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Lattice implementation of Abelian gauge theories with Chern–Simons number and an axion field

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Abstract

Real time evolution of classical gauge fields is relevant for a number of applications in particle physics and cosmology, ranging from the early Universe to dynamics of quark–gluon plasma. We present an explicit non-compact lattice formulation of the interaction between a *shift*-symmetric field and some $U(1)$ gauge sector, $a(x)F_{\mu\nu}\tilde{F}^{\mu\nu}$, reproducing the continuum limit to order $\mathcal{O}(dx_\mu^2)$ and obeying the following properties: (i) the system is gauge invariant and (ii) shift symmetry is exact on the lattice. For this end we construct a definition of the *topological number density* $\mathcal{K} = F_{\mu\nu}\tilde{F}^{\mu\nu}$ that admits a lattice total derivative representation $\mathcal{K} = \Delta_\mu^+ K^\mu$, reproducing to order $\mathcal{O}(dx_\mu^2)$ the continuum expression $\mathcal{K} = \partial_\mu K^\mu \propto \vec{E}\cdot\vec{B}$. If we consider a homogeneous field $a(x) = a(t)$, the system can be mapped into an Abelian gauge theory with Hamiltonian containing a Chern–Simons term for the gauge fields. This allow us to study in an accompanying paper the real time dynamics of fermion number non-conservation (or chirality breaking) in Abelian gauge theories at finite temperature. When $a(x) = a(\vec{x}, t)$ is inhomogeneous, the set of lattice equations of motion do not admit however a simple explicit local solution (while preserving an $\mathcal{O}(dx_\mu^2)$ accuracy). We discuss an iterative scheme allowing to overcome this difficulty.

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1. Introduction

Real-time evolution of classical fields has many applications in different areas of high energy physics and cosmology. These include the creation and evolution of topological defects in the early Universe [1–10], non-perturbative investigations of hot sphaleron transitions related to fermion number non-conservation in the electroweak theory [11–21], the analysis of inflationary preheating [22–31], the generation of cosmological perturbations [32–37] and gravitational waves [38–47] during preheating, and different aspects of quark–gluon plasma, see e.g. [48] and references therein. The classical approximation to quantum dynamics should work when the relevant distance scales of the problem exceed considerably the typical quantum distances, at finite temperatures T given by $1/T$ (distance between particles) and $1/(gT)$ (Debye screening length, where g is the gauge coupling).

The numerical procedures for Abelian or non-Abelian scalar-gauge theories, such as the Standard Model is well developed, see e.g. [49,12] for first studies in $1+1$ and $3+1$ dimensions. In the simplest realization it consists in the following steps (for inclusion in numerical simulations of hard thermal loops and Langevin-like dynamics see [50,51]). One uses the standard lattice formulation of the gauge theory action with exact lattice gauge invariance and Minkowski signature of the metric. The variation of the action with respect to the gauge fields (living at the links of the lattice) and scalar fields (living at the lattice sites) produce a system of equations in which the dynamical variables at time slice t_n are expressed via those at two preceding times t_{n-1} and t_{n-2}. So, giving an initial condition at t_0 and t_1 (the Cauchy problem) allows to follow the evolution of the system and address all sorts of questions one is interested in. The initial conditions are chosen depending on the physical system under consideration: for sphaleron transitions they are taken from an equilibrium ensemble at some temperature, for preheating from knowing the spectrum of initial fluctuations of the fields after inflation, etc.

It is very important that the procedure discussed above is gauge invariant. The variation of the action with respect to the zero component of the gauge field gives the lattice Gauss constraint, which is *exactly* conserved during the (lattice) time evolution. It is an empirical fact that the formulations that are not gauge invariant in discrete space-time (and only invariant when the lattice spacing and time step go to zero) are plagued with different non-physical numerical instabilities.

For a number of applications the simplest gauge-scalar actions should be extended by an addition of the pieces that contain the so called topological term or *Pontryagin* density, $\mathcal{K} = F_{\mu\nu}\tilde{F}^{\mu\nu}$, with $\tilde{F}_{\mu\nu} \equiv \frac{1}{2}\epsilon_{\mu\nu\alpha\beta}F^{\alpha\beta}$ the dual of the field strength. The most interesting examples contain an axion field coupled linearly to $\mathcal{K}$ as $a(x)F_{\mu\nu}\tilde{F}^{\mu\nu}$, and the theories with non-zero chemical potential μ for chiral fermions, leading to an effective bosonic Hamiltonian containing the Chern–Simons term for the gauge fields $\mu N_{\rm cs}$, with $N_{\rm cs} \propto \int d^4x\,\mathcal{K}$.

To investigate the time evolution of these systems one is faced with the following problem, realized already a long time ago [12,52,53]. The construction of $\mathcal{K}$ on the lattice should be done in such a way that the continuum topological properties of $\mathcal{K}$ hold: the integral of $\mathcal{K}$ over the volume of space-time can be expressed via an integral over the boundary. To put it in other words, in continuum one can write

$$\mathcal{K} = \partial_\mu K^\mu \ , \tag{1}$$

where K^μ is the Chern–Simons current. The lattice analogue of this relation is

$$\mathcal{K} = \Delta_\mu^+ K^\mu, \tag{2}$$

where Δ_μ^+ is the lattice difference in positive direction of μ axis (more details are provided in Sections 3, 4 and 5). If the lattice (gauge-invariant) definition of $\mathcal{K}$ does not satisfy this property, we will get unwanted lattice artifacts and the continuum extrapolation would be difficult. There are several interesting quantities which are very sensitive to the topological property (1). For example, it is Eq. (1) which makes the axion mass m_a to be zero in all orders of perturbation theory ($m_a \neq 0$ being a non-perturbative phenomenon). The extraction of the non-Abelian sphaleron rate in the symmetric phase of the electroweak theory from diffusion of Chern–Simons number requires a careful construction of the lattice version of $\mathcal{K}$ in which the property (1) is still approximate, but as precise as possible [15].

The aim of the present paper is to set up an explicit lattice gauge invariant formulation for real time simulations of *Abelian* gauge theories, respecting the topological property Eq. (2) of $\mathcal{K}$ *exactly*. For non-Abelian theories, the mission seems to be impossible due to well known difficulties of defining $\mathcal{K}$ obeying the property (2) on the lattice [54,55], though different ingenious techniques allowing to be closer to the continuum limit have been invented [52,53]. The statement that an implementation of $\mathcal{K}$ respecting the topological property Eq. (2) can be done exactly in Abelian lattice gauge theories goes back to the works of Guy Moore [52,53], where the motion of Chern–Simons number in SU(2) and SU(3) gauge at high temperatures under a chemical potential was investigated, significantly improving earlier studies [12]. Our work represents an explicit realization and extension of Moore remarks, providing all formulas necessary for numerical simulations.

The applications of our formulation include, for example, the study of the non-linear dynamics in axion-inflation models [56–63], the clarification of the role of Standard Model hypercharge group U(1) in baryogenesis and in magnetic field generation [64–67], the modeling the different aspects of chiral magnetic effects [68,64,69,70], or the study of the problem of chiral fermionic charge evolution in high temperature electrodynamics [71,72]. An accompanying paper [73] is devoted to the last subject.

This paper is organized as follows. In Sect. 2 we review the classical equations of motion in the continuum of an Abelian gauge theory with an axion field. We also discuss how to map that system into an Abelian gauge theory with chemical potential. In Sect. 3 we review the essence of the non-compact lattice formulation of an Abelian gauge theory, so that we set notation and conventions for the following sections. In Sect. 4 we build a lattice implementation of an axionic-interaction $a(x)\tilde{F}_{\mu\nu}F^{\mu\nu}$, deriving step by step the necessary ingredients to achieve a formulation consistent with the (lattice version) of the Bianchi identities, and solvable by an iterative scheme of evolution. We first consider in Sect. 4.1 the case of a homogeneous axion $a(x) = a(t)$, and later generalize to a fully inhomogeneous axion $a(x) = a(t, \mathbf{x})$ in Sect. 4.2. In Sect. 5 we finally discuss the lattice formulation of the Chern–Simons number $N_{\rm cs} \propto \int d^4x\, \mathcal{K}$ based on the lattice version(s) of $\mathcal{K} = \tilde{F}_{\mu\nu}F^{\mu\nu}$ developed in Sect. 4. We put special care in the need to achieve a lattice formulation that admits a total derivative representation for $\mathcal{K}$ as in Eq. (2). In Sect. 6 we summarize our results and discuss some of the potential applications in particle physics and cosmology.

2. Abelian gauge theory with an axion. Theory in the continuum

Let us begin by considering the action of an Abelian gauge theory in flat space-time. We chose metric signature $\eta_{\mu\nu} = \eta^{\mu\nu} = (-,+,+,+)$, and consider a 'Higgs' sector as $-\mathcal{L}_\varphi = (D_\mu\varphi)^*(D^\mu\varphi) + V(\varphi^*\varphi)$, with $\varphi = (\varphi_1 + i\varphi_2)/\sqrt{2}$ a $U(1)$ charged field [with $\varphi_i \in \Re$], $D_\mu \equiv \partial_\mu - ieA_\mu$ the covariant derivative, $A_\mu = (\phi, \vec{A})$ the gauge field, and e the gauge coupling strength. Including the presence of an axion-type field $a(x)$ linearly coupled to the *Pontryagin* density $F_{\mu\nu}\tilde{F}^{\mu\nu}$ of the U(1) gauge field, the action reads

$$\begin{aligned} S &= -\int d^4x \left(\mathcal{L}_\varphi + \frac{1}{4e^2}F_{\mu\nu}F^{\mu\nu} + \mathcal{L}_a - \frac{1}{(4\pi)^2}\frac{a}{M}F_{\mu\nu}\tilde{F}^{\mu\nu}\right) \\ &= \int d^4x \left(-\mathcal{L}_\varphi + \frac{1}{2e^2}\left(\vec{E}^2 - \vec{B}^2\right) + \frac{1}{2c_s^2}\dot{a}^2 - \frac{1}{2}|\nabla a|^2 + \frac{1}{4\pi^2}\frac{a}{M}\vec{E}\vec{B}\right), \end{aligned} \tag{3}$$

where $-\mathcal{L}_a \equiv \frac{1}{2c_s^2}(\partial_0 a)^2 - \frac{1}{2}(\partial_i a)(\partial_i a)$ represents the axion sector. The field strength and its dual are defined as usual by $F_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu$ and $\tilde{F}_{\mu\nu} \equiv \frac{1}{2}\epsilon_{\mu\nu\alpha\beta}F^{\alpha\beta}$, with $\epsilon_{\mu\nu\alpha\beta}$ the completely anti-symmetric tensor in four dimensions, with $\epsilon^{0123} = -\epsilon_{0123} \equiv +1$. We define the electric and magnetic fields as $E^i = E_i = \dot{A}_i - \partial_i\phi$ and $B^i = B_i = \epsilon_{ijk}\partial_j A_k$, so that $F_{\mu\nu} = (\delta_{\mu 0}\delta_{\nu i} - \delta_{\mu i}\delta_{\nu 0})E^i + (\delta_{\mu i}\delta_{\nu j} - \delta_{\mu j}\delta_{\nu i})\epsilon_{ijk}B^k$. Using $F_{\mu\nu}F^{\mu\nu} = 2(|\vec{B}|^2 - |\vec{E}|^2)$ and $F_{\mu\nu}\tilde{F}^{\mu\nu} = +4\vec{E}\vec{B}$, we arrive at the final vectorial expressions in Eq. (3).

Lagrangian Eq. (3) describes a system of scalar electro-dynamics in the presence of an axion-like field $a(x)$, with M some mass scale undetermined at this point. Note that we maintain explicitly the speed of propagation of the axion c_s^2 as a free parameter, as this will be convenient for us later on. Action Eq. (3) is invariant under the transformations $\varphi(x) \to e^{+i\beta(x)}\varphi(x)$, $A_\mu(x) \to A_\mu(x) + \partial_\mu\beta(x)$, with $\beta(x) \in \Re$ and $e^{i\beta(x)} \in U(1)$. Varying the action, one obtains the equations of motion (EOM)

$$D_\mu D^\mu \varphi = V_{,\varphi^*}\,, \tag{4}$$

$$\partial_\nu F^{\mu\nu} - \frac{e^2}{4\pi^2}\frac{a}{M}\partial_\nu\tilde{F}^{\mu\nu} = e^2 j^\mu + \frac{e^2}{4\pi^2}\frac{\partial_\nu a}{M}\tilde{F}^{\mu\nu}\,, \tag{5}$$

$$\partial_0\partial_0 a - c_s^2\partial_i\partial_i a = \frac{c_s^2}{(4\pi)^2 M}F_{\mu\nu}\tilde{F}^{\mu\nu}\,, \tag{6}$$

where the (unit-charge) current is defined as $j^\mu = 2\mathrm{Im}\{\varphi^* D^\mu\varphi\}$, so that

$$j_\mu = (\rho, \vec{J}) \equiv (2\mathrm{Im}\{\phi^*\dot{\phi}\}, 2\mathrm{Im}\{\phi^*\vec{D}\phi\}) \tag{7}$$

Eqs. (4)–(6) can be rewritten in a vectorial form as

$$D_o D_o\varphi - \vec{D}\vec{D}\varphi = -V_{,|\varphi|^2}\varphi \tag{8}$$

$$\dot{\vec{E}} + \vec{\nabla}\times\vec{B} + \frac{e^2}{4\pi^2}\frac{a}{M}(\dot{\vec{B}} - \vec{\nabla}\times\vec{E}) = e^2\vec{J} - \frac{e^2}{4\pi^2 M}\dot{a}\vec{B} + \frac{e^2}{4\pi^2 M}\vec{\nabla}a\times\vec{E} \tag{9}$$

$$\vec{\nabla}\vec{E} + \frac{e^2}{4\pi^2}\frac{a}{M}\vec{\nabla}\vec{B} = e^2\rho - \frac{e^2}{4\pi^2 M}\vec{\nabla}a\cdot\vec{B} \tag{10}$$

$$\ddot{a} - c_s^2\vec{\nabla}^2 a = \frac{c_s^2}{4\pi^2 M}\vec{E}\cdot\vec{B}\,, \tag{11}$$

with Eq. (10) representing the Gauss constraint in the presence of an axion.

As mentioned in Section 1, it is well known that the Pontryagin density represents a topological term, as it can be written as a total derivative $F_{\mu\nu}\tilde{F}^{\mu\nu} = \partial_\mu K^\mu$. This is reflected by the Bianchi identities, i.e. the term $\partial_\nu\tilde{F}^{\mu\nu} = 0$ in Eq. (5), or equivalently its vectorial counterparts $(\partial_t\vec{B} - \vec{\nabla}\times E) = 0$ in Eq. (9), and $\vec{\nabla}\vec{B} = 0$ in Eq. (10). Those terms simply represent vanishing contributions in the EOM, so it is customary to remove them. Despite their null contribution, it is nonetheless convenient for us to keep such terms in the EOM. The reason for this will become clear, however, only in Sec. 4, after we introduce the lattice discretization scheme(s) for the action Eq. (3).

For the time being, let us simply note now that due to the topological nature of $F_{\mu\nu}\tilde{F}^{\mu\nu}$, action Eq. (3) is also ('topologically') invariant under $a(x) \to a(x) + C$, with C an arbitrary constant. This is reflected in the fact that the linear coupling of $a(x)$ to the Pontryagin density, $\int d^4x\, a(x)\, F_{\mu\nu}\tilde{F}^{\mu\nu}$, represents a derivative coupling: the total derivative nature of $F_{\mu\nu}\tilde{F}^{\mu\nu} = \partial_\mu K^\mu$, after integration by parts, gives $\int d^4x\, K^\mu \partial_\mu a(x)$. Once the Bianchi identities are considered, the terms proportional to $a(x)$ in Eq. (5) [equivalently in Eqs. (9), (10)] disappear, as it should for a derivative coupling. As we will see later in Sec. 4, the lattice equivalent of the Bianchi identities, and hence the topological nature of the lattice equivalent of $F_{\mu\nu}\tilde{F}^{\mu\nu}$, depend crucially on the lattice discretization scheme. The lattice equivalent terms to $\propto \vec{\nabla}\vec{B}$, $\propto (\partial_t \vec{B} - \vec{\nabla} \times E)$ in the discrete EOM, are actually not granted to vanish by default. Achieving such a goal will represent, in fact, a guiding principle towards the construction of a correct lattice formulation of $F_{\mu\nu}\tilde{F}^{\mu\nu}$, admitting a total derivative representation on the lattice.

Let us remark that the *shift* symmetry enjoyed by $a(x)$, linearly coupled to the Pontryagin density, is at the heart of the original introduction of the axion as a solution for the strong CP problem (in that case the QCD axion is of course coupled to $\mathrm{Tr}\, \tilde{G}_{\mu\nu}G^{\mu\nu}$, with $G_{\mu\nu}$ the gluon field strength). Once $a(x)$ is considered as a dynamical field, the interaction $a(x)F_{\mu\nu}\tilde{F}^{\mu\nu}$ in Eq. (3) leads naturally to extra contributions in the EOM. Assuming a fully space-time dependent axion field, naturally leads to a contribution in Eq. (5) as $\propto \tilde{F}^{\mu\nu}\partial_\nu a$, or equivalently by the vectorial counterparts $\propto (-\dot{a}\vec{B} + \vec{\nabla}a \times \vec{E})$ and $\propto \vec{\nabla}a \cdot \vec{B}$ in Eq. (9) and Eq. (10), respectively. Besides, the Pontryagin density $F_{\mu\nu}\tilde{F}^{\mu\nu}$ acts as a source for $a(x)$ in the *rhs* of Eq. (11). The promotion of $a(x)$ into a dynamical field can therefore affect notably the dynamics of the system with respect to standard scalar electrodynamics described by Eq. (3) with $a(x) = 0$.

2.1. Mimicking a chemical potential

Interestingly, through an adequate interpretation of field variables and parameters, Eq. (3) can be mapped into the description of a gauge theory with a chemical potential μ for chiral fermions (for more details see [73]). Starting from Eq. (3) will allow us, through a formal trick, to bring up a Lagrangian formulation into this problem. In order to see this, let us begin by demanding that $a(x) = a(t)$ is a spatially homogeneous field, so that

$$\vec{\nabla}a = 0\,. \tag{12}$$

We then introduce the following convenient 'dimensionally reduced' variables

$$a \equiv \alpha M\,, \quad \dot{a} \equiv \mu M\,, \tag{13}$$

so that Eq. (3) is reduced to

$$\begin{aligned} S = \int d^4x \left\{ |D_0\varphi|^2 - (\vec{D}\varphi)^*(\vec{D}\varphi) - V(\varphi^*\varphi) + \frac{1}{2e^2}\left(\vec{E}^2 - \vec{B}^2\right) \right\} \\ + \lim_{V\to\infty} \left\{ \int dt\, \frac{\dot{\alpha}^2}{2c_s^2} \int_V M^2 d^3x + \int dt\, \frac{\alpha}{4\pi^2} \int_V d^3x\, \vec{E}\vec{B} \right\}. \end{aligned} \tag{14}$$

As we will see next, the requisite to describe a gauge theory at high temperatures and in the presence of a chemical potential, will fix the mass scale M and parameter c_s^2, see Eq. (21). We will describe first, however, the new dynamical equations that follow from minimizing the new re-written action.

Varying Eq. (14) we obtain the equations of motion of the system, which we write directly in a vectorial form as

$$D_o D_o \varphi - D_j D_j \varphi = -V_{,|\varphi|^2}\varphi \tag{15}$$

$$\dot{\vec{E}} + \vec{\nabla} \times \vec{B} = e^2 \vec{J} - \frac{e^2}{4\pi^2}\mu \vec{B} - \frac{e^2}{4\pi^2}\alpha(\dot{\vec{B}} - \vec{\nabla} \times \vec{E}) \tag{16}$$

$$\vec{\nabla}\vec{E} = e^2 \rho - \frac{e^2}{4\pi^2}\alpha \vec{\nabla}\vec{B} \quad \text{(Gauss Constraint)} \tag{17}$$

$$\dot{\mu} = \frac{c_s^2}{4\pi^2}\frac{1}{M^2}\lim_{V\to\infty}\frac{1}{V}\int_V d^3x\ \vec{E}\cdot\vec{B} \tag{18}$$

Once again, let us note that the terms $\propto \alpha(\dot{\vec{B}} - \vec{\nabla} \times E)$ in Eq. (9) and $\propto \alpha \vec{\nabla}\vec{B}$, which vanish in the continuum, are only maintained in the above equations for later convenience when discretising the system in Sect. 4.

We can now fix the mass scale M and the parameter c_s^2 to appropriate values, so that the set of Eqs. (15)–(18) properly describe an Abelian gauge theory with the chemical potential μ for chiral fermionic charge. In particular, the EOM of a chemical potential follows from the anomaly equation [74,75], and in our case has the form [72]

$$\dot{\mu} = \frac{3}{\pi^2}\frac{1}{T^2}\frac{1}{V}\int_{V\to\infty} d^3x\ \vec{E}\cdot\vec{B} \tag{19}$$

In light of Eq. (18), we can identify

$$\frac{c_s^2}{4M^2} = \frac{3}{T^2}\,, \tag{20}$$

so that we can fix the parameters (for instance) to

$$M^2 = \frac{T^2}{12}\,, \qquad c_s^2 = 1 \tag{21}$$

Let us note that in the original action Eq. (3), c_s^2 represents the speed of propagation of the axion field. However, as we are considering the axion now as a homogeneous field $a(x) = a(t)$, there is no propagation, only time evolution. Hence c_s^2 represents simply a free parameter of the theory. The identification in Eq. (21) with the speed of light is just a convenient choice. Had we chosen a relation between M^2 and T^2 different than in Eq. (21), we would require a value $c_s^2 \neq 1$ in order to satisfy Eq. (20), and yet we would be describing the same theory. Only the ratio Eq. (20) matters.

3. Part I. Lattice formulation of Abelian gauge theories to order $\mathcal{O}(dx_\mu^2)$, scalar-electrodynamics

In this section we briefly summarize the basics of the lattice formulation of a gauge theory. We focus, for convenience, in the non-compact formulation of an Abelian gauge theory (for related discussion see, e.g. [76]). We just intent to set notation and basic concepts, which we will be used later on when discussing the lattice formulation of an Abelian gauge theory with an axion. A reader already familiar with lattice gauge invariant techniques can skip this section and jump directly into Sect. 4.

Let us first set notation. A lattice point $n = (n_o, \vec{n}) = (n_o, n_1, n_2, n_3)$ displaced in the μ-direction by one unit lattice spacing, $n + \hat{\mu}$, will be often referred as $n + \mu$ or by $+\mu$, e.g. $\varphi_{+\mu} \equiv \varphi(n + \hat{\mu})$, $A_{\mu,+\nu} \equiv A_\mu(n + \frac{1}{2}\hat{\mu} + \hat{\nu})$, etc. We denote the lattice spacing as Δx and the time step as Δt, but we will we will speak loosely of a correction of order $\mathcal{O}(dx)$, independently or whether we are referring to $\mathcal{O}(\Delta t)$ or $\mathcal{O}(\Delta x)$. Note that we will not consider summation over repeated indices. We define lattice *links* as usual, with $U_\mu \equiv U_\mu(n + \frac{1}{2}\hat{\mu}) \equiv \exp\{-i \int_{x(n)}^{x(n+\hat{\mu})} A_\mu(x')dx'^\mu\} \simeq \exp\{-idx^\mu A_\mu(n + \frac{1}{2}\hat{\mu})\}$. We also define $U_{-\mu} \equiv U^*_{\mu,-\mu} \equiv U^*_\mu(n - \frac{1}{2}\hat{\mu}) \simeq \exp\{+idx^\mu A_\mu(n - \frac{1}{2}\hat{\mu})\}$. Forward (+) and backward (-), ordinary and covariant derivatives, are defined in the lattice by

$$\Delta^\pm_\mu \phi \equiv \tfrac{\pm 1}{dx}(\phi_{\pm\mu} - \phi)\,, \qquad (D^\pm_\mu \varphi) \equiv \tfrac{\pm 1}{dx}(U_{\pm\mu}\varphi_{\pm\mu} - \varphi)\,. \tag{22}$$

A lattice gauge transformation under $U(1)$ corresponds to

$$\varphi(n) \longrightarrow e^{+i\beta(n)}\varphi(n)\,, \quad A_\mu(n + \frac{1}{2}\hat{\mu}) \longrightarrow A_\mu(n + \frac{1}{2}\hat{\mu}) + \Delta^+_\mu \beta(n + \frac{1}{2}\hat{\mu})\,, \tag{23}$$

with β an arbitrary function of n. Links and covariant derivatives transform then as $U_{\pm\mu,n} \longrightarrow e^{i\beta}\, U_{\pm\mu,n}\, e^{-i\beta_{\pm\mu}}$, and $D^\pm_\mu \varphi \longrightarrow e^{i\beta}\, D^\pm_\mu \varphi$. We can build a gauge invariant lattice action (for the time being ignoring the axion field), using a non-compact formulation, like

$$\begin{aligned} S^L_{\rm AH} = \Delta t \Delta x^3 \sum_{\vec{n},t} \Big[&(D^+_o\varphi)^\dagger (D^+_o\varphi) - \sum_j (D^+_j\varphi)^\dagger (D^+_j\varphi) - V(\varphi\varphi^*, \phi) \\ &+ \frac{1}{2e^2}\sum_i \left(\Delta^+_o A_i - \Delta^+_i A_o\right)^2 - \frac{1}{4e^2}\sum_{i,j}(\Delta^+_i A_j - \Delta^+_j A_i)^2 \Big]. \end{aligned} \tag{24}$$

The lattice gauge invariance (based on the transformations defined above) of this action is rather explicit. We will refer to Eq. (24) as the *Abelian–Higgs* (AH) lattice action. Varying Eq. (24) with respect to the different fields, we obtain the lattice equivalent of the dynamical equations, which read (taking the Coulomb Gauge $A_o = 0 \leftrightarrow U_o = 1$)

$$\Delta^-_o \Delta^+_o \varphi - \sum_i D^-_i D^+_i \varphi + V_{,\varphi^*} = 0 \tag{25}$$

$$\Delta^-_o \Delta^+_o (A_i) - \sum_j \left(\Delta^-_j \Delta^+_j (A_i) - \Delta^+_i \Delta^-_j (A_j)\right) = 2e^2 {\rm Im}\{\varphi^* D_i \varphi\} \tag{26}$$

$$\sum_i \Delta^-_i \Delta^+_o (A_i) = 2e^2 {\rm Im}\{\varphi^* \Delta^+_o \varphi\} \quad \text{(Gauss constraint)} \tag{27}$$

Action Eq. (24), and hence the EOM Eqs. (25)–(27), reproduce to order $\mathcal{O}(dx^2)$ the continuum theory in the absence of an axion field ($a(x) = 0$). In order to see this, it is crucial to make a suitable interpretation of the lattice sites where each lagrangian operator naturally 'lives', so that all terms involved in a derived lattice EOM, live in the same lattice site (the lattice site where different equations live, do not need however to be the same). Denoting by l the natural lattice site where each operator lives, and by $\vec{x} \equiv l dx$ the physical coordinate where the continuum limit is reproduced, we can easily obtain the continuum limit of the lattice operators in Action Eq. (24) as

$$|D_\mu^+\varphi|^2(l)\big|_{l\equiv n+\frac{\hat\mu}{2}} \to |D_\mu\varphi|^2(x)\big|_{x=(n+\frac{1}{2}\hat\mu)dx} + \mathcal{O}(dx^2)\,, \tag{28}$$

$$\left(\Delta_\mu^+ A_\nu - \Delta_\nu^+ A_\mu\right)^2(l)\big|_{l\equiv n+\frac{\hat\mu}{2}+\frac{\hat\nu}{2}} \to F_{\mu\nu}^2(x)\big|_{x=(n+\frac{1}{2}\hat\mu+\frac{\hat\nu}{2})dx} + \mathcal{O}(dx^2)\,. \tag{29}$$

For the EOM Eqs. (25)–(27) we expect then a similar result. In the case of the charged scalar field EOM, $D_\mu^-(D_\mu^+\varphi)$ lives naturally at $l = \left(n + \frac{1}{2}\hat\mu\right) - \frac{1}{2}\hat\mu = n$, and thus we obtain

$$(D_\mu^- D_\mu^+\varphi)(l)\big|_{l\equiv n} \to (D_\mu D_\mu\varphi)(l)\big|_{x\equiv ndx} + \mathcal{O}(dx^2) \tag{30}$$

Consistently, the term $V_{,\varphi^*}$ in Eq. (27) [which reproduces the continuum to any order in dx], lives naturally at the same lattice site $l = n$. All terms in the discrete EOM Eq. (27) live therefore at $l = n$, so that Eq. (27) reproduces correctly the continuum Eq. (15) up to $\mathcal{O}(dx^2)$ corrections.

In the case of the EOM of the gauge fields, each term can be expanded as

$$\Delta_o^-\Delta_o^+ A_i(l)\big|_{l\equiv n+\frac{\hat i}{2}} \to (\ddot{A}_i)(x)\big|_{x\equiv ndx+\frac{\hat 0}{2}dt} + \mathcal{O}(dt^2) \tag{31}$$

$$\Delta_j^-\Delta_j^+ A_i(l)\big|_{l\equiv n+\frac{\hat i}{2}} \to (\partial_j^2 A_i)(x)\big|_{x\equiv(n+\frac{\hat i}{2})dx} + \mathcal{O}(dx^2) \tag{32}$$

$$\Delta_i^+\Delta_j^- A_j(l)\big|_{l\equiv n+\frac{\hat i}{2}} \to (\partial_i\partial_j A_j)(x)\big|_{x\equiv(n+\frac{\hat i}{2})dx} + \mathcal{O}(dx^2) \tag{33}$$

$$\mathrm{Im}\{\varphi^* D_i^+\varphi\}(l)\big|_{l\equiv n+\frac{\hat i}{2}} \to \mathrm{Im}\{\varphi^* D_i\varphi\}(x)\big|_{x\equiv(n+\frac{\hat i}{2})dx} + \mathcal{O}(dx^2)\,, \tag{34}$$

and a similar analysis applies for the terms in Eq. (27) [Gauss constraint] when expanded around their natural lattice site $l = n + \frac{1}{2}\hat 0$. Thus, interpreting the lattice operators involved in the gauge field discrete equations as living at $l = n + \frac{1}{2}\hat 0$ for the Gauss constraint Eq. (27), or at $l = n + \frac{1}{2}\hat i$ for the Dynamical Eq. (26), leads to reproduce correctly the continuum equations [in the absence of an axion] Eqs. (16)–(17), up to $\mathcal{O}(dx^2)$ corrections.

4. Part II. Lattice formulation of Abelian gauge theories to order $\mathcal{O}(dx_\mu^2)$, axionic-coupling

Let us now turn our discussion into the formulation of a proper lattice equivalent for the continuum interaction between the gauge fields and an axion, $S_{ac} \equiv -\frac{1}{(4\pi)^2}\int d^4x \frac{a}{M} F_{\mu\nu}\tilde{F}^{\mu\nu}$. In this section we aim to a general formulation of an Abelian gauge theory with an axion field. For simplicity we will first start dealing with the case of a homogeneous axion $\alpha(x) = \alpha(t)$ in Sect. 4.1. Our findings in Sect. 4.1 will be actually applicable as well to the case of a fully inhomogeneous axion $\alpha(x) = \alpha(t, \mathbf{x})$, but as the latter introduces further complications, we postpone the discussion about a fully spatially-dependent axion for Sect. 4.2.

We will introduce the dimensionally reduced variables $\alpha \equiv \frac{a}{M}$, $\mu \equiv \dot\alpha$ defined in Eq. (13), so we prevent this way having to drag the scale M along our derivations. Given our choice of metric signature $(-, +, +, +)$ and gauge field representation $A_\mu \equiv (\phi, \vec{A})$, we find $F_{\mu\nu}\tilde{F}^{\mu\nu} = +4\vec{E}\vec{B}$, so that we can write the above continuum action as

$$S_{ac} \equiv \frac{1}{4\pi^2}\int d^4x\, \alpha\, \vec{E}\vec{B}\,. \tag{35}$$

We will refer to the interaction described by Eq. (35) as an *axionic-coupling*. Our main aim now is to formulate a lattice version of the continuum action Eq. (35), from which to derive a discrete version of the EOM in the continuum Eqs. (8)–(11) [or Eqs. (15)–(18) in the case of a homogeneous axion mimicking a chemical potential]. In light of the EOM in the continuum, we can foresee three possible problems arising when formulating a lattice version of Eq. (35):

i) The terms $\alpha(-\dot{\vec{B}} + \vec{\nabla} \times \vec{E})$ and $\alpha\vec{\nabla}\vec{B}$ in Eqs. (16), (17), vanish in the continuum thanks to the Bianchi identities $\partial_\nu \tilde{F}^{\mu\nu} = 0$, which are equivalent to $\dot{\vec{B}} = \vec{\nabla} \times \vec{E}$ and $\vec{\nabla}\vec{B} = 0$. The equivalent terms in the discrete EOM are however not granted to vanish, as this depends on the lattice representation of the electric and magnetic fields, and on the choice of lattice derivatives. It is therefore crucial that we find a lattice representation of S_{ac} so that the equivalent discrete terms in the lattice EOM vanish identically (or at least to the same order in the lattice spacing to which the discrete EOM reproduce the continuum). In other words we seek a lattice formulation of S_{ac} so that the lattice expression of $\mathcal{K} = F_{\mu\nu}\tilde{F}^{\mu\nu}$ is topological admitting a total derivative representation $\mathcal{K} = \Delta_\mu^+ K^\mu$.

ii) Assuming that a correct version of the Bianchi identities follows naturally from a given topological lattice formulation of $F_{\mu\nu}\tilde{F}^{\mu\nu}$, another problem may arise. The terms $\propto \mu\vec{B}$ and $\propto \vec{E}\vec{B}$ in Eqs. (9), (11), indicate possible obstructions to achieving an explicit scheme to solve iteratively the set of lattice coupled equations reproducing the continuum Eqs. (8)–(11). Even though an implicit scheme for finite difference coupled equations can be solved by non-linear numerical methods (applied at every lattice site), this makes the continuum limit less transparent, and results typically in a computationally more expensive procedure (if not unfeasible). Therefore, achieving a simple explicit scheme for solving iteratively the set of lattice coupled equations that will mimic the continuum EOM, will be a strong requisite, unless we prove that such a scheme cannot be developed.

iii) When considering a fully inhomogeneous axion-like field $a(x)$, terms proportional to spatial variations $\propto \nabla a(x)$ appear in the EOM. In particular, the term $\nabla a \times \vec{E}$ in the rhs of electric field evolution equation Eq. (9) $\dot{E}_i = [...] + \frac{e^2}{4\pi^2}(\nabla a \times \vec{E})_i$, introduces a 'mixing' of the E_i component, naturally living in the i-th direction, with the components E_j, E_k, naturally living along the transverse directions to the ith axis. As electric field components live naturally in between lattice sites (at the *links*), this will imply a mixture of orthogonal links. Some spatial averaging over neighboring position along the i-th axis will be needed, to force the term $\nabla a \times \vec{E}$ (in the rhs of the equation) to live at the same location where E_i lives (in the lhs of the equation). This will create a non-local interaction, possibly preventing the development of an explicit iterative scheme to solve the resulting set of finite difference coupled equations.

In the following we will investigate various lattice versions of the interaction $\alpha\,\vec{E}\vec{B}$, determining their 'appropriateness' based on the ability of each lattice formulation to address the previous criteria *i)*–*iii)*.

4.1. Abelian gauge theory with a homogeneous axion

We will consider in this section the simplest case of a gauge theory with a homogeneous axion $\alpha(x) = \alpha(t)$. As discussed in Sect. 2, this case can be mapped into the description of a gauge theory in the presence of a chemical potential $\mu = \dot{\alpha}$. Both in Sect. 4.1.1 and 4.1.2 we will stick to $a(x) = a(t)$, simply to make more transparent the discussion about the importance of achieving a good lattice representation of the Bianchi identities, as well of an explicit iterative scheme to solve the set of coupled lattice EOM. The conclusions that will be reached in Sects. 4.1.1, 4.1.2 will be equally applicable to the case of a fully inhomogeneous axion $a(x) = a(t, \mathbf{x})$, which we will address in Sect. 4.2, building up from our previous findings on the homogeneous case.

4.1.1. Lattice formulation of the Bianchi identities

Let us first attempt to build S_{ac} using the basic lattice definition of electric and magnetic fields, $E_i \equiv (\Delta_o^+ A_i - \Delta_i^+ A_o)$ and $B_i \equiv \epsilon_{ijk}\Delta_j^+ A_k$, like

$$S_{ac}^{L(1)} \propto \sum_{\vec{n},n_o} \alpha \sum_i E_i B_i = \sum_{\vec{n},n_o} \alpha \sum_i (\Delta_o^+ A_i - \Delta_i^+ A_o)\epsilon_{ijk}\Delta_j^+ A_k \,. \tag{36}$$

This operator describes the continuum action up to order $\mathcal{O}(dx^2)$, as we showed in Sect. 3 that $F_{\mu\nu} \equiv (\Delta_\mu^+ A_\nu - \Delta_\nu^+ A_\nu)$ reproduces the continuum expression up to order $\mathcal{O}(dx^2)$, when interpreting that $F_{\mu\nu}$ lives at $n + \frac{1}{2}\hat{\mu} + \frac{1}{2}\hat{\nu}$. Varying Eq. (36) with respect A_i and A_o (recall that we are assuming now $\alpha(x) = \alpha(t)$ homogeneous), produces respectively terms as $\propto \alpha[\Delta_o^- B_i - (\nabla^- \times \vec{E})_i] \neq 0$ and $\propto \alpha \sum \Delta_i^- B_i \neq 0$. As expected, these resemble the continuum analogues $\propto \alpha(\partial_o \vec{B} - \vec{\nabla} \times \vec{E}) = 0$ and $\propto \alpha\vec{\nabla}\vec{B} = 0$ in Eqs. (16), (17). However, contrary to the continuum analogues, they do not vanish. As anticipated, generating the appropriated vanishing terms in the discrete EOM (due to the lattice version of the Bianchi identities), is not automatically granted.

The problem arises because the choice of Eq. (36) as an lattice operator is not consistent with the symmetries of the lattice. Note that Eq. (36) consists in the product of three fields, α, E_i and B_i that live, not only in different lattice sites, also at different time steps, e.g. E_i lives at $(n_o + \frac{1}{2}, \vec{n} + \frac{1}{2}\hat{\imath})$, whereas B_i lives at $(n_o, \vec{n} + \frac{1}{2}\hat{\jmath} + \frac{1}{2}\hat{k})$. The solution passes trough "symmetrizing" the factors in the operator, so that the factors built up from different fields, live nonetheless at the same site. Let us define

$$E_i^{(2)} \equiv \frac{1}{2}(E_i + E_{i,-i})(l)\Big|_{l\equiv n+\frac{\hat{0}}{2}} \tag{37}$$

$$E_i^{(4)} \equiv \frac{1}{4}(E_i + E_{i,-i} + E_{i,-0} + E_{i,-i-0})(l)\Big|_{l\equiv n} \tag{38}$$

$$B_i^{(4)} \equiv \frac{1}{4}(B_i + B_{i,-j} + B_{i,-k} + B_{i,-j-k})(l)\Big|_{l\equiv n}, \tag{39}$$

so that each of these fields reproduce the continuum expression to order $\mathcal{O}(dx^2)$. We note that $B_i^{(4)}$ corresponds to the well-known 'clover' definition of a magnetic field at a site. For later convenience we also define

$$E_i^{(8)} \equiv \frac{1}{2}\left(E_i^{(4)} + E_{i,+i}^{(4)}\right), \qquad B_i^{(8)} \equiv \frac{1}{2}\left(B_i^{(4)} + B_{i,+i}^{(4)}\right), \tag{40}$$

which also reproduce the continuum to order $\mathcal{O}(dx^2)$.

A 'symmetrized' operator that reproduces the continuum expression of S_{ac} at $l = (\vec{n}, n_o)$ to order $\mathcal{O}(dx^2)$, can be proposed based on the above expressions,

$$S_{ac}^{L(2)} \propto \sum_{\vec{n},n_o} \alpha \sum_i E_i^{(4)} B_i^{(4)} \,. \tag{41}$$

Varying Eq. (41) with respect A_i, produces a term in the discrete EOM of the gauge field as $\alpha[\sum_{j,k} \epsilon_{ijk}(\Delta_j^+ + \Delta_j^-)E_k^{(8)} - (\Delta_o^+ + \Delta_o^-)B_i^{(8)}] = 0$, which resembles the continuum term $\alpha(\epsilon_{ijk}\partial_j E_k - \partial_o B_i) = 0$ in Eq. (16), and it vanishes. Similarly, when varying Eq. (41) with respect A_o, we produce a vanishing term $\alpha \sum_i (2 + dt\Delta_t^+)\Delta_i^- B_i^{(8)} = 0$, which again resembles the term in the continuum $\alpha \partial_i B_i = 0$ in Eq. (17). This shows that Eq. (41) represents a good lattice candidate from which to derive [together with action Eq. (24)] a set of coupled finite difference equations reproducing correctly the functional form of continuum EOM. As we will see next, there is however another problem to be circumvented, related to the solubility of a set of coupled finite difference equations.

4.1.2. Explicit scheme for real time evolution

The operator Eq. (41) proposed to represent an axionic coupling, exhibits various features: *i*) it reproduces correctly the continuum term to order $\mathcal{O}(dx^2)$, and *ii*) it reproduces correctly a lattice version of the Bianchi identities, so that the discrete EOM reproduce correctly the functional form of the dynamical Eqs. (15)–(18) in the continuum. In fact, varying Eq. (41) with respect to the gauge fields, generates a term $\propto \frac{1}{2}(\mu_{-0}B_i^{(8)} + \mu B_{i,+0}^{(8)})$, which reduces correctly to the continuum term $\mu\vec{B}$ in Eq. (16), to order $\mathcal{O}(dx^2)$. At the same time, varying Eq. (41) with respect to $\alpha(t)$, generates a term $\propto \frac{1}{2}(E_i^{(2)} + E_{i,-0}^{(2)})B_i^{(4)}$ sourcing the chemical potential, which again reduces correctly to the continuum source term $\propto \vec{E}\vec{B}$ in Eq. (18), to order $\mathcal{O}(dx^2)$. The set of coupled discrete equations one obtains, cannot be put however in an explicit iterative scheme, because in order to find E_i we need μ and $A_{i,+0}$ (to obtain $B_{i,+0}^{(8)}$), and at the same time to find $A_{i,+0}$ and μ we need E_i. One would need to express the term $\mu B_{i,+0}^{(8)}$ in the gauge field EOM in terms of E_i, and then solve for E_i, but this would complicate the equations unnecessary. A simpler solution consists in choosing another lattice operator that upon variation over the gauge fields, prevents the duplication of the $\sim \mu B_i$ terms at the two different times. The duplication of these terms originated from Eq. (41) due to the fact that the electric field $E_i^{(4)}$ multiplying $\alpha B_i^{(4)}$ in the operator, is equivalent to the sum of electric fields at two time steps, $E_i^{(4)} \equiv \frac{1}{2}(E_i^{(2)} + E_{i,-0}^{(2)})$. Hence, when varying with respect to A_i, two terms of the form $\sim \mu B_i$ are generated, $(\mu_{-0}B_i^{(8)} + \mu B_{i,+0}^{(8)})$, each evaluated at a different time.

It is easy to build some lattice operator that verifies the last requisite, i.e. not involving the sum of two gauge field conjugate momenta (i.e. electric fields) at different times, like for example

$$S_{ac}^{L(3)} \propto \sum_{\vec{n},n_o} \alpha \sum_i E_i^{(2)} B_i^{(4)} \,. \tag{42}$$

This operator fails however in 'symmetrizing' the expression for $\vec{E}\cdot\vec{B}$ around a common time: as $B_i^{(4)}$ lives at integer times n_o whereas $E_i^{(2)}$ lives at time semi-integer times $(n_o + \frac{1}{2})$, the lattice equivalent to the terms that should be vanishing due to the discretized Bianchi identities, will fail to vanish, as it happened already with the operator $S_{ac}^{L(1)}$ Eq. (36).

A better solution is found if the lattice operator $\sim \alpha(E\cdot B)$ is built such that each element α, $\vec{E}$ and $\vec{B}$, live separately in a given common space-time site. In other words, contrary to the operator $S_{ac}^{L(3)}$ Eq. (42), where the electric and magnetic fields lived at different time steps separated away by half step $\frac{dt}{2}$, now both $\vec{E}$ and $\vec{B}$ must live at the same time step. As the natural time where electric fields live is $(n_o + \frac{1}{2})dt$, and given that we do not want to sum over electric fields at different times, the natural option will be to make the magnetic field to live in the same semi-integer time. There are 3 options for this,

$$S_{ac}^{L(4)} \propto \sum_{\vec{n},n_o} \alpha \sum_i E_i^{(2)} (B_i^{(4)} + B_{i+0}^{(4)}) \,, \tag{43}$$

$$S_{ac}^{L(5)} \propto \sum_{\vec{n},n_o} \alpha_{+0} \sum_i E_i^{(2)} (B_i^{(4)} + B_{i+0}^{(4)}) \tag{44}$$

$$S_{ac}^{L(6)} \propto \sum_{\vec{n},n_o}(\alpha+\alpha_{+0})\sum_i E_i^{(2)}(B_i^{(4)}+B_{i+0}^{(4)})\,. \tag{45}$$

Varying each of these action terms with respect to the gauge fields, we obtain correct vanishing versions of $\vec{\nabla}\vec{B}$ and $(\partial_t\vec{B}-\vec{\nabla}\times\vec{E})$ in the discrete equations of motion due to the lattice Bianchi identities, and generate the following terms in the gauge field EOM [recall that here we still consider $\alpha(x)=\alpha(t)$],

$$\begin{aligned}
\delta S_{ac}^{L(4)}=0 \quad &\Rightarrow \quad -\tfrac{e^2}{4\pi^2}\mu B_i^{(8)}\\
\delta S_{ac}^{L(5)}=0 \quad &\Rightarrow \quad -\tfrac{e^2}{4\pi^2}\mu B_i^{(8)}\\
\delta S_{ac}^{L(6)}=0 \quad &\Rightarrow \quad -\tfrac{e^2}{4\pi^2}\tfrac{1}{2}(\mu+\mu_{-0})B_i^{(8)}
\end{aligned}$$

From here we see that $S_{ac}^{L(6)}$ Eq. (45) does not allow for an explicit scheme of iteration[1], similarly as what it happened with $S_{ac}^{L(2)}$ Eq. (41). Only actions $S_{ac}^{L(4)}$ Eq. (43) and $S_{ac}^{L(5)}$ Eq. (44) allow for an explicit scheme of iteration, and in fact produce essentially an equivalent set of coupled discrete EOM.

In conclusion, although all operators $S_{ac}^{L(1)}$–$S_{ac}^{L(6)}$ reproduce correctly the continuum gauge-axionic interaction to order $\mathcal{O}(dx^2)$, $S_{ac}^{L(1)}$ Eq. (36) and $S_{ac}^{L(3)}$ Eq. (42) fail to generate vanishing terms in the discrete EOM from the lattice Bianchi identities, whereas $S_{ac}^{L(2)}$ Eq. (41) and $S_{ac}^{L(6)}$ Eq. (45) produce correctly null terms due to the lattice Bianchi identities, but fail to generate explicit iterative schemes for solving the set of coupled finite difference EOM. Only $S_{ac}^{L(4)}$ Eq. (43) and $S_{ac}^{L(5)}$ Eq. (44), produce correctly vanishing terms due to the lattice Bianchi identities, while maintaining an explicit iterative scheme for solving the set of lattice EOM. Actually, the functional form of $S_{ac}^{L(4)}$ Eq. (43) [equivalently $S_{ac}^{L(5)}$ Eq. (44)] indicates us something important: the natural time steps where a shift-symmetric field lives are also semi-integer times, and not integer steps as for ordinary scalar fields. Pseudo-scalar fields (independently of whether they are homogeneous as we have just required so far) must live in semi-integer times in the lattice. The kinetic term of the axion should therefore be defined differently compared to ordinary scalar fields, since we want to obtain a finite difference evaluated at integer times. In light of all this, we can interpret $S_{ac}^{L(4)}$ Eq. (43) and $S_{ac}^{L(5)}$ Eq. (44) as equivalent descriptions of a final suitable action.

Putting all together, the discretized action from where the dynamical effects of the presence of a homogeneous axion to be derived reads

$$S_{\alpha(t)}^{L}=\Delta t\Delta x^3\sum_{\vec{n},n_o}\left\{\frac{M^2}{2c_s^2}\left(\Delta_o^-\alpha\right)^2+\frac{1}{4\pi^2}\alpha\sum_i\frac{1}{2}E_i^{(2)}\left(B_i^{(4)}+B_{i,+0}^{(4)}\right)\right\}, \tag{46}$$

where it is important to note that α lives at space-time sites $(n_o+1/2,\vec{n})$.

It is perhaps relevant to stress that, at the end, the need for all the factors multiplying within a given operators living at the same space-time site $(l_o,\vec{l})$, is a crucial aspect for determining the right functional form the lattice operator. As we saw, however, this is not enough, as $S_{ac}^{L(2)}$ Eq. (41) verifies that, with $(l_o,\vec{l})=(n_o,\vec{n})$, but still has problems. One must first recognize the

[1] This occurs because even though there is a single electric field $E_i^{(2)}$ [hence defined at its natural time $(n_o+1/2)dt$], the latter is multiplied by $(\alpha+\alpha_{+0})$ with the axion-like field living at two different times.

natural space-time site where the operator lives. As we do not want to have the sum of electric fields at different times in the operator, the appropriate representation for the electric field is $E_i^{(2)}$, which lives in integer lattice sites, but semi-integer times, i.e. $(l_o, \vec{l}) = (n_o + 1/2, \vec{n})$. This implies, correspondingly, that the appropriate magnetic field representation must be $\frac{1}{2}(B_i^{(4)} + B_{i,+0}^{(4)})$, so that it also lives in $(l_o, \vec{l}) = (n_o + 1/2, \vec{n})$. The linear part in the (pseudo-)scalar field α, can then be made meaningfully defined only if α also lives at $(l_o, \vec{l}) = (n_o + 1/2, \vec{n})$.

The final set of equations of motion obtained from varying $S_{\rm AH}^L + S_{\alpha(t)}^L$ [Eq. (24) + Eq. (46)], mimicking a system with chemical potential $\mu \equiv \Delta_o^- \alpha$ at finite temperature T (recall $M = T/\sqrt{12}$, $c_s^2 = 1$), are (in the Coulomb gauge $A_o = 0$, i.e. $U_o = 1$)

$$
\begin{array}{rcll}
 & & \text{Equation} & \text{Natural site} \\
\pi & \equiv & \Delta_o^+ \varphi\,, & l \equiv (n_o + \frac{1}{2}, \vec{n}) \\
E_i & \equiv & \Delta_o^+ A_i\,, & l \equiv (n_o + \frac{1}{2}, \vec{n} + \frac{1}{2}\hat{i}) \\
\mu & \equiv & \Delta_o^- \alpha\,, & l \equiv (n_o, \vec{n}) \\
\Delta_o^- \pi & = & \sum_i D_i^- D_i^+ \varphi - V_{,\varphi^*} & l \equiv (n_o, \vec{n}) \\
\Delta_o^- E_i & = & 2e^2 {\rm Im}\{\varphi^* D_i^+ \varphi\} - (\Delta^- \times B)_i - \frac{e^2}{4\pi^2} \mu B_i^{(8)}\,, & l \equiv (n_o, \vec{n} + \frac{1}{2}\hat{i}) \\
\sum_i \Delta_i^- E_i & = & 2e^2 {\rm Im}\{\varphi^* \pi\} \quad \text{(Gauss constraint)}, & l \equiv (n_o + \frac{1}{2}, \vec{n}) \\
\Delta_o^+ \mu & = & \frac{3}{\pi^2}\frac{1}{T^2}\frac{1}{N^3} \sum_{\vec{n}} \frac{1}{2} \sum_i E_i^{(2)} (B_i^{(4)} + B_{i,+0}^{(4)})\,, & l \equiv (n_o + \frac{1}{2}, \vec{n})
\end{array}
\tag{47}
$$

Let us emphasize that the terms within each of the above equations live (as they should) at a given common natural space-time site (specifically indicated above in the rhs of each equation), around which we can expand each equation and reproduce the continuum analogue Eqs. (15)–(18), up to order $\mathcal{O}(dx^2)$.

4.2. Abelian gauge theory with an inhomogeneous axion

Let us just recall action Eq. (3) for a fully inhomogeneous axion-like field $a(x)$. Variation of this action produces the EOM Eqs. (8)–(11). Various differences arise with respect the set of Eqs. (15)–(11) describing an homogeneous field $a(x) = a(t)$. First, the gauge field EOM Eq. (9) includes now a term $\propto \vec{\nabla} a \times \vec{E}$. Secondly, the Gauss law Eq. (10) includes a term $\propto \vec{\nabla} a \cdot \vec{B}$. Third, the axion dynamics follows a (sourced) wave equation, where c_s^2 now plays the role of a real propagation speed. In other words, there are new terms affecting the dynamics (except in the Higgs sector) due to the spatial dependence of $a(x)$. Action Eq. (3) and the corresponding set of Eqs. (8)–(11), cannot be used anymore to describe the problem of an Abelian gauge theory with a chemical potential. They rather describe an Abelian gauge theory in the presence to a fully inhomogeneous axion field. We shall understand that from now on we are dealing with such scenario.

4.2.1. Implicit scheme for real time evolution

In order to find a lattice formulation for the interaction $a(x)\tilde{F}_{\mu\nu}F^{\mu\nu} \propto a\vec{E} \cdot \vec{B}$ where $a(x)$ is now an inhomogeneous field, we can proceed in the same manner as in Sect. 4.1, when $a(x) = a(t)$ was simply considered a homogeneous field. The same considerations apply now in order to find an appropriate lattice representation of the gauge-axion interaction. We can thus survey the same lattice implementations $S_{ac}^{L(1)}$–$S_{ac}^{L(6)}$ proposed in Sec. 4.1, as we know they all reproduce correctly the continuum interaction $a(x)\tilde{F}_{\mu\nu}F^{\mu\nu}$ to order $\mathcal{O}(dx^2)$. The spatial dependence of $a(x)$ does not change the fact that $S_{ac}^{L(1)}$ Eq. (36) and $S_{ac}^{L(3)}$ Eq. (42), fail again to generate vanishing terms in the discrete EOM due to the lattice Bianchi identities. We also find that $S_{ac}^{L(2)}$ Eq. (41) and $S_{ac}^{L(6)}$ Eq. (45) produce correctly null terms due to the lattice Bianchi identities, but fail again to generate explicit iterative schemes for solving the set of coupled finite difference EOM. The expressions $S_{ac}^{L(4)}$ Eq. (43) and $S_{ac}^{L(5)}$ Eq. (44) produce correctly vanishing terms in the gauge field discrete EOM due to the lattice Bianchi identities. However, contrary to the homogeneous $a(x) = a(t)$ case, $S_{ac}^{L(4)}$–$S_{ac}^{L(5)}$ do not lead now to an explicit iterative scheme for solving the set of lattice EOM when $a(x) = a(t, \mathbf{x})$ is inhomogeneous.

Let us see this more in detail, considering $S_{ac}^{L(4)}$ Eq. (43) as the lattice representation of the axion-gauge field interaction. We write the final lattice action mimicking to order $O(dx^2)$ the continuum action Eq. (3) as

$$\begin{aligned} S = S_{AH} + S_{axion} = \Delta t \Delta x^3 \sum_{\vec{n},t} \Bigg\{ & (D_o^+\varphi)^\dagger (D_o^+\varphi) - \sum_j (D_j^+\varphi)^\dagger (D_j^+\varphi) \\ & - V(\varphi\varphi^*, \phi) + \frac{1}{2e^2}\sum_i \left(\Delta_o^+ A_i - \Delta_i^+ A_o\right)^2 - \frac{1}{4e^2}\sum_{i,j}(\Delta_i^+ A_j - \Delta_j^+ A_i)^2 \\ & + \frac{1}{2c_s^2}\left(\Delta_o^- a\right)^2 - \frac{1}{2}\sum_i (\Delta_i^+ a)^2 + \frac{1}{4\pi^2}\frac{a}{M}\sum_i \frac{1}{2}E_i^{(2)}\left(B_i^{(4)} + B_{i,+0}^{(4)}\right) \Bigg\} \end{aligned} \tag{48}$$

Varying this action, we obtain a set of finite difference coupled equations,

$$\begin{aligned} \pi_\varphi &\equiv \Delta_o^+ \varphi\,, \\ E_i &\equiv \Delta_o^+ A_i\,, \\ \pi_a &\equiv \Delta_o^- a\,, \\ \Delta_o^- \pi_\varphi &= \sum_i D_i^- D_i^+ \varphi - V_{,\varphi^*}\,, \\ \Delta_o^- E_i &= 2e^2 \mathrm{Im}\{\varphi^* D_i^+ \varphi\} - \sum_{j,k}\epsilon_{ijk}\Delta_j^- B_k - \frac{e^2}{4\pi^2 M}\frac{1}{2}(\pi_a B_i^{(4)} + \pi_{a,+i} B_{i,+i}^{(4)}) \\ &\quad + \frac{e^2}{4\pi^2 M}\frac{1}{8}(2 + dx\Delta_i^+)\sum_\pm \sum_{jk}\epsilon_{ijk}\left\{[(\Delta_j^\pm a)E_{k,\pm j}^{(2)}] + [(\Delta_j^\pm a)E_{k,\pm j}^{(2)}]_{-0}\right\}, \\ \sum_i \Delta_i^- E_i &= 2e^2 \mathrm{Im}\{\varphi^* \pi\} - \frac{e^2}{4\pi^2 M}\frac{1}{8}\sum_\pm \sum_i (\Delta_i^\pm a)(B_i^{(4)} + B_{i,+0}^{(4)})_{\pm i}\,, \\ \Delta_o^+ \pi_a &= c_s^2 \sum_i \Delta_i^- \Delta_i^+ a + \frac{1}{4\pi^2}\frac{c_s^2}{M}\sum_i \frac{1}{2}E_i^{(2)}(B_i^{(4)} + B_{i,+0}^{(4)})\,, \end{aligned} \tag{49}$$

which reproduce to order $\mathcal{O}(dx^2)$ the set of continuum Eqs. (8)–(11), when expanding each equation around its natural lattice site. Note that the natural sites ascribed to each discrete EOM in Eqs. (49) coincide with those listed in the rhs of Eqs. (47), so we do not repeat them here. A simple inspection of the lhs of each equation suffices anyways to determine these sites, e.g. knowing that the lattice representation of the electric field $E_i = \Delta_o^+ A_i$ lives at $l = (n_o + 1/2, \vec{n} + \hat{i}/2)$, then equation $E_i \equiv [...]$ must be expanded around $x = ((n_o + 1/2)dt, (\vec{n} + \hat{i}/2)dx)$, $\Delta_o^- E_i = [...]$ around $x = (n_o dt, (\vec{n} + \hat{i}/2)dx)$, etc.

Unfortunately, the set of finite difference coupled Eqs. (49) cannot be solved with an explicit scheme. In fact, these equations can only be formally solved by a non-local solution, even though we started from a local Lagrangian Eq. (48). The reason for this is the following. Say we consider the $\hat{1}$-component of the curl product involving the electric field in the rhs of the gauge field EOM $\Delta_o^- E_1 = [...]$, i.e. $\sim [(\Delta a) \times \vec{E}^{(2)}]_1$. This term depends on $E_{2,+1}$ and $E_{3,+1}$, so the equation to update the $\hat{1}$-component of the electric field depends on $E_{2,+1}$ and $E_{3,+1}$, and analogously for the other electric field component equations. In other words, there is a first-neighbor coupling of the electric field components. This simply makes impossible to solve explicitly for the E_i components at a given lattice site (in a given time step), as we would need to know the electric field components at all other lattice sites (at the new time step).

The origin of this problem lies of course in the form of the interaction $\sim a\vec{E}\vec{B}$. In the moment $a(x) = a(\vec{x}, t)$ is inhomogeneous, this brings up the term $\vec{\nabla} a \times \vec{E}$ in the rhs of the gauge field continuum EOM Eq. (9), $\partial_t \vec{E} = [...]$. As in the lattice E_i lives at $\vec{n} + \hat{i}/2$, the equivalent lattice expression representing the continuum term $\sim (\vec{\nabla} a \times \vec{E})$ must be evaluated at both $\vec{n}$ and $\vec{n} + \hat{i}$. This explains in fact the $(2 + dx\Delta_i^+)$ operation in rhs of the equivalent discrete EOM $\Delta_o^- E_i = [...]$ within Eqs. (49). This turns non-local the set of coupled equations in finite differences Eqs. (49), hence making it unfeasible to solve them iteratively by an explicit scheme at each lattice site.

In conclusion, it does not seem possible to find a set of discrete equations reproducing to order $\mathcal{O}(dx^2)$ the dynamics of an Abelian gauge theory in the presence of a general axion-like field $a(x) = a(t, \mathbf{x})$, and at the same time being solvable by an explicit scheme. An approximate way around this difficulty can however be obtained by an implicit scheme as follows. Let us write the discrete equation evolving the electric fields, but writing down only the terms that prevented us from achieving an explicit scheme

$$\begin{aligned} E_{i,+\frac{\hat{0}}{2}} &= E_{i,-\frac{\hat{0}}{2}} + \Delta t\,[...] \\ &+ \Delta t \left(\frac{e^2}{4\pi^2 M} \frac{1}{8} (2 + dx\Delta_i^+) \sum_{\pm} \sum_{jk} \epsilon_{ijk} \left\{ [(\Delta_j^{\pm} a) E_{k,\pm j}^{(2)}]_{+\frac{\hat{0}}{2}} + [(\Delta_j^{\pm} a) E_{k,\pm j}^{(2)}]_{-\frac{\hat{0}}{2}} \right\} \right), \end{aligned} \tag{50}$$

where [...] represents all the terms in the rhs of the discrete equation which involve only the amplitude (or spatial gradients) of the gauge field A_i, but not the electric field. Now let us suppose that we approximate the electric field term in the rhs of Eq. (50) as

$$\left\{ [(\Delta_j^{\pm} a) E_{k,\pm j}^{(2)}]_{+\frac{\hat{0}}{2}} + [(\Delta_j^{\pm} a) E_{k,\pm j}^{(2)}]_{-\frac{\hat{0}}{2}} \right\} \simeq 2[(\Delta_j^{\pm} a) E_{k,\pm j}^{(2)}]_{-\frac{\hat{0}}{2}} \,. \tag{51}$$

Using this approximation, we obtain an approximate solution to Eq. (50) as

$$\begin{aligned} E_{i,+\frac{\hat{0}}{2}}\Big|_1 &= E_{i,-\frac{\hat{0}}{2}} + \Delta t\,[...] \\ &+ \Delta t \left(\frac{e^2}{4\pi^2 M} \frac{1}{4} (2 + dx\Delta_i^+) \sum_{\pm} \sum_{jk} \epsilon_{ijk} \left[(\Delta_j^{\pm} a) E_{k,\pm j}^{(2)} \right]_{-\frac{\hat{0}}{2}} \right). \end{aligned} \tag{52}$$

The solution for the updated electric field found this way makes Eq. (51) to reproduce the continuum Eq. (9) to order $\mathcal{O}(dt)$. We can however build now an iterative solution as

$$E_{i,+\frac{\hat{0}}{2}}\Big|_n = E_{i,+\frac{\hat{0}}{2}}\Big|_{n-1} + \Delta t\left(\frac{e^2}{4\pi^2 M}\frac{1}{4}(2+dx\Delta_i^+)\sum_{\pm}\sum_{jk}\epsilon_{ijk}\left[(\Delta_j^{\pm}a)\,E^{(2)}_{k,\pm j}\Big|_{n-1}\right]_{+\frac{\hat{0}}{2}}\right), \tag{53}$$

so that by successive iterations we approach closer an closer to the correct solution to Eq. (50) $E_{i,+\hat{0}/2}|_n \xrightarrow[n\to\infty]{} E_{i,+\hat{0}/2}$. Of course, it is enough, in principle, to iterate just two times, so that $E_{i,+\hat{0}/2} \simeq E_{i,+\frac{\hat{0}}{2}}|_2$ solves Eq. (50) reproducing the continuum Eq. (8) to order $\mathcal{O}(dt^2)$. On the other hand, the Gauss law within the set of Eqs. (49), should be exact (up to computer machine precision) as long as E_i is the exact solution to Eq. (50). However, as we are now approximating the electric field at each time step as $E_i \simeq E_i|_n$, it is not clear *a priori* the accuracy attained in the (now approximated) Gauss law

$$\sum_i \Delta_i^- \, E_i|_n \simeq 2e^2\mathrm{Im}\{\varphi^*\pi\} - \frac{e^2}{4\pi^2 M}\frac{1}{8}\sum_{\pm}\sum_i(\Delta_i^{\pm}a)(B_i^{(4)} + B_{i,+0}^{(4)})_{\pm i}\,, \tag{54}$$

particularly after only $n=2$ iterations. Even though successive solutions $E_i|_n$ with increasingly larger n, can never be better than order $\mathcal{O}(dt^2)$ with respect $E_i|_2$, it might very well be the case that, in order to fulfill the Gauss law with sufficient precision, $E_i|_n$ is required to an order $n \gg 2$. We have not investigated explicitly this aspect in simulations, as this will depend most likely on the specific scenario under study. We leave therefore this check as a future task to be considered when applying our formalism into specific scenarios where a time-dependent and fully-inhomogeneous axion may play a central role.

As a last comment, let us note that in relevant cosmological scenarios like e.g. axion-inflation [56–63], gauge fields are largely excited due to their axionic-coupling to a shift-symmetric field $a(x)$ which plays the role of the inflaton, and hence is (mostly) homogeneous. Only when the gauge fields are largely excited towards the end of inflation or during preheating, will they back react into the axion field, breaking its (classical) homogeneity. For most of the dynamics the axion-inflaton field remains therefore almost homogeneous. It is therefore conceivable that one may solve the system of Eqs. (49) simply using Eq. (52) to solve for the electric fields, i.e. with $E_i \simeq E_i|_1$, and yet maintain a good accuracy close to $\mathcal{O}(dt^2)$. The reason for this is that even though the approximated terms in the *rhs* of Eq. (52) have a reduced accuracy of $\mathcal{O}(dt)$ instead of $\mathcal{O}(dt^2)$, they are also suppressed by $\vec{\nabla}\alpha$. Thus, these terms may be negligible in the dynamics, allowing to solve iteratively the set of Eqs. (49) together with Eq. (52) to advance the electric fields, yet with $\mathcal{O}(dt^2)$ accuracy. As only dedicated simulations can resolve this issue, we leave as future work the test of this circumstance within these scenarios.

5. Lattice Chern–Simons number(s)

The Chern–Simons number in the continuum theory reads

$$N_{\rm cs} \equiv \frac{1}{(4\pi)^2}\int d^4x\, F_{\mu\nu}\tilde{F}^{\mu\nu} = \frac{1}{4\pi^2}\int dt\int d^3x\ \vec{E}\cdot\vec{B}\,. \tag{55}$$

In the lattice, we can define an equivalent quantity describing this topological number, by considering some lattice representation of $\vec{E}\cdot\vec{B}$, and substituting the space-time integral by finite sums, $\int d^4x \to \Delta t \Delta x^3 \sum_{n_o,\vec{n}}$. In order to do this, we just need to follow a similar logic as in Sect. 4, when we discussed the different lattice representations of an axionic-coupling. As we have already derived the lattice EOM reproducing the system continuum dynamics up to order $\mathcal{O}(dx^2)$, we should clearly aim now for a description of the Chern–Simons density to (at least) order $\mathcal{O}(dx^2)$. In order to build an appropriated lattice expression for $N_{\rm cs}$, let us review some of the properties the Chern–Simons number Eq. (55) verifies in the continuum, so that we demand our discretized version to verify analogous properties in the lattice.

A well known identity in the continuum is

$$4\pi^2 N_{\rm cs} \equiv \int_0^t dt \int d^3x\ \vec{E}\cdot\vec{B} = \frac{1}{2}\int d^3x\ (\vec{A}\cdot\vec{B})(t)\ \ + \mathcal{C}_o\,, \tag{56}$$

where the additive constant is simply given by the initial value

$$\mathcal{C}_o \equiv -\frac{1}{2}\int d^3x\,(\vec{A}\cdot\vec{B})(0)\,. \tag{57}$$

One can easily demonstrate identity Eq. (56) using integration by parts and the fact that fields vanish at infinity. Any good definition of a discrete Chern–Simons number should, therefore, verify an analogous property to Eq. (56). In the lattice, however, we rather take periodic boundary conditions in order to mimic an infinite volume. Hence, the lattice equivalent to Eq. (56) should rely on the use of periodic boundary conditions. For this purpose we define

$$A_i^{(2)} \equiv \frac{1}{2}(A_i + A_{i,-i}) = \frac{1}{2}(2 - dx\Delta_i^-)A_i\,, \tag{58}$$

which lives at $l = (n_o, \vec{n})$. Taking p, q as non-negative integer numbers, we observe that due to periodic boundary conditions, the following property holds

$$\sum_{\vec{n}}\sum_i A^{(2)}_{i,+p\hat{0}} B^{(4)}_{i,+q\hat{0}} = \sum_{\vec{n}}\sum_i B^{(4)}_{i,+p\hat{0}} A^{(2)}_{i,+q\hat{0}}\,. \tag{59}$$

Essentially, inside a lattice sum $\sum_{\vec{n}}\sum_i$, one can always exchange $A^{(2)}_{i,+p\hat{0}} B^{(4)}_{i,+q\hat{0}}$ by $A^{(2)}_{i,+q\hat{0}} B^{(4)}_{i,+p\hat{0}}$, precisely thanks to the periodicity of the boundary conditions. We will use shortly this property to verify that our lattice definition of Chern–Simons verify an analogous property to Eq. (56).

Another relevant property that any lattice implementation of $N_{\rm cs}$ should verify, is the following: in a theory (in the continuum) with chemical potential μ, after integrating in time the EOM Eq. (18), it follows the relation

$$\mu(t) = \mu(0) + \frac{12}{T^2}\lim_{V\to\infty}\frac{N_{\rm cs}}{V}\,. \tag{60}$$

Therefore, any lattice implementation of the Chern–Simons number should verify some discrete version of the relation Eq. (60).

From the evolution equation for the chemical potential in lattice, see Eqs. (47), we obtain that the chemical potential after p time steps is given by

$$\mu_{+p\hat{0}} = \mu_o + \frac{3}{\pi^2}\frac{1}{T^2 V_L^3}\frac{1}{2}\Delta t\Delta x^3 \sum_{n_o=0}^{p-1}\sum_{\vec{n}}\sum_i E_i^{(2)}(B_i^{(4)} + B_{i,+0}^{(4)})$$
$$\equiv \mu_o + \frac{12}{T^2 V_L^3} N_{\rm cs}^L\,, \tag{61}$$

where $\mu_o \equiv \mu(n_o = 0)$ is the initial chemical potential, and the lattice volume as $V_L \equiv (Ndx)^3$, with N is the number of lattice sites per dimension. Eq. (61) has lead us in fact to define a lattice Chern–Simons number as

$$4\pi^2 N_{\rm cs}^L \equiv \Delta t\Delta x^3 \sum_{n_o=0}^{p-1}\sum_{\vec{n}}\frac{1}{2}\sum_i E_i^{(2)}(B_i^{(4)} + B_{i,+0}^{(4)})$$
$$= \frac{\Delta x^3}{2}\sum_{\vec{n}}\sum_i A_{i,+p\hat{0}}^{(2)} B_{i,+p\hat{0}}^{(4)} \quad + \mathcal{D}_o\,, \tag{62}$$

with initial constant

$$\mathcal{D}_o = -\frac{1}{2}\Delta x^3 \sum_{\vec{n}}\sum_i A_i^{(2)} B_i^{(4)}\,. \tag{63}$$

Notice that in order to arrive at the final expression of Eq. (62) of the form $\sim \sum_{\vec{n}} AB$, from an initial expression of the form $\sim \sum_{n_o,\vec{n}} EB$, we have applied the trick expressed by Eq. (59).

In conclusion, we have defined a Chern–Simons number given by Eq. (62), as this expression is exactly linearly proportional to the chemical potential at arbitrary times, see Eq. (61), as required in order to mimic correctly the continuum relation Eq. (60). Besides, our definition of $N_{\rm cs}^L$ Eq. (62) verifies (by construction) a lattice analogue to the continuum relation Eq. (56) $\int dx^4\ \vec{E}\cdot\vec{B} = \frac{1}{2}\int dx^3 \vec{A}\cdot\vec{B} + \mathcal{C}_o$, and that the Pontryagin lattice density $\frac{1}{4}\mathcal{K}_L \equiv \frac{1}{2}\sum_i E_i^{(2)}(B_i^{(4)} + B_{i,+0}^{(4)})$ reproduces exactly the continuum expression $\vec{E}\cdot\vec{B}$ up to order $\mathcal{O}(dx^2)$. The starting expression in Eq. (62) in the form $\sim \sum_{n_o,\vec{n}} EB$, represents in fact the U(1) limit of the SU(2) expression for the Chern–Simons number introduced in [12,52,53].

Let us note that using the trick expressed by Eq. (59), we can write the lattice axionic-interaction term in the case of an Abelian gauge theory with chemical potential, in an alternative way to Eq. (46), like

$$S_{\alpha(t)}^L = \Delta t\Delta x^3 \sum_{\vec{n},n_o}\left\{\frac{M^2}{2c_s^2}\left(\Delta_o^-\alpha\right)^2 + \frac{1}{4\pi^2}\frac{\alpha}{2}\sum_i E_i^{(2)}\left(B_i^{(4)} + B_{i,+0}^{(4)}\right)\right\}$$
$$\equiv \Delta t\Delta x^3 \sum_{n_o}\left\{N^3\frac{M^2}{2c_s^2}\left(\Delta_o^-\alpha\right)^2 - \frac{1}{4\pi^2}(\Delta_o^-\alpha)\frac{1}{2}\sum_{\vec{n}}\vec{A}_i^{(2)}\vec{B}_i^{(4)}\right\}\,, \tag{64}$$

where we have discarded additive constants in the last expression of Eq. (64). One can check, of course, that from variations of the last expression in Eq. (64), we also obtain identical EOM as in Eq. (47), as it should be. Writing $S_{\alpha(t)}^L$ as in the last expression in Eq. (64), is perhaps the most natural thing to do in the presence of a chemical potential (homogeneous axion), as $\mu \equiv \Delta_o^-\alpha$ is simply given by the time derivative of an auxiliary variable α, but the latter plays no dynamical role. The last expression in Eq. (64) eliminates precisely the presence of α in the action, and maintains only terms involving explicitly $\mu = \Delta_o^-\alpha$.

5.1. Derivative representation of Pontryagin density $\tilde{F}_{\mu\nu}F^{\mu\nu}$

Our former demonstration(s) that the Chern–Simons number(s) can be written in either form $\sim \sum_{n_o,\vec{n}} \vec{E}\vec{B}$ or as $\sim \sum_{\vec{n}} \vec{A}\vec{B}$, indicates that we can find a derivative representation of our lattice expressions of the Pontragyn density. Whereas in the continuum we can write the identity $\mathcal{K} \equiv \tilde{F}_{\mu\nu}F^{\mu\nu} = \partial_\mu K^\mu$, with K^μ the Chern–Simons current, we expect that in the discrete some analogous relation may exist, so that $\mathcal{K}^L = \Delta_\mu^+ K_L^\mu$. If we redo the steps in Eq. (62), we realize that the lattice Chern–Simons number $N_{\rm cs}^L$ can be re-written like

$$16\pi^2 N_{\rm cs}^{L(2)} \equiv \Delta t \Delta x^3 \sum_{n_o=0}^{p-1} \sum_{\vec{n}} \mathcal{K}_L = \Delta t \Delta x^3 \sum_{n_o=0}^{p-1} \sum_{\vec{n}} \Delta_o^+ K_L^o \tag{65}$$

where

$$\mathcal{K}_L \equiv 4 \sum_i \frac{1}{2} E_i^{(2)} (B_i^{(4)} + B_{i,+0}^{(4)}), \tag{66}$$

$$K_L^0 = -K_0^L \equiv 2 \sum_i A_i^{(2)} B_i^{(4)}. \tag{67}$$

Note that this does not mean that we can locally substitute the expression of the lattice Pontryagin density $\mathcal{K}_L$ by $\Delta_o^+ K_L^o$, like if it was an identity at every lattice site. However, whenever summing over the lattice volume, we can do such a replacement locally inside the argument of the lattice sum, i.e.

$$\sum_{\vec{n}} \mathcal{K}_L = \sum_{\vec{n}} \Delta_o^+ K_L^o. \tag{68}$$

If we also sum over the time history of the system, we then arrive at

$$16\pi^2 N_{\rm cs}^L \equiv \Delta t \Delta x^3 \sum_{n_o=0}^{p-1} \sum_{\vec{n}} \mathcal{K}_L = \Delta x^3 \left(\sum_{\vec{n}} K_{L,+p\hat{0}}^o - \sum_{\vec{n}} K_L^o \right). \tag{69}$$

Using the definition of K_L^o in Eq. (67), we see that Eq. (69) coincides exactly, as it should, with the final expression of Eq. (62).

Let us find the spatial K_L^i components of the lattice representation of the Chern–Simons current. Starting from Eq. (66) for $\mathcal{K}_L$, we can write

$$\mathcal{K}_L = \frac{2}{\Delta t} \sum_i \left\{ \left(A_{i,+0}^{(2)} B_{i,+0}^{(4)} - A_i^{(2)} B_i^{(4)} \right) + \left(A_{i,+0}^{(2)} B_i^{(4)} - A_i^{(2)} B_{i,+0}^{(4)} \right) \right\}, \tag{70}$$

and recognize the first term in the *rhs* of Eq. (70) as equal to $\Delta_0^+ K_L^0$. The second term in the *rhs* of Eq. (70) can be re-written like

$$\frac{2}{\Delta t} \sum_i \left(A_{i,+0}^{(2)} B_i^{(4)} - A_i^{(2)} B_{i,+0}^{(4)} \right) = \sum_j \Delta_j^+ K_L^j, \tag{71}$$

where we have identified

$$K_L^i = K_i^L \equiv -\sum_{j,k} \epsilon_{ijk} \left(E_j^{(2)} A_{k,-i}^{(2)} + E_{j,-i}^{(2)} A_k^{(2)} \right). \tag{72}$$

We have demonstrated therefore that we can write

$$\mathcal{K}_L = \sum_{\mu} \Delta_\mu^+ K_L^\mu = \Delta_0^+ K_L^0 + \Delta_1^+ K_L^1 + \Delta_2^+ K_L^2 + \Delta_3^+ K_L^3\,, \tag{73}$$

as a local identity at every lattice site, with K_L^μ defined by components, K_L^0 given by Eq. (67) and K_L^i given by Eq. (72). Given that we consider periodic boundary conditions, let us note that it must be true that $\sum_{\vec{n}}\sum_i \Delta_i^+ K_L^i = 0$, no matter the expression for K_L^i. Therefore, the identity in Eq. (68) will not change if we just substitute $\Delta_o^+ K_L^o$ by $\sum_\mu \Delta_\mu^+ K_L^\mu$, in the rhs of such equation,

$$\sum_{\vec{n}} \mathcal{K}_L = \sum_{\vec{n}}\sum_{\mu} \Delta_\mu^+ K_L^\mu = \sum_{\vec{n}} \Delta_o^+ K_L^o\,. \tag{74}$$

This implies that the expression for the Chern–Simons number Eq. (69), given only in terms of K_L^0 (and not K_L^i's), is of course unchanged,

$$\begin{aligned} 16\pi^2 N_{\rm cs}^L &= \Delta t \Delta x^3 \sum_{n_o,\vec{n}}\sum_{\mu} \Delta_\mu^+ K_L^\mu \\ &= \Delta t \Delta x^3 \sum_{n_o,\vec{n}} \Delta_0^+ K_L^0 = \Delta x^3 \left(\sum_{\vec{n}} K^o_{L,+p\hat{0}} - \sum_{\vec{n}} K_L^o \right), \end{aligned} \tag{75}$$

as it should, independently of the expression Eq. (72) we found for K_L^i.

We have found, as promised, a lattice expression for the Pontryagin density $\mathcal{K}_L$ Eq. (66), that admits a total derivative representation as in Eq. (73), with K_L^0 and K_L^i given by Eqs. (67), (72), respectively.

5.2. Chern–Simons number in the presence of a magnetic field

Let us now turn our attention into the case where a background magnetic field is present in the system. Following [76], we can introduce a magnetic flux in the lattice by demanding that the boundary conditions of the gauge fields A_i are not periodic. Without loss of generality, we can consider an external magnetic field in the $\hat{z}$ direction, $\vec{B} = (0, 0, B)$. Such magnetic field can be introduced in the lattice, by demanding that only the component $A_1(n_1, n_2, n_3)$ of the gauge field is 'aperiodic' at a given x-site, say $n_1 = 1$, at the boundary of the lattice y-axis, independently of its location within the z-axis, i.e.

$$dx\left(A_j(n_1, 0, n_3) - A_j(n_1, N, n_z)\right) = 2\pi n_{\rm mag}\delta_{1j}\delta_{1n_1}\,. \tag{76}$$

This condition creates a flux of magnitude $\Phi_{\rm flux} \equiv 2\pi n_{\rm mag}$ orthogonal to the xy-plane of the lattice, with area $A \equiv (Ndx)^2$,

$$\int_A \vec{B}\, d^2\vec{x} = \int_A B\, dx_1 dx_2 = B(Ndx)^2 \equiv 2\pi n_{\rm mag}\,, \quad \Rightarrow \quad B \equiv \frac{2\pi n_{\rm mag}}{(dxN)^2}\,. \tag{77}$$

In principle, any flux can be generated. However, quantization of this flux is required for maintaining a periodic action in the non-compact formulation of a gauge theory, see [76] for details. We need therefore to take $n_{\rm mag}$ as a positive integer, with $n_{\rm mag} = 0$ simply representing the absence of magnetic field.

The 'twisted' boundary condition for A_1 Eq. (76) implies that whenever we want to calculate a (forward) magnetic field $B_3^+ = (\Delta_1^+ A_2 - \Delta_2^+ A_1)$ at the location $(n_1, n_2, n_3) = (1, N-1, n_3)$ [or equivalently a (backward) magnetic field $B_3^- = (\Delta_1^- A_2 - \Delta_2^- A_1)$ at the location $(n_1, n_2, n_3) = (1, 0, n_3)$], we should really make the substitution

$$B_3^+(n_1 = 1, n_2 = N-1, n_3) \quad \longrightarrow \quad (\Delta_1^+ A_2 - \Delta_2^+ A_1) + \frac{2\pi n_{\rm mag}}{dx^2} \tag{78}$$

$$B_3^-(n_1 = 1, n_2 = 0, n_3) \quad \longrightarrow \quad (\Delta_1^- A_2 - \Delta_2^- A_1) + \frac{2\pi n_{\rm mag}}{dx^2}. \tag{79}$$

This is equivalent to assume that the first component of the gauge field makes a 'discrete jump' from $n_2 = N-1$ to $n_2 = N$ as $A_1(1, N, n_3) = A_1(1, 0, n_3) - \frac{2\pi n_{\rm mag}}{dx}$, and from $n_2 = 0$ to $n_2 = N$ as $A_1(1, N, n_3) = A_1(1, N-1, n_3) + \frac{2\pi n_{\rm mag}}{dx}$, just as required by Eq. (76).

Let us now see how the Chern–Simons number Eq. (62) is modified in the presence of a background magnetic field, introduced in the lattice through the condition Eq. (76). Let us begin by noticing that the relation Eq. (59), used previously to relate the $\sim EB$ and $\sim AB$ expressions of the CS number [see Eq. (62)], does not hold anymore, as it relies on the (now lost) periodic boundary conditions of the gauge fields. When the gauge field follows instead the twisted boundary condition Eq. (76), Eq. (59) needs to be modified. Given some p, q integer numbers, we obtain now

$$\sum_{\vec{n}} \sum_i A^{(2)}_{i,+p\hat{0}} B^{(4)}_{i,+q\hat{0}} \equiv \sum_{\vec{n}} \sum_i B^{(4)}_{i,+p\hat{0}} A^{(2)}_{i,+q\hat{0}} + \mathcal{M}_p\,, \tag{80}$$

where $\mathcal{M}_p$ represents a magnetic correction given by

$$\mathcal{M}_p \equiv \frac{\pi n_{\rm mag}}{2\Delta x^2} \sum_{n_3} \Big\{ A^{(2)}_{3,+p\hat{0}}(1, 0, n_3) + A^{(2)}_{3,+p\hat{0}}(1, N-1, n_3) \\ + A^{(2)}_{3,+p\hat{0}}(2, 0, n_3) + A^{(2)}_{3,+p\hat{0}}(2, N-1, n_3) \Big\}\,. \tag{81}$$

Essentially, inside a lattice sum $\sum_{\vec{n}} \sum_i$, one can still substitute $A^{(2)}_{i,+p\hat{0}} B^{(4)}_{i,+q\hat{0}}$ by $A^{(2)}_{i,+q\hat{0}} B^{(4)}_{i,+p\hat{0}}$, as long as outside the sum one compensates by adding the magnetic correction $\mathcal{M}_p$. This correction is precisely a manifestation of the loss of periodic boundary conditions Eq. (76) for the gauge field component A_1.

In light of Eq. (80), the expression of the lattice Chern–Simons number Eq. (62), changes in the presence of an external magnetic field to

$$\begin{aligned} 4\pi^2 N^L_{\rm cs}\big|_{\rm mag} &\equiv \Delta t \Delta x^3 \sum_{n_o=0}^{p} \sum_{\vec{n}} \frac{1}{2} \sum_i E^{(2)}_i (B^{(4)}_i + B^{(4)}_{i,+0}) \\ &= \frac{\Delta x^3}{2} \sum_{\vec{n}} \sum_i A^{(2)}_{i,+p\hat{0}} B^{(4)}_{i,+p\hat{0}} \;+\; (\mathcal{D}_o - \mathcal{M}_0) + \mathcal{M}_p\,, \end{aligned} \tag{82}$$

with $\mathcal{D}_o$ the same constant as in Eq. (63), and $\mathcal{M}_0, \mathcal{M}_p$ given by Eq. (81), representing respectively initial and final (after p time steps) magnetic field corrections. Equivalently,

$$4\pi^2 N^L_{\rm cs}\big|_{\rm mag} = 4\pi^2 N^L_{\rm cs} + \mathcal{M}_p - \mathcal{M}_0\,. \tag{83}$$

6. Summary and discussion

In this paper we have derived a lattice representation of an axionic-interaction $a(x)\tilde{F}_{\mu\nu}F^{\mu\nu}$, presenting step by step the necessary ingredients to achieve a formulation that *i*) reproduces the continuum limit to order $\mathcal{O}(dx^2)$, *ii*) it is consistent with the (lattice version of the) Bianchi identities, and *iii*) it is solvable by an iterative scheme of evolution. We first considered in Sect. 4.1 the case of a homogeneous axion $a(x) = a(t)$, deriving a lattice representation of the axion-gauge interaction that leads to a set of discrete couple equations solvable by an explicit local iterative scheme, see Eqs. (47). We generalized our results afterwards, in Sect. 4.2, to the case of a fully inhomogeneous axion $a(x) = a(t, \mathbf{x})$. We showed that the set of discrete lattice Eqs. (49) do not admit a simple local explicit solution (while preserving the $\mathcal{O}(dx^2)$ difference with respect to the continuum). We have proposed an implicit scheme to overcome this difficulty. We have also introduced consistent lattice formulation(s) of the Chern–Simons number $N_{\rm cs} \propto \int d^4x\, \mathcal{K}$ (Sect. 5) based on the lattice version(s) of $\mathcal{K} = \tilde{F}_{\mu\nu}F^{\mu\nu}$ developed in Sect. 4. We put special care in the need to achieve a lattice formulation that admits a total derivative representation for $\mathcal{K}_L = \Delta_\mu^+ K_L^\mu$. We showed explicitly that such total derivative representation exists, and provided the expression for the K_L^μ components, see Eqs. (67), (72). Finally, we derived the analogous lattice expressions for the Chern–Simons number in the presence of an external magnetic field.

A number of potential applications of our lattice formalism has been already mentioned in the Introduction. In particular, in an accompanying paper [73] we study a number of questions one can address in high temperature electrodynamics with non-zero background magnetic field and fermion chemical potential. This theory was formulated on the lattice in Section 4.1. We investigate in [73] the random walk of the topological charge and show that it has a diffusive behavior in the presence of magnetic field B. This indicates that the mechanism for fermionic number non-conservation for $B \neq 0$ is similar to that in non-Abelian gauge theories. The diffusion rate is related to the rate of chiral charge non-conservation, and we present new results concerning the value of this rate. Our formulation allows us to study the dynamics of instabilities in the presence of non-zero μ and elucidate the role of thermal fluctuations of the gauge fields. We find several interesting behaviors that we did not expect $a\ priori$.

In addition, let us note that our formalism can be useful as well for the study of the non-linear dynamics in axion-inflation models [56–61]. In these scenarios, gauge fields coupled to a pseudo-scalar inflaton, are excited to high occupation states. Towards the last stages of inflation the system becomes non-linear: the gauge fields are so largely excited, that they significantly back-react into the inflaton dynamics, affecting also the inflationary expansion rate. The large amplification of the gauge fields leads to a very efficient generation of gravitational waves and scalar density perturbations, both with non-Gaussian statistics. If the amplitude of the scalar perturbations sourced by the gauge fields is too large, primordial black holes (PBHs) in excess to the current bounds may appear [60]. The details of both the gravitational waves and scalar perturbations (possibly leading to PBHs), depend very sensitively on the late non-linear stages of inflation, where analytical techniques can only provide an order of magnitude estimation of the dynamics. Our formalism, however, is suitable for solving the complicated non-linear dynamics numerically on a lattice, deviating from the continuum (classical) theory only to order $\mathcal{O}(dx^2)$. Besides, in axion-inflation scenarios, preheating is driven by the so called *tachyonic resonance* of the gauge fields, which occurs precisely due to the axionic-coupling with the inflaton [62, 63]. This represents a complicated non-linear evolution stage after inflation, for which our lattice formalism is particularly suitable.

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