Self-dual U(1) lattice field theory with a θ-term

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ABSTRACT: We study U(1) gauge theories with a modified Villain action. Such theories can naturally be coupled to electric and magnetic matter, and display exact electric-magnetic duality. In their simplest formulation without a θ-term, such theories are ultra-local. We extend the discussion to U(1) gauge theories with θ-terms, such that θ periodicity is exact for a free theory, and show that imposing electric-magnetic duality results in a local, but not ultra-local lattice action, which is reminiscent of the Lüscher construction of axial-symmetry preserving fermions in 4d. We discuss the coupling to electric and magnetic matter as well as to dyons. For dyonic matter the electric-magnetic duality and shifts of the θ-angle by 2π together generate an $\mathrm{SL}(2,\mathbb{Z})$ duality group of transformations, just like in the continuum. We finally illustrate how the $\mathrm{SL}(2,\mathbb{Z})$ duality may be used to explore theories at finite θ without a sign problem.

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Contents

1 Introduction

Abelian U(1) gauge theories are at the heart of electrodynamics, which, together with gravity, explains most of the world we experience. In modern high-energy physics, they are typically viewed as boring cousins of their non-abelian counterparts. The reason for this is that in four space-time dimensions they are infrared free and UV incomplete. In solid-state physics, however, U(1) gauge theories pop up as effective descriptions of many condensed matter systems with non-trivial and strongly coupled dynamics. Moreover they show up as effective descriptions of non-abelian gauge theories and were long hoped to

shed light on quark confinement and mass gap generation in those theories. While such abelian mechanisms have shown to be relevant in both supersymmetric [1, 2], and non-supersymmetric settings [3–6], a lot of justified skepticism remains about the potential of abelian gauge theories to give insights into the mysteries of 4d non-abelian gauge theories.

Both, in condensed matter applications as well as in the abelianized non-abelian gauge theories, monopoles play a crucial role. Monopoles have the ability to render the theory confining, and can therefore completely change the IR dynamics of the theory. The details of monopoles (e.g., their charge or mass) dictate whether or not they are important for the IR physics. Yet, on the lattice monopoles typically come as artifact rather than a feature, and are not under direct control. Two of us proposed a formalism of U(1) lattice gauge theories which allows electric and magnetic matter to be coupled simultaneously [7], and provides complete control over the matter content of the theory — both electric and magnetic. Moreover the formalism allows a duality transformation, mapping magnetic and electric content to each other, which is a well known feature of continuum theories. Such models were used for avoiding the complex action problem associated with the θ-term in 2d abelian gauge theories [8–12], and for formulating interacting exactly self-dual gauge theories [13, 14]. These modified Villain theories also found applications in fracton physics [15] and construction of theories with non-invertible symmetries [16, 17].

Furthermore 4d Villain theories allow for θ-terms. Indeed θ-terms in Villain-like models which have the correct continuum limit have been introduced long ago [18, 19], but generically they do not preserve exact θ-periodicity and self-duality, when applicable.[1] In [7] a class of θ-terms which preserve the exact 2π periodicity of the θ-angle in the pure gauge theory were introduced, but self-dual transformations in the presence of the θ-term were not discussed in detail. Here we find that insisting on exact θ-periodicity and on ultra-locality ruins self-duality. More precisely, if one performs a duality transformation with one of the θ-terms proposed in [7], a dual theory has a local, but not ultra-local[2] action, so that the theory is not self-dual for any choice of parameters.

On the other hand, one can restore self-duality by defining a local, but not ultra-local lattice action, which transforms covariantly under the duality transformation. We therefore reformulate the original U(1) lattice gauge theory in a local but non-ultra-local way, such that self-duality becomes exact. We recover the $SL(2, \mathbb{Z})$ duality, well known in continuum U(1) gauge theories [20].[3] Exploiting the $SL(2, \mathbb{Z})$ structure, we discuss interacting theories free from the sign problem. The situation is reminiscent of exactly massless Dirac

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[1]The θ-periodicity is lost in the presence of monopoles due to the Witten effect, since a monopole turns into a dyon which carries electric charge as well as a magnetic one. However, if the entire spectrum of dyons exists, whose masses correctly interchange under a 2π shift, the θ-periodicity can be valid even in the presence of magnetically charged matter. This is in fact what happens in abelianized non-abelian theories in 4d.

[2]A lattice action is called *ultra-local* when it couples only fields at a finite number of lattice distances. In a *local* lattice theory fields at arbitrary distances may couple, but the pre-factors decrease (at least) exponentially with the lattice separation.

[3]It is worth noting that [19] is the first proposal of the $SL(2, \mathbb{Z})$ structure for a lattice gauge theory, which, however, is only approximate.

fermions on the lattice. Exactly massless Dirac fermions have axial symmetries in addition to vector symmetries, which have mixed 't Hooft anomalies and are subject to the Nielsen-Ninomiya theorem [21–23]. This was widely interpreted as the inability to preserve axial symmetries on the lattice. However, Lüscher showed [24], using Neuberger's solution [25] of the Ginsparg-Wilson relation [26], that a lattice theory possesing an exact axial symmetry exists, at the expense of abandoning ultra-locality.

In fact also abelian gauge theories have 't Hooft anomalies [27–30] (see also [31]), so a straightforward implementation of symmetries is bound to face an obstructions, much like in the case of fermionic chiral symmetry. What is perhaps surprising is that the lattice action can still be made ultra-local when θ angle is vanishing [7], as we will review. Nevertheless we are forced to abandon ultra-locality when insisting on the θ-angle periodicity[4] and imposing self-duality in free abelian gauge theory. As is well known, these transformations form an $\mathrm{SL}(2, \mathbb{Z})$ group.

The paper is organized as follows: in the next section we review the approach to lattice discretization from [7] that gives rise to the Villain form with an additional closedness constraint for the 2-form Villain variables. This closedness constraint removes monopoles and we show that pure U(1) lattice gauge theory becomes self-dual. In section 3 we add electrically and magnetically charged matter and demonstrate that with our formulation self-duality can be extended to full QED with either bosonic or fermionic matter. For the case of bosonic matter we show that with a worldline formulation all sign problems are overcome (for fermionic matter the Grassmann nature of the matter fields may lead to a remaining sign problem). Based on the closedness constraint, in section 4 we define a topological charge in a consistent way and discuss its properties including the Witten effect. Using this topological charge we include a θ-term and discuss the generalized duality transformation that takes into account this term. To obtain self-duality with the θ-term we generalize the action to a non-ultra-local form which leads to a fully self-dual lattice discretization of QED with a θ-term. We discuss the resulting self-duality relations for several observables as well as the full $\mathrm{SL}(2, \mathbb{Z})$ duality. Finally we employ this duality to discuss theories with non-zero topological angle θ that can be simulated without complex action problem.

Some more technical parts are collected in several appendices: appendix A summarizes our notation and some results for differential forms on the lattice. In appendix B we discuss properties of our definition of the topological charge. In appendix C we discuss properties of the action kernels used in our paper and in appendix D we provide a short derivation of a generalized Poisson resummation formula. Appendix E shows how self dual QED can be mapped to a worldline representation that avoids the complex action problem and thus makes the theory accessible to Monte Carlo simulations. Finally, in appendix F we discuss a further generalization of the topological charge that implements all lattice symmetries.

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[4]The 2π θ-angle shifts are only an invariance of a theory without dynamical monopoles, because 2π shifts cause all monopoles to become dyons. Alternatively the theory can posses an entire tower of dynamical dyons of unit magnetic charge and all electric charges, in which case the 2π periodicity will be restored. This is precisely what happens in the abelianized regimes of the SU(N)-gauge theory.

2 Generalized Villain action for U(1) gauge fields and self-duality

In this section we briefly summarize the discretization strategy outlined in [7], which leads to a Villain form of the Boltzmann factor [32]. We implement additional closedness constraints for the Villain variables that suppress the artificial monopoles that plague the standard lattice discretization of U(1) gauge fields. We show that the construction leads to a self-dual discretization of the photon field which will be the starting point for more general self-dual theories in the subsequent sections.

2.1 Generalized Villain discretization with closedness constraints

When coupling U(1) gauge fields to matter in a gauge invariant way one uses the U(1)-valued compact link variables $U_{x,\mu} \in \mathrm{U}(1)$. The coupling between gauge and matter fields is then implemented via nearest neighbor terms such as $\phi_x^* U_{x,\mu} \phi_{x+\hat{\mu}}$. Under a U(1) gauge transformation the matter fields transform as $\phi_x \to e^{i\lambda_x}\phi_x$, such that the transformation $U_{x,\mu} \to e^{i\lambda_x} U_{x,\mu} e^{-i\lambda_{x+\hat{\mu}}}$ gives rise to gauge invariance of $\phi_x^* U_{x,\mu} \phi_{x+\hat{\mu}}$.

We now parameterize the link variables in the form[5]

$$U_{x,\mu} \equiv e^{iA_{x,\mu}^e} , \tag{2.1}$$

with the gauge fields $A_{x,\mu}^e \in [-\pi, \pi)$. We added the superscript ^{e} to mark the gauge fields as *electric gauge fields*, a notation that will turn out to be useful when studying electric-magnetic duality.

We may define the field strength tensor as the naive discretization of the continuum form $\partial_\mu A_\nu^e - \partial_\nu A_\mu^e$ and obtain

$$A_{x+\hat{\mu},\nu}^e - A_{x,\nu}^e - A_{x+\hat{\nu},\mu}^e + A_{x,\mu}^e \equiv (dA^e)_{x,\mu\nu} , \tag{2.2}$$

where in the last step we have defined the exterior lattice derivative d, here acting on the link variables. We will partly use the language of differential forms on the lattice and in appendix A briefly summarize our conventions and some of the results we use (for a more extensive presentation see the appendix of [7] or the mathematical standard literature such as [33]).

The compact link variables (2.1) are obviously invariant under the shifts

$$A_{x,\mu}^e \to A_{x,\mu}^e + 2\pi\, k_{x,\mu} , \quad k_{x,\mu} \in \mathbb{Z} . \tag{2.3}$$

However, the exterior derivative $(dA^e)_{x,\mu\nu}$ is not invariant under shifts, but instead transforms as

$$(dA^e)_{x,\mu\nu} \to (dA^e)_{x,\mu\nu} + 2\pi\, (dk)_{x,\mu\nu} , \tag{2.4}$$

i.e., $(dA^e)_{x,\mu\nu}$ is shifted by multiples of 2π. One way to establish invariance under the shift symmetry is to construct the action from the periodic function $\cos((dA^e)_{x,\mu\nu})$, which gives rise to the Wilson gauge action. Another option is to define the field strength as

$$F_{x,\mu\nu}^e \equiv (dA^e)_{x,\mu\nu} + 2\pi\, n_{x,\mu\nu} = (dA^e + 2\pi\, n)_{x,\mu\nu} , \tag{2.5}$$

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[5]To be specific, we consider a 4-d hypercubic lattice with lattice extents $N_\mu, \mu = 1, 2, 3, 4$ and a total number of sites $V \equiv N_1 N_2 N_3 N_4$. The lattice constant is set to $a = 1$ and all fields obey periodic boundary conditions.

where $n_{x,\mu\nu} \in \mathbb{Z}$ is a 2-form (i.e., plaquette based) variable which subsequently is summed over and obviously eats up a possible term $2\pi \, (dk)_{x,\mu\nu}$ generated by the shifts (2.3). In other words the Villain variables $n_{x,\mu\nu}$ can be viewed as gauge field of the shift symmetry [7]. In its simplest form this construction gives rise to a gauge field Boltzmann factor

$$B_\beta[A^e] \equiv \prod_{x \in \Lambda} \prod_{\mu < \nu} \sum_{n_{x,\mu\nu} \in \mathbb{Z}} e^{-\frac{\beta}{2} F^e_{x,\mu\nu} F^e_{x,\mu\nu}} = \prod_{x \in \Lambda} \prod_{\mu < \nu} \sum_{n_{x,\mu\nu} \in \mathbb{Z}} e^{-\frac{\beta}{2}(dA^e + 2\pi \, n)_{x,\mu\nu}(dA^e + 2\pi \, n)_{x,\mu\nu}} \, ,$$
(2.6)

which is known as the *Villain discretization* [32]. The first product runs over our 4-dimensional lattice Λ with periodic boundary conditions. We will refer to the variables $n_{x,\mu\nu}$ as *Villain variables*. As usual β is the inverse gauge coupling $\beta = 1/e^2$, where e is the electric charge.

The Boltzmann factor (2.6) is not only invariant under the shifts (2.3), (2.4), but also under the transformation $A^e_{x,\mu} \to A^e_{x,\mu} - \lambda_{x+\hat{\mu}} + \lambda_x$ which, up to a possible re-projection into the interval $[-\pi, \pi)$, corresponds to the gauge transformation of the gauge fields $A^e_{x,\mu}$.

A key insight is to note that the Villain variables $n_{x,\mu\nu}$ may be constrained further: they were introduced to implement the invariance of the Boltzmann factor $B_\beta[A^e]$ under the shifts (2.3), (2.4) which leads to a shift of the exterior derivative $(dA^e)_{x,\mu\nu}$ by $2\pi \, (dk)_{x,\mu\nu}$. Note that this shift obeys $(d(dk))_{x,\mu\nu\rho} = 0$ due to the nil-potency of the exterior derivative operator d , i.e., $d^2 = 0$ (compare appendix A). Thus we may constrain also the Villain variables $n_{x,\mu\nu}$ to obey

$$(dn)_{x,\mu\nu\rho} = 0 \quad \forall x \, , \ \mu < \nu < \rho \, .$$
(2.7)

This constraint implies that for all 3-cubes $(x, \mu < \nu < \rho)$ of the lattice the oriented sum over the Villain variables on the surface of the cube vanishes (appendix A). Using again the language of differential forms, the Villain variables are restricted to be a *closed* integer-valued 2-form. We point out that this constraint implies the absence of monopoles as we will discuss in more detail below.

Taking into account this closedness constraint we may formulate the partition sum of pure U(1) gauge theory in the form

$$Z(\beta) \equiv \int D[A^e] \sum_{\{n\}} e^{-\frac{\beta}{2} \sum_{x,\mu<\nu}(F^e_{x,\mu\nu})^2} \prod_x \prod_{\mu<\nu<\rho} \delta\big((dn)_{x,\mu\nu\rho}\big) \, .$$
(2.8)

Here we have defined the measure for the gauge fields and the sum over all configurations of the Villain variables as

$$\int D[A^e] \equiv \prod_x \prod_\mu \int_{-\pi}^{\pi} \frac{dA^e_{x,\mu}}{2\pi} \quad , \quad \sum_{\{n\}} \equiv \prod_x \prod_{\mu<\nu} \sum_{n_{x,\mu\nu} \in \mathbb{Z}} \, .$$
(2.9)

The product in (2.8) runs over all 3-cubes $(x, \mu < \nu < \rho)$ and implements the closedness constraint (2.7) using Kronecker deltas which we here denote with $\delta(j) \equiv \delta_{j,0}$.

It is useful to write the constraints in (2.8) by using the Fourier representation of the Kronecker deltas, such that

$$\prod_x \prod_{\mu<\nu<\rho} \delta\big((dn)_{x,\mu\nu\rho}\big) = \prod_x \prod_{\mu<\nu<\rho} \int_{-\pi}^{\pi} \frac{dA_{x,\mu\nu\rho}^m}{2\pi} e^{-iA_{x,\mu\nu\rho}^m (dn)_{x,\mu\nu\rho}}$$

$$= \int D[A^m] e^{-i \sum_x \sum_{\mu<\nu<\rho} A_{x,\mu\nu\rho}^m (dn)_{x,\mu\nu\rho}}, \qquad (2.10)$$

where we have introduced auxiliary fields $A_{x,\mu\nu\rho}^m \in \mathbb{R}$ assigned to the cubes $(x,\mu\nu\rho)$ of the lattice which, when integrated over, generate the closedness constraint (2.7) for the Villain variables. The notation A^m is chosen to reflect the fact that in the electric-magnetic duality transformations we discuss below, the auxiliary field A^m will take over the role of the vector potential, while in the dual form the vector field A^e will generate the dual closedness constraints. Due to this role in the duality transformation we will also use the nomenclature *magnetic gauge field* for A^m, while A^e is referred to as *electric gauge field* (see above).

For notational convenience, in the last step of (2.10) we have introduced the integral over all configurations of the magnetic gauge fields $A_{x,\mu\nu\rho}^m$,

$$\int D[A^m] \equiv \prod_x \prod_{\mu<\nu<\rho} \int_{-\pi}^{\pi} \frac{dA_{x,\mu\nu\rho}^m}{2\pi} . \qquad (2.11)$$

We thus may write the partition sum of our discretization of the U(1) gauge field in the form,

$$Z(\beta) = \int D[A^e] \int D[A^m] B_\beta[A^e, A^m] , \qquad (2.12)$$

where we have introduced the Boltzmann factor

$$B_\beta[A^e, A^m] \equiv \sum_{\{n\}} e^{-\frac{\beta}{2} \sum_x \sum_{\mu<\nu} (F_{x,\mu\nu}^e)^2} e^{-i \sum_x \sum_{\mu<\nu<\rho} A_{x,\mu\nu\rho}^m (dn)_{x,\mu\nu\rho}}, \qquad (2.13)$$

that depends on both, the electric gauge field A^e that in the Boltzmann factor $B_\beta[A^e, A^m]$ describes the photon dynamics, as well as on the magnetic gauge field A^m that here generates the constraints. As announced, in the duality transformation we discuss in the next subsection these two fields will interchange their role.

2.2 Proof of self-duality

The first step towards establishing self-duality is to rewrite the exponent of the second term in the Boltzmann factor (2.13),

$$\sum_x \sum_{\mu<\nu<\rho} A_{x,\mu\nu\rho}^m (dn)_{x,\mu\nu\rho} = \frac{1}{2\pi} \sum_x \sum_{\mu<\nu<\rho} A_{x,\mu\nu\rho}^m (d(dA^e + 2\pi n))_{x,\mu\nu\rho}$$

$$= -\frac{1}{2\pi} \sum_x \sum_{\mu<\nu} (\partial A^m)_{x,\mu\nu} (dA^e + 2\pi n)_{x,\mu\nu} , \qquad (2.14)$$

where in the first step we used $d^2 = 0$ (see appendix A) to insert the term dA^e. Subsequently we applied the partial integration formula (A.2). The Boltzmann factor (2.13)

thus can be written in the form of a product over all plaquettes (we here inserted $F^e_{x,\mu\nu} = (dA^e + 2\pi\,n)_{x,\mu\nu}$),

$$B_\beta[A^e, A^m] = \prod_x \prod_{\mu<\nu} \sum_{n_{x,\mu\nu}\in\mathbb{Z}} e^{-\frac{\beta}{2}\left((dA^e + 2\pi\,n)_{x,\mu\nu}\right)^2} e^{\frac{i}{2\pi}(dA^e + 2\pi n)_{x,\mu\nu}(\partial A^m)_{x,\mu\nu}}. \qquad (2.15)$$

Each factor in this product is 2π-periodic in the corresponding variable dA^e, where the periodicity is generated by the sum over the Villain variable on the plaquette. Thus we may use Poisson resummation (see appendix D for the proof of a more general result that collapses to the usual Poisson resummation when setting $N = 1$.),

$$\sum_{n\in\mathbb{Z}} e^{-\frac{\beta}{2}(dA^e + 2\pi\,n)^2} e^{\frac{i}{2\pi}(dA^e + 2\pi n)(\partial A^m)} = \frac{1}{\sqrt{2\pi\beta}} \sum_{p\in\mathbb{Z}} e^{-\frac{1}{2}\frac{1}{4\pi^2\beta}(\partial A^m + 2\pi\,p)^2} e^{-i\,p\,dA^e}\,, \quad (2.16)$$

where we have omitted the plaquette indices for notational convenience. Using this expression for all factors in the Boltzmann weight (2.15), we find

$$B_\beta[A^e, A^m] = \left(\frac{1}{2\pi\beta}\right)^{3V} \sum_{\{p\}} e^{-\frac{\widetilde\beta}{2}\sum_{x,\mu<\nu}\left((\partial A^m + 2\pi\,p)_{x,\mu\nu}\right)^2} e^{-i\sum_{x,\mu<\nu}(dA^e)_{x,\mu\nu}\,p_{x,\mu\nu}}, \quad (2.17)$$

where we have defined the dual gauge coupling

$$\widetilde\beta \equiv \frac{1}{4\pi^2\beta}\,, \qquad (2.18)$$

and denote the sum over all configurations of the newly introduced plaquette occupation numbers $p_{x,\mu\nu} \in \mathbb{Z}$ as

$$\sum_{\{p\}} \equiv \prod_x \prod_{\mu<\nu} \sum_{p_{x,\mu\nu}\in\mathbb{Z}}\,. \qquad (2.19)$$

The next step is to use again the partial integration formula (A.2) from appendix A to rewrite the second exponent in (2.17) such that the Boltzmann factor reads

$$B_\beta[A^e, A^m] = \left(\frac{1}{2\pi\beta}\right)^{3V} \sum_{\{p\}} e^{-\frac{\widetilde\beta}{2}\sum_{x,\mu<\nu}\left((\partial A^m + 2\pi\,p)_{x,\mu\nu}\right)^2} e^{-i\sum_{x,\mu} A^e_{x,\mu}\,(\partial p)_{x,\mu}}. \qquad (2.20)$$

We remark that we will use the form (2.20) of the Boltzmann factor to show that the self-dual formulation of scalar electrodynamics that we construct in the next section is free of any complex action problem. The self-dual formulation of pure gauge theory is already free of a complex action problem when the form (2.8) of the partition sum is used.

To complete the proof of self-duality of pure U(1) gauge theory, we now switch to the dual lattice. Using (A.4) we identify the r forms on the original lattice with $4-r$ forms on the dual lattice (when forms are considered on the dual lattice they are marked with "~" — compare appendix A),

$$A^e_{x,\mu} = \sum_{\nu<\rho<\sigma} \epsilon_{\mu\nu\rho\sigma}\, \widetilde{A}^e_{\tilde{x}-\hat\nu-\hat\rho-\hat\sigma,\nu\rho\sigma}\,, \;\; A^m_{x,\mu\nu\rho} = \sum_\sigma \epsilon_{\mu\nu\rho\sigma}\, \widetilde{A}^m_{\tilde{x}-\hat\sigma,\sigma}\,, \;\; p_{x,\mu\nu} = \sum_{\rho<\sigma} \epsilon_{\mu\nu\rho\sigma}\, \widetilde{p}_{\tilde{x}-\hat\rho-\hat\sigma,\rho\sigma}\,.$$
$$(2.21)$$

The d and ∂ operators interchange their role when switching to the dual lattice (see Equation (A.5) in appendix A), such that

$$(\partial A^m)_{x,\mu\nu} = \sum_{\rho<\sigma} \epsilon_{\mu\nu\rho\sigma} (d\widetilde{A}^m)_{\tilde{x}-\hat{\rho}-\hat{\sigma},\rho\sigma} \ , \ \ (\partial p)_{x,\mu} = \sum_{\nu<\rho<\sigma} \epsilon_{\mu\rho\sigma} (d\widetilde{p})_{\tilde{x}-\hat{\nu}-\hat{\rho}-\hat{\sigma},\nu\rho\sigma} \ . \quad (2.22)$$

Using (2.21) and (2.22) in (2.20) we find the following dual form of the Boltzmann factor,

$$\begin{aligned} B_\beta[A^e, A^m] &= \left(\frac{1}{2\pi\beta}\right)^{3V} \sum_{\{\widetilde{p}\}} e^{-\frac{\widetilde{\beta}}{2} \sum_{\tilde{x},\mu<\nu} \left((d\widetilde{A}^m + 2\pi\widetilde{p})_{\tilde{x},\mu\nu}\right)^2} e^{-i \sum_{\tilde{x},\mu<\nu<\rho} \widetilde{A}^e_{\tilde{x},\mu\nu\rho} (d\widetilde{p})_{\tilde{x},\mu\nu\rho}} \\ &= \left(\frac{1}{2\pi\beta}\right)^{3V} \sum_{\{\widetilde{p}\}} e^{-\frac{\widetilde{\beta}}{2} \sum_{\tilde{x},\mu<\nu} \left(\widetilde{F}^m_{\tilde{x},\mu\nu}\right)^2} e^{-i \sum_{\tilde{x},\mu<\nu<\rho} \widetilde{A}^e_{\tilde{x},\mu\nu\rho} (d\widetilde{p})_{\tilde{x},\mu\nu\rho}}, \quad (2.23) \end{aligned}$$

where we defined

$$\widetilde{F}^m_{\tilde{x},\mu\nu} \equiv (d\widetilde{A}^m + 2\pi\widetilde{p})_{\tilde{x},\mu\nu} \ , \quad (2.24)$$

and the sum over all configurations of the dual plaquette occupation numbers,

$$\sum_{\{\widetilde{p}\}} \equiv \prod_{\tilde{x}} \prod_{\mu<\nu} \sum_{\widetilde{p}_{\tilde{x},\mu\nu} \in \mathbb{Z}} = \sum_{\{p\}} \ , \quad (2.25)$$

where the identity on the right hand side is an obvious consequence of the last equation in (2.21). Thus, up to an overall factor the Boltzmann weights (2.13) and (2.23) have the same form.

Comparing (2.23) with (2.13) we can summarize the duality relation for the Boltzmann factor as

$$B_\beta[A^e, A^m] = \left(\frac{1}{2\pi\beta}\right)^{3V} \widetilde{B}_{\widetilde{\beta}}[\widetilde{A}^m, \widetilde{A}^e] \quad \text{with} \quad \widetilde{\beta} = \frac{1}{4\pi^2\beta} \ . \quad (2.26)$$

Equation (2.26) constitutes the self-duality relation for the generalized Boltzmann factor $B_\beta[A^e, A^m]$, where in the l.h.s. form of the Boltzmann factor the electric gauge field A^e describes the dynamics and the magnetic gauge field A^m generates the constraints. Under the duality transformation the gauge coupling β is replaced by the dual coupling $\widetilde{\beta}$, the Boltzmann factor picks up the overall factor $(2\pi\beta)^{-3V}$, all fields are replaced by their dual living on the dual lattice (thus the notation $\widetilde{B}_{\widetilde{\beta}}[\widetilde{A}^m, \widetilde{A}^e]$), and finally, the electric and the magnetic field interchange their role. This means that in the dual form on the r.h.s. of (2.26) the dual magnetic field $\widetilde{A}^m$ describes the dynamics, while the dual electric field $\widetilde{A}^e$ now generates the constraints.

To establish full duality of the partition sum $Z(\beta)$ we replace the integral measures $\int D[A^e]$ and $\int D[A^m]$ by the corresponding dual integral measures defined as,

$$\int D[\widetilde{A}^e] \equiv \prod_{\tilde{x}} \prod_{\mu<\nu<\rho} \int_{-\pi}^{\pi} \frac{d\widetilde{A}^e_{\tilde{x},\mu\nu\rho}}{2\pi} = \int D[A^e] \ ,$$

$$\int D[\widetilde{A}^m] \equiv \prod_{\tilde{x}} \prod_{\mu} \int_{-\pi}^{\pi} \frac{d\widetilde{A}^m_{\tilde{x},\mu}}{2\pi} = \int D[A^m] \ , \quad (2.27)$$

where again (2.21) ensures that the dual integration measures are equal to the ones on the original lattice. Thus we find

$$
\begin{aligned}
Z(\beta) &= \int D[A^e] \int D[A^m] \, B_\beta[A^e, A^m] \\
&= \left(\frac{1}{2\pi\beta}\right)^{3V} \int D[\widetilde{A}^e] \int D[\widetilde{A}^m] \, \widetilde{B}_\beta[\widetilde{A}^m, \widetilde{A}^e] \;=\; \left(\frac{1}{2\pi\beta}\right)^{3V} Z(\widetilde{\beta}) \,, \qquad (2.28)
\end{aligned}
$$

and identify the final form of the self-duality relation for the partition sum

$$
Z(\beta) = \left(\frac{1}{2\pi\beta}\right)^{3V} Z(\widetilde{\beta}) \qquad \text{with} \qquad \widetilde{\beta} = \frac{1}{4\pi^2\beta} \,. \qquad (2.29)
$$

Before we discuss properties and consequences of the self-duality relation (2.29) we note that iterating the duality relation gives the identity map, i.e.,

$$
Z(\beta) = \left(\frac{1}{2\pi\beta}\right)^{3V} Z(\widetilde{\beta}) = \left(\frac{1}{2\pi\beta}\right)^{3V} \left(\frac{1}{2\pi\widetilde{\beta}}\right)^{3V} Z\!\left(\widetilde{\widetilde{\beta}}\right) = Z(\beta) \,, \qquad (2.30)
$$

where in the last step we used the obvious properties $\beta\widetilde{\beta} = 1/4\pi^2$ and $\widetilde{\widetilde{\beta}} = \beta$. Equation (2.30) constitutes an important consistency check for the self-duality relation we constructed.

The self-duality relation (2.29) obviously maps the weak- and strong-coupling regions of the partition sum $Z(\beta)$ onto each other. Suitable derivatives of $\ln Z(\beta)$ thus will relate observables in the strong and the weak coupling region. To give an example, we consider the expectation value of the square of the field strength, which is proportional to the first derivative of $\ln Z(\beta)$:

$$
\begin{aligned}
\langle F^2 \rangle_\beta &\equiv -\frac{1}{3V} \frac{\partial}{\partial\beta} \ln Z(\beta) = -\frac{1}{3V} \frac{\partial}{\partial\beta} \ln\left((2\pi\beta)^{-3V} Z(\widetilde{\beta}) \right) \\
&= \frac{1}{\beta} - \frac{1}{3V} \left(\frac{\partial}{\partial\widetilde{\beta}} \ln Z(\widetilde{\beta}) \right) \frac{d\widetilde{\beta}}{d\beta} = \frac{1}{\beta} \;-\; \langle F^2 \rangle_{\widetilde{\beta}} \, \frac{1}{4\pi^2\beta^2} \,. \qquad (2.31)
\end{aligned}
$$

Multiplying the equation with β we can summarize the duality relation for $\langle F^2 \rangle$ in a sum rule that connects the weak and strong coupling results for $\langle F^2 \rangle$,

$$
\beta \, \langle F^2 \rangle_\beta + \widetilde{\beta} \, \langle F^2 \rangle_{\widetilde{\beta}} \;=\; 1 \,. \qquad (2.32)
$$

In a similar way one may relate the weak and strong coupling results of higher derivatives of $\ln Z(\beta)$, i.e., the susceptibility of the action density and higher moments. Self-duality relations for correlators of F^2 can be obtained by introducing an x-dependence of β (which leaves the duality transformation unchanged) and by performing local derivatives that generate the correlators.

3 Self-dual lattice QED

In this section we generalize our self-dual discretization of pure gauge theory to self-dual lattice QED, where we explicitly discuss the coupling of electrically and magnetically charged scalar fields. More particularly we first discuss in detail the case where we couple separate species of matter fields, one that is electrically charged and a second field with magnetic charges. Subsequently we briefly address the possibility of coupling dyonic matter in our formulation.

3.1 Coupling separate species for electric and magnetic matter

We here first present the construction for coupling separate species of electric and magnetic matter fields, then establish self-duality and finally discuss some of its consequences. We remark that in appendix E we show that one may switch to a worldline formulation that for the case of bosonic matter solves the complex action problem introduced by the closedness constraints, such that the worldline form can be used for numerical simulations.

We couple electrically charged matter to the electric gauge field A^e and magnetically charged matter to the magnetic gauge field A^m. Note that we have defined the magnetic gauge field A^m on the cubes of the original lattice, such that the corresponding dual form $\widetilde{A}^m$ corresponds to fields $\widetilde{A}^m_{\tilde{x},\mu}$ that live on the links $(\tilde{x}, \mu)$ of the dual lattice (compare (2.21)). We now use this dual form to couple the magnetically charged matter fields.

The partition function with gauge fields coupling to electric and magnetic matter fields reads

$$Z(\beta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m) \equiv \int D[A^e] \int D[A^m] \, B_\beta[A^e, A^m] \, Z_{M^e, \lambda^e, q^e}[A^e] \, \widetilde{Z}_{M^m, \lambda^m, q^m}[\widetilde{A}^m] \,, \tag{3.1}$$

where $B_\beta[A^e, A^m]$ is the gauge field Boltzmann factor in the form (2.13). We have introduced the partition function $Z_{M^e, \lambda^e, q^e}[A^e]$ for electrically charged matter ϕ^e that couples to the electric background gauge field A^e as

$$Z_{M^e, \lambda^e, q^e}[A^e] \equiv \int D[\phi^e] \, e^{-S_{M^e, \lambda^e, q^e}[\phi^e, A^e]} \,, \quad \int D[\phi^e] \equiv \prod_x \int_{\mathbb{C}} \frac{d\phi^e_x}{2\pi} \,, \tag{3.2}$$

$$S_{M^e, \lambda^e, q^e}[\phi^e, A^e] \equiv \sum_x \left[M^e |\phi^e_x|^2 + \lambda^e |\phi^e_x|^4 - \sum_\mu \left[\phi^{e*}_x \, e^{i \, q^e A^e_{x,\mu}} \, \phi^e_{x+\hat{\mu}} + \text{c.c.} \right] \right], \tag{3.3}$$

where we imparted the electric matter with a charge $q^e \in \mathbb{Z}$. As already announced, we couple bosonic matter, which for the electric field is a complex scalar $\phi^e_x \in \mathbb{C}$ that is assigned to the sites x of the original lattice. The path integral measure $\int D[\phi^e]$ is the usual product measure and the action $S_{M^e, \lambda^e, q^e}[\phi^e, A^e]$ is the free action plus a quartic term with coupling λ^e. The mass parameter M^e is related to the tree level mass m^e via $M^e = 8 + (m^e)^2$.

The magnetically charged scalar field $\widetilde{\phi}^m_{\tilde{x}} \in \mathbb{C}$ lives on the sites $\tilde{x}$ of the dual lattice and couples to the magnetic gauge field $\widetilde{A}^m_{\tilde{x},\mu}$ on the links of the dual lattice. The corresponding partition sum has the same form as the partition sum (3.2) for the electric matter but for the magnetic matter is defined entirely on the dual lattice,

$$\widetilde{Z}_{M^m, \lambda^m, q^m}[\widetilde{A}^m] \equiv \int D[\widetilde{\phi}^m] \, e^{-\widetilde{S}_{M^m, \lambda^m, q^m}[\widetilde{\phi}^m, \widetilde{A}^m]} \,, \quad \int D[\widetilde{\phi}^m] \equiv \prod_{\tilde{x}} \int_{\mathbb{C}} \frac{d\widetilde{\phi}^m_{\tilde{x}}}{2\pi} \,, \tag{3.4}$$

$$\widetilde{S}_{M^m, \lambda^m, q^m}[\widetilde{\phi}^m, \widetilde{A}^m] \equiv \sum_{\tilde{x}} \left[M^m |\widetilde{\phi}^m_{\tilde{x}}|^2 + \lambda^m |\widetilde{\phi}^m_{\tilde{x}}|^4 - \sum_\mu \left[\widetilde{\phi}^{m*}_{\tilde{x}} \, e^{i \, q^m \widetilde{A}^m_{\tilde{x},\mu}} \, \widetilde{\phi}^m_{\tilde{x}+\hat{\mu}} + \text{c.c.} \right] \right]. \tag{3.5}$$

Similarly to the electric matter, we chose to give the magnetic matter a charge $q^m \in \mathbb{Z}$. As before we allow for a quartic self-interaction term with corresponding coupling λ^m, and the relation of the mass parameter M^m to the tree level mass m^m is again given by $M^m = 8 + (m^m)^2$.

It is obvious that the construction can easily be generalized to coupling fermionic electric and magnetic matter fields, by simply replacing the partition sums $Z_{M^e, \lambda^e, q^e}[A^e]$ and $\widetilde{Z}_{M^m, \lambda^m, q^m}[\widetilde{A}^m]$ by the corresponding fermion determinants in the background fields A^e and $\widetilde{A}^m$ where for the latter case the corresponding discretized lattice Dirac operator lives entirely on the dual lattice.

The proof of self-duality is straightforward and is essentially a corollary of the self-duality relation (2.26) for the gauge field Boltzmann factor $B_\beta[A^e, A^m]$. Using (2.26) in the partition sum (3.1) we find (here $C = (1/2\pi\beta)^{3V}$)

$$
\begin{aligned}
Z(\beta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m) &= C\int D[A^e]\int D[A^m] B_{\widetilde{\beta}}[\widetilde{A}^m, \widetilde{A}^e] Z_{M^e, \lambda^e, q^e}[A^e]\widetilde{Z}_{M^m, \lambda^m, q^m}[\widetilde{A}^m] \\
&= C\int D[\widetilde{A}^m]\int D[\widetilde{A}^e] B_{\widetilde{\beta}}[\widetilde{A}^m, \widetilde{A}^e]\widetilde{Z}_{M^m, \lambda^m, q^m}[\widetilde{A}^m]\widetilde{\widetilde{Z}}_{M^e, \lambda^e, -q^e}\left[\widetilde{\widetilde{A}^e}\right],
\end{aligned}
\tag{3.6}
$$

where in the second step we have used (2.27) to replace the path integral measures by their dual counterparts, as well as the identity

$$
Z_{M^e, \lambda^e, q^e}[A^e] = \widetilde{\widetilde{Z}}_{M^e, \lambda^e, -q^e}\left[\widetilde{\widetilde{A}^e}\right] .
\tag{3.7}
$$

It is important to note that here the iterated duality relation gives rise to a flip of the sign of the electric charge q^e: for vector fields eq. (A.4) from appendix A implies

$$
A^e_{x,\mu} = \sum_{\nu < \rho < \sigma} \epsilon_{\mu\nu\rho\sigma}\widetilde{A}^e_{\tilde{x}-\hat{\nu}-\hat{\rho}-\hat{\sigma},\nu\rho\sigma} , \quad \widetilde{A}^e_{\tilde{x},\mu\nu\rho} = -\sum_\sigma \epsilon_{\mu\nu\rho\sigma}A_{x+\hat{s}-\hat{\sigma},\sigma} ,
\tag{3.8}
$$

where $\hat{s} = \hat{1}+\hat{2}+\hat{3}+\hat{4}$. As a consequence we find $\widetilde{\widetilde{A}}^e_{x,\mu} = -A^e_{x,\mu}$, such that the link variables $e^{iq^e A_{x,\mu}}$ in the electric mater action (3.3) become complex conjugate under iterated duality, which in turn is equivalent to changing the sign of the electric charge q^e.

Comparing the second line of (3.6) with the definition (3.1) of the full partition sum we can identify the self-duality relation for our discretization of QED

$$
\beta^{\frac{3V}{2}} Z(\beta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m) = \widetilde{\beta}^{\frac{3V}{2}} Z(\widetilde{\beta}, \widetilde{M}^e, \widetilde{q}^e, \widetilde{\lambda}^e, \widetilde{M}^m, \widetilde{\lambda}^m, \widetilde{q}^m) \qquad \text{with}
\tag{3.9}
$$

$$
\widetilde{\beta} = \frac{1}{4\pi^2\beta} , \ \widetilde{M}^e = M^m , \ \widetilde{\lambda}^e = \lambda^m , \ \widetilde{q}^e = q^m , \ \widetilde{M}^m = M^e , \ \widetilde{\lambda}^m = \lambda^e , \ \widetilde{q}^m = -q^e .
$$

Note that we have split the prefactor $C = (1/2\pi\beta)^{3V}$ of the partition sums in (3.6) by dividing it into equal powers of β and $\widetilde{\beta}$ to fully display the symmetry. As for the case of pure gauge theory, the duality transformation generates an overall factor, and the gauge coupling β is replaced by the dual coupling $\widetilde{\beta} = 1/(4\pi^2\beta)$, thus interchanging weak and strong coupling. In addition the parameters M^e, λ^e of electric matter are interchanged with the parameters M^m, λ^m of magnetic matter.[6] For the charge vector $\boldsymbol{q} = (q^e, q^m)^t$ (the superscript ^{t} denotes transposition) we find the following relation between the dual and the original charges,

$$
\widetilde{\boldsymbol{q}} = S\,\boldsymbol{q} \quad \text{with} \quad S = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} .
\tag{3.10}
$$

---

[6]When coupling fermionic matter only the bare fermion masses appear as parameters.

The self-duality symmetry described by (3.9) and (3.10) will be referred to as $\mathcal{S}$. However, we remark already now that in the next section we will extend the symmetry $\mathcal{S}$ to also include the θ-angle shifts by 2π, the so called $\mathcal{T}$ transformation.

Again we can generate self-duality relations for observables by evaluating derivatives of $\ln Z$ with respect to the couplings and when the couplings are considered to be space-time dependent suitable derivatives give rise to self-duality relations for correlation functions. We discuss two examples for such self-duality relations, the first being the generalization of the sum rule (2.32),

$$\beta \left\langle (F^e)^2 \right\rangle_{\beta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m} + \widetilde{\beta} \left\langle (F^e)^2 \right\rangle_{\widetilde{\beta}, \widetilde{M}^e, \widetilde{q}^e, \widetilde{\lambda}^e, \widetilde{M}^m, \widetilde{\lambda}^m, \widetilde{q}^m} = 1 \,. \tag{3.11}$$

The second term in the sum rule is evaluated with the dual parameters, i.e., with gauge coupling $\widetilde{\beta}$ and interchanged electric and magnetic coupling parameters.

Derivatives with respect to M^e and M^m generate field expectation values for the electric and magnetic matter fields. Exploring the duality relation (3.9) one finds

$$\begin{aligned}
\left\langle |\phi^e|^2 \right\rangle_{\beta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m} &\equiv -\frac{1}{V} \frac{\partial}{\partial M^e} \ln Z(\beta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m) \\
&= \left\langle |\widetilde{\phi}^m|^2 \right\rangle_{\widetilde{\beta}, \widetilde{M}^e, \widetilde{q}^e, \widetilde{\lambda}^e, \widetilde{M}^m, \widetilde{\lambda}^m, \widetilde{q}^m} \,,
\end{aligned} \tag{3.12}$$

with $\left\langle |\widetilde{\phi}^m|^2 \right\rangle = -1/V \partial \ln Z / \partial M^m$. According to the self-duality relation (3.12), the electric and magnetic field expectation values are converted into each other when changing from weak to strong coupling and simultaneously interchanging electric and magnetic coupling parameters. In a similar way self-duality relations for various observables and correlation functions can be obtained, where electric and magnetic fields and their parameters are interchanged, when switching between the weak and strong coupling domains of the theory. We stress once more, that the self-duality relations we discuss here hold identically for fermionic and for bosonic matter.

We remark again that the Boltzmann factor (2.13) which we use in (3.1) is complex, such that we cannot use Monte Carlo simulations for self-dual QED directly in the form (2.13), (3.1). This can be overcome by switching to a worldline representation, which we discuss in appendix E.

3.2 Comments on coupling dyons

In addition to purely electric and purely magnetic matter, one can also couple dyonic matter by identifying the lattice and its dual, e.g., by specifying a map $F : \Lambda \to \widetilde{\Lambda}$ which sends $x \in \Lambda$ to $x + \frac{\hat{s}}{2} \in \widetilde{\Lambda}$. We also define the map $\widetilde{F} : \widetilde{\Lambda} \to \Lambda$ which sends $\widetilde{x} \in \widetilde{\Lambda}$ to $\widetilde{x} + \frac{\hat{s}}{2} \in \Lambda$. The maps F and $\widetilde{F}$ do not have to necessarily be shifts by the same amount, and we could have just as well defined $\widetilde{F} : \widetilde{x} \to \widetilde{x} - \frac{\hat{s}}{2}$. We now work with only a single species of matter, the dyonic field $\phi_x \in \mathbb{C}$, that lives on the sites x of the lattice and carries both an electric charge q^e and a magnetic charge q^m. The corresponding action is obtained by replacing $\phi_x^e \to \phi_x$ in the mass and quartic terms of (3.3) and by replacing the hopping terms as follows,

$$\phi_x^{e*} \, e^{\,i\,q^e\,A_{x,\mu}^e} \, \phi_{x+\hat{\mu}}^e \;\to\; \phi_x \, e^{\,i\,q^e\,A_{x,\mu}^e + i\,q^m\,\tilde{A}_{F(x),\mu}^m} \, \phi_{x+\hat{\mu}} \,. \tag{3.13}$$

The field ϕ^m from the previous section is dropped completely.[7] Under a duality transformation the dyon field is mapped to the dual lattice, and since in the construction here we identify original and dual lattice, the duality relations (3.9) apply also to the dyonic case, of course with the modification that we have only a single mass parameter M and only a single quartic coupling λ. As in the previous subsection, also here the construction carries over to fermionic dyon matter in an obvious way.

Notice, however, that coupling dyons makes it difficult to eliminate the sign problem even if they are bosonic. In the previous subsection and appendix E the complex action problem was solved by switching to a worldline formulation for the magnetic matter, which converts the dependence of the magnetic matter action on the magnetic gauge field $\widetilde{A}^m$ into terms of the form $e^{i\,q^m\,\widetilde{A}^m_{\tilde{x},\mu}\,\widetilde{k}_{\tilde{x},\mu}}$ where the $\widetilde{k}_{\tilde{x},\mu} \in \mathbb{Z}$ are the flux variables that describe the dynamics of the magnetic matter in the worldline language (see appendix E). In this form the $\widetilde{A}^m$ then can be integrated out together with the constraint factors (2.10) to generate more general constraints that couple the Villain and the flux variables. However, when dyons are considered, the worldline expansion also generates terms of the form $e^{i\,q^e\,A^e_{x,\mu}\,k_{x,\mu}}$ that can not be integrated out, since the action for the electric gauge field A^e is quadratic. Further the $\mathcal{S}$-duality transformation does not change the situation, since it merely interchanges the form of the electric and the magnetic gauge action, i.e., one of the two is always quadratic. Hence dyons generically have a complex action problem.

However, it is well known that a θ-term can add or remove an electric charge from a monopole, which is the famous Witten effect [34], and we will exploit this effect to relate some dyonic theories to their simpler cousins discussed in the previous subsection, where indeed a worldline representation solves the complex action problem. We will review the Witten effect and its relation to the complex action problem in the next section when we introduce the θ-term for the Villain action. For the moment let us just note that when we change $\theta \to \theta \pm 2\pi$ we can absorb this shift by changing the dyonic charges $q^e \to q^e \mp q^m$ and $q^m \to q^m$. Obviously this can be used to relate theories with sign problem to theories that can be simulated without the sign problem. This idea becomes more powerful when the shift of θ is combined with the duality transformation such that the group of transformations becomes $\mathrm{SL}(2,\mathbb{Z})$. We will see that this allows us to connect some theories which have dyons[8] and a nonzero θ-term, to theories without the complex action problem. This will be discussed in detail in section 4.5.

4   QED with a θ-term

We generalize our formulation of self-dual U(1) lattice gauge theory and self-dual lattice QED further by adding a θ-term. We first construct a suitable discretization of the topological charge and analyze its properties. Subsequently we add the θ-term to the gauge field Boltzmann factor and identify the corresponding duality transformation. In yet another

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[7]We remark that we could have placed the dyonic field also on the dual lattice by coupling the dual of the electric field there.

[8]As we will see, such dyonic theories in general have smeared electric and magnetic charges, as the introduction of the θ-term will force the Witten effect to endow monopoles with electric charges which are generically spread across multiple lattice links.

generalization step we construct a self-dual Boltzmann factor at finite θ for the gauge fields, which then is the basis for fully self-dual U(1) lattice gauge theory and self-dual lattice QED both now containing also the θ-term.

Before we go through these steps, let us comment on our construction. It is well known that there are many ways to discretize a θ-term. We will, however, insist that the θ-term capturea the topological aspecta of the continuum U(1) theory. In the continuum the θ-term of the U(1) gauge theory is

$$S_\theta = i\theta\, Q \ , \tag{4.1}$$

where

$$Q = \frac{1}{8\pi^2} \int d^4x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} F_{\mu\nu} F_{\rho\sigma} \epsilon^{\mu\nu\rho\sigma} \ , \tag{4.2}$$

is the topological charge. It is well known that the θ-term does not depend on the local details of the gauge field A_μ, and only depends on the topological class of the gauge bundle. In other words, the variation of the above action with respect to small local changes of the gauge field A_μ is zero.

Moreover when θ is shifted $\theta \to \theta + 2\pi$, the Euclidean path integral weight is unchanged in the continuum, because[9] $Q \in \mathbb{Z}$.

The above features are both ruined in the presence of a dynamical monopole.[10] Indeed the Witten effect would endow the worldline of the monopole with electric charge $\theta/2\pi$, hence generating an explicit dependence on the gauge field A_μ along the monopole worldline, turning the monopole into a dyon. We will see a manifestation of this in our lattice construction below. The θ-periodicity can be restored if the theory contains an entire tower of dyons of all electric charges, but generically it will be destroyed by the presence of dynamical magnetic matter.

To construct the desired θ-term, we will therefore be guided by a theory without monopoles being gauge-invariant, independent of the local details of the gauge field $A_{x,\mu}$ and that has a 2π-periodicity in θ. To construct such a term it is sufficient to construct the appropriate topological charge Q. The most natural way to construct such a topological charge is to identify the lattice Λ and its dual $\widetilde{\Lambda}$ by defining a map $\Lambda \to \widetilde{\Lambda}$, as was discussed in [7]. Since such maps are not unique, the definition of the topological charge Q will not be unique either, and the most general definition of the topological charge will not be local. All of these definitions will turn out to be equivalent when monopoles are absent, because of the topological nature of Q.

We will see, however, that if such a θ term is introduced, any attempt to define an ultra-local kinetic term will fail to satisfy self-duality. In particular electric-magnetic duality transformation of such an ultra-local action would produce a local, but not ultra local action, and therefore violate the self-dual covariance. When we insist on self-duality we will be forced to consider local, but not ultra-local actions.

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[9]This is only true on spin manifolds. On non-spin manifolds the θ-periodicity is $\theta \to \theta + 4\pi$ because Q can be half-integer.

[10]Such an operator is constructed by excising a contour $\mathcal{C}$ from the space-time manifold, and imposing that on a small sphere linking the contour $\mathcal{C}$ the flux is $\int F = 2\pi q_m$, where $q_m \in \mathbb{Z}$ is the charge of the monopole operator.

It is well known that θ-periodicity and self-duality generate an $\mathrm{SL}(2,\mathbb{Z})$ duality group. Therefore, insisting on the exact $\mathrm{SL}(2,\mathbb{Z})$ structure of a lattice theory will force us to abandon ultra-locality.

4.1 Construction of a suitable topological charge

Following [7] we now introduce a topological charge for the Villain formulation but already generalize the discretization presented in [7] to a form that will turn out to be useful for the construction of self-dual theories with a θ-term. More specifically we introduce a whole family $Q_T[F^e]$ of lattice discretizations for the topological charge that are labelled by an integer-valued vector T,

$$
\begin{aligned}
Q_T[F^e] &\equiv \frac{1}{8\pi^2} \sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} F^e_{x,\mu\nu} \, \epsilon_{\mu\nu\rho\sigma} \, F^e_{x-\hat\rho-\hat\sigma+T,\,\rho\sigma} \\
&= \frac{1}{8\pi^2} \sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} (dA^e + 2\pi n)_{x,\mu\nu} \, \epsilon_{\mu\nu\rho\sigma} \, (dA^e + 2\pi n)_{x-\hat\rho-\hat\sigma+T,\,\rho\sigma} \,,
\end{aligned}
\tag{4.3}
$$

where we have introduced $T = \sum_\mu t_\mu \hat\mu$ with $t_\mu \in \mathbb{Z}$. Note that $F^e_{x,\mu\nu}$ is again given by the combination (2.5) of the exterior derivative and the Villain variable, i.e., $F^e_{x,\mu\nu} = (dA^e)_{x,\mu\nu} + 2\pi n_{x,\mu\nu}$. We now want to show that the definition has the desired properties of the continuum topological charge, when magnetic monopoles are not present. Since monopoles are not present, we will assume that Villain variables obey the closedness constraints (2.7). Thus the topological properties of $Q_T[F^e]$ as we define it in (4.3) are specific to the case when monopoles are absent.

For $T = 0$ the definition of $Q_0[F^e]$ is essentially a direct lattice discretization of the continuum topological charge $Q \propto \int d^4x \, F_{\mu\nu}(x) \epsilon_{\mu\nu\rho\sigma} F_{\rho\sigma}(x)$ with an additional shift of the second factor $F^e_{x,\rho\sigma}$ by one lattice unit in the negative ρ and σ directions.[11] This, in the absence of monopoles, will have as a consequence that the θ-term depends only on the villain variables $n_{x,\mu\nu}$ and not on gauge fields, and will also imply θ periodicity by 2π. Following [7], this θ-term may be interpreted as defining a map from a lattice to a dual lattice, and then making a natural product of $F^e_{x,\mu\nu}$ on a plaquette $(x,\mu\nu)$ with the corresponding dual field strength on the plaquette dual to $(x,\mu\nu)$. For $T \neq 0$ this definition from [7] is generalized to a product of $F^e_{x,\mu\nu}$ with the dual field strength on the dual plaquette shifted by T, which we implement by adding T in the argument of the second factor in (4.3). Note that when T becomes larger than the extent of the lattice the periodic boundary conditions will identify the shifted site $x + T$ with some site of the lattice, such that only a finite number of vectors T correspond to distinct definitions of $Q_T[F^e]$.

We will now show, that $Q_T[F^e]$ is topological in nature and that $Q_T[F^e]$ gives the same result for all vectors T as long as the Villain variables are closed. We proceed towards this goal in several steps where we discuss and use properties of $Q_T[F^e]$ that are partly proven in appendix B.

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[11]Without this shift we would not be able to show the topological properties of Q_T, and the θ-term in the absence of monopoles would lose the independence on $A^e_{x,\mu}$ and the θ-periodicity.

The first property shown in appendix B is the fact that $Q_T[F^e]$ is invariant under adding an arbitrary exterior derivative $(dB)_{x,\mu\nu}$ to the field strength $F^e_{x,\mu\nu}$, i.e.,

$$Q_T[F^e + dB] = Q_T[F^e] \,, \qquad (4.4)$$

where $B_{x,\mu}$ is an arbitrary 1-form, i.e., an arbitrary set of link-based fields. We stress again that this property only holds when the Villain variables $n_{x,\mu\nu}$ in $F^e_{x,\mu\nu} = (dA^e)_{x,\mu\nu} + 2\pi\, n_{x,\mu\nu}$ obey the closedness condition (2.7).

The property (4.4) immediately implies that $Q_T[F^e]$ is independent of the exterior derivative $(dA^e)_{x,\mu\nu}$ in $F^e_{x,\mu\nu} = (dA^e)_{x,\mu\nu} + 2\pi\, n_{x,\mu\nu}$. Thus the topological charge depends only on the Villain variables $n_{x,\mu\nu}$ and we may write (compare the definition (4.3))

$$Q_T[F^e] = \frac{1}{2} \sum_x \sum_{\substack{\mu < \nu \\ \rho < \sigma}} n_{x,\mu\nu}\, \epsilon_{\mu\nu\rho\sigma}\, n_{x-\hat{\rho}-\hat{\sigma}+T,\rho\sigma} \;\; \text{with} \;\; (dn)_{x,\mu\nu\rho} = 0 \;\; \forall x, \mu < \nu < \rho \,. \qquad (4.5)$$

The fact that the Villain variables obey the closedness condition (2.7) can be used together with the Hodge decomposition (see eq. (A.3) of appendix A) to write the Villain variables in the form

$$n_{x,\mu\nu} = (d\,l)_{x,\mu\nu} + h_{x,\mu\nu} \,, \qquad (4.6)$$

where the condition $(d\,n)_{x,\mu\nu\rho} = 0$ implies that we do not have a contribution $(\partial\,c)_{x,\mu\nu\rho}$ in the Hodge decomposition (A.3) of $n_{x,\mu\nu}$. In (4.6) $l_{x,\mu} \in \mathbb{Z}$ is an integer-valued 1-form which due to $d^2 l = 0$ does not contribute to dn. The second term in the Hodge decomposition (4.6) are the closed integer-valued harmonic contributions $h_{x,\mu\nu}$ which obey $(dh)_{x,\mu\nu\rho} = 0$ and cannot be written as exterior derivatives. We may parameterize them in the form ($\mu < \nu$)

$$h_{x,\mu\nu} = \omega_{\mu\nu} \sum_{i=1}^{N_\rho} \sum_{j=1}^{N_\sigma} \delta^{(4)}_{x,i\hat{\rho}+j\hat{\sigma}} \quad \text{with} \quad \rho \neq \mu, \nu \,; \sigma \neq \mu, \nu \,; \rho \neq \sigma \,, \qquad (4.7)$$

where N_ρ and N_σ denote the lattice extents in the ρ- and σ-directions and $\delta^{(4)}_{x,i\hat{\rho}+j\hat{\sigma}}$ is the 4-dimensional Kronecker delta. In other words $h_{x,\mu\nu}$ is the constant $\omega_{\mu\nu} \in \mathbb{Z}$ for μ-ν plaquettes $(x,\mu\nu)$ that have their root site x in the ρ-σ plane that is orthogonal to the μ-ν plane and contains the origin. For all other plaquettes $h_{x,\mu\nu} = 0$. It is easy to see that the harmonics $h_{x,\mu\nu}$ are closed forms, i.e., they obey $(dh)_{x,\mu\nu\rho} = 0$. We stress that our choice for the parameterization of the $h_{x,\mu\nu}$ is not unique, since they can be deformed by adding arbitrary exterior derivatives.

In appendix B we show the following result for the topological charge[12]

$$Q_T[2\pi n] = Q_T[2\pi h] = \omega_{12}\,\omega_{34} - \omega_{13}\omega_{24} + \omega_{14}\omega_{23} = \frac{1}{8}\epsilon_{\mu\nu\rho\sigma}\omega_{\mu\nu}\omega_{\rho\sigma} \in \mathbb{Z} \,, \;\; \forall\, T \,. \qquad (4.8)$$

The first identity follows already from (4.4) and shows that the topological charge depends only on the harmonic contributions to the Villain variables. The second step is the explicit evaluation of $Q_T[2\pi n] = Q_T[2\pi h]$ for the parameterization (4.7) of the harmonics, which,

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[12]In the notation for the final expression on the r.h.s. of (4.8) we assume antisymmetry of the $\omega_{\mu\nu}$.

as shown in appendix B, turns out to be independent of the vector T that appears as a parameter in the definitions (4.3) and (4.5). This completes the proof of our statement that for closed Villain variables $Q_T[F^e] = Q_T[2\pi n] = Q_T[2\pi h]$ is independent of T due to its topological nature. In addition the definition of the topological charge is integer-valued and can be computed uniquely from the harmonics in the Hodge decomposition of the Villain variables.

4.2 The Witten effect

Before we come to performing the duality transformation in the next section let us discuss an interesting physical aspect of the abelian θ-term, the Witten effect, which constitutes an important consistency check of our formulation. The Witten effect states that the θ-term endows a magnetic monopole with the minimal possible magnetic charge $m = 2\pi$ with an electric charge $q = \theta/2\pi$.

We here consider a general definition of the topological charge given by the superposition of different discretizations Q_T,

$$Q = \sum_T \gamma_T \, Q_T[dA^e + 2\pi n] \, , \tag{4.9}$$

where the Q_T are given by (4.3) and we require $\sum_T \gamma_T = 1$. Now consider a magnetic Wilson loop defined by

$$\prod_{(\tilde{x},\mu)\in\widetilde{C}} e^{\,i\,\widetilde{A}^m_{\tilde{x},\mu}} \, , \tag{4.10}$$

along some contour $\widetilde{C}$ on the dual lattice. Combining the Wilson loop with the closedness factor (2.10) and integrating over the $\widetilde{A}^m$ we find

$$\int D[\widetilde{A}^m] \, e^{-i\sum_x \sum_{\mu<\nu<\rho} A^m_{x,\mu\nu\rho}(dn)_{x,\mu\nu\rho}} \prod_{(\tilde{x},\mu)\in\widetilde{C}} e^{\,i\,\widetilde{A}^m_{\tilde{x},\mu}} \tag{4.11}$$

$$= \int D[\widetilde{A}^m] \prod_{(\tilde{x},\mu)\in\widetilde{C}} e^{\,i\,\widetilde{A}^m_{\tilde{x},\mu}[1+\sum_{\nu<\rho<\sigma} \epsilon_{\mu\nu\rho\sigma}(dn)_{x+\hat\mu,\nu\rho\sigma}]} \prod_{(\tilde{x},\mu)\notin\widetilde{C}} e^{\,i\,\widetilde{A}^m_{\tilde{x},\mu}\sum_{\nu<\rho<\sigma} \epsilon_{\mu\nu\rho\sigma}(dn)_{x+\hat\mu,\nu\rho\sigma}} ,$$

where in the second step we rewrote the A^m in terms of the dual fields $\widetilde{A}^m$. Obviously this integral imposes the new constraint

$$\sum_{\nu<\rho<\sigma} \epsilon_{\mu\nu\rho\sigma}(dn)_{x+\hat\mu,\nu\rho\sigma} = \begin{cases} -1 & \text{if } (\tilde{x},\mu)\in\widetilde{C} \ , \\ 0 & \text{if } (\tilde{x},\mu)\notin\widetilde{C} \ . \end{cases} \tag{4.12}$$

This constraint modifies the condition (2.7), which in its original form ensures the complete absence of monopoles, while now along the contour $\widetilde{C}$ of the magnetic Wilson loop (4.10) monopole charges are inserted.

Let us now inspect Q_T in the presence of the modified constraint (4.12) induced by the magnetic Wilson loop. We find (use $Q_T[dA^e] = 0$),

$$Q_T[dA^e + 2\pi n] = \frac{1}{4\pi} \sum_x \sum_{\substack{\mu < \nu \\ \rho < \sigma}} n_{x,\mu\nu} \epsilon_{\mu\nu\rho\sigma}(dA^e)_{x+T-\hat{\rho}-\hat{\sigma}, \rho\sigma}$$
$$+ \frac{1}{4\pi} \sum_x \sum_{\substack{\mu < \nu \\ \rho < \sigma}} (dA^e)_{x,\mu\nu} \epsilon_{\mu\nu\rho\sigma} n_{x+T-\hat{\rho}-\hat{\sigma}, \rho\sigma} + Q_T[2\pi n] . \tag{4.13}$$

Reorganizing the sums one finds

$$\sum_x \sum_{\substack{\mu < \nu \\ \rho < \sigma}} n_{x,\mu\nu} \epsilon_{\mu\nu\rho\sigma}(dA^e)_{x+T-\hat{\rho}-\hat{\sigma}, \rho\sigma} = \sum_x \sum_{\substack{\mu < \nu \\ \rho < \sigma}} n_{x-T+\hat{\rho}+\hat{\sigma},\mu\nu} \epsilon_{\mu\nu\rho\sigma}(dA^e)_{x, \rho\sigma} \tag{4.14}$$

$$= \sum_x \sum_{\rho < \sigma} N_{x,\rho\sigma}(dA^e)_{x, \rho\sigma} = \sum_x \sum_\mu A^e_{x,\mu}(\partial N)_{x,\mu} = \sum_x \sum_\mu A_{x+T,\mu} \sum_{\nu < \rho < \sigma} \epsilon_{\mu\nu\rho\sigma}(dn)_{x+\hat{\mu},\nu\rho\sigma} ,$$

where

$$N_{x,\rho\sigma} = \sum_{\mu < \nu} n_{x-T+\hat{\rho}+\hat{\sigma},\mu\nu} \epsilon_{\mu\nu\rho\sigma} . \tag{4.15}$$

In the third step of (4.14) we used the partial integration formula (A.2), and again some reordering of terms to get to the final form. In a similar way we find for the second sum in (4.13),

$$\sum_x \sum_{\substack{\mu < \nu \\ \rho < \sigma}} (dA^e)_{x,\mu\nu} \epsilon_{\mu\nu\rho\sigma} n_{x+T-\hat{\rho}-\hat{\sigma},\rho\sigma} = \sum_x \sum_\mu A_{x-T+\hat{s},\mu} \sum_{\nu < \rho < \sigma} \epsilon_{\mu\nu\rho\sigma}(dn)_{x+\hat{\mu},\nu\rho\sigma} , \tag{4.16}$$

so that inserting (4.13), (4.14) and (4.16) in (4.9) we find

$$Q[dA^e + 2\pi n] = \frac{1}{2\pi} \sum_x \sum_\mu \sum_T \gamma_T \frac{A_{x+T,\mu} + A_{x-T+\hat{s},\mu}}{2} \sum_{\nu < \rho < \sigma} \epsilon_{\mu\nu\rho\sigma}(dn)_{x+\hat{\mu},\nu\rho\sigma} + Q[2\pi n] . \tag{4.17}$$

Since in the presence of the magnetic Wilson loop $\prod_{(\tilde{x},\mu) \in \widetilde{C}} e^{i \widetilde{A}^m_{\tilde{x},\mu}}$ upon integrating over the $\widetilde{A}^m$ we have $\sum_{\nu < \rho < \sigma} \epsilon_{\mu\nu\rho\sigma}(dn)_{x,\nu\rho\sigma} = -1$ whenever $(\tilde{x}, \mu) \in \widetilde{C}$, and since Q comes with a weight $e^{-i\theta Q}$ in the partition function, a magnetic Wilson loop generates the contribution

$$\prod_{(\tilde{x},\mu) \in \widetilde{C}} e^{i \frac{\theta}{2\pi} \sum_T \gamma_T \frac{A^e_{x+T,\mu} + A^e_{x-T+\hat{s},\mu}}{2}} , \tag{4.18}$$

which is the A^e-dependent part of $Q[dA^e + 2\pi n]$ that gets added to the topological part $Q[2\pi n]$ given by the harmonic contributions as stated in (4.8). The interpretation of the above formula is that the monopole gets an electric charge $q^e = \frac{\theta}{2\pi}$, although smeared to the neighborhood of the dual link $(\tilde{x}, \mu)$. This is the famous Witten effect [34].

When we discussed the coupling of dyonic matter in subsection 3.2, we already announced, that in this context the Witten effect gives rise to a new duality $\mathcal{T}$ which relates shifts of the θ angle by 2π to a shift of the magnetic charge. The remainder of this subsection is devoted to discussing the duality $\mathcal{T}$.

Similar to the derivation of the worldline expansion of magnetic matter discussed in appendix E we may expand the hopping terms of the dyon action (compare (3.13)) to bring the dependence of the dyon partition sum on the two gauge fields into the form

$$\prod_{(x,\mu)} e^{i\left[q^e A^e_{x,\mu} + q^m \widetilde{A}^m_{F(x),\mu}\right] k_{x,\mu}} = \prod_{(x,\mu)} e^{i\,q^e A^e_{x,\mu} k_{x,\mu}} \prod_{(x,\mu)} e^{i\,q^m \widetilde{A}^m_{F(x),\mu} k_{x,\mu}} , \qquad (4.19)$$

where $k_{x,\mu} \in \mathbb{Z}$ are the flux variables for dyon matter (compare appendix E). Obviously the second factor on the r.h.s. generalizes the insertion of the magnetic Wilson loop considered in (4.10). Upon integrating out the magnetic gauge field this generates the modified constraint

$$\sum_{\nu < \rho < \sigma} \epsilon_{\mu\nu\rho\sigma} (dn)_{x+\hat{\mu},\nu\rho\sigma} = -q^m k_{x,\mu} \quad \forall\, (x,\mu) , \qquad (4.20)$$

which now replaces (4.12). However, the steps discussed in the previous paragraphs go through essentially unchanged also with the new constraint, and the additional term that is generated by the topological charge is a generalization of (4.18) given by

$$\prod_{(x,\mu)} e^{i\frac{\theta}{2\pi} q_m \sum_T \gamma_T \frac{A^e_{x+T,\mu} + A^e_{x-T+\hat{s},\mu}}{2} k_{x,\mu}} \prod_{(x,\mu)} \delta\left(\sum_{\nu < \rho < \sigma} \epsilon_{\mu\nu\rho\sigma} (dn)_{x+\hat{\mu},\nu\rho\sigma} + q^m k_{x,\mu} \right) e^{-i\theta Q[2\pi n]} , \qquad (4.21)$$

where we also wrote explicitly the constraint (4.20), using the already familiar product over Kronecker deltas. We also display the remaining topological contribution. The first factor in (4.18) may be combined with the flux terms (4.19) and we replace

$$\prod_{(x,\mu)} e^{i\left[q^e A^e_{x,\mu} + q^m \widetilde{A}^m_{F(x),\mu}\right] k_{x,\mu}} \;\rightarrow\; \prod_{(x,\mu)} e^{i\left[q^e A^e_{x,\mu} + q^m \sum_T \gamma_T \frac{A^e_{x+T,\mu} + A^e_{x-T+\hat{s},\mu}}{2} + q^m \widetilde{A}^m_{F(x),\mu}\right] k_{x,\mu}} , \qquad (4.22)$$

where we have reinstated the terms with $\widetilde{A}^m$ that upon integration generate the constraint in (4.21), given that the topological term is kept in the form $Q[2\pi n]$.

Note that the required 1-form gauge invariance [7]

$$\begin{aligned} A^e_{x,\mu} &\to A^e_{x,\mu} + 2\pi k_{x,\mu} , \\ n_{x,\mu\nu} &\to n_{x,\mu\nu} - (dk)_{x,\mu\nu} , \end{aligned} \qquad (4.23)$$

can be achieved by a shift of $A^m_{\tilde{x},\mu}$,

$$\widetilde{A}^m_{F(x),\mu} \to \widetilde{A}^m_{F(x),\mu} - \frac{\theta}{2} \sum_T \gamma_T \left(k_{x+T-\hat{\mu},\mu} + k_{x-T+s-\hat{\mu},\mu} \right) . \qquad (4.24)$$

Indeed the remainder of the action, has phase terms

$$i\theta Q[2\pi n] + i \sum_x \sum_{\mu < \nu < \rho} \epsilon^{\mu\nu\rho\sigma} (dn)_{x,\mu\nu\rho} \tilde{A}^m_{F(x)-\hat{\sigma},\sigma} , \qquad (4.25)$$

which are invariant under the transformations (4.23) and (4.24). Note that $Q[2\pi n]$ is now no longer necessarily an integer, because it is a sum of integers weighted by γ_T, and must

be kept in the action even if $\theta \in 2\pi\mathbb{Z}$. In fact it is crucial that this term is not dropped, as then the gauge symmetry (4.24) would be ruined.

The r.h.s. of (4.22) shows that in the presence of magnetic matter, the topological term generates an additional contribution to the electric charge, such that the combined electric charge is given by $q^e + q^m\theta/2\pi$, although this charge is generally smeared across multiple lattice links, weighted by γ_T. In fact, no choice of the coefficients γ_T in the definition (4.9) allows for an ultra-local Witten effect. Indeed, if even only a single γ_T is nonzero, i.e., $\gamma_T = 1$ with $\gamma_{T'} = 0 \; \forall \; T' \neq T$, this will produce the spread of the electric charge. However, independent of the details of the definition of Q we find that shifting $\theta \to \theta + 2\pi$ is equivalent to shifting the electric charge $q^e \to q^m + q^e$. Thus, if we shift $\theta \to \theta - 2\pi$ and simultaneously $q^e \to q^m + q^e$ this becomes an invariance. We will refer to this invariance as $\mathcal{T}$ duality, as is conventional, and summarize it as follows,

$$\theta \to \bar{\theta} = \theta - 2\pi \,, \;\; \boldsymbol{q} \to \bar{\boldsymbol{q}} = T\,\boldsymbol{q} \;\; \text{with} \;\; T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \,, \tag{4.26}$$

where again we use the vector of charges $\boldsymbol{q} = (q^e, q^m)^t$. We will later see that the $\mathcal{S}$ duality defined in (3.10), i.e., the self-dual transformation, and the duality $\mathcal{T}$ together generate the group $\mathrm{SL}(2,\mathbb{Z})$.

In the next two subsections we will see that a generalized form of the $\mathcal{S}$ duality holds also for the theory with a θ-term, but that the discretization we discussed so far will not map the action into the same form under a duality transformation. We will then go on to construct lattice actions which enjoy an exact self-duality, at the price of abandoning the ultra-local structure we so far employed. That such a non-ultra-local structure may be expected is already suggested by the discussion of the Witten effect in this subsection.

4.3 θ-term and duality transformation

We now generalize the partition sum (3.1) of self-dual lattice QED further by adding a θ-term and discuss the form of the duality transformation in the presence of such a term. This will not yet give rise to a self-dual theory, which will be identified only in the next subsection after another necessary generalization of the action.

We may write the partition sum that now also contains the θ-term in the form

$$Z(\beta, \theta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^e) \equiv \int D[A^e]\int D[A^m] B_{\beta,\theta}[A^e, A^m] Z_{M^e, \lambda^e, q^e}[A^e] \widetilde{Z}_{M^m, \lambda^m, q^m}\big[\widetilde{A}^m\big], \tag{4.27}$$

where we have generalized the Boltzmann factor (2.13) by adding the θ-term,

$$B_{\beta,\theta}[A^e, A^m] \equiv \sum_{\{n\}} e^{-\frac{\beta}{2}\sum_x \sum_{\mu<\nu}\left(F^e_{x,\mu\nu}\right)^2} \; e^{-i\,\theta\,Q_0[F^e]} \; e^{-i\sum_x\sum_{\mu<\nu<\rho} A^m_{x,\mu\nu\rho}(dn)_{x,\mu\nu\rho}} . \tag{4.28}$$

Note that for now we use the $T = 0$ discretization $Q_0[F^e]$ from the family $Q_T[F^e]$ of possible equivalent lattice forms of the topological charge we have introduced in subsection 4.1 in eq. (4.3). We will generalize the θ-term further in the next subsection when we construct the self-dual form of the Boltzmann factor.

Both, the gauge field action and the topological charge $Q_0[F^e]$ are quadratic in $F^e = dA^e + 2\pi\, n$, such that we can combine them in a quadratic form. The Boltzmann factor thus reads

$$B_{\beta,\theta}[A^e, A^m] = \sum_{\{n\}} e^{-\frac{\beta}{2} \sum_{\substack{x,\mu<\nu \\ y,\rho<\sigma}} F^e_{x,\mu\nu}\, M_{x,\mu\nu|y,\rho\sigma}\, F^e_{y,\rho\sigma}}\; e^{i\sum_{x,\mu<\nu}(\partial A^m)_{x,\mu\nu}\, n_{x,\mu\nu}}, \qquad (4.29)$$

where we used the partial integration formula (A.2) from appendix A to also rewrite the exponent of the last exponential that upon integration over A^m generates the constraints, which in the absence of magnetically charged matter are the closedness constraints (2.7) or, when magnetic matter is coupled, the modified constraints (4.12). The kernel $M_{x,\mu\nu|y,\rho\sigma}$ of the quadratic form (4.29) is defined as (note that in our notation $\mu < \nu$ and $\rho < \sigma$)

$$M_{x,\mu\nu|y,\rho\sigma} = \delta_{\mu\rho}\, \delta_{\nu\sigma}\, \delta^{(4)}_{x,y} + i\,\xi\, \epsilon_{\mu\nu\rho\sigma}\, \delta^{(4)}_{x-\hat\rho-\hat\sigma,y} \qquad \text{with} \quad \xi \equiv \frac{\theta}{4\pi^2\beta}\,. \qquad (4.30)$$

Using Fourier transformation (see appendix C for our conventions) we may diagonalize the lattice site dependence of M. Using (C.1) we find for the Fourier transform of M,

$$\widehat{M}(p)_{\mu\nu|\rho\sigma} = \sum_x e^{ip\cdot(x-y)} M_{x,\mu\nu|y,\rho\sigma} = \delta_{\mu\rho}\, \delta_{\nu\sigma} + i\,\xi\, \epsilon_{\mu\nu\rho\sigma}\, e^{ip_\rho + ip_\sigma}\,. \qquad (4.31)$$

It is straightforward to see that for $|\xi| < 1$ (this is a sufficient condition) we have $\det \widehat{M} \neq 0$, such that the matrix $\widehat{M}$ in Fourier space is invertible and thus also the real space matrix M. One finds (see appendix C),

$$\begin{aligned}
\widehat{M}(p)^{-1}_{\mu\nu|\rho\sigma} &= \frac{\delta_{\mu\rho}\, \delta_{\nu\sigma} - i\,\xi\, \epsilon_{\mu\nu\rho\sigma}\, e^{ip_\rho + ip_\sigma}}{1 + \xi^2\, e^{ip\cdot\hat{s}}} \\
&= \sum_{k=0}^{\infty} (-\xi^2)^k \left[\delta_{\mu\rho}\, \delta_{\nu\sigma}\, e^{ip\cdot k\hat{s}} - i\,\xi\, \epsilon_{\mu\nu\rho\sigma}\, e^{ip_\rho + ip_\sigma + ip\cdot k\hat{s}} \right],
\end{aligned} \qquad (4.32)$$

where $\hat{s} = \hat{1} + \hat{2} + \hat{3} + \hat{4}$ and in the second step we have expanded the denominator using the geometric series which converges exponentially for $|\xi| < 1$. Using this second form and (C.2) we can evaluate $M^{-1}_{x,\mu\nu|y,\rho\sigma}$ and obtain,

$$M^{-1}_{x,\mu\nu|y,\rho\sigma} = \sum_{k=0}^{\infty} (-\xi^2)^k \left[\delta_{\mu\rho}\, \delta_{\nu\sigma}\, \delta^{(4)}_{x-k\hat{s},y} - i\,\xi\, \epsilon_{\mu\nu\rho\sigma}\, \delta^{(4)}_{x-\hat\rho-\hat\sigma-k\hat{s},y} \right]. \qquad (4.33)$$

We now apply the generalized Poisson resummation formula proven in appendix D for $N = 6V$ and find[13] (use again eq. (2.14) to first rewrite the second exponent in (4.29))

$$B_{\beta,\theta}[A^e, A^m] =$$
$$C_M(\beta) \sum_{\{p\}} e^{-\frac{\widetilde{\beta}}{2} \sum_{\substack{x,\mu<\nu \\ y,\rho<\sigma}} (\partial A^m + 2\pi p)_{x,\mu\nu}\, M^{-1}_{x,\mu\nu|y,\rho\sigma}\, (\partial A^m + 2\pi p)_{y,\rho\sigma}}\; e^{-i\sum_{x,\mu<\nu}(dA^e)_{x,\mu\nu}\, p_{x,\mu\nu}}, \quad (4.34)$$

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[13] We remark that it is easy to show that for $|\xi| < 1$ all eigenvalues of M have positive real parts, which guarantees the existence of the Gaussian integral in the Poisson resummation.

with

$$\widetilde{\beta} \equiv \frac{1}{4\pi^2 \beta}\,, \qquad \sum_{\{p\}} \equiv \prod_{x,\mu<\nu} \sum_{p_{x,\mu\nu} \in \mathbb{Z}}\,, \qquad C_M(\beta) \equiv \frac{1}{(\sqrt{2\pi\beta})^{6V}\sqrt{\det M}}\,. \tag{4.35}$$

$\sum_{\{p\}}$ denotes the sum over all configurations of plaquette occupation numbers $p_{x,\mu\nu} \in \mathbb{Z}$.

Note that the first exponent in (4.34) with $M^{-1}_{x,\mu\nu|y,\rho\sigma}$ given by (4.33) gives rise to a lattice action that combines terms at arbitrary distances shifted relative to each other by $k\hat{s}$ with $k \in \mathbb{N}_0$, such that this action is not ultra-local, i.e., it connects terms at arbitrary distances $k\hat{s}$. However, the corresponding terms are suppressed exponentially with k, due to the condition $|\xi| < 1$. Such types of non-ultra local lattice actions with exponential suppression of shifted terms are widely used, with prominent examples being fixed point actions [35] or the overlap operator [25], and it is known that the exponential suppression of distant terms guarantees a local continuum limit [36]. As already mentioned, such lattice actions are referred to as local but non-ultra-local actions.

Let us now complete the duality transformation. The final step of the duality transformation is to express the electric and the magnetic gauge fields, as well as the plaquette occupation numbers in terms of their counterparts on the dual lattice, i.e., we again use eqs. (2.21) and (2.22). We find

$$B_{\beta,\theta}[A^e, A^m] = C_M(\beta)\sum_{\{p\}} e^{-\frac{\widetilde{\beta}}{2}\sum_{\substack{\tilde{x},\mu<\nu \\ \tilde{y},\rho<\sigma}} \widetilde{F}^m_{\tilde{x},\mu\nu} \widetilde{M}_{\tilde{x},\mu\nu|\tilde{y},\rho\sigma} \widetilde{F}^m_{\tilde{y},\rho\sigma}} \; e^{-i\sum_{\tilde{x},\mu<\nu<\rho} \widetilde{A}^e_{\tilde{x},\mu\nu\rho}(\widetilde{dp})_{\tilde{x},\mu\nu\rho}}, \tag{4.36}$$

where $\widetilde{F}^m_{\tilde{x},\mu\nu} = (d\widetilde{A}^m + 2\pi\tilde{p})_{\tilde{x},\mu\nu}$. The kernel $\widetilde{M}_{\tilde{x},\mu\nu|\tilde{y},\rho\sigma}$ is identified from $M^{-1}_{x,\mu\nu|y,\rho\sigma}$ when replacing $(\partial A^m + 2\pi p)_{x,\mu\nu}$ by the dual expression $\sum_{\mu'<\nu'} \epsilon_{\mu\nu\mu'\nu'}(d\widetilde{A}^m + 2\pi\tilde{p})_{\tilde{x}-\hat{\mu}'-\hat{\nu}',\mu'\nu'}$ in the exponent of (4.34) using (2.22), i.e.,

$$\widetilde{M}_{\tilde{x},\mu\nu|\tilde{y},\rho\sigma} \equiv \sum_{\substack{\mu'<\nu' \\ \rho'<\sigma'}} \epsilon_{\mu\nu\mu'\nu'} M^{-1}_{x+\hat{\mu}'+\hat{\nu}',\mu'\nu'|y+\hat{\rho}'+\hat{\sigma}',\rho'\sigma'} \epsilon_{\rho'\sigma'\rho\sigma} \bigg|_{\substack{x\to\tilde{x} \\ y\to\tilde{y}}}. \tag{4.37}$$

Inserting the explicit form (4.33) of $M^{-1}_{x,\mu\nu|y,\rho\sigma}$ and summing over the indices of the epsilon tensors that appear in (4.37) we obtain in a few lines of algebra

$$\widetilde{M}_{\tilde{x},\mu\nu|\tilde{y},\rho\sigma} = \sum_{k=0}^{\infty}(-\xi^2)^k \left[\delta_{\mu\rho}\,\delta_{\nu\sigma}\,\delta^{(4)}_{\tilde{x}-k\hat{s},\tilde{y}} \; - \; i\,\xi\,\epsilon_{\mu\nu\rho\sigma}\,\delta^{(4)}_{\tilde{x}-\hat{\rho}-\hat{\sigma}-k\hat{s},\tilde{y}} \right]\,. \tag{4.38}$$

It is important to note that as for the case without θ-term, the Boltzmann factor in its dual form (4.36) is structurally similar to the original form (4.29) we started from. The dual form lives on the dual lattice and the Villain variables n were replaced by the dual plaquette occupation numbers $\tilde{p}$. The electric and magnetic gauge fields interchanged their role, such that $\widetilde{A}^m$ now appears in the quadratic form, while $\widetilde{A}^e$ generates the constraints for the dual plaquette occupation numbers.

However, the original kernel $M_{x,\mu\nu|y,\rho\sigma}$ eq. (4.30) and the dual kernel $\widetilde{M}_{\tilde{x},\mu\nu|\tilde{y},\rho\sigma}$ eq. (4.38) differ. More specifically, the original kernel $M_{x,\mu\nu|y,\rho\sigma}$ is ultra-local, while the dual kernel $\widetilde{M}_{\tilde{x},\mu\nu|\tilde{y},\rho\sigma}$ is a sum over terms that are shifted relative to each other by $k\hat{s}$ with

$k \in \mathbb{N}_0$. Comparing this form with our definition of Q_T in eq. (4.3) we find that for a fixed k the second term in (4.38) gives rise to the topological charge $Q_T[\widetilde{F}^m]$ with $T = -k\hat{s}$, i.e., $Q_{-k\hat{s}}[\widetilde{F}^m]$, with $\widetilde{F}^m_{\tilde{x},\mu\nu} = (d\widetilde{A}^m)_{\tilde{x},\mu\nu} + 2\pi\widetilde{p}_{\tilde{x},\mu\nu}$. Since integrating over $\widetilde{A}^e$ in (4.36) generates the closedness constraints for the dual plaquette occupation numbers $\widetilde{p}_{\tilde{x},\mu\nu}$, the topological charge $Q_{-k\hat{s}}[\widetilde{F}^m]$ obeys all properties we showed for the original definition (4.3). In particular it is independent of $T = -k\hat{s}$, such that $Q_{-k\hat{s}}[\widetilde{F}^m] = Q_0[\widetilde{F}^m] \; \forall k \in \mathbb{Z}$. Thus we may sum up k in the term generated by the second factor of (4.38) such that the corresponding term in the exponent reads

$$-\frac{\widetilde{\beta}}{2} 8\pi^2 Q_0[\widetilde{F}^m] (-i\xi) \sum_{k=0}^{\infty} (-\xi^2)^k = i \frac{\theta}{4\pi^2\beta^2 + \theta^2/4\pi^2} Q_0[\widetilde{F}^m] = -i\,\theta'\, Q_0[\widetilde{F}^m]\,, \quad (4.39)$$

where $\theta' \equiv -\theta/(4\pi^2\beta^2 + \theta^2/4\pi^2)$. Thus we may rewrite the dual form (4.36) as

$$B_{\beta,\theta}[A^e, A^m] =$$
$$C_M \sum_{\{p\}} e^{-\frac{\widetilde{\beta}}{2} \sum_{k=0}^{\infty} (-\xi^2)^k \sum_{\tilde{x},\mu<\nu} \widetilde{F}^m_{\tilde{x},\mu\nu} \widetilde{F}^m_{\tilde{x}-k\hat{s},\mu\nu} - i\theta' Q_0[\widetilde{F}^m]} \; e^{-i \sum_{\tilde{x},\mu<\nu<\rho} \widetilde{A}^e_{\tilde{x},\mu\nu\rho} (d\widetilde{p})_{\tilde{x},\mu\nu\rho}}, \quad (4.40)$$

where we have again used the partial integration formula to re-express the exponent in the last factor. The dual form (4.40) has to be compared to the original form of the Boltzmann factor (4.28). One sees that after interchanging the gauge fields with their dual counterparts, multiplying the trivial overall factor, and replacing β by $\widetilde{\beta}$ and θ by θ', the two expressions are almost identical. The only remaining difference is that the gauge field action has the form

$$\frac{\widetilde{\beta}}{2} \sum_{k=0}^{\infty} (-\xi^2)^k \sum_{\tilde{x},\mu<\nu} \widetilde{F}^m_{\tilde{x},\mu\nu} \widetilde{F}^m_{\tilde{x}-k\hat{s},\mu\nu} = \frac{\widetilde{\beta}}{2} \sum_{k=0}^{\infty} (-\xi^2)^k \sum_{\tilde{x},\mu<\nu} (d\widetilde{A}^m + 2\pi\widetilde{p})_{\tilde{x},\mu\nu} (d\widetilde{A}^m + 2\pi\widetilde{p})_{\tilde{x}-k\hat{s},\mu\nu}\,,$$
$$(4.41)$$

i.e., the gauge field action is a superposition of terms where the two factors of the field strength $\widetilde{F}^m$ are shifted relative to each other by $k\hat{s}$ with $k \in \mathbb{N}_0$. The $k = 0$ term corresponds to the ultra-local action we have started from, but the duality transformation has generated the non-ultra-local extension, which for $|\xi| < 1$ still gives rise to a local continuum limit as we discussed above. We remark, however, that also the restriction $|\xi| < 1$, which corresponds to $\beta > |\theta|/4\pi^2$, is an unphysical restriction for a proper self-dual lattice version of U(1) lattice gauge theory with a θ-term we are aiming at.

4.4 Identification of the exactly self-dual theory

Having developed the duality transformation in the presence of a θ-term we are now ready to identify the fully self-dual discretization that includes the θ-term. We have seen that the duality transformation has converted the ultra-local lattice action of the original theory into a non-ultra-local lattice action for the dual theory. The key insight is that in order to obtain self-duality, we must not start with an ultra-local discretization for the original theory, but with a more general ansatz that allows terms at arbitrary distances with exponentially

decreasing coefficients. We write the Boltzmann factor in the form (compare (4.29))

$$B_{\beta,\theta}[A^e, A^m] \equiv \sum_{\{n\}} e^{-\frac{\beta}{2} \sum_{\substack{x,\mu<\nu \\ y,\rho<\sigma}} F^e_{x,\mu\nu} K_{x,\mu\nu|y,\rho\sigma} F^e_{y,\rho\sigma}} e^{i \sum_{x,\mu<\nu} (\partial A^m)_{x,\mu\nu} n_{x,\mu\nu}}, \qquad (4.42)$$

where K is a new kernel that we will specify below. Again the electric gauge field A^e describes the dynamics and the magnetic gauge field A^m generates the constraints.

The key step towards self-duality is to identify a kernel K that is form-invariant under inversion. This can be done directly in momentum space, and from inspection of (4.31) and (4.32) one finds that an ansatz of the form

$$\widehat{K}(p)_{\mu\nu|\rho\sigma} = \frac{\delta_{\mu\rho}\,\delta_{\nu\sigma} + i\,\frac{\gamma}{2}\,\epsilon_{\mu\nu\rho\sigma}\,[e^{ip_\rho+ip_\sigma} + e^{-ip_\mu-ip_\nu}]}{\sqrt{1 + \frac{\gamma^2}{2}\,[1 + \cos(p \cdot \hat{s})]}}\,, \qquad (4.43)$$

with

$$\widehat{K}(p)^{-1}_{\mu\nu|\rho\sigma} = \frac{\delta_{\mu\rho}\,\delta_{\nu\sigma} - i\,\frac{\gamma}{2}\,\epsilon_{\mu\nu\rho\sigma}\,[e^{ip_\rho+ip_\sigma} + e^{-ip_\mu-ip_\nu}]}{\sqrt{1 + \frac{\gamma^2}{2}\,[1 + \cos(p \cdot \hat{s})]}}\,, \qquad (4.44)$$

defines a gauge action and a topological term where the original kernel and the inverse kernel that is used in the dual theory have the same momentum dependence, and thus the same structure also in real space.[14] Here γ is a real parameter that we do not need to specify here and later will relate to the parameters β and θ. Note that we have symmetrized the part that generates the topological charge in K to $\epsilon_{\mu\nu\rho\sigma}\,[e^{ip_\rho+ip_\sigma} + e^{-ip_\mu-ip_\nu}]$, which is related to a combination of $Q_0[F^e]$ and $Q_{-\hat{s}}[F^e]$. With this choice the normalization factor in the denominator is regular for all γ, i.e., the argument of the square root is always positive, such that we have solved the problem of an unphysical restriction of β and θ we faced in the naive attempt in the previous subsection.

It is obvious, that the non-trivial denominator $\sqrt{1 + \frac{\gamma^2}{2}\,[1 + \cos(p \cdot \hat{s})]}$ that appears in the momentum space kernels (4.43) and (4.44) gives rise to non-ultra-local local real space kernels K and K^{-1}, which we now discuss. It is straightforward to identify the real space equivalent of $1 + \frac{\gamma^2}{2}\,[1 + \cos(p \cdot \hat{s})]$ which is the Helmholtz-type lattice operator

$$H_{x,y} = \delta^{(4)}_{x,y} + \frac{\gamma^2}{4}\,\left[\delta^{(4)}_{x+\hat{s},y} + 2\delta^{(4)}_{x,y} + \delta^{(4)}_{x-\hat{s},y}\right]\,. \qquad (4.45)$$

Thus we find in real space,

$$K_{x,\mu\nu|z,\rho\sigma} = \sum_z H^{-\frac{1}{2}}_{x,y}\left[\delta_{\mu\rho}\,\delta_{\nu\sigma}\,\delta^{(4)}_{y,z} + i\,\frac{\gamma}{2}\,\epsilon_{\mu\nu\rho\sigma}\,\left[\delta^{(4)}_{y-\hat{\rho}-\hat{\sigma},z} + \delta^{(4)}_{y+\hat{s}-\hat{\rho}-\hat{\sigma},z}\right]\right]\,, \qquad (4.46)$$

$$K^{-1}_{x,\mu\nu|y,\rho\sigma} = \sum_z H^{-\frac{1}{2}}_{x,y}\left[\delta_{\mu\rho}\,\delta_{\nu\sigma}\,\delta^{(4)}_{y,z} - i\,\frac{\gamma}{2}\,\epsilon_{\mu\nu\rho\sigma}\,\left[\delta^{(4)}_{y-\hat{\rho}-\hat{\sigma},z} + \delta^{(4)}_{y+\hat{s}-\hat{\rho}-\hat{\sigma},z}\right]\right]\,, \qquad (4.47)$$

where in real space the inverse square root $H^{-\frac{1}{2}}$ of the Helmholtz operator may be implemented with the spectral theorem or a series expansion. Since the denominator

---

[14]Note that (4.43) is not the only choice of a kernel that keeps the electric-magnetic duality of the theory, however, no ultra-local choice is possible. We remark that the choice (4.43) violates hypercubic symmetries. This can indeed be corrected, as we discuss in appendix (F).

$\sqrt{1 + \frac{\gamma^2}{2}\left[1 + \cos(p \cdot \hat{s})\right]}$ in the momentum space kernels $\widehat{K}(p)$ and $\widehat{K}(p)^{-1}$ is regular for all values of γ, the inverse Fourier transforms, i.e., the real space kernels K and K^{-1} will have entries that decrease exponentially with increasing lattice distance, i.e., they are local (but not ultra-local of course).

It is important to note that the operator $H_{x,y}^{-\frac{1}{2}}$ is composed from simple operators $\delta_{x+n\hat{s},y}$ for integers n. When applying these shifts on the terms with the epsilon tensor in (4.46) and (4.47) this generates terms proportional to $Q_{-\hat{s}k}[F^e]$ for different values of k. If there are no dynamical monopoles then we can replace all $Q_{-k\hat{s}}[F^e]$ by $Q_0[F^e]$.

Thus for the terms with the epsilon tensor in (4.46) and (4.47) we may replace the action of $H_{x,y}^{-\frac{1}{2}}$ simply by multiplication with $1/\sqrt{1+\gamma^2}$. We now use this fact to simplify the topological part of the quadratic form of the Boltzmann factor.

We may write the Boltzmann factor (4.42) in the form

$$B_{\beta,\theta}[A^e, A^m] \equiv \sum_{\{n\}} e^{-\beta S_g[F^e] - i\theta Q_0[F^e]} \, e^{i \sum_{x,\mu<\nu} (\partial A^m)_{x,\mu\nu} \, n_{x,\mu\nu}}, \qquad (4.48)$$

where the gauge field action is given by

$$S_g[F^e] = \frac{1}{2} \sum_{\substack{x,\mu<\nu \\ y,\rho<\sigma}} F_{x,\mu\nu}^e \, H_{x,\mu\nu|y,\rho\sigma}^{-\frac{1}{2}} \, F_{y,\rho\sigma}^e \,, \qquad (4.49)$$

and using the simplification of $H_{x,y}^{-\frac{1}{2}}$ for the topological part discussed above, we identify the topological angle θ as

$$\theta = \beta \, 4\pi^2 \, \frac{\gamma}{\sqrt{1+\gamma^2}} \quad \Rightarrow \quad \gamma = \frac{\theta}{\sqrt{(4\pi^2\beta)^2 - \theta^2}} \,. \qquad (4.50)$$

Note that while we obtained this for a model without dynamical magnetic matter, we can take the above formulas as the definition of the θ term even in this case.

In a similar way we may identify the bare electric charge parameter e through the pre-factor of the $F_{\mu\nu}^e F_{\mu\nu}^e$ term which gives rise to the relation (again replacing $H_{x,y}^{-\frac{1}{2}}$ by $1/\sqrt{1+\gamma^2}$)

$$\frac{1}{e^2} = \frac{\beta}{\sqrt{1+\gamma^2}} \,. \qquad (4.51)$$

Using (4.50) and (4.51) we may express the two auxiliary parameters β and γ in terms of the bare charge parameter e and the topological angle θ,

$$\beta = \frac{1}{2\pi}\sqrt{\left(\frac{2\pi}{e^2}\right) + \left(\frac{\theta}{2\pi}\right)^2}, \qquad \gamma = \frac{\theta \, e^2}{4\pi^2} \,. \qquad (4.52)$$

Repeating the steps of the duality transformation from the previous section we use the generalized Poisson resummation formula and find the dual form of the Boltzmann factor

$$B_{\beta,\theta}[A^e, A^m] = C_K(\beta) \sum_{\{p\}} e^{-\frac{\widetilde{\beta}}{2} \sum_{\substack{\tilde{x},\mu<\nu \\ \tilde{y},\rho<\sigma}} \widetilde{F}_{\tilde{x},\mu\nu}^m \, \widetilde{K}_{\tilde{x},\mu\nu|\tilde{y},\rho\sigma} \, \widetilde{F}_{\tilde{y},\rho\sigma}^m} \, e^{i \sum_{\tilde{x},\mu<\nu} (\partial\widetilde{A}^e)_{\tilde{x},\mu\nu} \, \tilde{p}_{\tilde{x},\mu\nu}}, \qquad (4.53)$$

where (it is straightforward to establish the result $\det K = 1$ we use here)

$$\tilde{\beta} \equiv \frac{1}{4\pi^2\beta} \qquad \text{and} \qquad C_K(\beta) \equiv \frac{1}{(\sqrt{2\pi\beta})^{6V}\sqrt{\det K}} = \frac{1}{(2\pi\beta)^{3V}} \; . \tag{4.54}$$

The dual kernel $\widetilde{K}_{\tilde{x},\mu\nu|\tilde{y}\rho\sigma}$ is identified in analogy to (4.37) and we find

$$\widetilde{K}_{\tilde{x},\mu\nu|\tilde{y},\rho\sigma} \equiv \sum_{\substack{\mu'<\nu' \\ \rho'<\sigma'}} \epsilon_{\mu\nu\mu'\nu'}\, K^{-1}_{x+\hat{\mu}'+\hat{\nu}',\mu'\nu'|y+\hat{\rho}'+\hat{\sigma}',\rho'\sigma'}\, \epsilon_{\rho'\sigma'\rho\sigma}\, \Big|_{\substack{x\to\tilde{x} \\ y\to\tilde{y}}}$$

$$= \sum_z H_{x,y}^{-\frac{1}{2}} \left[\delta_{\mu\rho}\,\delta_{\nu\sigma}\,\delta^{(4)}_{y,z} \;-\; i\,\frac{\gamma}{2}\,\epsilon_{\mu\nu\rho\sigma}\left[\delta^{(4)}_{y-\hat{\rho}-\hat{\sigma},z} + \delta^{(4)}_{y+\hat{s}-\hat{\rho}-\hat{\sigma},z} \right] \right] . \tag{4.55}$$

Obviously, up to the opposite sign of the imaginary part, also the dual kernel $\widetilde{K}_{\tilde{x},\mu\nu|\tilde{y},\rho\sigma}$ has the structure of the original kernel $K_{x,\mu\nu|y,\rho\sigma}$ in eq. (4.46), and comparing (4.42) and (4.53) we find that we have indeed constructed a self-dual Boltzmann factor that also includes the θ-term. Writing the dual form of the kernel as

$$B_{\beta,\theta}[A^e, A^m] = C_K(\beta)\sum_{\{p\}} e^{-\widetilde{\beta}S_g[\widetilde{F}^m] - i\,\widetilde{\theta}\,Q_0[\widetilde{F}^e]}\; e^{\,i\sum_{\tilde{x},\mu<\nu}(\partial\widetilde{A}^e)_{\tilde{x},\mu\nu}\,\widetilde{p}_{\tilde{x},\mu\nu}} \;, \tag{4.56}$$

we here identify the dual topological angle as

$$\widetilde{\theta} = -\,4\pi^2\widetilde{\beta}\,\frac{\gamma}{\sqrt{1+\gamma^2}} \; . \tag{4.57}$$

We now may summarize the self-duality relation of the Boltzmann factor with θ-term as

$$\beta^{\frac{3V}{2}}\, B_{\beta,\theta}[A^e, A^m] = \widetilde{\beta}^{\frac{3V}{2}}\, \widetilde{B}_{\widetilde{\beta},\widetilde{\theta}}[\widetilde{A}^m, \widetilde{A}^e] \;, \tag{4.58}$$

where we have again distributed the pre-factors symmetrically and use

$$\widetilde{\beta} = \beta f\,, \qquad \widetilde{\theta} = -\,\theta f \qquad \text{where} \qquad f \equiv \frac{1}{(2\pi\beta)^2} \; . \tag{4.59}$$

Alternatively we may write the transformation of the couplings completely in terms of the more physical parameters e and θ (use (4.50) and (4.51))

$$\frac{1}{\widetilde{e}^{\,2}} = \frac{1}{e^2}\,f\,, \qquad \widetilde{\theta} = -\,\theta f \qquad \text{with} \qquad f \equiv \frac{1}{\left(\frac{2\pi}{e^2}\right)^2 + \left(\frac{\theta}{2\pi}\right)^2} \; . \tag{4.60}$$

These equations constitute the generalization of the duality relation eq. (2.26) to the case of a Boltzmann factor that also includes the topological term. We remark at this point that the self-duality of QED with a θ-term can be extended to an even more general definition of the topological charge, that also fully implements all lattice symmetries. For the corresponding discussion see appendix F.

As before we check that repeating the duality transformation provides the identity map. This property follows from $\widetilde{\widetilde{A}}^e = -A^e$, $\widetilde{\widetilde{A}}^m = -A^m$ and the trivial identities

$$\widetilde{\widetilde{\beta}} = \beta\,, \quad \widetilde{\widetilde{\theta}} = \theta \qquad \text{and} \qquad C_K(\beta)\,C_K(\widetilde{\beta}) = 1 \; . \tag{4.61}$$

We may now use the Boltzmann factor (4.56) in the partition sum (4.27) and based on (4.58) obtain the self-duality relation for full QED with a θ-term,

$$\beta^{\frac{3V}{2}} Z(\beta, \theta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m) = \widetilde{\beta}^{\frac{3V}{2}} Z(\widetilde{\beta}, \widetilde{\theta}, \widetilde{M}^e, \widetilde{\lambda}^e, \widetilde{q}^e, \widetilde{M}^m, \widetilde{\lambda}^m, \widetilde{q}^m) , \qquad (4.62)$$

$$\text{with} \quad \widetilde{\beta} = \beta f , \quad \widetilde{\theta} = -\theta f , \quad f = \frac{1}{4\pi^2 \beta^2} ,$$

$$\widetilde{M}^e = M^m , \ \widetilde{\lambda}^e = \lambda^m , \ \widetilde{M}^m = M^e , \ \widetilde{\lambda}^m = \lambda^e ,$$

$$\widetilde{\mathbf{q}} = S \, \mathbf{q} , \quad S = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} ,$$

where again we use the vector of charges $\mathbf{q} = (q^e, q^m)^t$.

As before we can generate self-duality relations for observables by evaluating derivatives of $\ln Z$ with respect to the couplings. When considering observables for the matter fields, which are obtained from derivatives with respect to M^e, λ^e, M^m or λ^m, the self-duality relations generalize in a straightforward way. For example the relation (3.12) now reads,

$$\left\langle |\phi^e|^2 \right\rangle_{\beta, \theta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m} = \left\langle |\phi^m|^2 \right\rangle_{\widetilde{\beta}, \widetilde{\theta}, \widetilde{M}^e, \widetilde{\lambda}^e, \widetilde{q}^e, \widetilde{M}^m, \widetilde{\lambda}^m, \widetilde{q}^m} . \qquad (4.63)$$

However, self-duality relations for observables that contain the gauge fields, i.e., observables that are generated by derivatives with respect to β or θ require a little more work, since via γ as given in (4.50) the two parameters mix, and additional terms appear in the self-duality relations. We derive two such self-duality relations which for notational convenience we discuss without matter fields, i.e., we derive them for pure gauge theory with a θ-term (adding matter fields is trivial).

Applying a derivative with respect to β on the Boltzmann factor in the form of eq. (4.56) generates the insertion of the action S_g, such that we find (the matter couplings were omitted as arguments in all expressions since we discuss the pure gauge case),

$$-\frac{\partial \ln Z(\beta, \theta)}{\partial \beta} = \langle S_g \rangle_{\beta, \theta} + \beta \left\langle \frac{\partial S_g}{\partial \beta} \right\rangle_{\beta, \theta} = \langle S_g \rangle_{\beta, \theta} + \beta \frac{\partial \gamma}{\partial \beta} \langle S_g' \rangle_{\beta, \theta} = \langle S_g \rangle_{\beta, \theta} - \frac{\Gamma \theta}{\beta} \langle S_g' \rangle_{\beta, \theta}. \qquad (4.64)$$

The second terms on the right hand sides come from the β-dependence of the action S_g via the β-dependence of γ and we use the notation $S_g' = d \, S_g / d\gamma$. It is straightforward to compute the derivative $\frac{\partial \gamma}{\partial \beta}$ that appears after the second step from the explicit expression (4.50), and we write the result in the form

$$\frac{\partial \gamma}{\partial \beta} = -\frac{\Gamma \theta}{\beta} \qquad \text{with} \qquad \Gamma \equiv \frac{\beta^3 (4\pi^2)^2}{((4\pi^2 \beta)^2 - \theta^2)^{3/2}} = \frac{\widetilde{\beta}^3 (4\pi^2)^2}{((4\pi^2 \widetilde{\beta})^2 - \widetilde{\theta}^2)^{3/2}} \equiv \widetilde{\Gamma} , \qquad (4.65)$$

where we have factored out the combination Γ which is invariant under the duality transformation as follows immediately from the transformation properties (4.59). Using the self-duality relation (4.62) for the partition sum we can apply the derivative with respect

to β also on the dual form,

$$
\begin{aligned}
-\frac{\partial \ln Z(\beta,\theta)}{\partial \beta} &= -\frac{\partial}{\partial \beta} \ln\left((2\pi\beta)^{-3V} Z(\widetilde{\beta},\widetilde{\theta}) \right) = \frac{3V}{\beta} - \frac{d\widetilde{\beta}}{d\beta} \frac{\partial \ln Z(\widetilde{\beta},\widetilde{\theta})}{\partial \widetilde{\beta}} \\
&= \frac{3V}{\beta} - \frac{1}{4\pi^2 \beta^2} \left[\langle S_g \rangle_{\widetilde{\beta},\widetilde{\theta}} - \frac{\widetilde{\Gamma}\,\widetilde{\theta}}{\widetilde{\beta}} \langle S_g' \rangle_{\widetilde{\beta},\widetilde{\theta}} \right] .
\end{aligned}
\tag{4.66}
$$

Setting equal the right hand sides of (4.64) and (4.66) one obtains after a few steps of trivial reordering of terms (use also $\widetilde{\beta} = 1/4\pi^2\beta$ and $\widetilde{\Gamma} = \Gamma$) the final form of the self-duality relation

$$
\beta \langle S_g \rangle_{\beta,\theta} - \Gamma\,\theta \langle S_g' \rangle_{\beta,\theta} = 3V - \widetilde{\beta} \langle S_g \rangle_{\widetilde{\beta},\widetilde{\theta}} + \Gamma\,\widetilde{\theta} \langle S_g' \rangle_{\widetilde{\beta},\widetilde{\theta}} .
\tag{4.67}
$$

It is easy to check that for $\theta = 0$ this self-duality relation reduces to the self-duality relation (2.32) which we derived for pure gauge theory without θ-term (use $\theta = 0 \Rightarrow \gamma = 0$, the fact that S_g at $\gamma = 0$ reduces to the ultra-local action we used initially, and $\langle F^2 \rangle = \langle S_g|_{\gamma=0}\rangle/3V$). The generalization to the non-ultralocal action that is needed for $\theta \neq 0$ then generates the additional terms with S_g'.

In exactly the same way we may also study derivatives $i\partial/\partial\theta$ that generate expectation values of the topological charge Q_0, and following the same steps as above find the corresponding self-duality relation

$$
\beta \langle Q_0 \rangle_{\beta,\theta} - i\,\Gamma\,\beta \langle S_g' \rangle_{\beta,\theta} = -\widetilde{\beta} \langle Q_0 \rangle_{\widetilde{\beta},\widetilde{\theta}} + i\,\Gamma\,\widetilde{\beta} \langle S_g' \rangle_{\widetilde{\beta},\widetilde{\theta}} .
\tag{4.68}
$$

This self-duality relation vanishes for $\theta = 0$ (as expected), since $\langle Q_0 \rangle|_{\theta=0} = 0$ and due to $\theta = 0 \Rightarrow \gamma = 0$ also the second term disappears because of $S_g'|_{\gamma=0} = 0$.

4.5 The $\mathrm{SL}(2,\mathbb{Z})$ structure of dyonic lattice QED with a θ-term

In the course of this paper we have identified two transformations of our self-dual lattice version of QED with a θ-term. The first one is the duality transformation $\mathcal{S}$ itself, which we here write in terms of the bare charge parameter e, the topological angle θ and the vector of electric and magnetic charges $\boldsymbol{q} \equiv (q^e, q^m)^t$ (compare (4.60)),

$$
\frac{1}{e^2} \to \frac{1}{\widetilde{e}^{\,2}} = \frac{1}{e^2}\, f , \qquad \theta \to \widetilde{\theta} = -\theta\, f \qquad \text{where} \qquad f \equiv \frac{1}{\left(\frac{2\pi}{e^2}\right)^2 + \left(\frac{\theta}{2\pi}\right)^2} ,
$$

$$
\boldsymbol{q} \to \widetilde{\boldsymbol{q}} = S\,\boldsymbol{q} \qquad \text{with} \qquad S = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} .
\tag{4.69}
$$

The second transformation we identified is $\mathcal{T}$ which shifts θ by 2π that was discussed in subsection 4.2 in the context of the Witten effect. It acts only on θ and the charge vector $\boldsymbol{q}$ and is defined as follows (see (4.26))

$$
\theta \to \overline{\theta} = \theta - 2\pi ,
$$

$$
\boldsymbol{q} \to \overline{\boldsymbol{q}} = T\,\boldsymbol{q} \qquad \text{with} \qquad T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} .
\tag{4.70}
$$

We begin the discussion of the overall duality structure by noting that the matrices S and T are the generators[15] of the group $\mathrm{SL}(2,\mathbb{Z})$, which is the group of 2×2 matrices M

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[15]See for example [37] for an elementary introduction to the group $\mathrm{SL}(2,\mathbb{Z})$.

with integer-valued elements and determinant 1, i.e.,

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \text{with} \quad a, b, c, d \in \mathbb{Z} \quad \text{and} \quad ad - bc = 1 \,. \tag{4.71}$$

And since they are generators, combinations of the matrices S and T implement arbitrary $\mathrm{SL}(2, \mathbb{Z})$ transformations on the charge vector $\boldsymbol{q}$.

Furthermore, also the action of the dualities $\mathcal{S}$ and $\mathcal{T}$ on $1/e^2$ and θ can be identified with the group $\mathrm{SL}(2, \mathbb{Z})$. In order to see that, we combine the gauge coupling e and the topological angle θ into a joint complex-valued coupling τ, the so-called modular parameter of U(1) gauge theory (see, e.g., [19, 38, 39]), defined as

$$\tau \equiv i \frac{2\pi}{e^2} - \frac{\theta}{2\pi} \,. \tag{4.72}$$

It is straightforward to see from (4.69) and (4.70) that our two generators $\mathcal{S}$ and $\mathcal{T}$ act as

$$\mathcal{S}: \ \tau \rightarrow \widetilde{\tau} = -\frac{1}{\tau} \quad \text{and} \quad \mathcal{T}: \ \tau \rightarrow \overline{\tau} = \tau + 1 \,. \tag{4.73}$$

The action of a general $\mathrm{SL}(2, \mathbb{Z})$ transformation on a complex number τ is defined as[16]

$$\tau \ \rightarrow \ M\tau \equiv \frac{a\tau + b}{c\tau + d} \,, \tag{4.74}$$

where a, b, c, d are the entries of an $\mathrm{SL}(2, \mathbb{Z})$ matrix M as given in (4.71). It is straightforward to see that choosing the generators $M = S$ and $M = T$ gives rise to the transformations $\tau \rightarrow -1/\tau$ and $\tau \rightarrow \tau + 1$, i.e., the action of our symmetries $\mathcal{S}$ and $\mathcal{T}$ as stated in (4.73). Thus our transformations $\mathcal{S}$ and $\mathcal{T}$ generate the full set of group transformations (4.74). We conclude that combining our two transformations $\mathcal{S}$ and $\mathcal{T}$ as stated in (4.69) and (4.70) gives rise to a full $\mathrm{SL}(2, \mathbb{Z})$ invariance of our self-dual lattice formulation of QCD with a θ-term.

We now ignore the other couplings of the dyonic matter fields, such as M and λ, and only focus on the couplings $1/e^2$ and θ combined into the complex coupling τ, as well as the charge vector $\boldsymbol{q}$. Only those couplings are now listed as arguments of the partition function. Furthermore it is convenient to redefine the partition function as $\overline{Z}(\tau, \boldsymbol{q}) \equiv \beta^{\frac{3V}{2}} Z(\tau, \boldsymbol{q})$. Then the $\mathcal{S}$ and $\mathcal{T}$ symmetry relations are written as

$$\overline{Z}(\tau, \boldsymbol{q}) = \overline{Z}(S\tau, S\boldsymbol{q}) \qquad \text{and} \qquad \overline{Z}(\tau, \boldsymbol{q}) = \overline{Z}(T\tau, T\boldsymbol{q}) \,, \tag{4.75}$$

and according to the discussion above these two transformations generate the full $\mathrm{SL}(2, \mathbb{Z})$ invariance given by

$$\overline{Z}(\tau, \boldsymbol{q}) = \overline{Z}(M\tau, M\boldsymbol{q}) \qquad \text{with} \tag{4.76}$$
$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad a, b, c, d \in \mathbb{Z}, \ ad - bc = 1, \ M\tau = \frac{a\tau + b}{c\tau + d} \,.$$

These equations describe the symmetry content of dyonic self-dual QED with a θ-term.

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[16]Strictly speaking this implements the projected group $\mathrm{PSL}(2, \mathbb{Z})$, which is $\mathrm{SL}(2, \mathbb{Z})$ with matrices M and $-M$ identified.
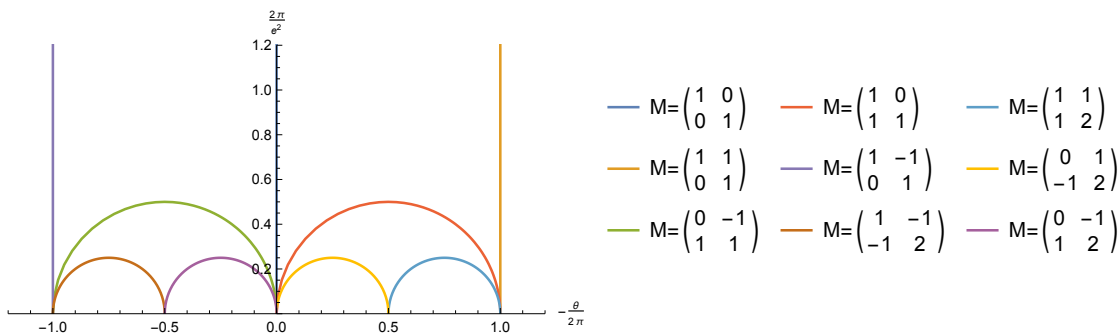
Figure 1. Mapping of theories in the complex τ plane that are related by different elements of $\mathrm{SL}(2,\mathbb{Z})$. On the vertical axis we plot $\mathrm{Im}\,\tau = 2\pi/e^2$ and on the horizontal axis $\mathrm{Re}\,\tau = -\theta/2\pi$. Theories that have $\theta = 0$ and thus can be directly simulated are located on the positive vertical axis (marked with a thick black line). Different elements of $\mathrm{SL}(2,\mathbb{Z})$ map this family of theories to equivalent theories with non-zero θ which are represented by the semi-circles (see the legend for which element M of $\mathrm{SL}(2,\mathbb{Z})$ was used).

As we have seen in section 3.2, dyonic theories generically have a sign problem. In addition, also theories with a θ-term have a sign problem. However, the $\mathrm{SL}(2,\mathbb{Z})$ structure we identified above allows us to map theories which can be recast in terms of wordlines without the sign-problem (i.e., with the purely electric and/or purely magnetic matter, at least one of which is bosonic and considered at $\theta = 0$) onto other theories that naively do have a sign problem. This map can be rather nontrivial. To illustrate the idea, let us discuss an example. We consider a matrix $M \in \mathrm{SL}(2,\mathbb{Z})$ given by

$$M = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} . \tag{4.77}$$

We have seen that a theory described by $(\tau, \boldsymbol{q})$ is equivalent to a theory with parameters $(M\tau, M\boldsymbol{q})$. Furthermore we can simulate the family of theories with $\tau = iy, y \in \mathbb{R}_+$ and, say a matter field with charge vector $\boldsymbol{q} = (n,0)^t$ with $n \in \mathbb{Z}$. This family of theories is dual to theories with $\bar{\tau} = M\tau = \frac{iy}{iy+1}$ and $\bar{\boldsymbol{q}} = M\boldsymbol{q} = (n,n)^t$. Identifying $\mathrm{Re}(\bar{\tau}) = \frac{\bar{\theta}}{2\pi}$ and $\mathrm{Im}(\bar{\tau}) = \frac{2\pi}{\bar{e}^2}$, we find that the dual theories have parameters and matter charges given by $(y \in \mathbb{R}_+)$

$$\bar{e}^2 = 2\pi \frac{1+y^2}{y} , \qquad \bar{\theta} = 2\pi \frac{y^2}{1+y^2} , \qquad \text{and} \qquad \bar{\boldsymbol{q}} = \begin{pmatrix} n \\ n \end{pmatrix} . \tag{4.78}$$

Obviously this is a family of theories that has a complex action problem, which, using our $\mathrm{SL}(2,\mathbb{Z})$ mapping we may study via simulating the corresponding sign free set of theories. The above family of theories is shown as an orange semi-circle in the τ plane in figure 1, or equivalently, in the (θ, e^2) plane in figure 2 (again the orange curve). Note that in particular the self-dual point of the original theory $y = 1$ is mapped to $e^2 = 4\pi$ and $\bar{\theta} = \pi$ of the dual theory.

Figures 1 and 2 show several $\mathrm{SL}(2,\mathbb{Z})$ families of theories that are dual to the family of theories which obeys $\mathrm{Im}(\tau) = 0$, i.e., the $\theta = 0$ theories, that can be simulated as long as the matter field is not dyonic, i.e., the matter fields are purely electric or purely
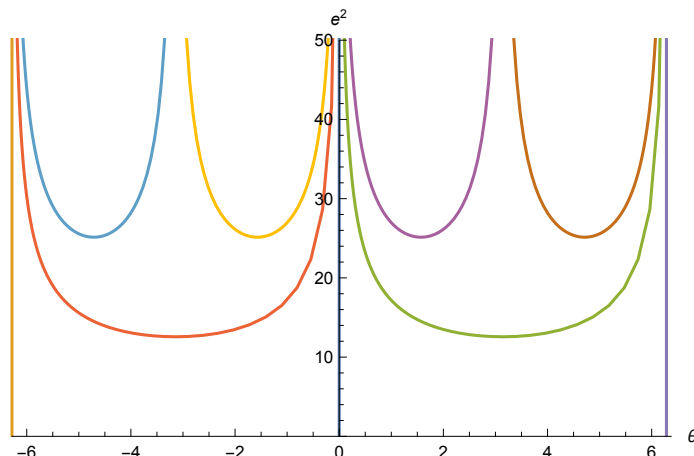
Figure 2. The same as figure 1, but now plotted in the (θ, e^2) plane.

magnetic. The legend shows the matrices M that need to be applied to the matter fields in the exactly same manner as in the example above. Note that all the interesting theories which are related to the sign-problem free theory are at strong electric coupling $\bar{e}^2 \geq 4\pi$, as is evident from figure 2.

5 Concluding remarks

In this work we discussed the construction of U(1) gauge theories in 4d on the lattice with θ-terms. We showed that modified Villain actions allow for a construction which admits the inclusion of θ-terms in a natural way. However, a naive ultra-local θ-term ruins the self-dual nature of the theory, mapping the ultra-local theory to a merely local one. We showed that by generalizing the modified Villain actions to include non-ultra-local terms, we can restore the exactly self-dual nature of the model. The construction is reminiscent of the inability to regulate a lattice theory in an ultra-local way, while preserving the axial symmetry in 4d lattice gauge theories. Indeed, the Nielsen-Ninomiya theorem [21–23] prohibits a lattice regularization for which the matrix γ^5 anti-commutes with the Dirac operator, which is essential for the axial symmetry. However, using the Ginsparg-Wilson relation [26] and its solution by Neuberger [25], Lüscher showed [24] that an axial symmetry can be defined. But such constructions, while local, are not ultra-local. In fact 4d U(1) gauge theories, both free and interacting, have anomalies [27–30] and it is not a priory a big surprise that for maintaining the correct symmetry and anomaly structure on the lattice one must resort to a local, but not ultra-local form of the action. Yet many examples exist of lattice discretization of theories with anomalies, which maintain their ultra-local form. One example is a $\theta = \pi$ 2d abelian gauge theory, whose lattice action was discussed in [7–12], and may be chosen ultra-local, even though such models may have 't Hooft anomalies involving their internal symmetries. Such models are also connected to half-integral spin-chains, which furnish a regulator of the Hilbert space.

It is well known, that the free abelian gauge theory has an $SL(2, \mathbb{Z})$ structure in the

continuum, generated by self-duality and shifts of the θ-angle by 2π. As Witten showed in [40], the free U(1) gauge theory partition function transforms as a modular form, with a modular weight determined by the Euler characteristic χ and the signature of the spin-for manifold σ. In [31] this was interpreted as a 't Hooft anomaly (see section 4.2.2 of [31]) at special points of the modular parameter τ, where the theory enjoys a $\mathbb{Z}_6$ symmetry, which is a subgroup of $\mathrm{SL}(2, \mathbb{Z})$. As explained by Honda and Tanizaki in [31], this $\mathbb{Z}_6$ symmetry has a mixed anomaly with gravity. On the other hand, the mixed axial-gravitational anomaly of fermions is also well known (see, e.g., [41–43]). Furthermore, the role of gravitational anomalies in lattice discretization was noted in [44], where it was proven (under some mild assumptions) that there exists no lattice discretization[17] in two dimensions unless its pure gravitational anomaly vanishes. One may then naturally wonder if the inability to write ultra-local actions is related to the involvement of mixed-gravitational anomalies.

Acknowledgments

A Notation and results for lattice differential forms

In this appendix we summarize the notation and some basic results for differential forms on the lattice, which we use in our paper. For a more general presentation see, e.g., [7, 33]. In the main part of the paper we work in $d = 4$ dimensions, but this appendix is kept general with arbitrary d.

We consider a d-dimensional hypercubic lattice Λ and set the lattice spacing to $a = 1$. The spatial extents of the lattice are denoted as N_μ, $\mu = 1, 2 \ldots d$ and we use periodic boundary conditions. Sites are denoted as x. Links are denoted as (x, μ), plaquettes as $(x, \mu\nu)$ with $\mu < \nu$, 3-cubes as $(x, \mu\nu\rho)$ with $\mu < \nu < \rho$ et cetera.

We can identify these elements with r-cells: sites are 0-cells. A link (x, μ) is a 1-cell and contains the 0-cells (sites) x and $x + \hat\mu$ where by $\hat\mu$ we denote the unit vector in direction μ. A plaquette $(x, \mu\nu)$ is a 2-cell and contains the sites x, $x + \hat\mu$, $x + \hat\nu$ and $x + \hat\mu + \hat\nu$, as well as the links (x, μ), $(x + \hat\mu, \nu)$, $(x + \hat\nu, \mu)$ and (x, ν). In an equivalent way 3-cells are the 3-cubes that contain 8 sites, 12 links and 6 plaquettes and similarly for higher r-cells. The site x in the definition of an r-cell we will sometimes refer to as *root site* or *root*.

We assign integers or real numbers to the r-cells and refer to these as r-forms. We denote r-forms as $f_{x, \mu_1 \mu_2 \ldots \mu_r} \in \mathbb{R}$ or $\mathbb{Z}$ with $\mu_1 < \mu_2 < \ldots < \mu_r$, i.e., the r-forms are labelled by the root site and the ordered indices μ_j, $j = 1, 2, \ldots r$ that label the corresponding r-cell. It is convenient to not only label the r-forms with the ordered indices $\mu_1 < \mu_2 < \ldots < \mu_r$ but allow for arbitrary ordering with the convention that $f_{x, \mu_1 \ldots \mu_j \ldots \mu_k \ldots \mu_r} = -f_{x, \mu_1 \ldots \mu_k \ldots \mu_j \ldots \mu_r}$, i.e., r-forms are antisymmetric in their indices.

---

[17]The proof was for a lattice discretization of Hilbert space, where time is viewed as continuous.

This also implies that an r-form vanishes when two or more of the indices are equal. One may use this generalized labelling with non-ordered indices also for the cells and the sign of the permutation of the indices defines an orientation for the cells.

We define two discrete differential operators that act on r-forms, the *exterior derivative* d that takes an r-form into an $(r+1)$-form with the definition that d acting on a d-form gives zero. The other differential operator is the *boundary operator* ∂ that takes an r-form into an $(r-1)$-form. When acting on a 0-form ∂ gives zero. The two differential operators are defined as

$$
(d\,f)_{x,\,\mu_1\mu_2\,...\,\mu_r} \equiv \sum_{j=1}^{r}(-1)^{j+1}\left[\,f_{x+\hat\mu_j,\,\mu_1\,...\,\overset{o}{\mu}_j\,...\,\mu_r} \,-\, f_{x,\,\mu_1\,...\,\overset{o}{\mu}_j\,...\,\mu_r}\,\right],
$$

$$
(\partial f)_{x,\,\mu_1\mu_2\,...\,\mu_r} \equiv \sum_{\nu=1}^{d}\left[\,f_{x,\,\mu_1\,...\,\mu_r\,\nu} \,-\, f_{x-\hat\nu,\,\mu_1\,...\,\mu_r\,\nu}\,\right], \tag{A.1}
$$

where in the first equation $\overset{o}{\mu}_j$ indicates that μ_j is dropped from the list of indices. We remark that due to the antisymmetry of the r-forms with respect to interchange of their indices, in the second line of (A.1) only those $(r+1)$-forms contribute to the sum where ν is different from all indices $\mu_1, \mu_2 \ldots \mu_r$. The ordering of these indices and ν determines the sign of the contribution.

Both differential operators are nilpotent, i.e., $d^2 = 0$ and $\partial^2 = 0$. Furthermore one may show the following partial integration formula, where f is an r-form and g an $(r-1)$-form,

$$
\sum_{\substack{x \\ \mu_1 < \ldots < \mu_r}} f_{x,\,\mu_1\,...\,\mu_r}\,(d\,g)_{x,\,\mu_1\,...\,\mu_r} = (-1)^r \sum_{\substack{x \\ \mu_1 < \ldots < \mu_{r-1}}} (\partial f)_{x,\,\mu_1\,...\,\mu_{r-1}}\,g_{x,\,\mu_1\,...\,\mu_{r-1}}. \tag{A.2}
$$

The *Hodge decomposition* states that an arbitrary r-form f can be written as the sum of the boundary operator ∂ acting on an $(r+1)$-form p, the exterior derivative operator d acting on an $(r-1)$-form q and a *harmonic* or *defect* r-form h that obeys $d\,h = 0$ and $\partial\,h = 0$,

$$
f_{x,\,\mu_1\,...\,\mu_r} = (\partial p)_{x,\,\mu_1\,...\,\mu_r} + (d\,q)_{x,\,\mu_1\,...\,\mu_r} + h_{x,\,\mu_1\,...\,\mu_r}. \tag{A.3}
$$

The *dual lattice* $\tilde\Lambda$ is defined by a one-to-one identification of the r-cells of the original lattice with the $(d-r)$-cells of the dual lattice. The sites $\tilde x$ of $\tilde\Lambda$ are at the centers of the d-cells of Λ, i.e., $\tilde x = x + \frac{1}{2}(\hat 1 + \hat 2 + \ldots + \hat d)$. There is a natural identification of the r-forms $f_{x,\,\mu_1\,...\,\mu_r}$ on Λ with the $(d-r)$-forms on $\tilde\Lambda$. We denote these as $\tilde f_{\tilde x,\,\nu_{r+1}\,...\,\nu_d}$ but stress that the numerical value is of course the same as the r-form $f_{x,\,\mu_1\,...\,\mu_r}$ we identify it with. The identification is given by

$$
f_{x,\,\mu_1\,...\,\mu_r} = \sum_{\nu_{r+1} < \nu_{r+2} < \ldots < \nu_d} \epsilon_{\mu_1\,...\,\mu_r\,\nu_{r+1}\,...\,\nu_d}\,\tilde f_{\tilde x - \hat\nu_{r+1} - \hat\nu_{r+2}\,...\,-\hat\nu_d,\,\nu_{r+1}\,...\,\nu_d}. \tag{A.4}
$$

Finally, when switching between the original lattice Λ and the dual lattice $\tilde\Lambda$ the exterior derivative d and the boundary operator are converted into each other,

$$
(\partial f)_{x,\,\mu_1\,...\,\mu_r} = \sum_{\nu_{r+1} < \nu_{r+2} < \ldots < \nu_d} \epsilon_{\mu_1\,...\,\mu_r\,\nu_{r+1}\,...\,\nu_d}\,(d\,\tilde f)_{\tilde x - \hat\nu_{r+1} - \hat\nu_{r+2}\,...\,-\hat\nu_d,\,\nu_{r+1}\,...\,\nu_d}. \tag{A.5}
$$

B Auxiliary results for the topological charge

In this appendix we collect some results for the topological charge $Q_T[F]$ which can be obtained with elementary although lengthy algebra. As a first result we show (4.4), i.e., the fact that the topological charge $Q_T[F]$ is invariant when adding the exterior derivative $(dB)_{x,\mu\nu}$ of an arbitrary 1-form $B_{x,\mu}$ to the field strength $F_{x,\mu\nu} = (dA^e)_{x,\mu\nu} + 2\pi\, n_{x,\mu\nu}$, as long as the Villain variables $n_{x,\mu\nu}$ obey the closedness condition (2.7), i.e., $(dn)_{x,\mu\nu\rho} = 0$. The expression $Q_T[F+dB]$ can be trivially decomposed into three contributions,

$$Q_T[F+dB] = \frac{1}{8\pi^2} \sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} (F+dB)_{x,\mu\nu}\, \epsilon_{\mu\nu\rho\sigma}\, (F+dB)_{x-\hat\rho-\hat\sigma+T,\rho\sigma} = Q_T[F] \,+\, Q_T[(dB)]$$

$$+ \frac{1}{8\pi^2} \sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} \Big[F_{x,\mu\nu}(dB)_{x-\hat\rho-\hat\sigma+T,\rho\sigma} + F_{x-\hat\rho-\hat\sigma+T,\rho\sigma}(dB)_{x,\mu\nu} \Big]\epsilon_{\mu\nu\rho\sigma}\,. \quad \text{(B.1)}$$

For proving the claimed independence of dB we need to show that the second and third terms on the right hand side vanish. We begin with the third term: after inserting the explicit definition of the exterior derivatives $(dB)_{x,\mu\nu}$ and reshuffling the summation indices the third term can be written in the form (a factor $1/8\pi^2$ was dropped)

$$\sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} \epsilon_{\mu\nu\rho\sigma}\Big[B_{x,\rho}\,(F_{x+\hat\rho+\hat\sigma-T,\mu\nu} - F_{x+\hat\rho-T,\mu\nu}) \,-\, B_{x,\sigma}\,(F_{x+\hat\rho+\hat\sigma-T,\mu\nu} - F_{x+\hat\sigma-T,\mu\nu}) \,+$$

$$B_{x,\mu}\,(F_{x-\hat\rho-\hat\sigma+T,\rho\sigma} - F_{x-\hat\rho-\hat\sigma-\hat\nu+T,\rho\sigma}) \,-\, B_{x,\nu}\,(F_{x-\hat\rho-\hat\sigma+T,\rho\sigma} - F_{x-\hat\rho-\hat\sigma-\hat\mu+T,\rho\sigma}\,) \Big]. \quad \text{(B.2)}$$

For a fixed site x we now may identify all the contributions that multiply $B_{x,\mu}$ for a fixed value of μ. For example, the terms that multiply $B_{x,1}$ are given by

$$F_{x+T-\hat3-\hat4,34} - F_{x+T-\hat2-\hat3-\hat4,34} - F_{x+T-\hat2-\hat4,24} + F_{x+T-\hat2-\hat3-\hat4,24} + F_{x+T-\hat2-\hat3,23}$$

$$- F_{x+T-\hat2-\hat3-\hat4,23} + F_{x-T+\hat1+\hat4,23} - F_{x-T+\hat1,23} - F_{x-T+\hat1+\hat3,24} \quad \text{(B.3)}$$

$$+ F_{x-T+\hat1,24} + F_{x-T+\hat1+\hat2,34} - F_{x-T+\hat1,34} \,=\, (dF)_{x+T-\hat2-\hat3-\hat4,234} - (dF)_{x-T+\hat1,234} = 0,$$

where in the last line we have combined the contributions into the exterior derivatives $(dF)_{x,\mu\nu\rho} = (d^2 A)_{x,\mu\nu\rho} + 2\pi(dn)_{x,\mu\nu\rho} = 0$, which vanish due to $d^2 = 0$ and the closedness condition $(dn)_{x,\mu\nu\rho} = 0$ we implemented for the Villain variables. The same steps can be repeated for the factors that multiply the other $B_{x,\mu}$ thus establishing that the third term on the r.h.s. of (B.1) vanishes.

Let us now explore the second term on the right hand side of (B.1), i.e., the term $Q[(dB)]$. Dropping again a factor of $1/8\pi^2$ the term reads

$$\sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} (dB)_{x,\mu\nu}\, \epsilon_{\mu\nu\rho\sigma}\, (dB)_{x-\hat\rho-\hat\sigma+T,\rho\sigma} = \sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} (dB)_{x+\hat\rho+\hat\sigma-T,\mu\nu}\, \epsilon_{\mu\nu\rho\sigma}\, (dB)_{x,\rho\sigma} \,=$$

$$\sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} \epsilon_{\mu\nu\rho\sigma}\Big[B_{x+\hat\rho,\sigma} - B_{x,\sigma} - B_{x+\hat\sigma,\rho} + B_{x,\rho}\Big]\, (dB)_{x+\hat\rho+\hat\sigma-T,\mu\nu} \,=$$

$$\sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} \epsilon_{\mu\nu\rho\sigma}\Big[B_{x,\rho}\Big((dB)_{x+\hat\rho+\hat\sigma-T,\mu\nu} - (dB)_{x+\hat\rho-T,\mu\nu}\Big)$$

$$- B_{x,\sigma}\Big((dB)_{x+\hat\rho+\hat\sigma-T,\mu\nu} - (dB)_{x+\hat\sigma-T,\mu\nu}\Big)\Big], \quad \text{(B.4)}$$

where we performed trivial shifts of site indices, explicitly wrote out one of the exterior derivatives, and organized the terms such that we identify the factors multiplying $B_{x,\rho}$ and $B_{x,\sigma}$. As with the third term we now collect all factors that multiply $B_{x,\mu}$ for a fixed μ. For the case of $B_{x,1}$ this factor is given by

$$(dB)_{x-T+\hat{1}+\hat{4},23} - (dB)_{x-T+\hat{1},23} - (dB)_{x-T+\hat{1}+\hat{3},24} + (dB)_{x+T+\hat{1},24} \tag{B.5}$$
$$+(dB)_{x-T+\hat{1}+\hat{2},34} - (dB)_{x-T+\hat{1},34} = (d^2B)_{x-T+\hat{1},234} = 0 \, .$$

In the second line we have identified the terms with $(d^2B)_{x-T+\hat{1},234}$, which vanishes due to the nilpotency of the exterior derivative. In a similar way one can treat the terms that multiply $B_{x,\mu}$ for all values of μ and show that also the second term on the r.h.s. of (B.1) vanishes. Thus we have proven (4.4), i.e., $Q_T[F+dB] = Q_T[F]$ for configurations of the Villain variables that obey the closedness condition $(dn)_{x,\mu\nu\rho} = 0$.

The second result we show in this appendix is the fact that when using the Hodge decomposition (4.6) for the Villain variables the result for the topological charge $Q_T[F]$ at arbitrary T is given by (4.8) when the harmonic contribution is parameterized as in (4.7). Obviously

$$Q_T[F] = Q_T[2\pi n] = Q_T[2\pi dl + 2\pi h] = Q_T[2\pi h] = \frac{1}{2} \sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} \epsilon_{\mu\nu\rho\sigma} h_{x,\mu\nu} h_{x-\hat{\rho}-\hat{\sigma}+T,\rho\sigma} \, ,$$
$$\tag{B.6}$$

where in the first step we used (4.5), then inserted the Hodge decomposition (4.6) and subsequently used (4.4). In the final step $Q_T[2\pi h]$ was written explicitly. Inserting the parametrization (4.7) for the harmonic contribution h we find

$$Q_T[2\pi h] = \frac{1}{2} \sum_x \sum_{\substack{\mu<\nu \\ \rho<\sigma}} \epsilon_{\mu\nu\rho\sigma} \, \omega_{\mu\nu} \, \omega_{\rho\sigma} \sum_{i=1}^{N_\rho} \sum_{j=1}^{N_\sigma} \delta_{x,i\hat{\rho}+j\hat{\sigma}} \sum_{n=1}^{N_\mu} \sum_{l=1}^{N_\nu} \delta_{x-\hat{\rho}-\hat{\sigma}+T, n\hat{\mu}+l\hat{\nu}} \tag{B.7}$$

$$= \frac{1}{2} \sum_{\substack{\mu<\nu \\ \rho<\sigma}} \epsilon_{\mu\nu\rho\sigma} \, \omega_{\mu\nu} \, \omega_{\rho\sigma} \sum_{n=1}^{N_\mu} \sum_{l=1}^{N_\nu} \sum_{i=1}^{N_\rho} \sum_{j=1}^{N_\sigma} \delta_{i\hat{\rho}+j\hat{\sigma}-\hat{\rho}-\hat{\sigma}+T, n\hat{\mu}+l\hat{\nu}}$$

$$= \frac{1}{2} \sum_{\substack{\mu<\nu \\ \rho<\sigma}} \epsilon_{\mu\nu\rho\sigma} \, \omega_{\mu\nu} \, \omega_{\rho\sigma} \sum_{n=1}^{N_\mu} \sum_{l=1}^{N_\nu} \sum_{i=1}^{N_\rho} \sum_{j=1}^{N_\sigma} \delta_{0,(n-t_\mu)\hat{\mu}+(l-t_\nu)\hat{\nu}+(1-i)\hat{\rho}+(1-j)\hat{\sigma}} \, .$$

In the first step we summed over x to remove the first Kronecker delta. In the second step we used that $T = t_\mu\hat{\mu} + t_\nu\hat{\nu} + t_\rho\hat{\rho} + t_\sigma\hat{\sigma}$ for mutually distinct μ,ν,ρ,σ. Then it is obvious that only a single term remains where the Kronecker deltas give 1, such that the topological charge reduces to

$$Q_T[2\pi h] = \frac{1}{2} \sum_{\substack{\mu<\nu \\ \rho<\sigma}} \epsilon_{\mu\nu\rho\sigma} \, \omega_{\mu\nu} \, \omega_{\rho\sigma} = \omega_{12}\omega_{34} - \omega_{13}\omega_{24} + \omega_{14}\omega_{23} \in \mathbb{Z} \, , \tag{B.8}$$

which is the result (4.8).

C Properties of the kernels M and K from Fourier transformation

In sections 4.1 and 4.3 we combine the gauge field action and the θ-term into quadratic forms with kernels $M_{x,\mu\nu|y,\rho\sigma}$ defined in eq. (4.30) and similarly in section 4.3 with a new kernel $K_{x,\mu\nu|y,\rho\sigma}$ defined in eq. (4.46). In order to diagonalize the space-time dependence of these kernels, which we here generically denote as $A_{x,\mu\nu|y,\rho\sigma}$, we use Fourier transformation, i.e., a similarity transformation with the unitary matrices $U_{p,x} \equiv V^{-1/2} e^{-ip\cdot x}$, where the momenta are given by $p_\mu = 2\pi n_\mu/N_\mu$, $n_\mu = 0, 1, 2 \ldots N_\mu - 1$ (we use periodic boundary conditions). We find

$$\sum_{x,y} U^\star_{p,x} A_{x,\mu\nu|y,\rho\sigma} U_{q,y} = \delta^{(4)}_{p,q} \, \widehat{A}(p)_{\mu\nu|\rho\sigma} \, , \tag{C.1}$$

such that

$$A^{-1}_{x,\mu\nu|y,\rho\sigma} = \frac{1}{V} \sum_p e^{ip(y-x)} \, \widehat{A}(p)^{-1}_{\mu\nu|\rho\sigma} \, . \tag{C.2}$$

The Fourier transform $\widehat{A}(p)_{\mu\nu|\rho\sigma}$ is a 6×6 matrix (we order the indices $\mu < \nu$, $\rho < \sigma$). Both, the Fourier transforms of M and of K have a similar structure given by[18] (again we use the generic notation $\widehat{A}$ for both kernels),

$$\widehat{A}(p)_{\mu\nu|\rho\sigma} = f(p)[\delta_{\mu\rho}\,\delta_{\nu\sigma} \, + \, i\,a\,\epsilon_{\mu\nu\rho\sigma}\,e^{ip_\rho + ip_\sigma}] \, , \tag{C.3}$$

where $f(p)$ is some function of the momenta and $a \in \mathbb{R}$ some real-valued parameter. It is straightforward to show that

$$\sum_{\rho<\sigma}[\delta_{\mu\rho}\,\delta_{\nu\sigma} + i\,a\,\epsilon_{\mu\nu\rho\sigma}\,e^{ip_\rho + ip_\sigma}][\delta_{\rho\tau}\,\delta_{\sigma\omega} - i\,a\,\epsilon_{\rho\sigma\tau\omega}\,e^{ip_\tau + ip_\omega}] = \delta_{\mu\tau}\,\delta_{\nu\omega}(1 + a^2 e^{ip\cdot\hat{s}}) \, , \tag{C.4}$$

where again we use $\hat{s} \equiv \hat{1} + \hat{2} + \hat{3} + \hat{4}$. As a consequence, the inverse momentum space kernel is given by

$$\widehat{A}(p)^{-1}_{\mu\nu|\rho\sigma} = \frac{\delta_{\mu\rho}\,\delta_{\nu\sigma} \, - \, i\,a\,\epsilon_{\mu\nu\rho\sigma}\,e^{ip_\rho + ip_\sigma}}{f(p)(1 + a^2 e^{ip\cdot\hat{s}})} \, , \tag{C.5}$$

and with (C.2) one finds the inverse kernel in real space.

D Generalized Poisson resummation

In this appendix we present a short derivation of the generalized Poisson resummation formula. We consider a function $b(x_1, x_2, \ldots x_N)$ of N real variables x_j that has the form

$$b(x_1, x_2, \ldots x_N) \equiv \left(\prod_{j=1}^N \sum_{n_j \in \mathbb{Z}}\right) e^{-\frac{\beta}{2}\sum_{j,k=1}^N (x_j + 2\pi n_j)\,M_{jk}\,(x_k + 2\pi n_k)} \, e^{-i\sum_{j=1}^N \zeta_j(x_j + 2\pi n_j)} \, . \tag{D.1}$$

---

[18]For K we actually use a symmetrized version of the term with the ϵ-tensor, but the inversion strategy is identical to the one outlined here.

M_{jk} is an invertible matrix that has eigenvalues with positive real parts and ζ_j are some real parameters. The generalized Poisson resummation formula states that $b(x_1, x_2, \ldots x_N)$ can be expressed as

$$b(x_1, x_2 \ldots x_N) = \left(\frac{1}{\sqrt{2\pi\beta}}\right)^N \frac{1}{\sqrt{\det M}} \left(\prod_{j=1}^N \sum_{p_j \in \mathbb{Z}}\right) e^{-\frac{1}{2\beta} \sum_{j,k=1}^N (\zeta_j + p_j) M_{jk}^{-1} (\zeta_k + p_k)} e^{i \sum_{j=1}^N p_j x_j}.$$

(D.2)

To prove (D.2) we first note that $b(x_1, x_2 \ldots x_N)$ given in (D.1) is 2π-periodic in each of its arguments. This implies that it has the Fourier representation

$$b(x_1, x_2 \ldots x_N) = \left(\prod_{j=1}^N \sum_{p_j \in \mathbb{Z}}\right) \widehat{b}(p_1, p_2 \ldots p_N) e^{i \sum_{j=1}^N p_j x_j},$$

(D.3)

with the Fourier transforms $\widehat{b}(p_1, p_2 \ldots p_N)$ given by

$$\widehat{b}(p_1, p_2 \ldots p_N) = \left(\prod_{j=1}^N \int_{-\pi}^{\pi} \frac{dx_j}{2\pi}\right) b(x_1, x_2 \ldots x_N) e^{-i \sum_{j=1}^N p_j x_j}.$$

(D.4)

Inserting the explicit form (D.1) we find

$$\begin{aligned}
\widehat{b}(p_1, p_2 \ldots p_N) &= \left(\prod_{j=1}^N \sum_{n_j \in \mathbb{Z}} \int_{-\pi}^{\pi} \frac{dx_j}{2\pi}\right) e^{-\frac{\beta}{2} \sum_{j,k=1}^N (x_j + 2\pi n_j) M_{jk} (x_k + 2\pi n_k)} e^{-i \sum_{j=1}^N (\zeta_j + p_j)(x_j + 2\pi n_j)} \\
&= \left(\prod_{j=1}^N \int_{-\infty}^{\infty} \frac{dy_j}{2\pi}\right) e^{-\frac{\beta}{2} \sum_{j,k=1}^N y_j M_{jk} y_k} e^{-i \sum_{j=1}^N (\zeta_j + p_j) y_j} \\
&= \left(\frac{1}{\sqrt{2\pi\beta}}\right)^N \frac{1}{\sqrt{\det M}} e^{-\frac{1}{2\beta} \sum_{j,k=1}^N (\zeta_j + p_j) M_{jk}^{-1} (\zeta_k + p_k)},
\end{aligned}$$

(D.5)

where in the first step we have inserted factors $e^{-i2\pi p_j n_j} = 1$ (note that the p_j are integer) and in the second step have switched to new integration variables $y_j = x_j + 2\pi n_j$. In the last step the N-dimensional Gaussian integral was solved. Inserting this result for $\widehat{b}(p_1, p_2 \ldots p_N)$ in (D.3) completes the proof of (D.2).

E The dual worldline formulation

In the section 3 we have generalized the self-dual U(1) gauge theory from section 2 to include electric and magnetic matter and showed that the construction is self-dual. However, the form of self-dual lattice QED discussed in section 3 is not directly suitable for a numerical simulation, since the gauge field Boltzmann factor (2.13) obviously is complex and does not give rise to a real and positive weight factor that may be used in a Monte Carlo simulation. In this apppendix we now show that for bosonic matter this complex action problem can

be overcome by switching to a worldline formulation for the magnetic matter.[19] First numerical results for self-dual QED based on this representation were presented in [13].

In order to prepare the Boltzmann factor (2.13) for the worldline formulation we rewrite the second exponent in (2.13) by switching to the dual lattice using (2.21) and the identity

$$(dn)_{x,\mu\nu\rho} = -\sum_\sigma \epsilon_{\mu\nu\rho\sigma} \left(\partial \widetilde{n} \right)_{\tilde{x}-\hat{\sigma},\sigma} , \tag{E.1}$$

which is a direct consequence of (A.5). Thus the gauge field Boltzmann factor assumes the form

$$B_\beta[A^e, A^m] = \sum_{\{n\}} e^{-\frac{\beta}{2} \sum_x \sum_{\mu<\nu} \left(F^e_{x,\mu\nu} \right)^2} \prod_{\tilde{x},\mu} e^{i\widetilde{A}^m_{\tilde{x},\mu}(\partial \widetilde{n})_{\tilde{x},\mu}} , \tag{E.2}$$

where we have converted the sum in the second exponent of the Boltzmann factor into a product over all links of the dual lattice.

The second step is to use the well known worldline representation of the charged scalar in a background U(1) gauge field (see, e.g., [46, 47]). It is straightforward to convert this worldline representation to the dual lattice where the magnetic matter partition sum (3.4) is defined. The worldline representation then reads (compare the appendix of [7] for the notation used here)

$$\widetilde{Z}_{M^m, \lambda^m, q^m}[\widetilde{A}^m] \equiv \sum_{\{\widetilde{k}\}} W_{M^m, \lambda^m}[\widetilde{k}] \left[\prod_{\tilde{x}} \delta\left((\partial \widetilde{k})_{\tilde{x}} \right) \right] \left[\prod_{\tilde{x},\mu} e^{i\,q^m\,\widetilde{A}^m_{\tilde{x},\mu}\,\widetilde{k}_{\tilde{x},\mu}} \right] . \tag{E.3}$$

The partition function is a sum over configurations of the dual flux variables $\widetilde{k}_{\tilde{x},\mu} \in \mathbb{Z}$ assigned to the links $(\tilde{x}, \mu)$ of the dual lattice, where

$$\sum_{\{\widetilde{k}\}} \equiv \prod_{\tilde{x},\mu} \sum_{\widetilde{k}_{\tilde{x},\mu}\in\mathbb{Z}} . \tag{E.4}$$

The flux variables are subject to vanishing divergence constraints

$$(\partial \widetilde{k})_{\tilde{x}} \equiv \sum_{\mu=1}^d \left[\widetilde{k}_{\tilde{x},\mu} - \widetilde{k}_{\tilde{x}-\hat{\mu},\mu} \right] = 0 \quad \forall \tilde{x} , \tag{E.5}$$

which in (E.3) are implemented with the product of Kronecker deltas. These constraints enforce flux conservation at each site $\tilde{x}$ of the dual lattice, such that the $\widetilde{k}_{\tilde{x},\mu}$ form closed loops of flux on the dual lattice. At every link $(\tilde{x}, \mu)$ of the dual lattice the dual magnetic gauge field $\widetilde{A}^m_{\tilde{x},\mu}$ couples in the form $e^{i\,q^m\,\widetilde{A}^m_{\tilde{x},\mu}\,\widetilde{k}_{\tilde{x},\mu}}$, which gives rise to the second product in (E.3).

---

[19]We remark that also for fermionic matter one may switch to a worldline formulation that solves the complex action problem from the gauge field Boltzmann factor. However, for fermions the worldline configurations come with signs that are due to the Pauli principle and the spinor properties of the fermions. Thus the worldline formulation of fermions generates its own challenges that for some examples could be overcome with other techniques such as resummation or density of states techniques (see, e.g., [45]).

The configurations of the dual flux variables $\widetilde{k}_{\tilde{x},\mu}$ come with real and positive weight factors $W_{M^m,\lambda^m}[\widetilde{k}]$, that are themselves sums (defined analogously to (E.4)) over configurations $\sum_{\{\tilde{a}\}}$ of auxiliary variables $\widetilde{a}_{\tilde{x},\mu} \in \mathbb{N}_0$. The weights are given by

$$W_{M^m,\lambda^m}[\widetilde{k}] \equiv \sum_{\{\tilde{a}\}} \left[\prod_{\tilde{x},\mu} \frac{1}{\left(|\widetilde{k}_{\tilde{x},\mu}|+\widetilde{a}_{\tilde{x},\mu}\right)!\,\widetilde{a}_{\tilde{x},\mu}!}\right] \left[\prod_{\tilde{x}} I_{M^m,\lambda^m}(f_{\tilde{x}})\right] \qquad \text{with} \qquad (\text{E.6})$$

$$I_{M^m,\lambda^m}(f_{\tilde{x}}) \equiv \int_0^\infty \!\!dr\, r^{f_{\tilde{x}}+1} e^{-M^m r^2 - \lambda^m r^4}, \quad f_{\tilde{x}} \equiv \sum_\mu \left[|\widetilde{k}_{\tilde{x},\mu}|+|\widetilde{k}_{\tilde{x}-\hat\mu,\mu}| + 2\left(\widetilde{a}_{\tilde{x},\mu}+\widetilde{a}_{\tilde{x}-\hat\mu,\mu}\right)\right].$$

The $f_{\tilde{x}}$ are non-negative integer-valued combinations of the flux variables $\widetilde{k}_{\tilde{x},\mu}$ and the auxiliary variables $\widetilde{a}_{\tilde{x},\mu}$. For a numerical simulation the integrals $I_{M^m,\lambda^m}(f_{\tilde{x}})$ may be pre-computed numerically and stored for sufficiently many values of $f_{\tilde{x}}$. The updates of the auxiliary variables can be implemented with standard techniques (see, e.g., [48, 49] for details).

With the gauge field Boltzmann factor in the form (E.2) and the dependence of the partition sum $\widetilde{Z}_{M^m,\lambda^m,q^m}$ on the dual magnetic gauge field $\widetilde{A}^m_{\tilde{x},\mu}$ given by the last factor in (E.3) we can now completely integrate out the dual magnetic gauge field. The corresponding integral reads (compare (3.1) and use $\int D[A^m] = \int D[\widetilde{A}^m]$)

$$\int D[\widetilde{A}^m] \left[\prod_{\tilde{x},\mu} e^{i\widetilde{A}^m_{\tilde{x},\mu}(\partial n)_{\tilde{x},\mu}}\right]\left[\prod_{\tilde{x},\mu} e^{i\,q^m\,\widetilde{A}^m_{\tilde{x},\mu}\,\widetilde{k}_{\tilde{x},\mu}}\right] = \prod_{\tilde{x},\mu} \int_{-\pi}^{\pi} \frac{d\widetilde{A}^m_{\tilde{x},\mu}}{2\pi} e^{i\widetilde{A}^m_{\tilde{x},\mu}\left[q^m\,\widetilde{k}_{\tilde{x},\mu}+(\partial\widetilde{n})_{\tilde{x},\mu}\right]}$$

$$= \prod_{\tilde{x},\mu} \delta\!\left(q^m\,\widetilde{k}_{\tilde{x},\mu} + (\partial\widetilde{n})_{\tilde{x},\mu}\right). \qquad (\text{E.7})$$

Integrating out the dual magnetic gauge fields has generated link-based constraints that relate the flux variables and the dual Villain variables via

$$q^m\,\widetilde{k}_{\tilde{x},\mu} = -(\partial\widetilde{n})_{\tilde{x},\mu} \qquad \forall(\tilde{x},\mu). \qquad (\text{E.8})$$

Note that the constraints (E.8) are consistent with the vanishing divergence constraints $\partial\widetilde{k} = 0$ from (E.5), due to $\partial^2 = 0$ (see appendix A).

Thus we may summarize the final form of self-dual scalar lattice QED with a worldline representation for the magnetic matter:

$$Z(\beta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m) = \int D[A^e] \sum_{\{n\}}\sum_{\{\tilde{k}\}}\sum_{\{\tilde{a}\}} \left[\prod_{\tilde{x},\mu} \delta\!\left(q^m\,\widetilde{k}_{\tilde{x},\mu} + (\partial\widetilde{n})_{\tilde{x},\mu}\right)\right] \qquad (\text{E.9})$$

$$e^{-\frac{\beta}{2}\sum_x \sum_{\mu<\nu} \left(F^e_{x,\mu\nu}\right)^2} Z_{M^e,\lambda^e,q^e}[A^e] \left[\prod_{\tilde{x},\mu} \frac{1}{\left(|\widetilde{k}_{\tilde{x},\mu}|+\widetilde{a}_{\tilde{x},\mu}\right)!\,\widetilde{a}_{\tilde{x},\mu}!}\right]\left[\prod_{\tilde{x}} I_{M^m,\lambda^m}(f_{\tilde{x}})\right],$$

with $F^e_{x,\mu\nu} = (dA^e + 2\pi\,n)_{x,\mu\nu}$ and

$$f_{\tilde{x}} = \sum_\mu \left[|\widetilde{k}_{\tilde{x},\mu}|+|\widetilde{k}_{\tilde{x}-\hat\mu,\mu}| + 2\left(\widetilde{a}_{\tilde{x},\mu}+\widetilde{a}_{\tilde{x}-\hat\mu,\mu}\right)\right]. \qquad (\text{E.10})$$

Obviously all weight factors in (E.9) are real and positive, such that this form now is accessible to numerical Monte Carlo simulations. Note that for $q^m = \pm 1$ one may use the constraints (E.8) to completely eliminate the flux variables $\widetilde{k}_{\tilde{x},\mu}$ such that in that case the Villain variables are not subject to any constraints, which in some aspects makes a numerical simulation of (E.9) simpler than the simulation of the pure gauge theory (2.8), where configurations of the Villain variables need to obey the closedness constraint (2.7).

We conclude the discussion of the worldline form by expressing the expectation value $\langle |\phi^m|^2 \rangle$ that appears in the duality relation (3.12) in terms of the worldline variables. The expectation value is obtained from a derivative of $\ln Z$ with respect to M^m, and this derivative can of course also be applied to Z in the form (E.9), (E.10). A few lines of algebra give (use $-\partial/\partial M^m I_{M^m,\lambda^m}(f_{\tilde{x}}) = I_{M^m,\lambda^m}(f_{\tilde{x}} + 2)$),

$$
\begin{aligned}
\left\langle |\phi^m|^2 \right\rangle_{\beta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m} &= -\frac{1}{V}\frac{\partial}{\partial M^m} \ln Z(\beta, M^e, q^e, \lambda^e, M^m, \lambda^m, q^m) \\
&= \frac{1}{V} \left\langle \sum_{\tilde{x}} \frac{I_{M^m,\lambda^m}(f_{\tilde{x}} + 2)}{I_{M^m,\lambda^m}(f_{\tilde{x}})} \right\rangle_{\beta, M^e, \lambda^e, q^e, M^m, \lambda^m, q^m}.
\end{aligned}
\tag{E.11}
$$

F Self-duality with a generalized topological charge

In this appendix we briefly discuss how the construction of the self-dual theory with a θ-term in subsection 4.4 can be generalized further, such that the topological charge fully implements all lattice symmetries.

The general form of the self-dual kernel we consider (this generalizes the kernel defined in (4.43)) is in momentum space written as

$$
\widehat{K}_{\mu\nu|\rho\sigma}(p) = \frac{1}{\widehat{G}(p)} \left(\delta_{\mu\rho}\delta_{\nu\sigma} - i \sum_T \gamma_T \, \epsilon_{\mu\nu\rho\sigma} \, e^{ip_\rho + ip_\sigma + iT\cdot p} \right) ,
\tag{F.1}
$$

where $T = \sum_\mu t_\mu \hat{\mu}$ with $t_\mu \in \mathbb{Z}$, and γ_T are some coefficients. Now note that (compare also appendix C)

$$
\begin{aligned}
&\left(\delta_{\mu\rho}\delta_{\nu\sigma} + i \sum_T \gamma_T \, \epsilon_{\mu\nu\rho\sigma} \, e^{ip_\rho + ip_\sigma - iT\cdot p} \right) \left(\delta_{\rho\mu'}\delta_{\sigma\nu'} - i \sum_T \gamma_T \, \epsilon_{\rho\sigma\mu'\nu'} \, e^{ip'_\mu + ip'_\nu - iT\cdot p} \right) \\
&= \delta_{\mu\mu'}\delta_{\nu\nu'} + \sum_{T,T'} \gamma_T \, \gamma_{T'} \, \epsilon_{\mu\nu\rho\sigma} \, \epsilon_{\rho\sigma\mu'\nu'} \, e^{ip_\rho + ip_\sigma + ip_\mu + ip_\nu - iT\cdot p - iT'\cdot p} \\
&= \delta_{\mu\mu'}\delta_{\nu\nu'} \left(1 + \sum_{T,T'} \gamma_T\gamma_{T'} e^{i\hat{s}\cdot p - iT\cdot p - iT'\cdot p} \right),
\end{aligned}
\tag{F.2}
$$

where again $\hat{s} = \hat{1} + \hat{2} + \hat{3} + \hat{4}$. So by choosing

$$
\widehat{G}(p) = \sqrt{1 + \sum_{T,T'} \gamma_T\gamma_{T'} e^{i(\hat{s}-T-T')\cdot p}} ,
\tag{F.3}
$$

we find that $\hat{K}$ is form-covariant under inversion, i.e.,

$$\widehat{K}_{\mu\nu|\rho\sigma}(p) = \frac{\delta_{\mu\rho}\delta_{\nu\sigma} + i\sum_T \gamma_T\,\epsilon_{\mu\nu\rho\sigma}\,e^{ip_\rho + ip_\sigma + iT}}{\sqrt{1 + \sum_{T,T'}\gamma_T\gamma_{T'}e^{i(\hat{s}-T-T')\cdot p}}}\;, \tag{F.4}$$

$$\widehat{K}^{-1}_{\mu\nu|\rho\sigma}(p) = \frac{\delta_{\mu\rho}\delta_{\nu\sigma} - i\sum_T \gamma_T\,\epsilon_{\mu\nu\rho\sigma}\,e^{ip_\rho + ip_\sigma + iT}}{\sqrt{1 + \sum_{T,T'}\gamma_T\gamma_{T'}e^{i(\hat{s}-T-T')\cdot p}}}\;. \tag{F.5}$$

Now a convenient choice of the coefficients γ_T is such that $\gamma_{-T+\hat{s}} = \gamma_T$, which implies that the argument in the square root of $\widehat{G}(p)$ is real. This argument is given by

$$1 + \sum_{T,T'}\gamma_T\gamma_{T'}e^{i(\hat{s}-T-T')\cdot p} = 1 + \left|\sum_T \gamma_T e^{-iT\cdot p}\right|^2. \tag{F.6}$$

In real space this corresponds to the operator

$$H_{x,y} = \sum_{T,T'}\gamma_T\,\gamma_{T'}\,\delta^{(4)}_{x+T,y+T'}\;, \tag{F.7}$$

which generalizes the Helmholtz lattice operator introduced in (4.45).

We point out that the above result does not depend on the vector $\hat{s}$ which singles out a direction on the lattice, such that now, with a suitable choice of the coefficients γ_T the lattice symmetries can be implemented in H. The full θ-term, however, does not seem to be manifestly invariant due to the appearance of the vectors $\hat{\sigma}$ and $\hat{\rho}$ in (F.1). In a free theory, however, the θ-term is topological, and hence lattice symmetries are exact in this case too.

The action density is now given by

$$\sum_y \sum_{\mu<\nu}\sum_{\rho<\sigma} F_{x,\mu\nu}(H^{-1/2})_{x,z}\left(\delta_{y,z} + i\sum_T \gamma_T\,\epsilon_{\mu\nu\rho\sigma}\,\delta_{y,z-\hat{\rho}-\hat{\sigma}+T}\right)F_{z,\rho\sigma}\;. \tag{F.8}$$

As announced, the theory can be made fully invariant under all lattice symmetries if, in addition to the conditions $\gamma_{-T+\hat{s}} = \gamma_T$ from above, we implement the following relations among the coefficients,[20]

$$\gamma_T = \gamma_{R\left(T-\frac{\hat{s}}{2}\right)+\frac{\hat{s}}{2}}\;, \tag{F.9}$$

where R is an arbitrary lattice rotation.

---

[20] This is easiest to see as follows: the generic θ-term is defined as $Q_W = \sum_p F_p F_{\star W(p)}$, where W is an arbitrary translation operator from the lattice to the dual lattice, p is a plaquette of the lattice and $\star$ is the Hodge-star analogue mapping of the lattice to the dual lattice (compare [7]). The lattice rotation R commutes with the $\star$ operator, but not with W. We now consider $R: F_p \to F_{R(p)}$, but then $Q_W \to \sum_p F_{R(p)}F_{R(\star W R^{-1}R(p))} = Q_{RWR^{-1}}$. So if we now define a general topological charge as $\sum_W \kappa_W Q_W$, with coefficients κ_W that respect $\kappa_{RWR^{-1}} = \kappa_W$, the θ-term will obey the lattice symmetries. Writing explicitly

$$\sum_W \kappa_W Q_W = \sum_x \sum_{\mu<\nu}\sum_{\rho<\sigma}\sum_{\boldsymbol{W}} \kappa_{\boldsymbol{W}} F_{x,\mu\nu}\epsilon_{\mu\nu\rho\sigma}F_{x+\frac{\hat{s}}{2}+\boldsymbol{W}-\hat{\rho}-\hat{\sigma}}\;,$$

where $\boldsymbol{W}$ is now a vector which corresponds to the map W. Now, setting a lattice vector, $T = \boldsymbol{W} + \frac{\hat{s}}{2}$, this form can be written as

$$\sum_{\boldsymbol{W}} \kappa_{\boldsymbol{W}} Q_{\boldsymbol{W}} = \sum_x \sum_{\mu<\nu}\sum_{\rho<\sigma}\sum_T \kappa_T F_{x,\mu\nu}\epsilon_{\mu\nu\rho\sigma}F_{x+T-\hat{\rho}-\hat{\sigma}}\;,$$

where $\kappa_{T-\frac{\hat{s}}{2}} = \kappa_T$, and the condition $\kappa_{R(\boldsymbol{W})} = \kappa_{\boldsymbol{W}}$ translates to $\gamma_T = \gamma_{R\left(T-\frac{\hat{s}}{2}\right)+\frac{\hat{s}}{2}}$ as stated in (F.9).

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