWORDS

finite element, Maxwell–Klein–Gordon, numerical analysis

1 | INTRODUCTION

The Standard Model of physics and Einstein's theory of Gravitation, which describe the fundamental forces and particles in nature, involve nonlinear partial differential equations. In the Standard

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Model the particles are either fermions or bosons. The fermions are described by spinors, and the forces between them by connections on vector bundles. The connections model bosons. In quantum electrodynamics (QED) these are photons. In particular, in scalar QED, one models spin zero bosons that interact with photons. The equations are derived through a variational principle from a Lagrangian function. The form of the Lagrangian is determined by the symmetry (gauge) group of the theory. If, in addition, one demands the theory to be renormalizable, the maximal order of derivatives in the Lagrangian is reduced to one, see [25]. Through Noether's theorem (see [24]) one can show that gauge symmetry implies preservation of constraints on the solutions of the Euler–Lagrange equations. The Maxwell–Klein–Gordon (MKG) equations are an example of such equations modelling the interaction of an electromagnetic wave with a particle. The corresponding Lagrangian is invariant under a gauge transformation and the resulting Euler–Lagrange equations are a set of coupled nonlinear time-dependent wave equations verifying a charge preservation constraint, consequence of gauge symmetry. We focus on this set of equations for our study.

Gauge symmetry makes the theory consistent, one should thus strive to preserve this symmetry when discretizing the model. However, standard discretization techniques can break this symmetry. As an example, for the related Yang–Mills equation it was shown in [10] that standard FE discretizations produce approximate solutions that strongly violate the constraints. The field of structure preserving discretization addresses this issue. It is now successfully applied in various area of numerical analysis and applied physics (see e.g., [4, 5, 14, 16, 19, 20, 29] and references therein). The idea is that the preservation of the underlying geometric structure will reveal itself through both stability and good qualitative properties of the solutions.

Nonlinear wave equations such as, also, the sine-Gordon equations [1, 15], provide a particularly interesting test-bed for such approaches.

In the MKG equations, the coupling between the electromagnetic field and scalar complex field describing the evolution of the particle arises through covariant derivatives. Conventional discretization methods, such as standard finite difference methods (FDM) or finite element methods (FEM), approximate the gradient part and the part containing the electromagnetic field separately. Consequently, the resulting approximation of the covariant derivative has no local transformation law, and the gauge symmetry is broken at the discrete level. This implies a violation of the constraint. The key to preserve the gauge symmetry is to approximate the covariant derivative directly, and not as the sum of the gradient and the product of the gauge field with the scalar field/spinor. This was achieved by Kenneth Wilson [32] in 1974 in the field of high energy physics. He was doing calculations on quarks on a lattice, and the theory he developed is now known as lattice gauge theory (LGT). LGT approximates the covariant derivative in a consistent way and at the same time preserves the local gauge symmetry. The essence in the procedure is to localize the nonlocal terms arising in finite difference methods: the nonlocal terms which are to be compared, are parallel transported to a common reference point with the gauge potential. By doing this, the discrete theory becomes gauge invariant. In this context, one motivation of this work is to exploit this technique in a finite element framework to design gauge invariant schemes. As a result, we propose and analyze a numerical LGT scheme for the Maxwell–Klein–Gordon equations that satisfies the discrete constraint by preserving the gauge symmetry at the discrete level.

Some LGT schemes have already been proposed in the literature. In two other articles [6, 7], two of the authors already considered LGT discretization techniques for Maxwell-type equations. In [7], the convergence of the LGT scheme applied to pure Maxwell theory was studied. This was done by comparing the LGT scheme with the classical Yee scheme [33] which is known to converge. In [6], a LGT scheme and a standard Finite Difference discretization for the Maxwell–Klein–Gordon equations were compared. A discrete Noether theorem ensures that the constraint (charge) is preserved. However no

proof of convergence of the scheme was provided in that paper. With a more applicative perspective, in [29], lattice schemes are also used (with a Yee-type scheme for the electromagnetic part) to investigate some numerical simulations for the massive Maxwell–Klein–Gordon equation in the context of QED. Here again no numerical analysis is provided. LGT type discretizations have also been studied for other equations, in particular the Ginzburg–Landau equation [13].

Apart from LGT type discretizations, and regarding numerical analysis works in this context (MKG), in [8], two of the authors proposed a finite element semidiscrete energy preserving scheme in the temporal gauge where gauge symmetry is lost but the constraint preservation is recovered using a Lagrange multiplier. The complete semidiscrete numerical analysis is provided. Let us also mention the recent study [17] considering Maxwell–Klein–Gordon equations in the Coulomb gauge. There, a discretization framework is proposed, based on Finite Elements in space and a modified Crank–Nicolson scheme in time that is energy preserving but not constraint preserving. A complete convergence study and some academical test cases are provided. To the best knowledge of the authors, these are the only studies where a complete numerical analysis work is tackled in the precise context of Maxwell–Klein–Gordon equations.

In this article, we propose a discrete numerical framework for the massive and renormalizable MKG equations in the temporal gauge, based on conforming finite elements (FE) and LGT, aiming at preserving gauge symmetry at the discrete level. The Klein–Gordon (KG) part is discretized as in [6] with LGT techniques, while the Maxwell part is discretized using conforming Nédélec Finite Elements. The resulting semidiscrete scheme preserves a discrete constraint, namely the electric charge. We then prove the convergence of this semidiscrete scheme in two space dimensions. This is done with some inspiration from the methodology used in [8] using compactness arguments and energy principles. Discrete constraint preservation plays a central role in the proof to achieve the adequate bounds to obtain convergence. In a second step, we furthermore propose a fully discrete scheme based on a leapfrog time integration that also preserves the constraint at the discrete level. The fully discrete scheme is implemented and some academic numerical results are given for validation.

The paper is organized as follows: In Section 2, the continuous model is introduced from a variational point of view. In Section 3, we set the discretization in space using the lowest order Nédélec elements [23] on rectangles. The discrete gauge invariant Lagrangian is developed through both LGT and FE. Constraint and energy conservation are shown leading to the proof of the convergence of the scheme in Section 4. Finally, Section 5 numerically assess the fully discrete scheme.

2 | THE MAXWELL–KLEIN–GORDON EQUATION

We first set the equations in a quite general setting of differential forms. Let M be a compact Riemannian manifold without boundary. The space of real-valued k -forms will be denoted $\Omega^k(M)$. We will often identify one-forms and vector-fields. The real valued L^2 -product on differential forms on M is denoted $\langle \cdot, \cdot \rangle$, and the associated L^2 -norm $\| \cdot \|$. Similar notations will be used for complex valued forms. All adjoints, denoted $(\cdot)^*$, will be taken with respect to these L^2 products.

2.1 | Formulation

2.1.1 | The Klein–Gordon action

The unknown of the Klein–Gordon theory is a complex scalar field, $t \mapsto \phi(t)$ (an element in $\Omega^0(M) \otimes \mathbb{C}$), and the corresponding action functional is given by

$$S[\phi] = \frac{1}{2} \int_0^T \left(\|\dot{\phi}\|^2 - \|d\phi\|^2 - m^2 \|\phi\|^2 - \frac{\gamma}{2} \|\phi\|^4 \right) dt, \quad (1)$$

where the dot represents time derivative and $d : \Omega^k(M) \otimes \mathbb{C} \rightarrow \Omega^{k+1}(M) \otimes \mathbb{C}$ is the exterior derivative acting on complex valued forms. The third term is the mass term ($\mathbf{m} \geq 0$ is the mass) and the fourth term is the self-coupling term with $\gamma \geq 0$.

Remark 2.1 The case $\gamma < 0$ will not be envisaged in this work and should deserve a specific study, since it leads to possible nonpositive energy.

2.1.2 | The Maxwell–Klein–Gordon action

In this section, we formally explain the classical physical steps to achieve the gauge invariant MKG action. The MKG-equation is obtained by imposing a local $U(1)$ -symmetry, that is, by demanding the action (or more precisely the Lagrangian) to be invariant under the transformation

$$\phi \rightsquigarrow e^{i\beta} \phi, \quad (2)$$

where β is a real valued function on M , $\beta \in \Omega^0(M)$. The Lagrangian given in Equation (1) is clearly not invariant under this transformation.

This is resolved by replacing the usual derivatives with covariant derivatives, that is, $\partial_t \rightsquigarrow D_\alpha := \partial_t + iq\alpha$ and $d \rightsquigarrow D_A := d + iqA$, with q the coupling constant. Here $t \mapsto \alpha(t)$ is a real valued function on M , that is, $\alpha \in \Omega^0(M)$, and $t \mapsto A(t)$ is a real valued one-form on M , that is, $A \in \Omega^1(M)$.

The function α is usually called the *electric potential* while A is called the *magnetic potential*. They are related to the electric and magnetic fields by the following equations

$$\mathbf{E} = -\dot{A} + d\alpha, \quad \mathbf{B} = dA,$$

and they transform as

$$\begin{aligned} \alpha &\rightsquigarrow \alpha - \dot{\beta}, \\ A &\rightsquigarrow A - d\beta, \end{aligned}$$

simultaneously with (2). This constitutes the gauge transformation of the field (ϕ, α, A) given as $(\phi, \alpha, A) \rightsquigarrow (e^{i\beta} \phi, \alpha - \dot{\beta}, A - d\beta)$.

It is then easy to check that the following action

$$S_{KG}[\phi, \alpha, A] = \frac{1}{2} \int_0^T \left(\|D_\alpha \phi\|^2 - \|D_A \phi\|^2 - \mathbf{m}^2 \|\phi\|^2 - \frac{\gamma}{2} \|\phi\|^2 \right) dt,$$

is locally $U(1)$ -invariant.

To complete the action we add the $U(1)$ -invariant Maxwell action given by

$$S_M[\alpha, A] = \frac{1}{2} \int_0^T (\|\dot{A} - d\alpha\|^2 - c^2 \|dA\|^2) dt,$$

with c the speed of propagation. The full MKG-action is then given by (cf. [18, 25, 26, 28])

$$S_{MKG}[\phi, \alpha, A] = S_{KG}[\phi, \alpha, A] + S_M[\alpha, A].$$

One can finally check that this action is invariant under the gauge transformation.

2.1.3 | Euler–Lagrange equations

The stationary points of this action with respect to the different fields are given by the following Euler–Lagrange equations

$$\langle D_\alpha D_\alpha \phi, \phi' \rangle + \langle D_A \phi, D_A \phi' \rangle + \mathbf{m}^2 \langle \phi, \phi' \rangle + \gamma \langle |\phi|^2 \phi, \phi' \rangle = 0, \quad \forall \phi' \in \Omega^0(M) \otimes \mathbb{C},$$

$$\begin{aligned} \langle \dot{\mathbf{E}}, A' \rangle - c^2 \langle dA, dA' \rangle + \langle i\phi^* D_A \phi, A' \rangle &= 0, & \forall A' \in \Omega^1(M), \\ \langle \mathbf{E}, d\alpha' \rangle - \langle i\phi^* D_\alpha \phi, \alpha' \rangle &= 0, & \forall \alpha' \in \Omega^0(M). \end{aligned} \tag{3}$$

In a strong formulation, the Euler–Lagrange equations are also given by

$$D_\alpha D_\alpha \phi + D_A^* D_A \phi + \mathbf{m}^2 \phi + \gamma |\phi|^2 \phi = 0, \tag{4}$$

$$\dot{\mathbf{E}} - c^2 d^* dA + i \frac{1}{2} (\phi^* D_A \phi - \phi (D_A \phi)^*) = 0, \tag{5}$$

$$d^* \mathbf{E} - i \frac{1}{2} (\phi^* D_\alpha \phi - \phi (D_\alpha \phi)^*) = 0, \tag{6}$$

where d^* is the adjoint to d and $D_A^* = d^* - iqA$.

We see that the Euler–Lagrange-equations consist of two evolution equations given by (7)–(8) and a constraint equation given by Equation (6). Due to the local gauge invariance, Noether’s second theorem can be applied to conclude that the constraint is preserved on the solution of the evolution equations (see [6]), which makes the equations consistent. See [24] for the continuous version(s) of Noether’s theorem(s).

These equations together with the differential Bianchi identity (cf. [31])

$$d \mathbf{B} = 0, \quad \dot{\mathbf{B}} = -d \mathbf{E},$$

which is satisfied by construction of the electromagnetic field from a gauge potential, constitute the complete set of the MKG-equations.

In the rest of the article, we consider unitary constants $q = 1, c = 1$. For the mass \mathbf{m} and self-coupling constant γ , we will consider that they are either 1 or 0 in the mathematical proofs to allow for variations on the system of equations considered. All the proofs are of course valid for nonunitary cases.

2.2 | In the temporal gauge

We restrict the equations to the temporal gauge, $\alpha = 0$, allowed by the gauge symmetry for the rest of the paper. We also now focus on domains in \mathbb{R}^2 . From this section, we also leave the differential forms notation behind (namely d) and use rather the usual notation $\text{grad} = \nabla, \text{curl} = \nabla \times, \text{div} = \nabla \cdot$.

2.2.1 | Strong form of the equation

In the temporal gauge, the strong form of the equations is to find (A, ϕ) such that

$$\ddot{\phi} + D_A^* D_A \phi + \mathbf{m}^2 \phi + \gamma |\phi|^2 \phi = 0, \tag{7}$$

$$\ddot{A} + \text{curl}(\text{curl} A) - \mathfrak{I}(\phi^* D_A \phi) = 0, \tag{8}$$

where $D_A^* \cdot = -\text{div} \cdot -iA \cdot$ and \mathfrak{I} is the imaginary part of a complex.

The constraint is

$$\text{div}(\dot{A}) = \mathfrak{I}(\dot{\phi} \bar{\phi}).$$

2.2.2 | Notations and definition of weak solutions

We let S be a bounded contractible domain in \mathbb{R}^2 with C^1 boundary.

We use the classical notations for $L^p(S)$ spaces and Sobolev spaces $W^{1,s}(S)$, $H^1(S)$, $H_0^1(S)$ (with seminorm $|\cdot|_{H^1(S)}$), and $H(\text{curl}, S)$ is the space of vector potentials in \mathbb{R}^2 considered as vector fields or one forms, with square integrable curl; the analogue space for the divergence will be denoted $H(\text{div}, S)$. We also denote

$$H_0(\text{curl}, S) := \{ \mathbf{A} \in H(\text{curl}, S) \mid \gamma_\tau \mathbf{A} = 0 \text{ on } \partial S \},$$

where $\gamma_\tau \mathbf{A}$ is the tangential component of \mathbf{A} on ∂S , and

$$V := \{ v \in H_0(\text{curl}, S) \mid \text{div } v = 0 \text{ in } \Omega \},$$

Time dependent spaces are defined as follows.

For closed intervals $I \subseteq [0, T]$, $C(I; X)$ is the space of continuous functions from I to X , and $C(0, T; X)$ will denote $C([0, T]; X)$.

We also define for $1 \leq p \leq +\infty$, the Bochner spaces $L^p(0, T; X)$ for X a Banach space as in [30].

We now give a rigorous sense to a weak solution in the temporal gauge and use a similar notion as in [8].

Definition 1 (E, A, ψ, ϕ) is said to be a **weak solution** of (80) in the temporal gauge, if

- There exists $q < 2$, such that
 - $E \in L^\infty(0, T; L^2(S))$,
 - $A \in C(0, T; L^2(S)) \cap L^\infty(0, T; H_0(\text{curl}, S) \cap W^{1,q}(S)^2)$,
 - $\psi \in L^\infty(0, T; L^2(S))$,
 - $\phi \in C(0, T; L^2(S)) \cap L^\infty(0, T; H_0^1(S))$.
- $\begin{cases} \dot{A} &= -E, \\ \dot{\phi} &= -\psi. \end{cases}$
- For every $(E', \psi') \in C_c^\infty([0, T] \times S)^2 \times C_c^\infty([0, T] \times S)$, there holds

$$\begin{aligned} - \int_0^T \langle E, \dot{E}' \rangle dt - \int_0^T \langle \psi, \dot{\psi}' \rangle dt &= \int_0^T \langle \nabla \times A, \nabla \times E' \rangle dt \\ &+ \int_0^T \langle D_A \phi, i\phi E' \rangle dt + \int_0^T \langle D_A \phi, D_A \psi' \rangle dt \\ &+ m^2 \int_0^T \langle \phi, \psi' \rangle dt + \gamma \int_0^T \langle |\phi|^2 \phi, \psi' \rangle dt. \end{aligned} \tag{9}$$

We now turn to the discretization of this equation.

3 | SEMIDISCRETE SETTING

3.1 | Finite Element discretization and gauge invariance

3.1.1 | Finite element discretization

We discretize the spatial part of the continuous action. Let $h > 0$. We assume S to be a rectangular domain with a Cartesian mesh \mathcal{T}_h , and we will assume homogeneous boundary conditions. Furthermore, for $(k, l) \in \mathbb{N} \times \mathbb{N}$, $\mathcal{Q}_{k,l}(\mathbb{C})$ is defined as the space of polynomials with complex coefficients in two variables $(x_1, x_2) \in \mathbb{R}^2$ with maximum degree k with respect to x_1 and l with respect to x_2 .

The discretization is based on three finite dimensional spaces Z_h^0 , Z_h^1 , and Z_h^2 defined as (see [22, 23] for properties of these spaces)

$$\left\{ \begin{aligned} Z_h^0 &= \{u_h \in H_0^1(S) \mid \forall K \in \mathcal{T}_h, u_h|_K \in Q_{1,1}(\mathbb{C})\} \\ &\text{the space of piecewise } Q_{1,1}(\mathbb{C}) \text{ continuous scalar} \\ &\text{functions on } S. \\ Z_h^1 &= \{v_h \in H_0(\text{curl}, S) \mid \forall K \in \mathcal{T}_h, v_h|_K \in Q_{0,1}(\mathbb{C}) \times Q_{1,0}(\mathbb{C})\}, \\ Z_h^2 &= \{v_h \in L^2(S) \mid \forall K \in \mathcal{T}_h, v_h|_K \in Q_{0,0}(\mathbb{C})\}. \end{aligned} \right. \tag{10}$$

We denote by Y_h^0 , Y_h^1 , Y_h^2 (respectively) the analogues of Z_h^0 , Z_h^1 , Z_h^2 constructed with real valued functions. These spaces are equipped with real basis functions (w_n^h) , (w_e^h) and (w_f^h) respectively, which we choose as the tensor product of the one dimensional Whitney forms [22, 23]. With these choices of basis functions, scalar fields ϕ_h have degrees of freedom at the nodes of the mesh, ϕ_n^h , edge-vector-fields/one-forms A_h have degrees of freedom at the edges of the mesh, A_e^h , while face-vector-fields/two-forms B_h have degrees of freedom at the faces of the mesh.

Moreover, the *grad* and *curl* operators in 2D relate the finite dimensional spaces Z_h^0 , Z_h^1 , and Z_h^2 , so that we have a complex:

$$Z_h^0 \xrightarrow{\nabla} Z_h^1 \xrightarrow{\nabla \times} Z_h^2.$$

They also induce matrices $G = (G_{en})$ and $R = (R_{fe})$ in the chosen bases, such that

$$\mathbb{R}^N \xrightarrow{G} \mathbb{R}^E \xrightarrow{R} \mathbb{R}^F,$$

where N, E , and F are the sets of vertices, edges and faces respectively.

Remark 3.1 Since $\text{curl grad} = 0$, we analogously have $RG = 0$.

Thus, for a node element function ϕ_h and an edge element function A_h we can write

$$\begin{aligned} \phi_h &= \sum_n \phi_n^h w_n^h, & \nabla \phi_h &= \sum_e (G\phi^h)_e w_e^h, & \phi_n^h, (G\phi^h)_e &\in \mathbb{C}, \\ A_h &= \sum_e A_e^h w_e^h, & \nabla \times A_h &= \sum_f (RA^h)_f w_f^h, & A_e^h, (RA^h)_f &\in \mathbb{R}. \end{aligned}$$

Here, ϕ_n^h and $(G\phi^h)_e$ are vertex and edge degrees of freedom, while A_e^h and $(RA^h)_f$ are edge and face degrees of freedom. The quantity $(G\phi^h)_e$ represents the differential of the scalar field along the edge e , and has the form $(\phi_m^h - \phi_n^h)$, where the edge e goes from node m to node n . Since we are considering rectangles, a natural orthogonal coordinate system can be associated to the mesh, and in such a coordinate system the expression $(\phi_m^h - \phi_n^h)$ represents the differential in one of the two directions (see [6] for a more explicit formulation).

The notation $e = \{m, n\}$ will denote the edge e which goes from node m to node n .

3.1.2 | Scalar products and norms

The information about the shape and size of the rectangles is encoded in the *mass matrices*. For two edges e and e' , we define

$$(M_1^h)_{ee'} = \int_S w_e^h \cdot w_{e'}^h,$$

where \cdot denotes the scalar product in \mathbb{R}^2 . We also define

$$(M_k^h)_{ss'} = \int_S w_s^h w_{s'}^h,$$

in the cases $k = 0$ and $k = 2$, where s and s' are respectively two nodes or two faces of the mesh.

We note that the matrices M_k^h are square, symmetric and positive definite. We also note that the nonzero entries in M_0^h, M_1^h, M_2^h are of the order h^2, h^0, h^{-2} , where h denotes the maximum diameter of the elements in the mesh.

These matrices M_k^h are the representative matrices of the L^2 -products in the corresponding bases w^h . Thus, for example, for two edge element fields u_h and v_h written as

$$u_h = \sum_e \mathbf{u}_e^h w_e^h, \quad v_h = \sum_e \mathbf{v}_e^h w_e^h,$$

where \mathbf{u}_e^h and \mathbf{v}_e^h are the edge degrees of freedom (DoF), we have

$$\begin{aligned} \langle u_h, v_h \rangle &= \frac{1}{2} \sum_{e, e' \in E} (\overline{\mathbf{u}_e^h \mathbf{v}_{e'}^h} + \overline{\mathbf{u}_{e'}^h \mathbf{v}_e^h}) \int_S w_e^h \cdot w_{e'}^h \\ &= \Re(\overline{\mathbf{u}^h}^T M_1^h \mathbf{v}^h) = (M_1^h \mathbf{u}^h, \mathbf{v}^h). \end{aligned}$$

We use (\cdot, \cdot) to denote the real valued scalar product of vectors.

3.1.3 | Norm estimates

One can establish estimates between norms and degrees of freedom as in the following Lemmas

Lemma 3.2 *If $u_h \in Y_h^1$, then*

$$|\mathbf{u}_e^h| \leq C \|u_h\|_{L^2(S)}.$$

Furthermore, with $p > 2$, $q > 2$ and $\frac{1}{p} + \frac{1}{q} = \frac{1}{2}$, we have:

$$|\mathbf{u}_e^h| \leq Ch^{\frac{2}{q}} \|u_h\|_{L^p(S)}.$$

Proof. Let $u_h \in Y_h^1$. There exists a constant C , independent of u and h such that

$$\frac{1}{C} (\mathbf{u}^h)^T \mathbf{u}^h \leq \|u_h\|_{L^2}^2 = (M_1^h \mathbf{u}^h, \mathbf{u}^h) \leq C (\mathbf{u}^h)^T \mathbf{u}^h, \quad (\mathbf{u}^h)^T \mathbf{u}^h = \sum_e (\mathbf{u}_e^h)^2.$$

Thus

$$|\mathbf{u}_e^h| \leq \sqrt{\sum_{e' \in K} (\mathbf{u}_{e'}^h)^2} \leq C \|u_h\|_{L^2(K)} \leq C \|u_h\|_{L^2(S)}.$$

This estimate together with Hölder's inequality gives

$$|\mathbf{u}_e^h| \leq Ch^{\frac{2}{q}} \|u_h\|_{L^p(S)}. \quad \blacksquare$$

3.1.4 | Gauge symmetry

We can redo the formal derivation of the gauge invariant action at the discrete level. This amounts to understand how the natural analogue of the action at the discrete level would transform under the gauge and correct the terms to obtain a gauge invariant action.

With the notation developed in the previous sections, we can express the discrete version of the Lagrangian from (1) as

$$\langle \dot{\phi}_h, \dot{\phi}_h \rangle - \langle \nabla \phi_h, \nabla \phi_h \rangle = (M_0^h \dot{\phi}^h, \dot{\phi}^h) - (M_1^h G \phi^h, G \phi^h).$$

where $\dot{\phi}^h$ and ϕ^h are degrees-of-freedom vectors. As in the continuous model we want to impose a local $U(1)$ gauge symmetry. We would like the theory to be invariant under the set of transformations

$$\phi_h \rightsquigarrow e^{i\beta_h} \phi_h, \tag{11}$$

where $t \mapsto \beta_h(t) \in Y_h^0$ is a real valued function, but with $\phi_h \in Z_h^0, e^{i\beta_h} \phi_h \notin Z_h^0$.

We thus modify $\langle \dot{\phi}_h, \dot{\phi}_h \rangle = (M_0^h \dot{\phi}^h, \dot{\phi}^h)$ in two steps.

- (a) First, as in the continuous case, we replace the ordinary time derivative by the covariant time derivative, that is, $\partial_0 \rightsquigarrow D_{\alpha_h} = \partial_0 + i\alpha_h$, where α_h is a real valued function, $\alpha_h \in Y_h^0$. Furthermore, $\alpha_h \rightsquigarrow \alpha_h - \dot{\beta}_h$ under a gauge transformation, implying that $D_{\alpha_h} \phi_h$ transforms as

$$D_{\alpha_h} \phi_h \rightsquigarrow e^{i\beta_h} D_{\alpha_h} \phi_h.$$

- (b) Next, we replace the mass matrix M_0^h with a mass lumped version H_0^h , which is both diagonal and positive definite. Its entries are given by

$$(H_0^h)_{nm} = \begin{cases} \sum_k (M_0^h)_{nk}, & n = m, \\ 0, & n \neq m. \end{cases}$$

Let u, v be continuous scalar functions, and \mathbf{u}, \mathbf{v} their vectors of nodal degrees-of-freedom. We define the associated bilinear form by $\langle \cdot, \cdot \rangle_{0,h}$ (which gives the scalar product associated to the matrix H_0^h on Z_h^0) by

$$\begin{aligned} \langle u, v \rangle_{0,h} &= \sum_{n \in N} \Re(u_n (H_0^h)_{nn} \bar{v}_n) = (H_0^h \mathbf{u}, \mathbf{v}) \\ &= \Re \left(\int_S \Pi_{0,h}(u\bar{v}) dS \right) = \sum_{K \in \mathcal{T}_h} \frac{|K|}{4} \sum_{x \in K} \Re(u(x) \bar{v}(x)), \end{aligned} \tag{12}$$

where the points x appearing in the sum are the vertices of K and (\cdot, \cdot) denotes the real valued scalar product for nodal DoF vectors.

Consistency. H_0^h is consistent with M_0^h . More precisely, we have the following error estimate (see [9, 11]).

For real $l > 1$, and all $u \in H^l(S)$ and $v_h \in Z_h^0$, there exists a constant C depending on l such that

$$|\langle u, v_h \rangle_{0,h} - \langle u, v_h \rangle| \leq Ch \|u\|_{H^l(S)} \|v_h\|_{L^2(S)}. \tag{13}$$

Hölder type inequality. Furthermore, for p and p' such that $\frac{1}{p} + \frac{1}{p'} = 1$, for all u, v in Z_h^0 (even u, v continuous scalar fields on S),

$$|\langle u, v \rangle_{0,h}| \leq \|u\|_{h,p} \|v\|_{h,p'}, \tag{14}$$

where for $p > 1$, one defines

$$\|u\|_{h,p} = \left(\int_S \Pi_{0,h}(|u|^p) dS \right)^{\frac{1}{p}},$$

which is uniformly equivalent on Z_h^0 to the true L^p norm [3], that is, there exists a constant C (independent of h) such that for all $u \in Z_h^0$,

$$\frac{1}{C} \|u\|_{L^p(S)} \leq \|u\|_{h,p} \leq C \|u\|_{L^p(S)}.$$

As a conclusion, we have modified the term $\langle \dot{\phi}_h, \dot{\phi}_h \rangle$ as $\langle D_{\alpha_n} \phi_h, D_{\alpha_n} \phi_h \rangle_{0,h}$.

As for the term $\langle \dot{\phi}_h, \dot{\phi}_h \rangle = (M_0^h \dot{\phi}^h, \dot{\phi}^h)$, we get a gauge invariant expression approximating $\langle \nabla \phi_h, \nabla \phi_h \rangle = (M_1^h G \phi^h, G \phi^h)$ in two steps.

- (a) The mass matrix M_1^h defines the L^2 -product for fields with edge degrees-of-freedom. We lump this matrix with the same numerical quadrature as we used for M_0^h in Equation (12), as follows.

Define the scalar product $\langle \cdot, \cdot \rangle_{1,h}$ on $Z_h^1 \times Z_h^1$ by a diagonal matrix H_1^h in the basis w_e^h indexed over the edges in the mesh. Let u, v be continuous vector fields/one-forms, and \mathbf{u}, \mathbf{v} their edge degrees-of-freedom. Then

$$\begin{aligned} \langle u, v \rangle_{1,h} &= \mathfrak{R} \left(\int_S \Pi_{0,h}(u \cdot \bar{v}) dS \right) = \sum_{K \in \mathcal{T}_h} \frac{|K|}{4} \sum_{x \in K} \mathfrak{R}(u(x) \bar{v}(x)) \\ &= \sum_{e \in E} \mathfrak{R}(u_e H_{1,ee}^h \bar{v}_e) = (H_1^h \mathbf{u}, \mathbf{v}). \end{aligned}$$

Here (\cdot, \cdot) denotes the real valued scalar product for edge DoF vectors, $(\mathbf{u}, \mathbf{v}) = \sum_{e \in E} \mathfrak{R}(u_e \bar{v}_e)$. We observe that H_1^h is both symmetric and positive-definite.

Consistency. We have the following error estimate (see [9, 11]). For real $l > 1$, and all $u \in H^l(S)$ and $v_h \in Z_h^1$,

$$|\langle u, v_h \rangle - \langle u, v_h \rangle_{1,h}| \leq C(D)h \|u\|_{H^l(S)} \|v_h\|_{L^2(S)}. \tag{15}$$

Henceforth, the mass matrix M_1^h is replaced with the above described mass lumped version H_1^h in the inner products.

However, we observe that

$$(G \phi^h)_{e=\{m,n\}} = \phi_n^h - \phi_m^h \rightsquigarrow e^{i\beta_n^h} \phi_n^h - e^{i\beta_m^h} \phi_m^h$$

under a gauge transformation, so the expression $(H_1^h G \phi^h, G \phi^h)$ is not gauge invariant.

- (b) This can be resolved by inspiration from Lattice Gauge Theory (LGT) [12, 27, 32], that is, we make the replacement

$$(G \phi^h)_{e=\{m,n\}} \rightarrow (G_{A_h} \phi^h)_{e=\{m,n\}} = \phi_n^h - U^h(m, n) \phi_m^h, \quad U^h(m, n) = e^{-i \int_m^n A_h},$$

where $U^h(m, n)$ is called a link variable.

The vector-field $A_h \in Y_h^1$ transforms as

$$A_h \rightsquigarrow A_h - \nabla \beta_h,$$

under a gauge transformation, implying that $(G_{A_h} \phi^h)_{e=\{m,n\}} \rightsquigarrow e^{i\beta_n^h} (G_{A_h} \phi^h)_{e=\{m,n\}}$.

We will denote $G_{A_h} \phi^h$ the vector of degrees of freedom $(\phi_n^h - U^h(m, n) \phi_m^h)_{e=\{m,n\}}$ and $G_{A_h} \phi_h$ the corresponding element of Z_h^1 (i.e., that has the vector $G_{A_h} \phi^h$ of degrees of freedom). Furthermore, we define $U_h \in Z_h^1$ that has vector of degrees of freedom $(e^{-iA_e})_{e=\{m,n\}}$.

In conclusion, we have thus replaced $\langle \nabla \phi_h, \nabla \phi_h \rangle$ with the expression $\langle G_{A_h} \phi_h, G_{A_h} \phi_h \rangle_{1,h}$.

3.2 | Discrete formulation of the Maxwell–Klein–Gordon equation

3.2.1 | Gauge invariant discrete Maxwell–Klein–Gordon action

The LGT inspired discretely gauge invariant Klein–Gordon action is therefore given by

$$S_h^{KG}[\phi_h, \alpha_h, A_h] = \frac{1}{2} \int_0^T \left(\|D_{\alpha_h} \phi_h\|_{h,2}^2 - \|G_{A_h} \phi_h\|_{h,2}^2 - \mathbf{m}^2 \|\phi_h\|_{h,2}^2 - \frac{\gamma}{2} \|\phi_h\|_{h,2}^2 \right) dt.$$

To complete the construction of the Maxwell–Klein–Gordon action, we add the Maxwell action

$$S^M[\alpha_h, A_h] = \frac{1}{2} \int_0^T \left(\|\dot{A}_h - \nabla \alpha_h\|_{L^2(S)}^2 - \|\nabla \times A_h\|_{L^2(S)}^2 \right) dt. \tag{16}$$

The discretization of the Maxwell part of the action is well understood (see e.g., [2, 21–23]), so the gauge invariant action we are going to use is

$$S_h^{MKG}[\phi_h, \alpha_h, A_h] = S_h^M[\alpha_h, A_h] + S_h^{KG}[\phi_h, \alpha_h, A_h]. \tag{17}$$

With the above considerations, S_h^{MKG} is invariant under the discrete gauge transformation $\mathcal{G}_{\beta_h} : (\phi_h, \alpha_h, A_h) \mapsto (\Pi_{0,h}(e^{i\beta_h} \phi_h), \alpha_h - \beta_h, A_h - \nabla \beta_h)$, with $t \mapsto \beta_h(t) \in Y_h^0$ and $\Pi_{0,h}$ the nodal interpolant onto Z_h^0 .

3.2.2 | Weak formulation of the discretized equations

The variation of S_h^{MKG} at (ϕ_h, α_h, A_h) in the direction $(\phi'_h, \alpha'_h, A'_h)$ is given by

$$DS_h^{MKG}[\phi_h, \alpha_h, A_h](\phi'_h, 0, 0) = \int_0^T \left(\langle D_{\alpha_h} \phi_h, D_{\alpha_h} \phi'_h \rangle_{0,h} - \langle G_{A_h} \phi_h, G_{A_h} \phi'_h \rangle_{1,h} \right) dt + \mathbf{m}^2 \int_0^T \left(\langle \phi_h, \phi'_h \rangle_{0,h} + \gamma \langle |\phi_h|^2 \phi_h, \phi'_h \rangle_{0,h} \right) dt \tag{18}$$

$$DS_h^{MKG}[\phi_h, \alpha_h, A_h](0, \alpha'_h, 0) = \int_0^T \left(-\langle \dot{A}_h - \nabla \alpha_h, \nabla \alpha'_h \rangle + \langle D_{\alpha_h} \phi_h, i\alpha'_h \phi_h \rangle_{0,h} \right) dt, \tag{19}$$

$$DS_h^{MKG}[\phi_h, \alpha_h, A_h](0, 0, A'_h) = \int_0^T \left(\langle \dot{A}_h - \nabla \alpha_h, \dot{A}'_h \rangle - \langle \nabla \times A_h, \nabla \times A'_h \rangle - \langle G_{A_h} \phi_h, i\mathcal{R}_h(U_h, \phi_h, A'_h) \rangle_{1,h} \right) dt, \tag{20}$$

where $\mathcal{R}_h : Z_h^1 \times Z_h^0 \times Y_h^1 \rightarrow Z_h^1$, and for all $(\tilde{U}, \tilde{\phi}, \tilde{A})$ in $Z_h^1 \times Z_h^0$, $\mathcal{R}_h(\tilde{U}, \tilde{\phi}, \tilde{A})$ is the edge element uniquely defined by its edge degrees of freedom

$$(\mathcal{R}_h(\tilde{U}, \tilde{\phi}, \tilde{A}))_e := \tilde{U}_e \tilde{\phi}_m \tilde{A}_e,$$

for $e = \{m, n\}$.

The Euler–Lagrange equations are given by the stationarity of the action, that is,

$$DS_h^{MKG}[\phi_h, \alpha_h, A](\phi'_h, \alpha'_h, A'_h) = 0.$$

By defining the electric field E_h as

$$E_h = \nabla \alpha_h - \dot{A}_h, \tag{21}$$

and by a partial integration in time, the Euler–Lagrange equations read

$$\begin{aligned} \langle D_\alpha^2 \phi_h, \phi'_h \rangle_{0,h} + \langle G_{A_h} \phi_h, G_{A_h} \phi'_h \rangle_{1,h} + \mathbf{m}^2 \langle \phi_h, \phi'_h \rangle_{0,h} + \gamma \langle |\phi_h|^2 \phi_h, \phi'_h \rangle_{0,h} &= 0, & \forall \phi'_h \in Z_h^0, \\ \langle \dot{E}_h, A'_h \rangle - \langle \nabla \times A_h, \nabla \times A'_h \rangle - \langle G_{A_h} \phi_h, i\mathcal{R}_h(U_h, \phi_h, A'_h) \rangle_{1,h} &= 0, & \forall A'_h \in Y_h^1, \end{aligned} \quad (22)$$

and

$$\langle E_h, \nabla \alpha'_h \rangle + \langle D_\alpha \phi_h, i\alpha'_h \phi_h \rangle_{0,h} = 0, \quad \forall \alpha'_h \in Y_h^1. \quad (23)$$

We see that these equations consist of two evolution equations, Equation (22), and one constraint equation, Equation (23) (corresponding to Equation (80)).

Remark 3.3 If one had considered a classical Finite Element discretization, the covariant derivative would have been discretized using $D\phi_h + \Pi_{1,h}(A_h\phi_h)$ which would break the gauge invariance.

We suppose that the following initial conditions, $A^0 \in H^1(S)$, $E^0 \in L^2(S)$, $\phi^0 \in H_0^1(S)$, $\psi^0 \in L^2(S)$ are given.

Then we consider the following discrete initial conditions

$$\begin{aligned} A_h(0, \cdot) &= A_h^0 \in Y_h^1, \\ E_h(0, \cdot) &= E_h^0 \in Y_h^1, \\ \phi_h(0, \cdot) &= \phi_h^0 \in Z_h^0, \\ \psi_h(0, \cdot) &= \psi_h^0 \in Z_h^0. \end{aligned} \quad (24)$$

Furthermore, we suppose that they are chosen such that

$$A_h^0 \xrightarrow{h \rightarrow 0} A^0 \text{ in } (H_0(\text{curl}, S)) \cap L^q, \quad E_h^0 \xrightarrow{h \rightarrow 0} E^0 \text{ in } L^2(S), \quad (25)$$

$$\phi_h^0 \xrightarrow{h \rightarrow 0} \phi^0 \text{ in } H_0^1(S), \quad \psi_h^0 \xrightarrow{h \rightarrow 0} \psi^0 \text{ in } L^2(S). \quad (26)$$

In the rest of Section 3.2, for simplicity of notations we drop the indices h , and consider the situation where h is fixed.

3.2.3 | Constraint preservation

One important feature of this scheme concerns the constraint equation (23). The discrete MKG action (17) is gauge invariant, since both terms are. One can therefore use a discrete Noether's theorem to prove constraint preservation, in a similar manner as in [6].

We can also show this by a direct calculation.

Theorem 1 Suppose $(\mathbf{E}, \mathbf{A}, \alpha, \phi)$ solves Equation (22) on a time interval $[0, T]$. Suppose furthermore that the constraint (23) is satisfied at $t = 0$. Then the constraint (23) is satisfied for all $t \in [0, T]$.

Proof. We start out by a differentiation in time of the left hand side of Equation (23), denoted κ . This gives

$$\dot{\kappa} = \langle \dot{E}, \nabla \alpha' \rangle + \langle D_\alpha \dot{\phi}, i\alpha' \phi \rangle_{0,h} + \langle D_\alpha \phi, i\alpha' \dot{\phi} \rangle_{0,h} + \langle i\dot{\alpha} \phi, i\alpha' \phi \rangle_{0,h}. \quad (27)$$

By the evolution equation for the electric field, Equation (22), we have

$$\langle \dot{E}, \nabla \alpha' \rangle = \langle G_{A_h} \phi, i\mathcal{R}(U, \phi, \nabla \alpha') \rangle_{1,h}. \quad (28)$$

Furthermore,

$$D_\alpha^2 \phi = D_\alpha \dot{\phi} + i\alpha D_\alpha \phi + i\dot{\alpha} \phi, \tag{29}$$

and we can apply the nodal interpolator to both sides of this equality. Then (27) can be rewritten

$$\dot{\kappa} = \langle G_A \phi, i\mathcal{R}(U, \phi, \nabla \alpha') \rangle_{1,h} + \langle D_\alpha^2 \phi, i\alpha' \phi \rangle_{0,h} + \langle D_\alpha \phi, i\alpha' \dot{\phi} \rangle_{0,h} - \langle i\alpha D_\alpha \phi, i\alpha' \phi \rangle_{0,h}. \tag{30}$$

The evolution equation for the Klein–Gordon scalar field gives

$$\begin{aligned} \dot{\kappa} = & \langle G_A \phi, i\mathcal{R}(U, \phi, \nabla \alpha') \rangle_{1,h} - \langle G_A \phi, G_A(i\Pi_{0,h}(\alpha' \phi)) \rangle_{1,h} \\ & + m^2 \langle \phi, i\Pi_{0,h}(\alpha' \phi) \rangle_{0,h} + \gamma \langle |\phi|^2 \phi, i\Pi_{0,h}(\alpha' \phi) \rangle_{0,h} \\ & + \langle D_\alpha \phi, i\alpha' \dot{\phi} \rangle_{0,h} - \langle i\alpha D_\alpha \phi, i\alpha' \phi \rangle_{0,h}. \end{aligned} \tag{31}$$

Since our scalar product is real valued, we obtain

$$\langle D_\alpha \phi, i\alpha' \dot{\phi} \rangle_{0,h} - \langle i\alpha D_\alpha \phi, i\alpha' \phi \rangle_{0,h} = \langle D_\alpha \phi, i\alpha' D_\alpha \phi \rangle_{0,h} = 0 \tag{32}$$

In a same manner, since

$$\langle |\phi|^2 \phi, i\Pi_{0,h}(\alpha' \phi) \rangle_{0,h} = \langle |\phi|^2 \phi, i\alpha' \phi \rangle_{0,h}, \tag{33}$$

one has

$$\langle |\phi|^2 \phi, i\Pi_{0,h}(\alpha' \phi) \rangle_{0,h} = 0, \tag{34}$$

and

$$\langle \phi, i\Pi_{0,h}(\alpha' \phi) \rangle_{0,h} = \langle \phi, i\alpha' \phi \rangle_{0,h} = 0 \tag{35}$$

This gives

$$\dot{\kappa} = \langle G_A \phi, i\mathcal{R}(U, \phi, \nabla \alpha') \rangle_{1,h} - \langle G_A \phi, G_A(i\Pi_{0,h}(\alpha' \phi)) \rangle_{1,h}. \tag{36}$$

where,

$$(G_A(i\Pi_{0,h}(\alpha' \phi)))_e = i\alpha'_n \phi_n - iU_e \alpha'_m \phi_m, \tag{37}$$

$$= i\alpha'_n (\phi_n - U_e \phi_m) - iU_e (G\alpha')_e \phi_m, \tag{38}$$

$$= i\alpha'_n (G_A \phi)_e - iU_e (G\alpha')_e \phi_m. \tag{39}$$

This gives that

$$\langle G_A \phi, G_A(i\Pi_{0,h}(\alpha' \phi)) \rangle_{1,h} = \langle G_{A_h} \phi, i\mathcal{R}(U, \nabla \alpha', \phi) \rangle. \tag{40}$$

Thus $\dot{\kappa} = 0$.

This concludes the proof. ■

3.2.4 | Energy conservation

We define the energy of the system at any time with

$$\mathcal{H}(t) = \frac{1}{2} \left(\|D_\alpha \phi\|_{0,h}^2 + \|G_A \phi\|_{1,h}^2 + \|E\|^2 + \|\nabla \times A\|^2 + m^2 \|\phi\|_{0,h}^2 + \frac{\gamma}{2} \|\ |\phi|^2 \phi \|^2_{0,h} \right).$$

We will show through a direct formal calculation that this energy is preserved by the flow.

Proposition 3.4 Suppose (E, A, α, ϕ) solves the evolution equations (21, 22). Then the energy is conserved.

Proof. The proof is a mere calculation. We have

$$\begin{aligned} \dot{\mathcal{H}}(t) = & \langle D_\alpha \dot{\phi}, D_\alpha \phi \rangle_{0,h} + \langle i\dot{\alpha}\phi, D_\alpha \phi \rangle_{0,h} + \langle G_A \phi, G_A \dot{\phi} \rangle_{1,h} + \langle G_A \phi, \mathcal{R}(iU, \phi, \dot{A}) \rangle_{1,h} \\ & + \langle \dot{E}, E \rangle + \langle \nabla \times A, \nabla \times \dot{A} \rangle + \mathfrak{m}^2 \langle \phi, \dot{\phi} \rangle_{0,h} + \gamma \langle |\phi|^2 \phi, \dot{\phi} \rangle_{0,h}. \end{aligned} \quad (41)$$

Using (29), we deduce that

$$\langle D_\alpha^2 \phi, D_\alpha \phi \rangle_{0,h} = \langle D_\alpha \dot{\phi}, D_\alpha \phi \rangle_{0,h} + \langle i\dot{\alpha}\phi, D_\alpha \phi \rangle_{0,h}. \quad (42)$$

So that

$$\begin{aligned} \dot{\mathcal{H}}(t) = & \langle D_\alpha^2 \phi, D_\alpha \phi \rangle_{0,h} + \langle G_A \phi, G_A \dot{\phi} \rangle_{1,h} + \langle G_A \phi, \mathcal{R}(iU, \phi, \dot{A}) \rangle_{1,h} + \langle \dot{E}, E \rangle + \langle \nabla \times A, \nabla \times \dot{A} \rangle \\ & + \mathfrak{m}^2 \langle \phi, \dot{\phi} \rangle_{0,h} + \gamma \langle |\phi|^2 \phi, \dot{\phi} \rangle_{0,h}. \end{aligned} \quad (43)$$

Using (22), we find

$$\begin{aligned} \dot{\mathcal{H}}(t) = & -\langle G_A \phi, G_A \Pi_{0,h}(D_\alpha \phi) \rangle_{0,h} - \mathfrak{m}^2 \langle \phi, D_\alpha \phi \rangle_{0,h} - \gamma \langle |\phi|^2 \phi, D_\alpha \phi \rangle_{0,h} \\ & + \langle G_A \phi, G_A \dot{\phi} \rangle_{1,h} + \langle G_A \phi, \mathcal{R}(iU, \phi, \dot{A}) \rangle_{1,h} \\ & - \langle G_A \phi, i\mathcal{R}(U, \phi, \dot{A}) \rangle_{1,h} + \langle G_A \phi, i\mathcal{R}(U, \phi, \nabla \alpha) \rangle_{1,h} \\ & + \mathfrak{m}^2 \langle \phi, \dot{\phi} \rangle_{0,h} + \gamma \langle |\phi|^2 \phi, \dot{\phi} \rangle_{0,h}. \end{aligned} \quad (44)$$

Since the scalar product is real, one has that $\langle \phi, i\alpha\phi \rangle_{0,h}$ and $\langle |\phi|^2 \phi, i\alpha\phi \rangle_{0,h}$ vanish. This gives

$$\dot{\mathcal{H}}(t) = -\langle G_A \phi, G_A(i\alpha\phi) \rangle_{0,h} + \langle G_A \phi, i\mathcal{R}(U, \phi, \nabla \alpha) \rangle_{1,h} \quad (45)$$

Using the computation done in the proof of Theorem 1, we conclude that $\dot{\mathcal{H}} \equiv 0$, so that the energy is preserved in time. ■

3.2.5 | Choice of gauge and existence

We choose to work in the temporal gauge, that is, $\alpha \equiv 0$ (as in definition 1) and, for the discretization, $\alpha_h \equiv 0$. This implies

$$\begin{aligned} \dot{A}_h &= -E_h, \\ D_{\alpha_h} \phi_h &= \dot{\phi}_h. \end{aligned}$$

Let $T > 0$. Since we are working on a finite dimensional space, we have local existence of solutions of (22), (23), and (24). Conservation of energy assures that the local solution is a global one: the discrete solutions are defined on the whole interval $[0, T]$.

4 | CONVERGENCE OF THE SEMIDISCRETE SCHEME

In the rest of the paper, C will denote a generic constant (independent of t and h). In the proof of convergence, we will need some results concerning the convergence of approximations. We state them here and postpone their proofs to Appendix A.1.

4.1 | Preliminary results

Lemma 4.1 *Let $\Pi_{1,h}$ be the edge interpolant. For $p > 2$, the following inequalities hold. There exists $C > 0$ such that for all $(F_h, \zeta_h) \in Z_h^1 \times Z_h^0$,*

$$(i) \quad \|F_h \zeta_h - \Pi_{1,h}(F_h \zeta_h)\|_{L^2(S)} \leq Ch^{1-\frac{2}{p}} \|F_h\|_{L^p(S)} |\zeta_h|_{H^1(S)}. \tag{46}$$

Furthermore there exists $C > 0$ such that for all $t \in [0, T]$,

$$(ii) \quad \sqrt{\sum_{K \in \mathcal{T}_h} |A_h|_{H^1(K)}^2} \leq C \left(\|\nabla \times A_h\|_{L^2(S)} + \sup_{r_h \in Y_h^0} \frac{|\langle A_h, \nabla r_h \rangle|}{\|r_h\|_{L^2(S)}} \right), \tag{47}$$

$$(iii) \quad \sqrt{\sum_{K \in \mathcal{T}_h} |\Pi_{1,h}(A_h \phi_h)|_{H^1(K)}^2} \leq Ch^{-\frac{2}{p}} \left[\left(\|\nabla \times A_h\|_{L^2(S)} + \sup_{r_h \in Y_h^0} \frac{|\langle A_h, \nabla r_h \rangle|}{\|r_h\|_{L^2(S)}} \right) \|\phi_h\|_{L^p(S)} + \|A_h\|_{L^p(S)} |\phi_h|_{H^1(S)} \right]. \tag{48}$$

The following result allows, by the constraint (23), to control the weak divergence of A_h appearing in (47) and (48).

Lemma 4.2 *Let $p > 2$. There exists $C > 0$ such that for all $t \in [0, T]$:*

$$\sup_{r_h \in Y_h^0} \frac{|\langle A_h, \nabla r_h \rangle|}{\|r_h\|_{L^2(S)}} \leq Ch^{-\frac{2}{p}} \|\phi_h\|_{L^\infty(0,T,L^p(S))} \|\dot{\phi}_h\|_{L^\infty(0,T,L^2(S))}.$$

With these results at hand, we are ready to prove the convergence of the weak solution of (22).

4.2 | Study of convergence

4.2.1 | Boundedness in the energy norm

The initial energy is bounded uniformly in h , as can be seen from (25), (26), and since it is conserved in time, we can immediately conclude that E_h and $\nabla \times A_h$ are bounded in $L^\infty(0, T; L^2(S))$, that is,

$$\begin{aligned} \|E_h\|_{L^\infty(0,T,L^2(S))} &\leq C, \\ \|\nabla \times A_h\|_{L^\infty(0,T,L^2(S))} &\leq C. \end{aligned} \tag{49}$$

We can also conclude that $\phi_h, \dot{\phi}_h$ and $G_{A_h} \phi_h$ are bounded in time in the following sense.

$$\begin{aligned} \sup_{[0,T]} \|\dot{\phi}_h\|_{0,h} &\leq C, \\ \sup_{[0,T]} \|G_{A_h} \phi_h\|_{1,h} &\leq C. \end{aligned} \tag{50}$$

Furthermore if $m \neq 0$,

$$\sup_{[0,T]} \|\phi_h\|_{h,2} \leq C, \tag{51}$$

and if $\gamma > 0$,

$$\sup_{[0,T]} \|\phi_h\|_{h,4} \leq C, \tag{52}$$

4.2.2 | Convergence of ϕ_h

This is obtained in three steps. First, one bounds the $H^1(S)$ -norm of $|\phi_h|$, then one obtains a bound on the $L^p(S)$ ($p > 2$) norm of the gauge potential A_h . In a third step, this is used to conclude that ϕ_h is bounded in H^1 .

Boundedness of the H^1 -norm of $|\phi_h|$.

We would like to deduce that

$$\|G_{A_h} \phi_h\|_{1,h}^2 \leq C \text{ implies } \|\nabla |\phi_h|\|_{L^2}^2 \leq C.$$

One has

$$(G_{A_h} \phi^h)_{e=\{m,n\}} = \phi_m^h - U^h(m,n) \phi_n^h,$$

with

$$U^h(m,n) = \exp(-i \int_m^n A_h) = \exp(-i \mathbf{A}_e^h),$$

where \mathbf{A}_e^h is the degree of freedom relative to the edge e .

Since $i\mathbf{A}_e^h$ is purely imaginary, we have the following estimate

$$\|\phi_m\| - \|\phi_n\| \leq |(G_{A_h} \phi^h)_{e=\{m,n\}}|,$$

so that by positivity of the diagonal matrix H_1^h , one can conclude that

$$\|\nabla \Pi_{0,h} |\phi_h|\|_{1,h}^2 \leq \|G_{A_h} \phi_h\|_{1,h}^2.$$

We recall that $\nabla \Pi_{0,h} |\phi_h|$ is the edge element vector field whose degrees of freedom are given by the vector $G|\phi^h|$. By previous estimates,

$$\|\nabla \Pi_{0,h} |\phi_h|\|_{L^2(S)}^2 \leq C \|\nabla \Pi_{0,h} |\phi_h|\|_{1,h}^2.$$

This implies

$$\|\nabla \Pi_{0,h} |\phi_h|\|_{L^\infty(0,T,L^2(S))}^2 \leq C,$$

which gives that $\Pi_{0,h} |\phi_h|$ is bounded in $L^\infty(0,T,H_0^1(S))$.

In order to extract estimates on the H^1 -norm of ϕ_h rather than on the H^1 -norm of its modulus $|\phi_h|$, one needs a control of the L^p -norm of A_h .

Boundedness of the gauge potential. Along the same lines as in [8], one can obtain a bound on A_h in the L^p norm. To this aim, we consider the discrete Helmholtz decomposition of A_h

$$A_h = \mathring{A}_h + \nabla p_h. \quad (53)$$

We bound each part in L^p .

Bound on the discrete divergence-free part. The discrete divergence free part \mathring{A}_h is bounded in L^p by the L^2 -norm of the curl of the gauge potential,

$$\|\mathring{A}_h\|_{L^\infty(0,T,L^p(S))} \leq C \|\nabla \times A_h\|_{L^\infty(0,T,L^2(S))}. \quad (54)$$

We won't give any details on this estimate as it can be extracted exactly as in proposition 2.5. of [8].

Bound on the gradient part. One has from the constraint Equation (23)

$$\langle \nabla p_h, \nabla v_h \rangle = \langle u_h, v_h \rangle_{0,h}, \quad (55)$$

with

$$u_h(t) = \int_0^t \dot{\phi}_h \bar{\phi}_h dt.$$

We would like to bound p_h in $L^\infty(0, T; W^{1,p}(S))$ for $p > 2$. By classical estimates that can be found in [3], we have

$$\|p_h\|_{W^{1,p}(S)} \leq C \sup_{v_h \in Y_h^0} \frac{|\langle u_h, v_h \rangle_{0,h}|}{\|v_h\|_{W^{1,p'}(S)}} \text{ at any } t \in [0, T],$$

where $\frac{1}{p} + \frac{1}{p'} = 1$, with $p > 2$ and $p' < 2$.

Let us choose q' such that $\frac{1}{q'} = \frac{1}{p'} - \frac{1}{2}$. For any q such that $\frac{1}{q} + \frac{1}{q'} = 1$, we have

$$|\langle u_h, v_h \rangle_{0,h}| \leq \|u_h\|_{h,q} \|v_h\|_{h,q'}.$$

Furthermore,

$$\|u_h\|_{h,q} \leq C \int_0^t \|\dot{\phi}_h\|_{h,2} \|\bar{\phi}_h\|_{h,p} \leq C \int_0^t \|\dot{\phi}_h\|_{L^2(S)} \|\phi_h\|_{L^p(S)}.$$

Since $\frac{1}{2} + \frac{1}{p} = \frac{1}{q}$, from the energy bound (52), we deduce that $\|\dot{\phi}_h\|_{L^2(S)} \leq C$ and $\|\phi_h\|_{L^p(S)} \leq C$. This implies that

$$|\langle u_h, v_h \rangle_{0,h}| \leq C \|v_h\|_{L^{q'}(S)},$$

independently of $t \in [0, T]$.

By the Sobolev embeddings $W^{1,p'}(S) \hookrightarrow L^{q'}(S)$, we deduce

$$|\langle u_h, v_h \rangle_{0,h}| \leq C \|v_h\|_{W^{1,p'}(S)},$$

which implies that p_h is bounded in $W^{1,p}(S)$, and

$$\|A_h\|_{L^\infty(0,T,L^p(S))} \leq C.$$

Remark 4.3 If $\gamma > 0$, we can also directly prove (without having to use the boundedness in the H^1 norm of $|\phi_h|$) that A_h is bounded in $L^\infty(0, T, L^4(S))$, using that in this case ϕ_h is bounded in $L^\infty(0, T, L^4(S))$.

Convergence of ϕ_h . From this, we deduce that ϕ_h is bounded in $H^1(S)$. Indeed,

$$(G_{A^h} \phi^h)_e = \frac{1 + \exp(-iA_e^h)}{2} (G\phi^h)_e + \frac{1 - \exp(-iA_e^h)}{2} (\phi_m^h + \phi_n^h),$$

so that

$$(G\phi^h)_e = \frac{2}{1 + \exp(-iA_e^h)} (G_{A^h} \phi^h)_e - \frac{1 - \exp(-iA_e^h)}{1 + \exp(-iA_e^h)} (\phi_m^h + \phi_n^h),$$

which implies

$$|(G\phi^h)_e| \leq \frac{1}{\left| \cos\left(\frac{A_e^h}{2}\right) \right|} \left| (G_{A^h} \phi^h)_e \right| + \left| \frac{\sin\left(\frac{A_e^h}{2}\right)}{\cos\left(\frac{A_e^h}{2}\right)} \right| \left(\left| \phi_m^h \right| + \left| \phi_n^h \right| \right).$$

In the last section we obtained

$$\|A_h\|_{L^\infty(0,T,L^p(S))} \leq C,$$

which yields

$$|A_e^h| \leq Ch^{\frac{2}{q}}, \tag{56}$$

where $\frac{1}{q} + \frac{1}{p} = \frac{1}{2}$. This means that for h sufficiently small, $h \leq \varepsilon_0$ with $\varepsilon_0 > 0$ given,

$$\left| \cos\left(\frac{|\mathbf{A}_e^h|}{2}\right) \right| \geq C > 0.$$

We also make use of the following inequality

$$\sin\left(\frac{|\mathbf{A}_e^h|}{2}\right) \leq \frac{|\mathbf{A}_e^h|}{2}.$$

As a consequence

$$|(G\phi^h)_e| \leq C|(G_{A_h}\phi^h)_e| + C|\mathbf{A}_e^h|(|\phi_m^h| + |\phi_n^h|).$$

Furthermore, $\mathbf{A}_e^h(\frac{|\phi_m^h|+|\phi_n^h|}{2})$ are the degrees of freedom of the product $A_h\Pi_{0,h}(|\phi_h|)$, and one can then conclude that

$$\|\nabla\phi_h\|_{h,2}^2 \leq C\|G_{A_h}\phi_h\|_{h,2}^2 + C\|\Pi_{1,h}(A_h\Pi_{0,h}(|\phi_h|))\|_{h,2}^2.$$

Using Lemma 4.1 with $A_h\Pi_{0,h}(|\phi_h|)$ and bounds obtained on both A_h and $|\phi_h|$, we can conclude that

$$\|\nabla\phi_h\|_{1,h}^2 \leq C.$$

Finally since $\|\nabla\phi_h\|_{L^2(S)} \leq C\|\nabla\phi_h\|_{1,h}$, it follows that

$$\|\phi_h\|_{L^\infty(0,T,H^1_0(S))} \leq C.$$

Remark 4.4 Following Remark 4.3, if $\gamma > 0$, we can also directly obtain this result (without having to use the boundedness in the H^1 norm of $|\phi_h|$) using the boundedness of A_h in $L^\infty(0, T, L^4(S))$.

By following [8] and using the bound on the energy, we arrive the convergence of ϕ_h in $L^\infty(0, T; L^p(S))$ (up to a subsequence) using the compactness result from [30] and interpolation estimates on $L^p(S)$ spaces.

4.2.3 | Convergence of the gauge potential A_h

The convergence of the gauge potential is obtained by considering the discrete divergence free part and the gradient part of the discrete Helmholtz decomposition (53) separately.

Discrete divergence free part.

We follow again [8]. By a Kikuchi type result, one obtains the convergence of \hat{A}_h in $L^\infty(0, T, L^2(S))$. Interpolation estimates then give the convergence in $L^\infty(0, T, L^p(S))$, since one has (54). *Gradient part.* The equation we are considering is (Equation(55))

$$\langle \nabla p_h, \nabla v_h \rangle = \langle u_h, v_h \rangle_{0,h} =: l_h(v_h), \quad \forall v_h \in Y_h^0.$$

We have $l_h \in (Y_h^0)^*$, and one can then find, by the Riesz representation theorem, $f_h \in Y_h^0$ such that $\forall v_h \in Y_h^0$,

$$\langle f_h, v_h \rangle = l_h(v_h).$$

Let $q > 2$ be given. We choose $r > 0$ such that $\frac{1}{2} < \frac{1}{r} < \frac{1}{2} + \frac{1}{q}$. One has

$$\|f_h\|_{L^r(S)} = \sup_{v \in L^r(S)} \frac{|\langle f_h, v \rangle|}{\|v\|_{L^r(S)}} = \sup_{v \in L^r(S)} \frac{|\langle f_h, v_h \rangle|}{\|v\|_{L^r(S)}} = \sup_{v \in L^r(S)} \frac{|l_h(v_h)|}{\|v\|_{L^r(S)}} \leq C\|u_h\|_{h,r},$$

where $\frac{1}{r} + \frac{1}{r'} = 1$, and $v_h = P_h(v)$ is the L^2 orthogonal projection on Y_h^0 (which is stable in $L^r(S)$). As already shown in a previous section, this implies

$$\|f_h\|_{L^\infty(0,T;L^r(S))} \leq C \|\dot{\phi}_h\|_{L^\infty(0,T;L^2(S))} \|\phi_h\|_{L^\infty(0,T;L^q(S))}.$$

Furthermore, $\forall t \in [0, T]$,

$$\langle \dot{f}_h, v_h \rangle = \langle \dot{u}_h, v_h \rangle_{0,h},$$

which means that

$$\|\dot{f}_h\|_{L^\infty(0,T;L^r(S))} \leq C \|\dot{\phi}_h\|_{L^\infty(0,T;L^2(S))} \|\phi_h\|_{L^\infty(0,T;L^q(S))}.$$

From this one concludes that there exists $w \in L^\infty(0, T; W^{-1,q}(S))$ such that

$$f_h \xrightarrow{h \rightarrow 0} w \text{ in } L^\infty(0, T; W^{-1,q}(S)),$$

where we used the compact embedding from $L^r(S)$ into $W^{-1,q}(S)$, and the compactness result of [30].

Define $p \in W^{1,q}(S)$ as the unique solution of

$$\langle \nabla p, \nabla v \rangle = \langle w, v \rangle =: l(v), \quad \forall v \in W^{1,q'}(S), \quad \frac{1}{q} + \frac{1}{q'} = 1.$$

We would like to prove that

$$\|p_h - p\|_{L^\infty(0,T;W^{1,q}(S))} \xrightarrow{h \rightarrow 0} 0.$$

In order to prove this, we use a version of the Strang lemma, that is,

$$\sup_{v_h \in Z_h^0} \frac{|l_h(v_h) - l(v_h)|}{\|v_h\|_{W^{1,q'}(S)}} \xrightarrow{h \rightarrow 0} 0,$$

which is verified by construction of l , and we can conclude that $p_h \xrightarrow{h \rightarrow 0} p$ in $L^\infty(0, T; W^{1,q}(S))$ for all $q > 2$.

4.3 | The limit equation

4.3.1 | Summary of convergences obtained

(a) Convergence obtained for A_h . We have that

$$A_h \xrightarrow{h \rightarrow 0} A \text{ in } L^\infty(0, T; L^p(S)), \quad \forall 2 < p,$$

and from energy bound we directly have

$$\nabla \times A_h \rightharpoonup \nabla \times A \text{ in } L^\infty(0, T; L^2(S)) \text{ weak-}^*,$$

and

$$\dot{A}_h \rightharpoonup \dot{A} \text{ in } L^\infty(0, T; L^2(S)) \text{ weak-}^*.$$

(b) Convergence of ϕ_h . We have that

$$\phi_h \xrightarrow{h \rightarrow 0} \phi \text{ in } L^\infty(0, T; L^p(S)), \quad \forall p < +\infty,$$

and from energy bound, we directly have

$$\phi_h \rightharpoonup \phi \text{ in } L^\infty(0, T; H_0^1(S)) \text{ weak-}^*,$$

and

$$\phi_h \rightharpoonup \phi \text{ in } L^\infty(0, T; L^2(S)) \text{ weak-}^*.$$

4.3.2 | Limit equations

Let $\phi' \in C_c^\infty([0, T] \times S)$ and $A' \in (C_c^\infty([0, T] \times S))^2$. Define $\phi'_h = \Pi_{0,h}(\phi') \in C_c^\infty(0, T; Z_h^0)$ and $A'_h = \Pi_{1,h}(A') \in C_c^\infty(0, T; Y_h^1)$. We denote by ϕ^{th} and A^{th} the vectors of the degrees of freedom associated to ϕ'_h and A'_h respectively.

In the temporal gauge, the semidiscrete equations (22) read

$$\int_0^T \langle \ddot{\phi}_h, \phi'_h \rangle_{0,h} + \int_0^T \langle G_{A_h} \phi_h, G_{A_h} \phi'_h \rangle_{1,h} + m^2 \int_0^T \langle \phi_h, \phi'_h \rangle_{0,h} + \gamma \int_0^T \langle |\phi_h|^2 \phi_h, \phi'_h \rangle_{0,h} = 0, \tag{57}$$

$$\int_0^T \langle \dot{E}_h, A'_h \rangle - \int_0^T \langle \nabla \times A_h, \nabla \times A'_h \rangle - \int_0^T \langle G_{A_h} \phi_h, i\mathcal{R}_h(U_h, \phi_h, A'_h) \rangle_{1,h} = 0. \tag{58}$$

Study of Equation (57). We have $\int_0^T \langle \ddot{\phi}_h, \phi'_h \rangle_{0,h} = -\int_0^T \langle \dot{\phi}_h, \dot{\phi}'_h \rangle_{0,h} = -\int_0^T \langle \dot{\phi}_h, \dot{\phi}' \rangle_{0,h}$, and by weak- * convergence of $\dot{\phi}_h$,

$$\int_0^T \langle \dot{\phi}_h, \dot{\phi}' \rangle \xrightarrow{h \rightarrow 0} \int_0^T \langle \dot{\phi}, \dot{\phi}' \rangle.$$

Furthermore from (13) and uniform L^2 bound on $\dot{\phi}_h$

$$\left| \int_0^T \langle \dot{\phi}_h, \dot{\phi}' \rangle_{0,h} - \int_0^T \langle \dot{\phi}_h, \dot{\phi}' \rangle \right| \leq \int_0^T Ch \|\dot{\phi}_h\|_{L^2(S)} \|\dot{\phi}'\|_{H^1(S)} \leq Ch.$$

The convergence of the terms $\int_0^T \langle \phi_h, \phi' \rangle_{0,h}$ and $\int_0^T \langle |\phi_h|^2 \phi_h, \phi' \rangle_{0,h}$ directly follows from the convergence of ϕ_h in $L^\infty(0, T; L^p(S))$ and the convergence for the test functions. We now study the convergence of the term $\int_0^T \langle G_{A_h} \phi_h, G_{A_h} \phi'_h \rangle_{1,h}$ to $\int_0^T \langle D_A \phi, D_A \phi' \rangle$. It will be obtained in several steps.

First, we decompose the quantity of interest $\langle G_{A_h} \phi_h, G_{A_h} \phi'_h \rangle_{1,h} - \langle D_A \phi, D_A \phi' \rangle$ into three terms as

$$\begin{aligned} \langle G_{A_h} \phi_h, G_{A_h} \phi'_h \rangle_{1,h} - \langle D_A \phi, D_A \phi' \rangle &= \underbrace{\langle G_{A_h} \phi_h, G_{A_h} \phi'_h \rangle_{1,h} - \langle \Pi_{1,h}(D_{A_h} \phi_h), G_{A_h} \phi'_h \rangle_{1,h}}_{I_1} \\ &+ \underbrace{\langle \Pi_{1,h}(D_{A_h} \phi_h), G_{A_h} \phi'_h \rangle_{1,h} - \langle \Pi_{1,h}(D_{A_h} \phi_h), \Pi_{1,h}(D_{A_h} \phi'_h) \rangle_{1,h}}_{I_2} \\ &+ \underbrace{\langle \Pi_{1,h}(D_{A_h} \phi_h), \Pi_{1,h}(D_{A_h} \phi'_h) \rangle_{1,h} - \langle D_A \phi, D_A \phi' \rangle}_{J}. \end{aligned} \tag{59}$$

We first concentrate on I_1 and I_2 . We need the two following Lemma. Their proofs are postponed to Appendix B.1.

Lemma 4.5 *There exist $\eta > 0$ and $C > 0$ such that if $h < \eta$,*

$$\sup_{[0, T]} \|G_{A_h} \phi_h - \Pi_{1,h} D_{A_h} \phi_h\|_{h,2}^2 \leq Ch^{2-4/p},$$

so that

$$\sup_{[0, T]} \|G_{A_h} \phi_h - \Pi_{1,h} D_{A_h} \phi_h\|_{h,2} \xrightarrow{h \rightarrow 0} 0.$$

Furthermore, from the bound on the energy we directly have the following.

Lemma 4.6 *There exists $C > 0$ such that*

$$\sup_{[0,T]} \|G_{A_h} \phi_h\|_{h,2} \leq C. \tag{60}$$

We can in a same manner obtain the analogous Lemma with ϕ_h replaced by ϕ'_h . Using Lemma 4.5, 4.6, and 4.1 (and their analogous counter part for ϕ'_h), one proves that I_1 and I_2 converges uniformly in time to 0 as $h \rightarrow 0$.

The estimation of J rely on the following decomposition

$$J = \underbrace{\langle \Pi_{1,h}(D_{A_h} \phi_h), \nabla \phi'_h \rangle_{1,h} - \langle \Pi_{1,h}(D_{A_h} \phi_h), \nabla \phi' \rangle}_{J_1} \tag{61}$$

$$+ \underbrace{\langle \nabla \phi_h, iA_h \phi'_h \rangle_{1,h} - \langle \nabla \phi_h, iA_h \phi'_h \rangle}_{J_2} \tag{62}$$

$$+ \underbrace{\langle \nabla \phi_h, \Pi_{1,h}(iA_h \phi'_h) - iA_h \phi'_h \rangle_{1,h}}_{J_3} \tag{63}$$

$$+ \underbrace{\langle \Pi_{1,h}(D_{A_h} \phi_h), iA_h \phi'_h \rangle - \langle \Pi_{1,h}(D_{A_h} \phi_h), iA \phi' \rangle}_{J_4} \tag{64}$$

$$+ \underbrace{\langle \Pi_{1,h}(iA_h \phi_h), \Pi_{1,h}(iA_h \phi'_h) \rangle_{1,h} - \langle \Pi_{1,h}(iA_h \phi_h), \Pi_{1,h}(iA_h \phi'_h) \rangle}_{J_5} \tag{65}$$

$$+ \underbrace{\langle \Pi_{1,h}(iA_h \phi_h), \Pi_{1,h}(iA_h \phi'_h) \rangle - \langle \Pi_{1,h}(iA_h \phi_h), iA_h \phi'_h \rangle}_{J_6} \tag{66}$$

$$+ \underbrace{\langle \Pi_{1,h}(D_{A_h} \phi_h), \nabla \phi' \rangle - \langle D_A \phi, D_A \phi' \rangle + \langle \Pi_{1,h}(D_{A_h} \phi_h), iA \phi' \rangle}_{J_7}. \tag{67}$$

To estimate these terms, one needs the four following Lemma. To ease the reading, we postponed their proofs to Appendix B.1.

Lemma 4.7

$$\| \langle \Pi_{1,h}(D_{A_h} \phi_h), \nabla \phi'_h \rangle_{1,h} - \langle \Pi_{1,h}(D_{A_h} \phi_h), \nabla \phi' \rangle \|_{L^\infty(0,T)} \xrightarrow{h \rightarrow 0} 0.$$

Lemma 4.8

$$\| \langle \nabla \phi_h, A_h \phi'_h \rangle_{1,h} - \langle \nabla \phi_h, A_h \phi'_h \rangle \|_{L^\infty(0,T)} \xrightarrow{h \rightarrow 0} 0.$$

Lemma 4.9

$$\| \langle \Pi_{1,h}(A_h \phi_h), \Pi_{1,h}(A_h \phi'_h) \rangle_{1,h} - \langle \Pi_{1,h}(A_h \phi_h), \Pi_{1,h}(A_h \phi'_h) \rangle \|_{L^\infty(0,T)} \xrightarrow{h \rightarrow 0} 0.$$

Lemma 4.10

$$\int_0^T \langle \Pi_{1,h} D_{A_h} \phi_h, \Pi_{1,h} D_{A_h} \phi'_h \rangle dt \xrightarrow{h \rightarrow 0} \int_0^T \langle D_A \phi, D_A \phi' \rangle dt.$$

Let us briefly describe how the seven terms of the decomposition of J are treated. The first term J_1 is estimated using Lemma 4.7. Lemma 4.8 gives an estimation of J_2 . The terms $J_3, J_4,$ and J_6 are estimated using 4.1 and bounds on the discrete solution. Lemma 4.9 gives an estimation of J_5 . Finally, since $J_7 = \langle \Pi_{1,h}(D_{A_h} \phi_h), D_A \phi' \rangle - \langle D_A \phi, D_A \phi' \rangle$, we deduce that this terms converges to 0 as $h \rightarrow 0$ with the help of Lemma 4.1 and the convergences obtained and summarized at the beginning of Section 4.3.

Study of Equation (58). The two first terms in Equation (58) are classical and are treated in a same manner as for Equation (57). Thus, the only remaining term to estimate is the nonlinear term of Equation (58). We use the following lemma

Lemma 4.11

$$\langle \mathcal{R}_h(U_h, \phi_h, A'_h) - \Pi_{1,h}(A'_h \phi), \mathcal{R}_h(U_h, \phi_h, A'_h) - \Pi_{1,h}(A'_h \phi) \rangle_{1,h} \xrightarrow{h \rightarrow 0} 0.$$

The proof is postponed to Appendix B.1.

We write

$$\begin{aligned} \langle G_{A_h} \phi_h, i\mathcal{R}_h(U_h, \phi_h, A'_h) \rangle_{1,h} - \langle D_A \phi, i\phi A' \rangle &= \underbrace{\langle G_{A_h} \phi_h, i\mathcal{R}_h(U_h, \phi_h, A_h) \rangle_{1,h} - \langle D_{A_h} \phi_h, i\Pi_{1,h}(\phi_h A'_h) \rangle}_{I} \\ &+ \langle D_{A_h} \phi_h, i\Pi_{1,h}(\phi_h A'_h) \rangle - \langle D_A \phi, i\phi A' \rangle \end{aligned} \quad (68)$$

Using convergences summarized at the beginning of Section 4.3 and Lemma 4.1, we can prove that

$$\int_0^T \langle D_{A_h} \phi_h, i\Pi_{1,h} \phi_h A'_h \rangle \xrightarrow{h \rightarrow 0} \int_0^T \langle D_A \phi, i\phi A' \rangle,$$

Furthermore,

$$\begin{aligned} I &= \underbrace{\langle G_{A_h} \phi_h, i\mathcal{R}_h(U_h, \phi_h, A_h) - i\Pi_{1,h}(\phi_h A'_h) \rangle_{1,h}}_{I_1} \\ &+ \underbrace{\langle G_{A_h} \phi_h - \Pi_{1,h}(D_{A_h} \phi_h), i\Pi_{1,h}(\phi_h A'_h) \rangle_{1,h}}_{I_2} \\ &+ \underbrace{\langle \Pi_{1,h}(D_{A_h} \phi_h), i\Pi_{1,h}(\phi_h A'_h) - i\phi_h A'_h \rangle_{1,h}}_{I_3} \\ &+ \underbrace{\langle \Pi_{1,h}(D_{A_h} \phi_h), i\phi_h(A'_h - A') \rangle_{1,h}}_{I_4} \\ &+ \underbrace{\langle \Pi_{1,h}(D_{A_h} \phi_h), i(\phi_h - \phi)A' \rangle_{1,h}}_{I_5} \end{aligned}$$

$$\begin{aligned}
 & + \underbrace{\langle \Pi_{1,h}(D_{A_h} \phi_h), i\phi A' \rangle_{1,h} - \langle \Pi_{1,h}(D_{A_h} \phi_h), i\phi A' \rangle}_{I_6} \\
 & + \underbrace{\langle (\Pi_{1,h}(D_{A_h} \phi_h) - D_{A_h} \phi_h), i\phi A' \rangle}_{I_7} \\
 & + \underbrace{\langle (D_{A_h} \phi_h - D_A \phi), i\phi A' \rangle}_{I_8}.
 \end{aligned} \tag{69}$$

Each of the terms converges to 0 as $h \rightarrow 0$. Indeed, for

- I_1 , we use the energy norm estimate and Lemma 4.11,
- I_2 , we use Lemma 4.7, Lemma 4.1 (i) and estimates on A'_h and ϕ_h ,
- I_3 , we use estimates on A_h , ϕ_h , A'_h , Lemma 4.1 and the fact that $\|\Pi_{1,h}(D_{A_h} \phi_h)\|_{1,h}$ is bounded (combination of Lemma 4.1 and bounds on the fields),
- I_4 , we use the estimates on A_h , ϕ_h , the convergence properties of A'_h and bound on $\|\Pi_{1,h}(D_{A_h} \phi_h)\|_{1,h}$,
- I_5 , we use the estimates on A_h , ϕ_h , the convergence properties of ϕ'_h and bound on $\|\Pi_{1,h}(D_{A_h} \phi_h)\|_{1,h}$,
- I_6 , we use the consistency estimate (15),
- I_7 , we use Lemma (4.1) and estimates on A_h , ϕ_h ,
- I_8 , we use the convergence properties of A_h and ϕ_h .

Thus we can state that

$$\int_0^T \langle G_{A_h} \phi_h, i\mathcal{R}_h(U_h, \phi_h, A'_h) \rangle_{1,h} \xrightarrow{h \rightarrow 0} \int_0^T \langle D_A \phi, i\phi A' \rangle.$$

The limit equation. To conclude,

$$\begin{aligned}
 & - \int_0^T \langle \dot{\phi}, \dot{\phi}' \rangle + \int_0^T \langle D_A \phi, D_A \phi' \rangle = 0, \\
 & - \int_0^T \langle E, \dot{A}' \rangle - \int_0^T \langle dA, dA' \rangle - \int_0^T \langle D_A \phi, i\phi A' \rangle = 0,
 \end{aligned} \tag{70}$$

which means that (A, ϕ) is a weak solution of the Maxwell–Klein–Gordon equation in the sense of Definition 1.

5 | NUMERICAL RESULTS

In this section, we provide some numerical results to assess the theory. To this end, we first propose a fully discrete scheme and then study two types of test cases in two dimensions.

5.1 | Fully discrete setting

We consider a time-discretization that consists of a uniform subdivision of $N_T + 1$ ($N_T \in \mathbb{N}^*$) points of the interval $[0, T]$. The time step will be denoted $\Delta t := \frac{T}{N_T}$. We propose the following simple time discretization of leap-frog type.

For all $k \in \{0, \dots, N_T\}$, find $(\psi_h^k, \phi_h^k, E_h^k, A_h^k) \in Z_h^0 \times X_h^0 \times Y_h^1 \times Y_h^1$ such that for all $(\phi'_h, A'_h) \in Z_h^0 \times Y_h^0$,

$$\begin{cases} \langle d_t \psi_{0,h}^k, \psi'_{0,h} \rangle - \langle G_{A_h^k} \phi_h^k, G_{A_h^k} \phi' \rangle_{1,h} - \mathbf{m}^2 \langle \phi_h^k, \phi'_h \rangle_{0,h} - \gamma \langle |\phi_h^k|^2 \phi_h^k, \phi'_h \rangle_{0,h} = 0 \\ \langle d_t E_h^k, A'_h \rangle - \langle \text{curl } A_h^k, \text{curl } A'_h \rangle - \langle G_{A_h^k} \phi_h^k, U_h^k \phi'_h A'_h \rangle_{1,h} = 0 \end{cases}$$

with

- $E_h^{k+\frac{1}{2}} := -\frac{A_h^{k+1} - A_h^k}{\Delta t}$ and $\psi_h^{k+\frac{1}{2}} := -\frac{\phi_h^{k+1} - \phi_h^k}{\Delta t}$
- $d_t E_h^k := \frac{E_h^{k+\frac{1}{2}} - E_h^{k-\frac{1}{2}}}{\Delta t}$ and $d_t \psi_h^k := \frac{\psi_h^{k+\frac{1}{2}} - \psi_h^{k-\frac{1}{2}}}{\Delta t}$
- $E_h^k := \frac{E_h^{k+\frac{1}{2}} + E_h^{k-\frac{1}{2}}}{2}$ and $\psi_h^k := \frac{\psi_h^{k+\frac{1}{2}} + \psi_h^{k-\frac{1}{2}}}{2}$

For a given sequence B^k , we will also use the following notations $d_t B^k = \frac{B^{k+1} - B^k}{\Delta t}$.

We initialize the algorithm with values $A_h^0, A_h^1, \psi_h^0, \psi_h^1$.

In this work, we focus on first numerical results and postpone a more thorough fully-discrete numerical analysis for a future work.

5.2 | Constraint preservation

One can straightforwardly check that the constraint is verified.

Proposition 5.1 *If $\langle E_h^{\frac{1}{2}}, \nabla \beta' \rangle = \langle \psi_h^{\frac{1}{2}}, \phi^1 \beta' \rangle_{0,h}$, the constraint is verified that is,*

$$\langle E_h^{k-\frac{1}{2}}, \nabla \beta'_h \rangle = \langle \psi_h^{k-\frac{1}{2}}, \phi_h^k \beta'_h \rangle_{0,h}, \quad \forall k \in \{0, \dots, N_T\} \tag{71}$$

Proof. If one expresses the discrete differential, one obtains

$$\begin{aligned} & d_t \left(\langle E_h^{k-\frac{1}{2}}, \nabla \beta'_h \rangle - \langle \psi_h^{k-\frac{1}{2}}, \phi_h^k \beta'_h \rangle_{0,h} \right) \\ &= \frac{1}{\Delta t} \left[\langle E_h^{k+\frac{1}{2}}, \nabla \beta'_h \rangle - \langle E_h^{k-\frac{1}{2}}, \nabla \beta'_h \rangle - \langle \psi_h^{k+\frac{1}{2}}, \phi_h^{k+1} \beta'_h \rangle_{0,h} + \langle \psi_h^{k-\frac{1}{2}}, \phi_h^k \beta'_h \rangle_{0,h} \right] \end{aligned} \tag{72}$$

But from the definition $\psi_h^{k+\frac{1}{2}}$ and the scalar product,

$$\begin{aligned} \frac{1}{\Delta t} \left[\langle \psi_h^{k+\frac{1}{2}}, \phi_h^{k+1} \beta'_h \rangle_{0,h} - \langle \psi_h^{k-\frac{1}{2}}, \phi_h^k \beta'_h \rangle_{0,h} \right] &= \left\langle \frac{\psi_h^{k+\frac{1}{2}} - \psi_h^{k-\frac{1}{2}}}{\Delta t}, \phi_h^k \beta'_h \right\rangle_{0,h} + \langle \psi_h^{k+\frac{1}{2}}, \frac{(\phi_h^{k+1} - \phi_h^k)}{\Delta t} \beta'_h \rangle_{0,h} \\ &= \langle d_t \psi_h^k, \phi_h^k \beta'_h \rangle_{0,h} \end{aligned} \tag{73}$$

So that

$$d_t (\langle E_h^{k-\frac{1}{2}}, \nabla \beta' \rangle - \langle \psi_h^{k-\frac{1}{2}}, \phi^k \beta' \rangle_{0,h}) = \langle d_t E^k, \nabla \beta' \rangle - \langle d_t \psi^k, \phi^k \beta' \rangle_{0,h}. \tag{74}$$

Similar arguments as in Section 3.2.3 apply to prove that the constraint is preserved even in discrete time. This implies that

$$\langle E_h^{k-\frac{1}{2}}, \nabla \beta' \rangle - \langle \psi_h^{k-\frac{1}{2}}, \phi^k \beta' \rangle_{0,h} = 0 \tag{75}$$

if the constraint is verified at initial time, that is, for $k = 1$. ■

5.3 | Numerical tests

We have implemented the proposed fully-discrete scheme using a dedicated module that we developed using the Finite Element library Firedrake.¹ Let us point out that these results are preliminary and used as first assessments of the method. We consider a two dimensional domain given by a square $[0, 1] \times [0, 1]$. The scheme defined in the previous section is explicit. Thus, as expected in each of our test cases, we observe that the stability of the scheme is guaranteed by a CFL type condition $\Delta t \leq \text{CFL} h$. The CFL constant has been empirically fixed according to our tests to 0.25.

5.3.1 | Artificial test case and convergence order

One does not have access to an exact solution as such. In order to assess our implementation, we propose to design an artificial test case as explained in the following. We consider for all $(t, x, y) \in [0, T] \times [0, 1] \times [0, 1]$,

$$\phi_{art}(t, x, y) = \sin(\omega t) \sin(\pi x) \sin(\pi y), \tag{76}$$

$$A_{art}(t, x, y) = (\cos(\sqrt{2}\pi t) \cos(\pi x) \sin(\pi y), -\cos(\sqrt{2}\pi t) \sin(\pi x) \cos(\pi y)), \tag{77}$$

with $\omega = \sqrt{2\pi^2 + m^2}$. Then we define

$$J_{\phi_{art}} = \partial_{tt}\phi_{art} + (D_{A_{art}})^* D_{A_{art}} \phi_{art} + m^2 \phi_{art} + \gamma |\phi_{art}|^2 \phi_{art} \tag{78}$$

$$J_{A_{art}} = \partial_{tt}A_{art} + d^* dA_{art} - i\phi_{art}^* D_{A_{art}} \phi_{art} \tag{79}$$

In this way, (A_{art}, ϕ_{art}) is a solution of the following set of equations:

$$\begin{aligned} \partial_{tt}\phi + (D_A)^* D_A \phi + m^2 \phi + \gamma |\phi|^2 \phi &= J_{\phi_{art}}, \\ \partial_{tt}A + d^* dA - i\phi^* D_A \phi &= J_{A_{art}}. \end{aligned} \tag{80}$$

with initial conditions

$$\phi(0, \cdot) = \phi_{art}(0, \cdot), \tag{81}$$

$$A(0, \cdot) = A_{art}(0, \cdot). \tag{82}$$

We then use the discretization proposed above, add the external currents $(J_{A_{art}}, J_{\phi_{art}})$ on the right hand side, and compute the corresponding solution $(A_h^n, \phi_h^n)_{n \in \{0, \dots, N_T\}}$. Doing so, we are able to compute the $L^\infty L^2$ error as

$$\text{err}_h^{L^2} = \max_{n \in \{0, \dots, N_T\}} \left(\|\phi_h^n - \Pi_{0,h}(\phi_{art}(t_n, \cdot))\|_{L^2(S)}^2 + \|A_h^n - \Pi_{1,h}(A_{art}(t_n, \cdot))\|_{L^2(S)}^2 \right)^{\frac{1}{2}} \tag{83}$$

We computed the solution for 4 types of (m, γ) couples: $(0, 0)$, $(1, 0)$, $(0, 1)$ and $(1, 1)$. In Figure 1, we plot for several values of the number of points, the values of the respective error defined in (83). The error analysis is performed using mesh parameters that fulfill $\Delta t = \text{CFL}h$. Doing so, we compute the minimum order in time and space of the scheme.

In Figure 2, we plot the results in logarithmic scales. We infer an order of convergence of 1 (a linear regression would even give slopes of ≈ 1.5). Local orders are presented in Table 1.

¹<https://www.firedrakeproject.org/>.

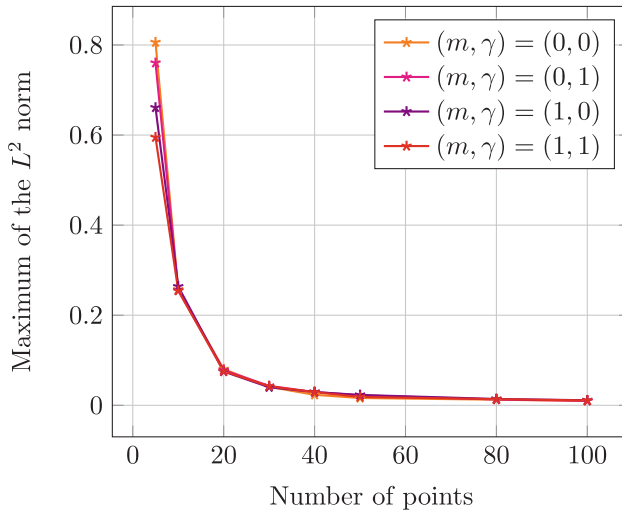


FIGURE 1 Maximum in time of L^2 errors versus number of points.

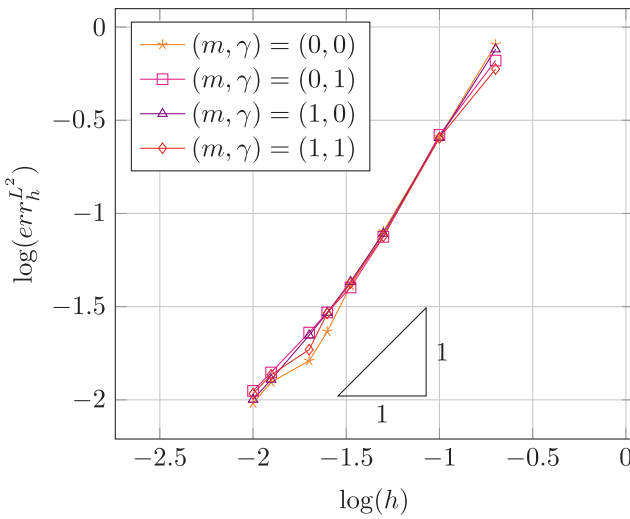


FIGURE 2 Convergence order.

TABLE 1 Approximate numerical orders obtained for various values of the couples (m, γ) $((0, 0), (0, 1), (1, 0), (1, 1))$.

h	$(0, 0)$	$(0, 1)$	$(1, 0)$	$(1, 1)$
0.2	–	–	–	–
0.1	1.64	1.57	1.33	1.23
0.05	1.68	1.71	1.82	1.75
0.033	1.65	1.47	1.54	1.43
0.025	1.96	1.33	1.07	1.30
0.02	1.62	1.25	1.11	2.01
0.0125	0.56	1.16	1.05	0.66
0.01	1.16	1.10	1.02	1.04

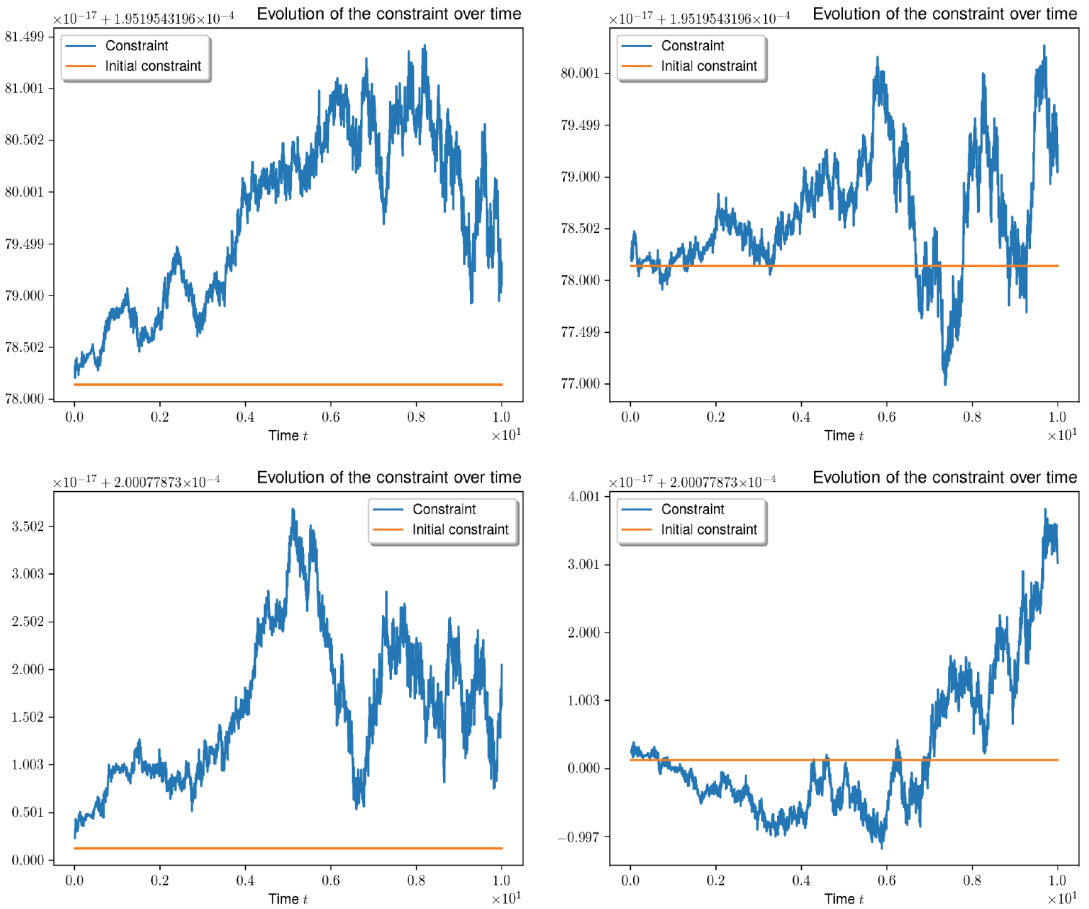


FIGURE 3 Evolution of the constraint in time for several couples (\mathbf{m}, γ) : $(0, 0)$ upper left, $(0, 1)$ upper right, $(1, 0)$ bottom left, $(1, 1)$ bottom right. The initial constraint is nonzero and is represented by the orange horizontal line.

Although this is out of the scope of this work to obtain a theoretical proof of the convergence orders, one can however try to find, through our analysis, some indication of first order convergence for this test case using regular fields. Indeed the approximation of the discrete covariant derivative $D_{A_h} \phi_h$ by the LGT gauge compatible discretization come at the price of the estimate such as (4.5) where we do not hope to obtain more than first order of approximation of the covariant derivative.

Regarding the constraint κ , in this case, one has instead of (23), the following equation.

$$\langle \kappa(t), \alpha' \rangle = \langle \kappa(0), \alpha' \rangle + \int_0^t (\langle J_{\phi_{arr}}, \Pi_{0,h}(-i\alpha' \phi) \rangle + \langle J_{A_{arr}}, \nabla \alpha' \rangle) ds. \tag{84}$$

Hence, except if currents are chosen such that the right hand side vanishes, we do not expect preservation of the constraint in this artificial case. We will not compute the constraint for this precise test case and postpone the tests to the next section.

5.3.2 | Second test case and preservation of the constraint

For this second test case, we propose to initialize the system with an electromagnetic plane wave for A and a 2D-Gaussian initial profile for ϕ centered at the center of the domain. In other words, we consider a focalized density profile for the modulus of the complex Klein–Gordon field. In Figure 3,

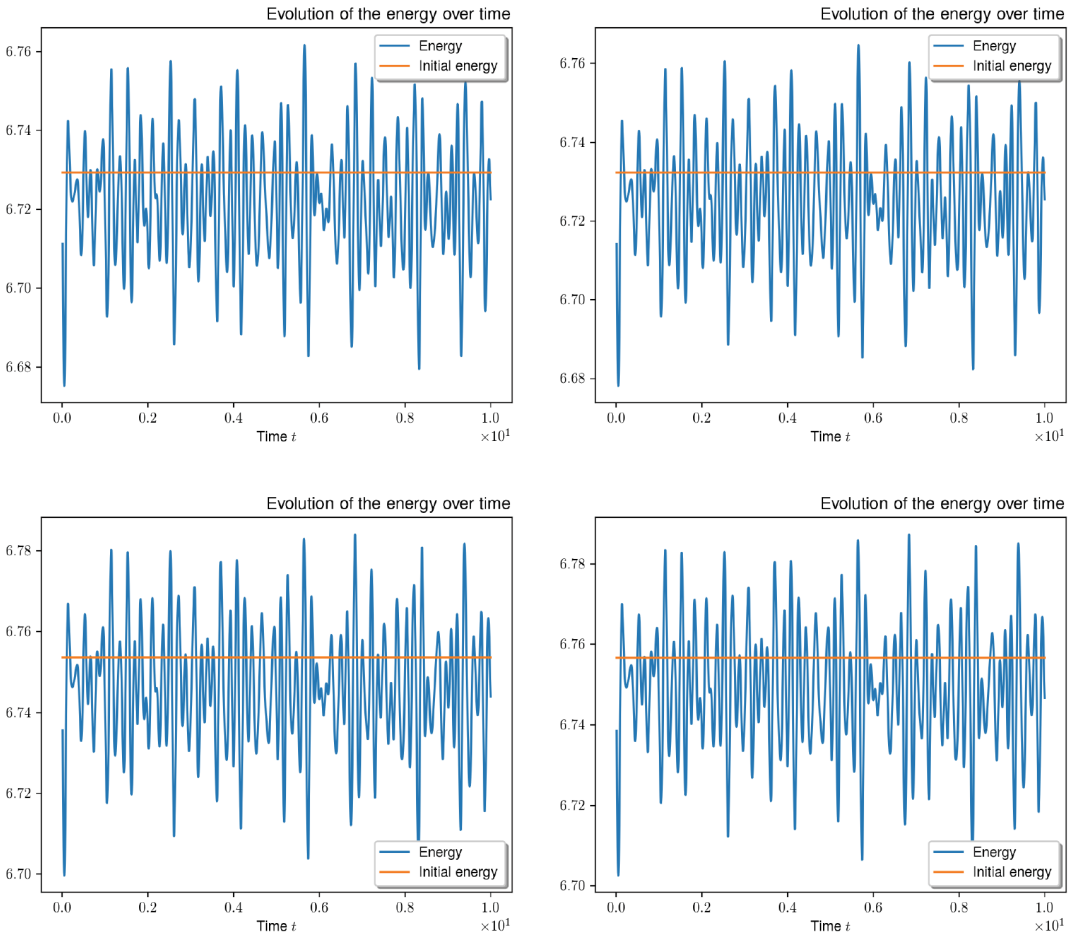


FIGURE 4 Evolution of the energy over time for several couples (m, γ) : $(0, 0)$ upper left, $(0, 1)$ upper right, $(1, 0)$ bottom left, $(1, 1)$ bottom right. The initial energy is represented by the orange horizontal line.

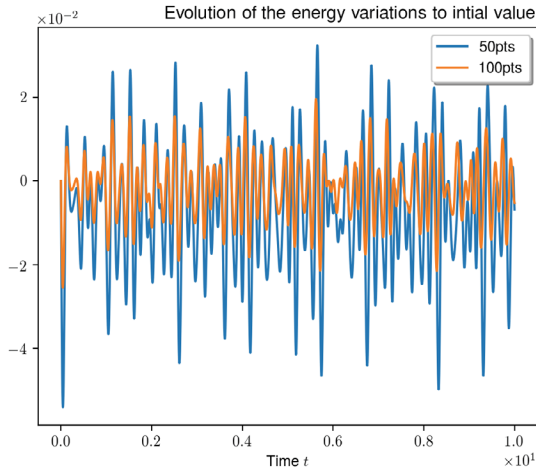


FIGURE 5 Absolute variations of the energy with respect to its initial value over time for a space discretization made of 50 and 100 pts.

10982426, 2023, 4, Downloaded from https://onlinelibrary.wiley.com/doi/10.1002/mm.23008 by University Of Oslo, Wiley Online Library on [29/02/2024]. See the Terms and Conditions (https://onlinelibrary.wiley.com/terms-and-conditions) on Wiley Online Library for rules of use; OA articles are governed by the applicable Creative Commons License

we observe that the constraint is preserved up to machine precision. This is in accordance with the theory developed in previous sections.

The energy is not preserved by the time-integration scheme, however relative variations of the energy from its initial value are relatively small (see Figure 4) and this variation gets consistently smaller as the discretization parameters decrease (see Figure 5).

To conclude, we represent in Figure 6 some ϕ modulus profiles and their evolution with time (the initial profile is represented in Figure 7). At this stage of our investigations, we cannot really interpret these profiles since we work on a toy academic model. This will be part of future works to improve the physical relevance of the setting considered here and the corresponding test cases. The way we use these profiles here is to show the effect of the introduction of mass and self-coupling term. Even if, again, the physical relevance of the values chosen are not discussed here, we propose to test the use of nonunitary values of the mass and self-coupling term.

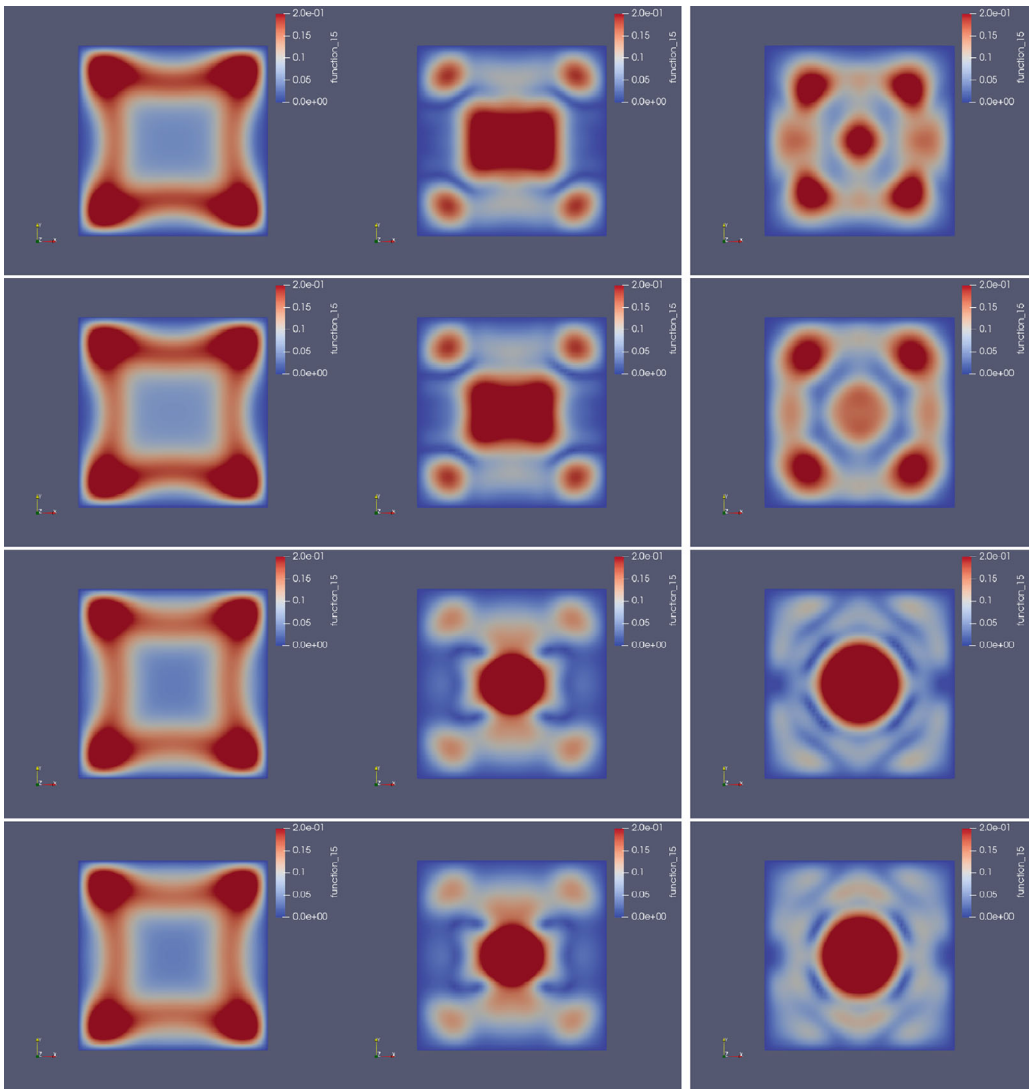


FIGURE 6 Evolution of the profile of the modulus of the Klein–Gordon complex field with $(m, \gamma) = (0, 0)$ (first row), $(m, \gamma) = (0, 10)$ (second row), $(m, \gamma) = (10, 0)$ (third row) and $(m, \gamma) = (10, 10)$ (fourth row): $t = 0.125$ left, $t = 0.225$ middle, $t = 0.985$ right, with $t = 1$ being the end of simulation time.

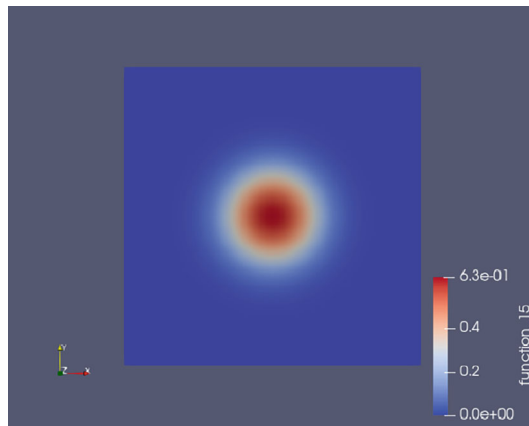


FIGURE 7 Initial profile of the modulus of the Klein–Gordon complex field.

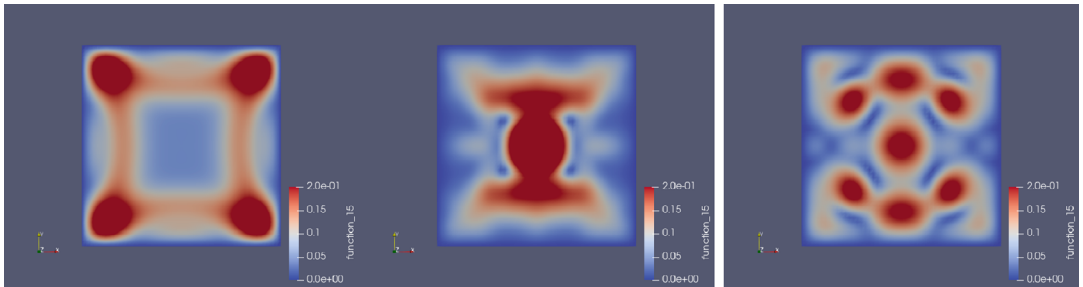


FIGURE 8 Evolution of the profile of the modulus of the Klein–Gordon complex field with $(m, \gamma) = (10, 100)$: $t = 0.125$ left, $t = 0.225$ center, $t = 0.985$ right, with $t = 1$ being the end of simulation time.

What we observe is that the effect of mass and/or self-coupling occurs after some elapsed time and that the effect of self-coupling seems to be weak. We therefore also tested a situation where self-coupling is ten times bigger than mass. In this case, we significantly see self-coupling effects over mass on the profiles patterns (see Figure 8).

6 | CONCLUSION

In this work, we studied the Maxwell–Klein–Gordon equation in dimension two and focused on the semidiscrete analysis of a discretization scheme based on lattice gauge theory (LGT) combined with Nédélec finite elements. The special feature of this scheme is that it ensures gauge invariance at the discrete level therefore respecting the geometrical structure of the original equation through the preservation of the constraint. Our analysis is not an a priori analysis, but concentrates on sequential compactness arguments without the a priori knowledge of a solution of the continuous equations. We use the discrete energy principle combined to constraint preservation to extract bounds in the appropriate spaces and extract convergent subsequences. At last, we implement a fully discrete numerical scheme based on a leap frog type time integration. We provide first academical test cases to extract convergence orders and assess the method. Future works include more relevant physical test cases and the fully discrete analysis of the proposed scheme.

ACKNOWLEDGMENT

This research was supported by the European Research Council through the FP7-IDEAS-ERC Starting Grant scheme, project 278011 STUCCOFIELDS.

DATA AVAILABILITY STATEMENT

The software used to generate the numerical results is not shared, but the parameters used and the results obtained are reported in Section 5.

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How to cite this article: S. H. Christiansen, T. G. Halvorsen, and C. Scheid, *Convergence of a discretization of the Maxwell–Klein–Gordon equation based on finite element methods and lattice gauge theory*, Numer. Methods Partial Differ. Eq. **39** (2023), 3271–3308. <https://doi.org/10.1002/num.23008>

APPENDIX A: PROOFS OF THE PRELIMINARY LEMMA 4.1 AND A.2.

Lemma A.1 *Let $\Pi_{1,h}$ be the edge interpolant. For $p > 2$, the following inequalities hold. There exists $C > 0$ such that for all $(F_h, \zeta_h) \in Y_h^1 \times Z_h^0$*

$$(i) \quad \|F_h \zeta_h - \Pi_{1,h}(F_h \zeta_h)\|_{L^2(S)} \leq Ch^{1-\frac{2}{p}} \|F_h\|_{L^p(S)} |\zeta_h|_{H^1(S)}, \tag{A1}$$

Furthermore there exists $C > 0$ such that

$$(ii) \quad \sqrt{\sum_{K \in \mathcal{T}_h} |A_h|_{H^1(K)}^2} \leq C \left(\|\nabla \times A_h\|_{L^2(S)} + \sup_{r_h \in Y_h^0} \frac{|\langle A_h, \nabla r_h \rangle|}{\|r_h\|_{L^2(S)}} \right), \tag{A2}$$

$$(iii) \quad \sqrt{\sum_{K \in \mathcal{T}_h} |\Pi_{1,h}(A_h \phi_h)|_{H^1(K)}^2} \leq Ch^{-\frac{2}{p}} \left[\left(\|\nabla \times A_h\|_{L^2(S)} + \sup_{r_h \in Y_h^0} \frac{|\langle A_h, \nabla r_h \rangle|}{\|r_h\|_{L^2(S)}} \right) \|\phi_h\|_{L^p(S)} + \|A_h\|_{L^p(S)} \|\phi\|_{H^1(S)} \right]. \tag{A3}$$

Proof. Let $\hat{\Pi}$ be the projector on the reference domain \hat{K} corresponding to $\Pi_{1,h}$ on Z_h^1 , and $\hat{F}_h, \hat{\zeta}_h$ the corresponding functions classically defined on the reference element \hat{K} .

One has

$$\|\hat{F}_h \hat{\zeta}_h - \hat{\Pi} \hat{F}_h \hat{\zeta}_h\|_{L^2(\hat{K})} \leq C \inf_{p \in Q} \|\hat{F}_h \hat{\zeta}_h - p\|_{H^1(\hat{K})},$$

where $Q = Q_{0,1}(\mathbb{C}) \times Q_{1,0}(\mathbb{C})$ is the space of polynomials we will consider on \hat{K} . Furthermore

$$\inf_{p \in Q} \|\hat{F}_h \hat{\zeta}_h - p\|_{H^1(\hat{K})} \leq \inf_{p \in \mathbb{P}_0} \|\hat{F}_h(\hat{\zeta}_h - p)\|_{H^1(\hat{K})},$$

where \mathbb{P}_0 are complex constant functions on \hat{K} . In addition,

$$\begin{aligned} & \inf_{p \in \mathbb{P}_0} \|\hat{F}_h(\hat{\zeta}_h - p)\|_{H^1(\hat{K})} \\ & \leq C \left[\|\hat{F}_h\|_{L^p(\hat{K})} \inf_{p \in \mathbb{P}_0} \|\hat{\zeta}_h - p\|_{H^1(\hat{K})} + |\hat{F}_h|_{H^1(\hat{K})} \right. \\ & \quad \left. \inf_{p \in \mathbb{P}_0} \|\hat{\zeta}_h - p\|_{H^1(\hat{K})} + |\hat{\zeta}_h|_{H^1(\hat{K})} \|\hat{F}_h\|_{L^p(\hat{K})} \right], \end{aligned}$$

which gives

$$\begin{aligned} \inf_{p \in \mathbb{P}_0} \|\hat{F}_h(\hat{\zeta}_h - p)\|_{H^1(\hat{K})} & \leq C \|\hat{F}_h\|_{L^p(\hat{K})} |\hat{\zeta}_h|_{H^1(\hat{K})} + |\hat{F}_h|_{H^1(\hat{K})} |\hat{\zeta}_h|_{H^1(\hat{K})} + |\zeta_h|_{H^1(\hat{K})} \|\hat{F}_h\|_{L^p(\hat{K})} \\ & \leq C \|\hat{F}_h\|_{L^p(\hat{K})} |\hat{\zeta}_h|_{H^1(\hat{K})}. \end{aligned}$$

So on any rectangle K , one deduces by scaling

$$\|F_h \zeta_h - \Pi_{1,h}(F_h \zeta_h)\|_{L^2(K)} \leq Ch^{1-\frac{2}{p}} \|F_h\|_{L^p(K)} |\zeta_h|_{H^1(K)} \leq Ch^{1-\frac{2}{p}} \|F_h\|_{L^p(S)} |\zeta_h|_{H^1(K)},$$

and by summing up the squares of each part of this inequality (i) is proved. By inverse inequality one also has

$$\|F_h \zeta_h - \Pi_{1,h}(F_h \zeta_h)\|_{H^1(K)} \leq Ch^{-\frac{2}{p}} \|F_h\|_{L^p(K)} |\zeta_h|_{H^1(K)}.$$

Furthermore, on the reference square \hat{K} ,

$$|\hat{F}_h \hat{\zeta}_h|_{H^1(\hat{K})} \leq C \left[|\hat{F}_h|_{H^1(\hat{K})} \|\hat{\zeta}_h\|_{L^p(\hat{K})} + |\hat{\zeta}_h|_{H^1(\hat{K})} \|\hat{F}_h\|_{L^p(\hat{K})} \right],$$

which gives on any rectangle K ,

$$|F_h \zeta_h|_{H^1(K)} \leq Ch^{-\frac{2}{p}} \left[|F_h|_{H^1(K)} \|\zeta_h\|_{L^p(K)} + |\zeta_h|_{H^1(K)} \|F_h\|_{L^p(K)} \right].$$

This implies

$$\sqrt{\sum_{K \in \mathcal{T}_h} |\Pi_{1,h}(F_h \zeta_h)|_{H^1(K)}^2} \leq Ch^{-\frac{2}{p}} \left[\left(\sqrt{\sum_{K \in \mathcal{T}_h} |F_h|_{H^1(K)}^2} \right) \|\zeta_h\|_{L^p(S)} + \|F_h\|_{L^p(S)} |\phi|_{H^1(S)} \right]. \tag{A4}$$

Turning to the proof of (ii). The discrete Helmholtz decomposition of A_h is written (see 22)

$$A_h = \mathring{A}_h + \nabla p_h, \tag{A5}$$

where

- \mathring{A}_h is discrete divergence free, that is, $\mathring{A}_h \in V_h := \{u_h \in Y_h^1 | \langle u_h, \nabla \beta_h \rangle = 0, \forall \beta_h \in Y_h^0\}$,
- $p_h \in Y_h^0$.

First, we consider the term \mathring{A}_h . We would like to prove that

$$\sqrt{\sum_{K \in \mathcal{T}_h} |\mathring{A}_h|_{H^1(K)}^2} \leq C \|\nabla \times \mathring{A}_h\|_{L^2(S)}. \tag{A6}$$

Let us define P_V the L^2 projection on the space of divergence free vectors fields. By inverse inequality

$$\sqrt{\sum_{K \in \mathcal{T}_h} |\mathring{A}_h - P_V \mathring{A}_h|_{H^1(K)}^2} \leq Ch^{-1} |\mathring{A}_h - P_V \mathring{A}_h|_{L^2(S)},$$

and following 8 (the proof of Proposition 2.5.), one has

$$|\mathring{A}_h - P_V \mathring{A}_h|_{L^2(S)} \leq Ch \|\nabla \times \mathring{A}_h\|_{L^2(S)}.$$

This yields

$$\sqrt{\sum_{K \in \mathcal{T}_h} |\mathring{A}_h - P_V \mathring{A}_h|_{H^1(K)}^2} \leq C \|\nabla \times \mathring{A}_h\|_{L^2(S)}.$$

Furthermore $P_V(\mathring{A}_h) \in H^1(S)$ and one has

$$|P_V \mathring{A}_h|_{H^1(S)} \leq C \|\nabla \times P_V \mathring{A}_h\|_{L^2(S)} = C \|\nabla \times \mathring{A}_h\|_{L^2(S)},$$

and (A6) is proved. Let us study the gradient part. From the expression of the constraint (23), there exists, from Riesz representation theorem, $u_h \in Y_h^0$ such that

$$\langle \nabla p_h, \nabla r_h \rangle = \langle u_h, r_h \rangle, \quad \forall r_h \in Y_h^0,$$

and

$$\|u_h\|_{L^2(S)} = \sup_{r_h \in Y_h^0} \frac{|\langle \nabla p_h, \nabla r_h \rangle|}{\|r_h\|_{L^2(S)}}.$$

Define $p \in H_0^1(S)$ as the unique solution of the following equation

$$\langle \nabla p, \nabla r \rangle = \langle u_h, r \rangle, \quad \forall r \in H_0^1(S).$$

Since $u_h \in L^2(S)$, then $p \in H^2(S) \cap H_0^1(S)$ and the following inequality holds

$$\|p\|_{H^2(S)} \leq C \|u_h\|_{L^2(S)}.$$

Furthermore, by standard estimates

$$\|p_h - \Pi_{0,h} p\|_{H^1(S)} \leq Ch \|p\|_{H^2(S)}.$$

We would like to prove that

$$\sqrt{\sum_{K \in \mathcal{T}_h} |\nabla p_h|_{H^1(K)}^2} \leq C \|u_h\|_{L^2(S)}.$$

One has

$$\sqrt{\sum_{K \in \mathcal{T}_h} |\nabla p_h|_{H^1(K)}^2} \leq \sqrt{\sum_{K \in \mathcal{T}_h} |\nabla p_h - \nabla \Pi_{0,h} p_h|_{H^1(K)}^2} + \sqrt{\sum_{K \in \mathcal{T}_h} |\nabla \Pi_{0,h} p_h|_{H^1(K)}^2} \tag{A7}$$

$$\leq Ch^{-1} \sqrt{\sum_{K \in \mathcal{T}_h} |\nabla p_h - \nabla \Pi_{0,h} p|_{L^2(K)}^2} + \sqrt{\sum_{K \in \mathcal{T}_h} |\nabla \Pi_{0,h} p|_{H^1(K)}^2} \tag{A8}$$

$$\leq C \|p\|_{H^2(S)} + C \|\nabla p\|_{H^1(S)} \tag{A9}$$

$$\leq C \|u_h\|_{L^2(S)}, \tag{A10}$$

where we used inverse inequalities and the continuity arguments.

Using the estimates established, one concludes that

$$\sqrt{\sum_{K \in \mathcal{T}_h} |A_h|_{H^1(K)}^2} \leq C \left(\|\nabla \times A_h\|_{L^2(S)} + \sup_{r_h \in Y_h^0} \frac{|\langle A_h, \nabla r_h \rangle|}{\|r_h\|_{L^2(S)}} \right),$$

and (ii) is proved.

Inequality (iii) follows directly from (ii) and (A4). ■

The following result allows by the constraint (23) to control the weak divergence of A_h appearing in (47) and (48).

Lemma A.2 For any $p > 2$,

$$\sup_{r_h \in Y_h^0} \frac{|\langle A_h, \nabla r_h \rangle|}{\|r_h\|_{L^2(S)}} \leq Ch^{-\frac{2}{p}} \|\phi_h\|_{L^\infty(0,T,L^p(S))} \|\dot{\phi}_h\|_{L^\infty(0,T,L^2(S))}.$$

Proof. One has from the constraint (23)

$$|\langle A_h, \nabla r_h \rangle| = \left| \left\langle \int_0^t \dot{\phi}_h \bar{\phi}_h, r_h \right\rangle_{0,h} \right|, \quad \forall r_h \in Y_h^0,$$

implying that

$$\begin{aligned} \sup_{r_h \in Y_h^0} \frac{|\langle A_h, \nabla r_h \rangle|}{\|r_h\|_{L^2(S)}} &= \sup_{r_h \in Y_h^0} \frac{|\langle \int_0^t \dot{\phi}_h \bar{\phi}_h, r_h \rangle_{0,h}|}{\|r_h\|_{L^2(S)}} \leq \sup_{r_h \in Y_h^0} \frac{\|\int_0^t \dot{\phi}_h \bar{\phi}_h\|_{0,h} \|r_h\|_{0,h}}{\|r_h\|_{L^2(S)}} \\ &\leq C \left\| \int_0^t \dot{\phi}_h \bar{\phi}_h \right\|_{0,h} \leq C \int_0^t \|\dot{\phi}_h\|_{L^p(S)} \|\phi_h\|_{L^q(S)} \\ &\leq Ch^{-\frac{2}{p}} \|\phi_h\|_{L^\infty(0,T,L^p(S))} \|\dot{\phi}_h\|_{L^\infty(0,T,L^2(S))}, \end{aligned}$$

with $1/p + 1/q = 1/2$. ■

APPENDIX B: PROOF OF LEMMA 4.5 TO LEMMA 4.11

We will use the following decomposition of $G_{A_h} \phi_h$ in terms of its gradient part and its nonlinear part, that upon requiring h to be sufficiently small, is close to $iA_h \phi_h$.

Let $e = \{m, n\}$ denote an oriented edge of the mesh. The following decomposition holds

$$(G_{A_h} \phi^h)_e = \frac{1 + \exp(-i\mathbf{A}_e^h)}{2} (\phi_n^h - \phi_m^h) + \frac{1 - \exp(-i\mathbf{A}_e^h)}{2} (\phi_m^h + \phi_n^h). \tag{B1}$$

Let us denote

- $N_h \in Z_h^1$ the edge element such that its edge degrees of freedom are $\mathbf{N}_e^h = 1 - \exp(-i\mathbf{A}_e^h)$.
- $\mathbf{N}\phi^h$ the vector of the degrees of freedom of the vector $N_h \phi_h$, that is, $(\mathbf{N}\phi^h)_e = \mathbf{N}_e^h (\frac{\phi_m^h + \phi_n^h}{2})$.
- \mathbf{P}^h the vector such that $\mathbf{P}_e^h := -\frac{1}{2} \mathbf{N}_e^h (G\phi^h)_e$, and $P_h \in Z_h^1$ its associated edge element vector field.

This gives

$$(G_{A_h} \phi^h)_e = (G\phi^h)_e + \mathbf{P}_e^h + (\mathbf{N}\phi^h)_e.$$

We first prove the following

Lemma B.1 *There exist $\eta > 0$ and $C > 0$ such that if $h < \eta$,*

$$\sup_{[0,T]} \|G_{A_h} \phi_h - \Pi_{1,h}(D_{A_h} \phi_h)\|_{1,h}^2 \leq Ch^{2-4/p},$$

so that

$$\sup_{[0,T]} \|G_{A_h} \phi_h - \Pi_{1,h}(D_{A_h} \phi_h)\|_{1,h} \xrightarrow{h \rightarrow 0} 0.$$

Proof. Let $e = \{m, n\}$ be an oriented edge of the mesh, one has,

$$(G_{A_h} \phi^h - \Pi_{1,h}(D_{A_h} \phi^h))_e = (\mathbf{P}^h)_e + (\mathbf{N}_e^h - i\mathbf{A}_e^h) \frac{\phi_m^h + \phi_n^h}{2},$$

and

$$\|P_h + (N_h - iA_h)\phi_h\|_{1,h} \leq \|P_h\|_{1,h} + \|(N_h - iA_h)\phi_h\|_{1,h}.$$

Furthermore,

$$\begin{aligned} \|P_h\|_{1,h}^2 &= \sum_e (H_1^h)_{ee} \left| \frac{\exp(-i\mathbf{A}_e^h) - 1}{2} (G\phi^h)_e \right|^2 \\ &\leq \sum_e (H_1^h)_{ee} \frac{|\mathbf{A}_e^h|^2}{4} |(G\phi^h)_e|^2 \\ &\leq Ch^{2-\frac{4}{p}} \|A_h\|_{L^\infty(0,T,L^p(S))}^2 \sum_e (H_1^h)_{ee} |(G\phi^h)_e|^2 \\ &\leq Ch^{2-\frac{4}{p}} \|\nabla\phi_h\|_{1,h}^2 \leq Ch^{2-\frac{4}{p}} \|\nabla\phi_h\|_{L^\infty(0,T,L^2(S))}^2 \leq Ch^{2-\frac{4}{p}}, \end{aligned}$$

since $\nabla\phi_h$ is uniformly bounded in $L^\infty(0, T, L^2(S))$. In addition,

$$\|(N_h - iA_h)\phi_h\|_{1,h}^2 = \sum_e (H_1^h)_{ee} \left| \frac{1 - \exp(-i\mathbf{A}_e^h) - i\mathbf{A}_e^h}{2} (\phi_m^h + \phi_n^h) \right|^2$$

There exists $\eta > 0$, such that $|\mathbf{A}_e^h|$ is sufficiently small (from (56)) so that the following inequalities hold for $h < \eta$

$$\begin{aligned} \|(N_h - iA_h)\phi_h\|_{1,h}^2 &\leq C \sum_e (H_1^h)_{ee} |\mathbf{A}_e^h|^2 \left| \frac{\mathbf{A}_e^h}{2} (\phi_m^h + \phi_n^h) \right|^2 \\ &\leq Ch^{2-\frac{4}{p}} \|A_h\|_{L^\infty(0,T,L^p(S))}^2 \sum_e (H_1^h)_{ee} \left| \frac{\mathbf{A}_e^h}{2} (\phi_m^h + \phi_n^h) \right|^2 \\ &\leq Ch^{2-\frac{4}{p}} \|A_h\|_{L^\infty(0,T,L^p(S))}^2 \|\Pi_{1,h}(A_h\phi_h)\|_{1,h}^2 \\ &\leq Ch^{2-\frac{4}{p}} \|A_h\|_{L^\infty(0,T,L^p(S))}^2 \|\Pi_{1,h}(A_h\phi_h)\|_{L^\infty(0,T,L^2(S))}^2 \\ &\leq Ch^{2-\frac{4}{p}}, \end{aligned}$$

where we used Lemma A.1, and uniform bounds on the L^p -norm of A_h and the H^1 -norm on ϕ_h . \blacksquare

The following Lemma is a direct consequence of the estimate on the energy.

Lemma B.2 *There exists $C > 0$ such that*

$$\sup_{[0,T]} \|G_{A_h} \phi_h\|_{1,h} \leq C. \tag{B2}$$

Lemma B.3

$$\| \langle \Pi_{1,h}(D_{A_h} \phi_h), \nabla \phi'_h \rangle_{1,h} - \langle \Pi_{1,h}(D_{A_h} \phi_h), \nabla \phi' \rangle \|_{L^\infty(0,T)} \xrightarrow{h \rightarrow 0} 0.$$

Proof. From the consistency estimate, one has

$$| \langle \Pi_{1,h}(D_{A_h} \phi_h), \nabla \phi' \rangle_{1,h} - \langle \Pi_{1,h}(D_{A_h} \phi_h), \nabla \phi' \rangle | \leq Ch \| \Pi_{1,h}(D_{A_h} \phi_h) \|_{L^2(S)} \| \nabla \phi' \|_{H^1(S)},$$

for $l > 1$, and from bounds established in Lemma A.1, one deduces for $p > 2$ a bound on $\| \Pi_{1,h}(D_{A_h} \phi_h) \|_{L^2(S)}$ in terms of $\| A_h \|_{L^\infty(0,T;L^p(S))}$ and $\| \phi_h \|_{L^\infty(0,T;H^1(S))}$ which concludes the proof using the obtained bounds and convergence of discrete test functions. ■

Lemma B.4

$$\| \langle \nabla \phi_h, A_h \phi'_h \rangle_{1,h} - \langle \nabla \phi_h, A_h \phi'_h \rangle \|_{L^\infty(0,T)} \xrightarrow{h \rightarrow 0} 0.$$

Proof. Mapping consistency estimates from the reference square to any rectangle K of the mesh (as is done in 9) gives

$$\begin{aligned} & | \langle \nabla \phi_h, A_h \phi'_h \rangle_{1,h} - \langle \nabla \phi_h, A_h \phi'_h \rangle | \\ & \leq C \left(h \sqrt{\sum_{K \in \mathcal{T}_h} |A_h \phi'_h|_{H^1(K)}^2} + h^2 \sqrt{\sum_{K \in \mathcal{T}_h} |A_h \phi'_h|_{H^2(K)}^2} \right) \| \nabla \phi_h \|_{L^2(S)}. \end{aligned}$$

The two terms $\sqrt{\sum_{K \in \mathcal{T}_h} |A_h \phi'_h|_{H^1(K)}^2}$ and $\sqrt{\sum_{K \in \mathcal{T}_h} |A_h \phi'_h|_{H^2(K)}^2}$ can be estimated by standard techniques on the reference simplex as in Lemma A.1. It will not be detailed here since arguments are similar to those already used in previous proofs.

One obtains

$$h \sqrt{\sum_{K \in \mathcal{T}_h} |A_h \phi'_h|_{H^1(K)}^2} + h^2 \sqrt{\sum_{K \in \mathcal{T}_h} |A_h \phi'_h|_{H^2(K)}^2} \leq Ch^{1-\frac{2}{p}} \sqrt{\sum_{K \in \mathcal{T}_h} |A_h|_{H^1(K)}^2} \| \phi'_h \|_{H^1(S)}.$$

Using Lemma A.1 and A.2 and previously obtained bounds, we obtain

$$\| \langle \nabla \phi_h, A_h \phi'_h \rangle_{1,h} - \langle \nabla \phi_h, A_h \phi'_h \rangle \|_{L^\infty(0,T)} \leq Ch^{1-\frac{4}{p}}.$$

Choosing $p > 4$ gives the result. ■

Lemma B.5

$$\| \langle \Pi_{1,h}(A_h \phi_h), \Pi_{1,h}(A_h \phi'_h) \rangle_{1,h} - \langle \Pi_{1,h}(A_h \phi_h), \Pi_{1,h}(A_h \phi'_h) \rangle \|_{L^\infty(0,T)} \xrightarrow{h \rightarrow 0} 0.$$

Proof. From error estimates in 11, one deduces that

$$\begin{aligned} & | \langle \Pi_{1,h}(A_h \phi_h), \Pi_{1,h}(A_h \phi'_h) \rangle_{1,h} - \langle \Pi_{1,h}(A_h \phi_h), \Pi_{1,h}(A_h \phi'_h) \rangle | \\ & \leq Ch \sum_{K \in \mathcal{T}_h} \left(\| \Pi_{1,h}(A_h \phi_h) \|_{L^2(K)} | \Pi_{1,h}(A_h \phi'_h) |_{H^1(K)} \right. \\ & \quad \left. + \| \Pi_{1,h}(A_h \phi'_h) \|_{L^2(K)} | \Pi_{1,h}(A_h \phi_h) |_{H^1(K)} \right). \end{aligned}$$

So by Lemma A.1, Lemma A.2 and the bounds on A_h , ϕ_h and ϕ'_h the result follows. ■

Lemma B.6

$$\int_0^T \langle \Pi_{1,h}(D_{A_h} \phi_h), \Pi_{1,h}(D_{A_h} \phi'_h) \rangle dt \xrightarrow{h \rightarrow 0} \int_0^T \langle D_A \phi, D_A \phi' \rangle dt.$$

Proof. This follows from Lemma A.1, weak-* convergence of $\nabla \phi_h$ to $\nabla \phi$ in $L^\infty(0, T; L^2(S))$ and strong convergence of A_h and ϕ_h in $L^\infty(0, T; L^p(S))$. ■

Last

Lemma B.7

$$\|\mathcal{R}_h(U_h, \phi_h, A'_h) - \Pi_{1,h}(A'_h \phi_h)\|_{1,h} \xrightarrow{h \rightarrow 0} 0.$$

Proof. For h sufficiently small

$$\begin{aligned} & \|\mathcal{R}_h(U_h, \phi_h, A'_h) - \Pi_{1,h}(A'_h \phi_h)\|_{1,h}^2 \\ &= \sum_e (H_1^h)_{ee} \left| \mathbf{A}_e^{th} \exp(-i\mathbf{A}_e^h) \phi_m^h - \mathbf{A}_e^{th} \frac{\phi_m^h + \phi_n^h}{2} \right|^2 \\ &= \sum_e (H_1^h)_{ee} \left| \mathbf{A}_e^{th} \exp(-i\mathbf{A}_e^h) \frac{\phi_n^h + \phi_m^h}{2} - \mathbf{A}_e^{th} \exp(-i\mathbf{A}_e^h) \frac{\phi_n^h - \phi_m^h}{2} - \mathbf{A}_e^{th} \frac{\phi_m^h + \phi_n^h}{2} \right|^2 \\ &= \sum_e (H_1^h)_{ee} \left| \mathbf{A}_e^{th} (1 - \exp(-i\mathbf{A}_e^h)) \frac{\phi_n^h + \phi_m^h}{2} - \mathbf{A}_e^{th} \exp(-i\mathbf{A}_e^h) \frac{\phi_n^h - \phi_m^h}{2} \right|^2 \\ &\leq C \sum_e (H_1^h)_{ee} \left(|\mathbf{A}_e^{th}|^2 |\mathbf{A}_e^h|^2 \left| \frac{\phi_n^h + \phi_m^h}{2} \right|^2 + |\mathbf{A}_e^{th}|^2 \left| \frac{\phi_n^h - \phi_m^h}{2} \right|^2 \right) \\ &\leq Ch^{2-\frac{4}{p}} \sum_e (H_1^h)_{ee} \left(|\mathbf{A}_e^h|^2 \left| \frac{\phi_n^h + \phi_m^h}{2} \right|^2 + |\phi_n^h - \phi_m^h|^2 \right) \\ &\leq Ch^{2-\frac{4}{p}} \left(\|\Pi_{1,h}(A_h \phi_h)\|_{L^\infty(0,T;L^2(S))}^2 + \|\nabla \phi_h\|_{L^\infty(0,T;L^2(S))}^2 \right). \end{aligned}$$

The same arguments as in Lemma 4.9 gives the result. ■