Density of states approach for lattice gauge theory with a θ-term

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Abstract

We discuss a new strategy for treating the complex action problem of lattice field theories with a θ-term based on density of states (DoS) methods. The key ingredient is to use open boundary conditions where the topological charge is not quantized to integers and the density of states is sufficiently well behaved such that it can be computed precisely with recently developed DoS techniques. After a general discussion of the approach and the role of the boundary conditions, we analyze the method for 2-d U(1) lattice gauge theory with a θ-term, a model that can be solved in closed form. We show that in the continuum limit periodic and open boundary conditions describe the same physics and derive the DoS, demonstrating that only for open boundary conditions the density is sufficiently well behaved for a numerical evaluation. We conclude our proof of principle analysis with a small test simulation where we numerically compute the density and compare it with the analytical result.

1. Introduction

Although Quantum Chromodynamics (QCD) is considered the well-established and well-tested theory of the strong interaction, there are several aspects that should be understood considerably better. One open issue is the role of topology, in particular of the so-called θ-term, which is introduced by generalizing the gauge field action $S_G[A]$ to

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$$S_G[A] + i\,\theta\,Q[A]\,, \tag{1}$$

where θ is the vacuum angle and $Q[A]$ the topological charge. The physics of the θ-term is non-perturbative in nature such that non-perturbative methods are needed for exploring it. In principle lattice field theory could provide a suitable non-perturbative approach, but obviously the presence of the θ-term makes the action (1) complex, such that the Boltzmann factor e^{-S} has a complex phase and thus cannot be used as a probability in a Monte Carlo simulation.

Similar complex action problems appear also in other physically interesting settings, in particular for lattice field theories with a chemical potential. For this case a possible approach for overcoming the complex action problem are density of states (DoS) techniques that were originally introduced to lattice field theory in [1,2] and over the years were used in a wide range of applications [3–23]. Based on an idea by Wang and Landau [7] a new considerably improved modern DoS approach was introduced in [8] and further developed for lattice field theories at finite density [8–23].

It is interesting to note that so far only a single application of DoS techniques to lattice gauge theory with a θ-term can be found in the literature [19]. The problem with applying DoS techniques to lattice gauge theories with a θ-term is the fact that the density for the topological charge Q becomes concentrated on integers in the continuum limit.[1] Thus towards the continuum limit the density of states turns into a sum of Dirac delta functions, i.e., it has a very non-smooth form that also for the powerful new techniques [8–23] is very hard to evaluate. As a consequence, in the test study [19] the results for the density are far from the continuum limit, which cannot be reached with that approach.

In this paper we argue that DoS techniques may be used if one works with open boundary conditions. For that choice the topological charge is not quantized to integers [24,25] and as a consequence the density of states will not converge towards a sum of Dirac delta functions, but instead is expected to approach a form that vaguely resembles a Gaussian distribution with a width proportional to $\chi_t V$, where χ_t is the topological susceptibility and V the 4-volume. Such a distribution is much better conditioned for a DoS approach and is expected to be well accessible with the techniques [8–23].

Using open boundary conditions for simulations of lattice QCD has been proposed in [24,25] as a method to overcome topological freezing. In the infinite volume limit physics becomes independent of the boundaries and the open boundary conditions thus will give rise to the same physical results, as has been established in various studies (see, e.g., [26] for the analysis of topological properties that is relevant for the discussion here).

In the next section we formulate lattice field theory with a θ-term in the DoS approach and briefly summarize the techniques [8–23] for numerically evaluating the density. Subsequently we discuss the role of the boundary conditions and argue that open boundary conditions indeed give rise to a much better conditioned density of states.

To illustrate in more detail the idea of DoS with open boundary conditions for lattice gauge theory with a θ-term we then consider 2-d U(1) lattice gauge theory with a topological term. We use the Villain formulation [27] with a θ-term [28–31] where, using a dual formulation, the model can essentially be solved in closed form. We discuss the system for periodic and for open boundary conditions and show that the large volume physics is the same for both boundary conditions. Subsequently we compute the densities for both types of boundary conditions and

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[1] For a fermionic definition or also the so-called *geometrical definition*, the topological charge is already integer-valued at finite lattice spacing.

indeed find that the density for open boundary conditions remains well conditioned, while for periodic boundary conditions it assumes the form of a sum of Dirac delta functions.

In a small test simulation we compute the density for 2-d U(1) lattice gauge theory with a topological term, now using the Wilson formulation. More specifically we use the DoS Functional Fit Approach (FFA) [19–21] to determine the density. For the case of open boundary conditions we compare the numerical data to analytic results for the density and find excellent agreement, indicating that using modern DoS techniques combined with open boundary conditions indeed is an interesting approach to simulating lattice field theory with a θ-term.

2. Density of states for θ-terms

We begin our discussion with a general formulation of the problem with DoS and then briefly summarize the recently developed techniques [8–23] for computing the densities. Finally we analyze the influence of the boundary conditions on the structure of the densities.

2.1. DoS formulation of the problem

Formally it is straightforward to set up the DoS formulation of lattice field theory with a θ-term. The partition sum Z_θ and vacuum expectation values $\langle \mathcal{O} \rangle_\theta$ of observables $\mathcal{O}$ at finite topological angle θ are given by

$$Z_\theta = \int D[A] \, e^{-S_{eff}[A] - i\theta \, Q[A]} \, , \quad \langle \mathcal{O} \rangle_\theta = \frac{1}{Z_\theta} \int D[A] \, e^{-S_{eff}[A] - i\theta \, Q[A]} \, \mathcal{O}[A] \, , \qquad (2)$$

where $\int D[A]$ denotes the path integral over all configurations of the gauge fields. The effective action $S_{eff}[A]$ consists of the gauge field action and the logarithm of the fermion determinant,[2] or in the case of pure gauge theory is simply given by only the gauge field action. $Q[A]$ denotes a suitable lattice discretization of the topological charge, and $\mathcal{O}[A]$ is some observable.

We now define generalized densities $\rho^{(\mathcal{J})}(x)$ of the form

$$\rho^{(\mathcal{J})}(x) = \int D[A] \, e^{-S_{eff}[A]} \, \mathcal{J}[A] \, \delta\Big(x - Q[A]\Big) \, . \qquad (3)$$

Note that in the definition of the densities we have allowed for the insertion of a functional $\mathcal{J}[A]$ in the path integral, which we will either choose to be the unit operator $\mathbb{1}$ or one of the observables $\mathcal{O}[A]$ we want to study. In order to make clear which observable we refer to, we indicate the insertion chosen for a density $\rho^{(\mathcal{J})}(x)$ with a corresponding superscript. One may use charge conjugation to show that the $\rho^{(\mathcal{J})}(x)$ are either even or odd functions of x, depending on the charge conjugation symmetry of the insertion $\mathcal{J}[A]$. Thus in a practical implementation the density has to be determined only for positive values of x.

It is straightforward to write the partition sum and the vacuum expectation values (2) as integrals over the densities (3),

$$Z_\theta = \int dx \, \rho^{(\mathbb{1})}(x) \, e^{-i\theta x} \, , \quad \langle \mathcal{O} \rangle_\theta = \frac{1}{Z_\theta} \int dx \, \rho^{(\mathcal{O})}(x) \, e^{-i\theta x} \, . \qquad (4)$$

For both, the partition sum Z_θ and vacuum expectation values $\langle \mathcal{O} \rangle_\theta$ the corresponding densities need to be integrated over with the oscillating factors factors $e^{-i\theta x}$ such that they have to be

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[2] Also in the framework of the DoS techniques outlined below standard pseudo-fermion and hybrid Monte Carlo techniques can be used to take into account the fermion determinant.

computed with very high precision. Obtaining the necessary precision is exactly what may be achieved with the new DoS techniques [8–23] and we now briefly summarize the key steps. We remark at this point that if the observables are moments of the topological charge Q it is sufficient to compute only the density $\rho^{(1)}(x)$, since the moments $\langle Q^n \rangle$ can be converted into factors x^n inserted in the first integral in (4).

2.2. Determination of the densities with modern DoS techniques

For the evaluation of the densities $\rho^{(\mathcal{J})}(x)$ we parameterize them in the form

$$\rho^{(\mathcal{J})}(x) = \exp\Big(-L^{(\mathcal{J})}(x)\Big). \tag{5}$$

Here $L^{(\mathcal{J})}(x)$ are continuous functions that are piecewise linear on intervals $I_n = [x_n, x_{n+1}]$, $n = 0, 1, \dots$, where by Δ_n we denote the length of the interval I_n. The functions $L^{(\mathcal{J})}(x)$ are normalized to $L^{(\mathcal{J})}(0) = 0$, which implies the normalization $\rho^{(\mathcal{J})}(0) = 1$ for the densities. Using the continuity and the normalization of the $L^{(\mathcal{J})}(x)$ one may show that the $L^{(\mathcal{J})}(x)$ depend only on the slopes $k_n^{(\mathcal{J})}$, $n = 0, 1, \dots$ of the piecewise linear functions, one slope $k_n^{(\mathcal{J})}$ for each interval I_n, such that in terms of the $k_n^{(\mathcal{J})}$ the density is given by

$$\rho^{(\mathcal{J})}(x) = A_n^{(\mathcal{J})} e^{-x k_n^{(\mathcal{J})}} \quad \text{for} \quad x \in I_n \quad \text{with} \quad A_n^{(\mathcal{J})} = e^{-\sum_{j=0}^{n-1} \left(k_j^{(\mathcal{J})} - k_n^{(\mathcal{J})}\right)\Delta_j}. \tag{6}$$

With the DoS methods [8–23] the slopes $k_n^{(\mathcal{J})}$ can be computed with very high precision. The slopes $k_n^{(\mathcal{J})}$ uniquely determine the densities $\rho^{(\mathcal{J})}(x)$ and vacuum expectation values are then obtained via (4). The determination of the slope $k_n^{(\mathcal{J})}$ for a given interval I_n makes use of so-called *restricted vacuum expectation values* defined as

$$\langle Q \rangle_n^{(\mathcal{J})}(\lambda) = \frac{1}{Z_n^{(\mathcal{J})}(\lambda)} \int D[A] e^{-S_{eff}[A]} \, \mathcal{J}[A] \, e^{\lambda Q[A]} \, Q[A] \, \Theta_n\Big(Q[A]\Big). \tag{7}$$

The support function $\Theta_n(x)$ equals 1 for $x \in I_n$ and vanishes outside the interval I_n. The corresponding Monte Carlo simulation thus contains a reject step for proposal configurations where $Q[A]$ would leave the interval I_n. The parameter $\lambda \in \mathbb{R}$ plays two roles: Varying λ allows one to probe the density in the whole interval I_n. Furthermore, when using the parameterized form (5), one may find a closed expression of the restricted vacuum expectation value (7) in terms of the density, which depends only on the single slope k_n corresponding to the interval I_n. As a consequence we may determine the slopes from comparing the data for $\langle Q \rangle_n^{(\mathcal{J})}(\lambda)$ with a known function $h(s)$,

$$\frac{\langle Q \rangle_n^{(\mathcal{J})}(\lambda) - x_n}{\Delta_n} - \frac{1}{2} = h\Big(\Delta_n \big[\lambda - k_n^{(\mathcal{J})}\big]\Big), \tag{8}$$

where $h(s)$ turns out to be given by

$$h(s) \equiv \frac{1}{1 - e^{-s}} - \frac{1}{s} - \frac{1}{2}, \tag{9}$$

and has the properties $h(0) = 0$, $h'(0) = 1/12$, $\lim_{s \to \pm\infty} h(s) = \pm 1/2$. The LLR approach [8–16] computes the slopes $k_n^{(\mathcal{J})}$ by finding the zeros of the lhs. of Eq. (8) using an iterative process, while the FFA method [17–23] combines simulations at different values of λ and determines

the $k_n^{(\mathcal{J})}$ from one-parameter fits of the data with the rhs. of (8). Both approaches have been demonstrated to provide very accurate determinations of the densities for several different types of applications in systems plagued by sign problems.

2.3. Implications of the boundary conditions for the DoS

Let us now briefly discuss the implications of the boundary conditions for the densities and the consequences for their determination with modern DoS techniques [8–23]. We here focus on the densities with insertion $\mathcal{J} = \mathbb{1}$ (the upper index $(\mathcal{J})$ is dropped now to simplify the notation), i.e., the densities that determine the partition sum, as well as moments of the topological charge. Other densities where for $\mathcal{J}$ some observable is inserted can be treated identically.

We begin this discussion with the case of periodic boundary conditions where the discretized $Q[A]$ either is already integer valued or becomes so in the continuum limit. As a consequence, near the continuum limit the partition sum for periodic boundary conditions $Z_\theta^{(per)}$ becomes 2π-periodic and thus has a Fourier representation of the form

$$Z_\theta^{(per)} = \sum_{n \in \mathbb{Z}} Z_n \, e^{-i\theta n} \,, \tag{10}$$

with the coefficients Z_n given by

$$Z_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta \, Z_\theta^{(per)} \, e^{i\theta n} \,. \tag{11}$$

Comparing (10) with Eq. (4) we can read off the form of the density $\rho^{(per)}(x)$ for periodic boundary conditions in the continuum limit,

$$\rho^{(per)}(x) = \frac{1}{2\pi} \sum_{n \in \mathbb{Z}} Z_n \, \delta(x - n) \,. \tag{12}$$

Obviously the density converges towards a sum of Dirac deltas (or already has this form if an integer-valued lattice discretization of $Q[A]$ is used), which clearly is a functional form that cannot be determined with the DoS techniques [8–23], since the slopes k_n jump between the values 0 and $\pm\infty$.

For open boundary conditions the situation is different. In that case the topological charge does not become quantized at integers and the partition sum (2) does not converge towards a 2π-periodic function. Thus the partition sum with open boundary conditions has the representation

$$Z_\theta^{(open)} = \int dx \, \rho^{(open)}(x) \, e^{-i\theta x} \,, \tag{13}$$

with

$$\rho^{(open)}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\theta \, Z_\theta^{(open)} \, e^{i\theta x} \,. \tag{14}$$

For the density with open boundary conditions we do not expect convergence towards a sum of Dirac deltas and instead expect a smooth dependence on x that can be evaluated with the modern DoS techniques presented in the previous subsection.

3. DoS for 2-d U(1) lattice gauge theory with a θ-term

As outlined, we will now discuss the case of 2-d U(1) lattice field theory where the general arguments presented in the previous section can be made explicit in a theory that is analytically solvable. More specifically we consider the density of states approach for 2-d $U(1)$ lattice gauge theory with Villain action [27] and a θ-term. Using dual variables this model can be solved in closed form and the properties as a function of θ can be discussed in detail. In particular also the densities can be determined for different boundary conditions such that this system is ideal for discussing very transparently different aspects of the approach outlined in the previous section.

3.1. Definition of the model and the topological charge

The continuum action for 2-d U(1) gauge fields with a topological term is given by (as usual $F_{12}(x) = \partial_1 A_2(x) - \partial_2 A_1(x)$)

$$S_G[A] + i\,\theta\,Q[A] = \frac{1}{2\,e^2} \int_{T_2} d^2x\; F_{12}(x)^2 + i\,\theta\,\frac{1}{2\pi} \int_{T_2} d^2x\; F_{12}(x)\,, \tag{15}$$

where the integration runs over the 2-torus T_2. In the Villain form of the lattice discretization the continuum gauge fields $A_\mu(x) \in \mathbb{R}$ are replaced by fields $A_{x,\mu} \in [-\pi, \pi]$ based on the links of the lattice. A discretized version of the exterior derivative may be defined as

$$dA_x = A_{x,1} + A_{x+\hat{1},2} - A_{x+\hat{2},1} - A_{x,2}\,, \tag{16}$$

i.e., the oriented sum of the gauge fields along the boundary links of a plaquette, which on our 2-d lattice we can label with the coordinate of its lower left corner x. The lattice version of the field strength may then be defined as

$$F_x = dA_x + 2\pi\,n_x\,, \tag{17}$$

where the Villain variables $n_x \in \mathbb{Z}$ assigned to the plaquettes are summed over all integers. They serve to make the theory invariant under reparameterization of the gauge links $e^{i A_{x,\mu}}$ needed for coupling matter fields, i.e., shifts $A_{x,\mu} \to A_{x,\mu} + 2\pi j_{x,\mu}$ with $j_{x,\mu} \in \mathbb{Z}$ (for details of the underlying symmetries see the discussion in [28–31]).

We define the gauge field action $S_G[A, n]$ and the topological charge $Q[A, n]$ as

$$S_G[A, n] = \frac{\beta}{2} \sum_x \left(dA_x + 2\pi n_x \right)^2 \quad , \qquad Q[A, n] = \frac{1}{2\pi} \sum_x \left(dA_x + 2\pi n_x \right), \tag{18}$$

where the sums run over all plaquettes labeled by their lower left corner x and the inverse gauge coupling is given by $\beta = 1/e^2$. The partition sum on the lattice (which here we consider to be of size $L \times L$) then is given by

$$\begin{aligned} Z_{\theta,\beta,L} &= \int D[A] \sum_{\{n\}} e^{-S_G[A,n] - i\,\theta\,Q[A,n]} \\ &= \int D[A] \prod_x \sum_{n_x \in \mathbb{Z}} e^{-\frac{\beta}{2}(dA_x + 2\pi n_x)^2 - i\frac{\theta}{2\pi}(dA_x + 2\pi n_x)}\,, \end{aligned} \tag{19}$$
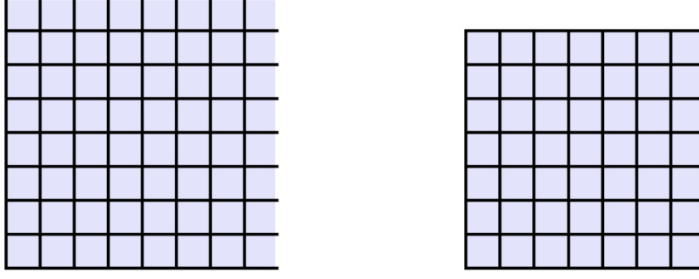
Fig. 1. Illustration of the boundary conditions we use (the thick lines are the links and the shaded areas the plaquettes). In the lhs. plot we show a 8×8 lattice with periodic boundary conditions, where the links with open ends on the right and the top of the lattice connect periodically to the sites on the left and the bottom respectively. In the rhs. plot we show the 8×8 lattice with open boundary conditions, where the periodically connecting links and the plaquettes bounded by them are omitted.

with

$$\int D[A] = \prod_{x,\mu} \int_{-\pi}^{\pi} \frac{dA_{x,\mu}}{2\pi} \quad , \quad \sum_{\{n\}} = \prod_x \sum_{n_x \in \mathbb{Z}} . \tag{20}$$

The lattice definition of the topological charge (18) in terms of the gauge fields $A_{x,\mu}$ and the Villain variables n_x allows one to discuss the role of the boundary conditions in a very transparent way. The two types of boundary conditions we consider here are illustrated in Fig. 1. In the lhs. plot we show the links (thick lines) and plaquettes (shaded area) of an 8×8 lattice with periodic boundary conditions. The links with open ends on the right and at the top periodically connect to the sites on the left and the bottom respectively. For the open boundary conditions[3] shown in the rhs. plot of Fig. 1 the links that connect periodically are omitted, as well as the plaquettes bounded by them.

The different boundary conditions give rise to different results for the topological charge $Q[A, n]$. For periodic boundary conditions the sum $\sum_x dA_x$ over the exterior derivatives dA_x defined in (16) vanishes since every gauge field variable $A_{x,\mu}$ appears twice in the sum over all plaquettes, and the two terms have opposite sign since in the two neighboring plaquettes that contain a given $A_{x,\mu}$ the corresponding link (x, μ) is run through in opposite direction. Thus for periodic boundary conditions the topological charge reduces to the sum over the Villain variables which obviously is integer [28–31] and can be shown to obey the index theorem [32].

For open boundary conditions the plaquettes that were bounded by the links that closed periodically are absent. Thus the links in the boundary ∂ of the lattice appear in only a single plaquette and thus the corresponding $A_{x,\mu}$ do not cancel. As a consequence the topological charge receives a contribution that has the form of an oriented sum over the gauge fields $A_{x,\mu}$ on ∂, corresponding to a Wilson loop around the boundary. We may summarize our finding as

$$Q^{(per)}[A, n] = \sum_x n_x \in \mathbb{Z} \quad , \quad Q^{(open)}[A, n] = \sum_x n_x + \frac{1}{2\pi} \sum_{(x,\mu)\in\partial} A_{x,\mu} \notin \mathbb{Z} . \tag{21}$$

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[3] We here use open boundaries for both directions, but remark that our analysis is essentially unchanged when using open boundary conditions for only one of the directions.

It is interesting to note that with fixed boundary conditions the topological charge becomes integer again. For that case all links in the boundary are set to the same value, such that the oriented sum over the boundary vanishes and the topological charge again reduces to the sum over Villain variables, although for only the $(L-1)^2$ plaquettes of the lattice with fixed boundary conditions.

Equation (21) shows that the effect of the boundary conditions is exactly as expected: periodic boundary conditions give rise to a topological charge that is integer, while for open boundary conditions no such quantization occurs. Thus U(1) gauge theory in 2-d with a θ-term is an interesting toy model for analyzing the use of DoS techniques with open boundary conditions we propose here. We remark once more that the formulation with the Villain action is more transparent for the discussion of the topological charge, but of course also with the Wilson gauge action the same physical picture emerges in the continuum limit, i.e., integer values for the topological charge for periodic boundary conditions, while no quantization is introduced with open boundary conditions.

3.2. Solution of the model with dual variables

2-d U(1) lattice gauge theory with a θ-term can essentially be solved in closed form by switching to dual variables. The first step is to rewrite the contributions to the Boltzmann factor from a single plaquette (compare the second line of Eq. (19)) using Poisson resummation (see the appendix of [28] for details)

$$\sum_{n_x \in \mathbb{Z}} e^{-\frac{\beta}{2}(dA_x + 2\pi n_x)^2 - i\frac{\theta}{2\pi}(dA_x + 2\pi n_x)} = \sqrt{\frac{1}{2\pi\beta}} \sum_{p_x \in \mathbb{Z}} e^{-\frac{1}{2\beta}(p_x + \frac{\theta}{2\pi})^2} e^{i\,p_x\,dA_x} . \tag{22}$$

In this form the contribution of the plaquette with lower left corner x is the sum over a plaquette occupation number $p_x \in \mathbb{Z}$ that enters a Gaussian weight factor, where the topological angle determines the mean. Inserting the form (22) of the Boltzmann factors into the partition sum (19) we find (overall constants were dropped)

$$
\begin{aligned}
Z_{\theta,\beta,L} &= \sum_{\{p\}} \prod_x e^{-\frac{1}{2\beta}(p_x + \frac{\theta}{2\pi})^2} \int D[A] \prod_x e^{i\,dA_x\,p_x} \\
&= \sum_{\{p\}} \prod_x e^{-\frac{1}{2\beta}(p_x + \frac{\theta}{2\pi})^2} \prod_x \int_{-\pi}^{\pi} \frac{dA_{x,1}}{2\pi} e^{i\,A_{x,1}(p_x - p_{x-\hat{2}})} \int_{-\pi}^{\pi} \frac{dA_{x,2}}{2\pi} e^{-i\,A_{x,2}(p_x - p_{x-\hat{1}})} \\
&= \sum_{\{p\}} \prod_x e^{-\frac{1}{2\beta}(p_x + \frac{\theta}{2\pi})^2} \prod_{x,\mu} \delta_{p_x, p_{x-\hat{\mu}}} ,
\end{aligned}
\tag{23}
$$

where in the first line $\sum_{\{p\}}$ denotes the sum over all configurations of the plaquette occupation numbers $p_x \in \mathbb{Z}$ which is defined as $\sum_{\{p\}} = \prod_x \sum_{p_x \in \mathbb{Z}}$. In the second line we have inserted the explicit form (16) of the exterior derivative dA_x which gives rise to products of phase factors such as $e^{ip_x A_{x,1}}$ et cetera. These products were then organized with respect to links and after using the explicit form (20) of the measure $\int D[A]$ lead to the integrals at the end of the second line. These integrals give rise to Kronecker deltas on all links that force the plaquette occupation numbers of the two neighboring plaquettes that share a link to be equal.

For the constraints implemented by the Kronecker deltas the boundary conditions play an important role. For periodic boundary conditions, i.e., the case illustrated in the lhs. plot of Fig. 1

each link on the lattice has two plaquettes that contain it such that the constraints simply imply $p_x = p \in \mathbb{Z} \ \forall x$. Considering an $L \times L$ lattice, such that for the periodic case we have L^2 plaquettes, we find for the partition sum with periodic boundary conditions

$$Z_{\theta,\beta,L}^{(per)} = \sum_{p\in\mathbb{Z}} e^{-\frac{1}{2}\frac{L^2}{\beta}(p+\frac{\theta}{2\pi})^2} . \tag{24}$$

The partition function is a sum over all occupation numbers $q \in \mathbb{Z}$ that due to the constraints are the same for all plaquettes. The weight factors are simply the weight factors of a single plaquette raised to the power L^2, i.e., the number of plaquettes.

For open boundary conditions the situation is different. In that case the links that constitute the boundary of the lattice have only a single plaquette that contains them. The corresponding integrals over these gauge links in the second line of (23) are of the type $\int_{-\pi}^{\pi} dA_{x,1}/2\pi \ e^{iA_{x,1}p_x} = \delta_{p_x,0}$, i.e., for open boundary conditions the plaquettes that touch the boundary are forced to have vanishing plaquette occupation numbers $p_x = 0$. The constraints on the links in the interior of the lattice then force also all other plaquette occupation numbers to 0. Thus only the configuration with $p_x = 0 \ \forall x$ remains. The partition sum for open boundary conditions then reads

$$Z_{\theta,\beta,L}^{(open)} = e^{-\frac{1}{2}\frac{(L-1)^2}{\beta}(\frac{\theta}{2\pi})^2} . \tag{25}$$

Note that here the single plaquette weight is raised to a different power $(L-1)^2$, which is the number of plaquettes on a $L \times L$ lattice with open boundary conditions.

We stress at this point that the exact results which in this section were obtained for the Villain action can also be obtained from the Wilson action when the continuum limit is considered (see, e.g., [33–35]). Consequently also the relations between results for periodic and for open boundary conditions that we discuss in the next section hold for Wilson fermions in the continuum limit, and actually for the numerical tests in Section 4 we use the Wilson formulation and compare to the respective analytical results [33–35].

3.3. Comparing physics for periodic and open boundary conditions

One expects that in the large volume limit physics becomes independent of the boundary conditions. Thus we now discuss in more detail the relation between the partition sums as well as observables for periodic and open boundary conditions. Obviously (see (24), (25))

$$Z_{\theta,\beta,L}^{(per)} = Z_{\theta,\beta,L+1}^{(open)} \, Q_{\theta,\beta,L} \qquad \text{with} \qquad Q_{\theta,\beta,L} = \sum_{p\in\mathbb{Z}} e^{-\frac{1}{2}\frac{L^2}{\beta}(p^2+2p\frac{\theta}{2\pi})} . \tag{26}$$

The factor $Q_{\theta,\beta,L}$ that relates the partition sums with periodic and open boundary conditions can be rewritten as

$$Q_{\theta,\beta,L} = 1 + 2\sum_{p=1}^{\infty} e^{-\frac{R}{2}p^2} \cosh\left(2p\frac{R}{2}\frac{\theta}{2\pi}\right)$$

$$= \theta_3\left(e^{-\frac{R}{2}}, i\frac{R}{2}\frac{\theta}{2\pi}\right) = 1 + O(e^{-R/2}) . \tag{27}$$
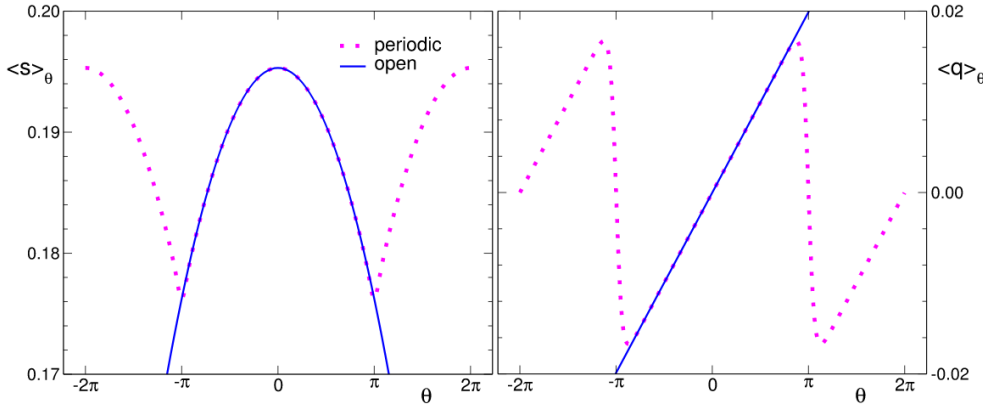
Fig. 2. Exact results for $\langle s \rangle_\theta$ (lhs. plot) and $\langle q \rangle_\theta$ (rhs.) as a function of θ. We compare the results for periodic (dashed curves) to those from open (full curves) boundary conditions. The parameters are $L = 16$ and $\beta = 2.56$, giving rise to $R = 100$.

In the second step we have used the definition of the theta function θ_3 [36]. $Q_{\theta,\beta,L}$ can be expanded around 1, where the factor R in the exponent of the correction is given by

$$R = \frac{L^2}{\beta} = V e^2 .\tag{28}$$

The continuum limit towards a continuum system with physical volume V and charge e is reached by sending $L \to \infty$ and $\beta \to \infty$ at a fixed ratio $R = L^2/\beta$, which in 2-d is dimensionless and is given by the continuum expression $V e^2$. Thus we find that the factor $Q_{\theta,\beta,L}$ that relates the partition sums with periodic and open boundary conditions has the expansion $Q_{\theta,\beta,L} = 1 + O(\exp(-\frac{1}{2} V e^2))$. This implies that the free energy densities $f = -\ln Z/L^2$ for the two boundary conditions are related by

$$f^{(per)}_{\theta,\beta,L} = f^{(open)}_{\theta,\beta,L+1} + O\left(e^{-\frac{1}{2}Ve^2}/L^2\right) .\tag{29}$$

As expected, the discrepancy between the free energies for periodic and open boundary conditions is a finite size effect that decreases exponentially with the physical volume. An additional factor $1/L^2$ suppresses the correction with the lattice size L^2 that goes to infinity in the combined limit $L \to \infty$, $\beta \to \infty$ at a fixed ratio $R = L^2/\beta$.

Thus one expects that also bulk observables, which are given by derivatives of the free energy density with respect to the couplings, differ only by finite volume effects. To illustrate this property we here consider the expectation values of the action density and of the topological charge density, which are defined as

$$\langle s \rangle_\theta = -\frac{1}{L^2} \frac{\partial}{\partial \beta} \ln Z_{\theta,\beta,L} \quad , \quad \langle q \rangle_\theta = -\frac{1}{L^2} \frac{\partial}{\partial \theta} \ln Z_{\theta,\beta,L} .\tag{30}$$

It is straightforward to obtain these observables for periodic and open boundary conditions by computing the respective derivatives of the partition sums (24) and (25) and evaluating the resulting expressions numerically.

In Fig. 2 we show the results for $\langle s \rangle_\theta$ (lhs. plot) and $\langle q \rangle_\theta$ (rhs.) as a function of θ for $L = 16$ and $\beta = 2.56$ (i.e., $R = 100$). The results for periodic boundary conditions are shown with

dashed curves, those for open boundary conditions with full curves. The observables for periodic boundary conditions show the expected 2π-periodicity, while for open boundary conditions periodicity is absent (as it should be). However, we find that the open boundary condition results very accurately reproduce those in the fundamental interval $\theta \in [-\pi, \pi]$ with slight deviations visible only near the boundaries of the interval, i.e., for $\theta \sim \pm\pi$. Thus in our 2-d theory we nicely confirm with an analytic calculation the expectation that the physics of the θ-term can be reliably determined from a calculation with open boundary conditions.

3.4. Exact evaluation of the DoS

Having discussed the exact solution of 2-d U(1) lattice gauge theory with a θ-term and how periodic and open boundary conditions give rise to the same physics up to boundary terms, we now address the densities for the two types of boundary conditions. Also they can be computed in closed form and we will see that for periodic boundary conditions we obtain a sum of Dirac deltas, while for open boundary conditions a smooth density is found. Again we focus on the densities with trivial insertion $\mathcal{J} = \mathbb{1}$, i.e., the densities that determine the partition sum and moments of the topological charge Q.

The partition sum for periodic boundary conditions (24) obviously is 2π-periodic in θ such that the density of states is given by (12), i.e., it is a sum of Dirac deltas with the coefficients Z_n given by (11). Inserting the partition sum (24) into (11) we obtain for these coefficients

$$Z_n = \frac{1}{2\pi} \int\limits_{-\pi}^{\pi} d\theta \, Z_{\theta,\beta,L}^{(per)} \, e^{i\theta n} = \frac{1}{2\pi} \int\limits_{-\pi}^{\pi} d\theta \sum_{p\in\mathbb{Z}} e^{-\frac{1}{2}\frac{L^2}{\beta}\left(p+\frac{\theta}{2\pi}\right)^2} e^{i\theta n} \tag{31}$$

$$= \frac{1}{2\pi} \sum_{p\in\mathbb{Z}} \int\limits_{-\pi}^{\pi} d\theta \, e^{-\frac{L^2}{8\pi^2\beta}(2\pi p+\theta)^2 + i(2\pi p+\theta)n} = \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} d\xi \, e^{-\frac{L^2}{8\pi^2\beta}\xi^2 + i\xi n} = C \, e^{-\frac{2\pi^2\beta}{L^2} n^2},$$

where we performed a change of variables $\xi = 2\pi p + \theta$, and in the last step we collected the factor of the gaussian integral and the factor $1/2\pi$ in the irrelevant constant C. The proper value of C can be determined in the end by implementing a suitable normalization of the density. Inserting the coefficients Z_n in (12) we obtain the result for the density with periodic boundary conditions,

$$\rho_{\beta,L}^{(per)}(x) = C \sum_{n\in\mathbb{Z}} e^{-\frac{2\pi^2}{R} n^2} \, \delta(x-n) \,, \tag{32}$$

where we used (28) to replace the ratio L^2/β by the combination $R = V e^2$.

For open boundary conditions the corresponding partition sum (25) is not 2π-periodic, such that the density is given by (14). We find (again we consider lattice extent $L+1$ for simpler comparison with the periodic case)

$$\rho_{\beta,L+1}^{(open)}(x) = \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} d\theta \, Z_{\theta,\beta,L+1}^{(open)} \, e^{i\theta x} = \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} d\theta \, e^{-\frac{L^2}{8\pi^2\beta}\theta^2 + i\theta x} = C \, e^{-\frac{2\pi^2}{R} x^2}. \tag{33}$$

Comparing the density for periodic boundary conditions (32) with its counterpart for open boundary conditions (33), we find that both densities are described by the same gaussian that has a width given by $\sqrt{R}/2\pi = \sqrt{V}e/2\pi$. However, for periodic boundary conditions the density has

support only on the integers, while for open boundary conditions a continuous Gaussian distribution is found. The fact that the width is the same for both densities underlines again the fact that the same physics can be retrieved with both choices for the boundary conditions.

4. An exploratory numerical test with the FFA approach

As announced we conclude the paper with an exploratory numerical test of a calculation of the density with the FFA approach [19–21]. This merely serves to illustrate that for open boundary conditions the density can indeed be reliably determined with FFA. For this test we again focus on the density for $\mathcal{J} = \mathbb{1}$.

4.1. Setting of the calculation

For the numerical studies presented here we use the standard Wilson formulation of U(1) lattice gauge theory with a θ-term, i.e., action and topological charge are given by

$$S[U] + i\theta \, Q[U] = -\beta \sum_x \mathrm{Re}\, U_{x,12} + i \frac{\theta}{2\pi} \sum_x \mathrm{Im}\, U_{x,12} \,, \tag{34}$$

where by $U_{x,12} \equiv U_{x,1} U_{x+\hat{1},2} U^*_{x+\hat{2},1} U^*_{x,2}$ we denote the plaquettes built from the link variables $U_{x,\mu} \in$ U(1). Also for the Wilson action the system can be solved in closed form (see, e.g., [33–35]) following the strategy in Section 3.2. For an $L \times L$ lattice with open boundary conditions one obtains for the partition sum

$$Z^{(open)}_{\theta,\beta,L} = I_0 \left(\sqrt{ \beta^2 - \left(\frac{\theta}{2\pi} \right)^2 } \right)^{(L-1)^2} \,, \tag{35}$$

where I_0 denotes a modified Bessel function. Using this expression in (14) gives rise to the analytic result for the density (up to an overall normalization) which we use for comparison with our numerical FFA determination. The corresponding integral (14) has been solved numerically with Mathematica.

For the numerical determination of the density we apply the FFA approach [19–21] following the strategy outlined in Section 3.2. We divide the range of x where we want to evaluate the density into intervals I_n of size Δ_n and subsequently evaluate the restricted expectation values $\langle Q \rangle_n^{(\mathcal{J})}(\lambda)$ of Eq. (7) for several values of λ. After normalization to the form (8) we fit the data with $h(\Delta_n[\lambda - k_n])$ to determine the slopes k_n from which we compute the density using (6).

We consider different lattice sizes, 4×4, 8×8, 12×12, 16×16 and 24×24 and work at a ratio of $R = L^2/\beta = 10$ which gives rise to $\beta = 1.6, 6.4, 14.4, 25.6$ and $\beta = 57.6$. We simulate the system using sweeps of local Metropolis updates which for the simple 2-d system is sufficiently efficient, in particular since we work with open boundary conditions where autocorrelation from topological freezing is absent. We typically use statistics of 5×10^5 measurements for each set of couplings separated by 10 sweeps for decorrelation after an initial equilibration phase of 2.5×10^4 sweeps. The errors we show are statistical errors determined with Jackknife combined with a blocking analysis.
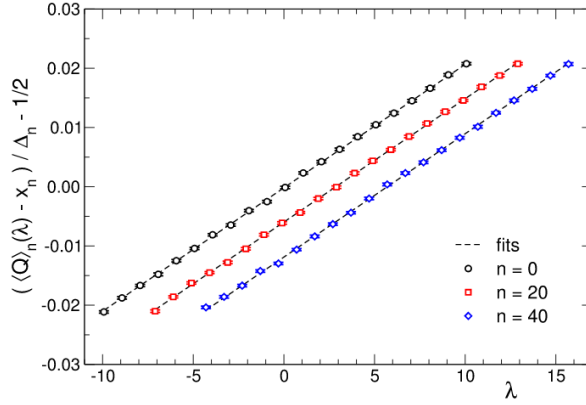
Fig. 3. Results for the restricted expectation values $\langle Q \rangle_n^{(\mathcal{J})}(\lambda)$ as a function of λ. We use the normalized form (8) and fit the Monte Carlo data (symbols) with the functions $h(\Delta_n[\lambda - k_n])$ (dashed lines). We show results for three different intervals with $n = 0$, $n = 20$ and $n = 40$ using $\Delta_n = 0.025$. The parameters are parameters $L = 8$ and $\beta = 6.4$.
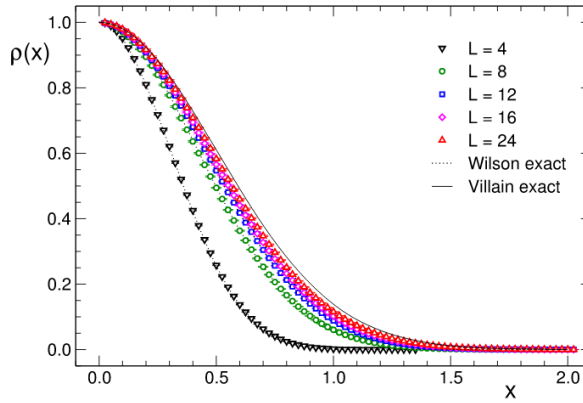

Fig. 4. Results for the density $\rho^{(open)}(x)$ as a function of x. We show the numerical results from the FFA determination (symbols) for different lattice sizes $L \times L$ at fixed $R = L^2/\beta = 10$ for $\Delta_n = 0.025$ and compare them to the corresponding exact results for the Wilson action (dotted curves). For illustration we also show the exact result for the Villain action (full curve), which constitutes the infinite volume limit at fixed R (here $R = 10$).

4.2. Numerical results

We begin the presentation of our results with showing data for the restricted expectation values $\langle Q \rangle_n^{(\mathcal{J})}(\lambda)$ in the normalization (8). In Fig. 3 we show the results for a 8×8 lattice at $\beta = 6.4$ for three different intervals, I_0, I_{20}, I_{40} using a constant size $\Delta_n = 0.025$ for all intervals. The data for different values are plotted with symbols and the curves represent the fits with $h(\Delta_n[\lambda - k_n])$ according to (8) and obviously the data are well described by the fits.

After determining the slopes k_n from the fits the density was evaluated using (6). In Fig. 4 the results for the density $\rho^{(open)}(x)$ for our different lattice sizes between 4×4, and 24×24 at $R = 10$ are shown as a function of x (symbols). For comparison we also show the corresponding analytic results for Wilson action (dashed curves) obtained from the integrals (14) with the exact
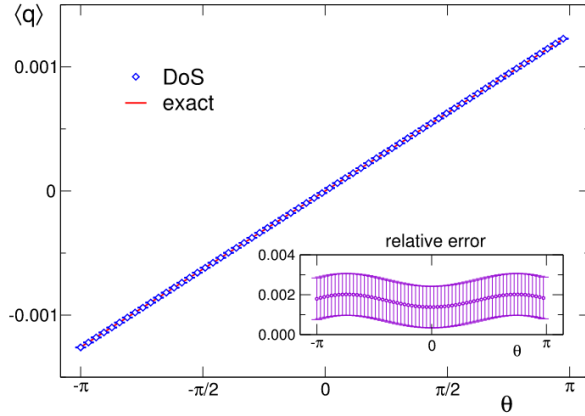
Fig. 5. Results for the topological charge density $\langle q \rangle$ as a function of the topological angle λ. We show the DoS data for our $L = 24$ lattices at $R = 10$ (symbols) and compare them to the exact results (red line). In the insert we show the corresponding relative error from the comparison of the DoS data with the exact results. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

partition sum (35). We find that the FFA determination agrees very well with the analytic results. In addition we display the exact result for the Villain action at $R = 10$ (full curve) which can be shown to be the limiting form for the sequence of Wilson results.

Finally, in Fig. 5 we show our $L = 24$ results for the topological charge density $\langle q \rangle$ as a function of θ. The expectation value $\langle q \rangle$ can be computed by replacing $\rho^{(\mathcal{O})}(x)$ by $x\,\rho^{(1)}(x)$ in the rhs. of Eq. (4), such that no additional density has to be evaluated. The integrals in (4) were computed numerically after fitting the density determined from DoS with the exponential of an even polynomial, where already a second order polynomial turned out to be the optimal choice here. Fig. 5 illustrates that the DoS data (symbols) very nicely match the exact result (red curve), and the corresponding relative error in the insert shows that with the numerical effort used here we obtain an accuracy in the 2 per mill range. We conclude from our exploratory numerical test that our strategy for treating the θ term with DoS techniques qualifies as an interesting new approach, ready for tests in 4-d.

5. Summary and outlook

In this paper we have explored the use of new DoS techniques for studying lattice field theories with a θ-term, a class of systems where a complex action problem spoils direct lattice simulations. The key observation is that using open boundary conditions gives rise to a much better behaved density of states, such that it can be reliably determined with recently developed modern DoS methods. We have set up the framework for applying these DoS techniques and argued that indeed the density remains sufficiently smooth for open boundary conditions also in the continuum limit.

To better study different aspects of our proposal we analyzed 2-d U(1) lattice gauge theory with a θ-term, a theory that can be solved in closed form with the help of dual variables, both for periodic, as well as for open boundary conditions. We established that the free energies for periodic and for open boundary conditions approach each other in the large volume limit. Observables for periodic boundary conditions are 2π-periodic in θ, while for open boundary conditions

no periodicity emerges. However, the results from open boundary conditions reproduce those from periodic boundary conditions very well in the fundamental interval $\theta \in [-\pi, \pi]$ with slight deviations visible only near the boundaries $\theta \sim \pm\pi$. We finally computed the densities in closed form, finding them to be sums of Dirac deltas for periodic boundary conditions, while they remain smooth for open boundary conditions.

Our exploratory study in 2-d U(1) gauge theory with a θ-term thus confirmed that the same physics emerges for different boundary conditions, and that for periodic boundary conditions the density of states is indeed accessible with modern DoS techniques. This latter statement was also confirmed in a small Monte Carlo simulation of 2-d U(1) gauge theory with a θ-term where the density for open boundary conditions was computed with the FFA DoS method and shown to agree very well with the analytic results.

Thus the successful proof of principle study in the 2-d U(1) gauge theory with a θ-term sets the stage for more ambitious applications of the new approach. Several interesting systems come to mind: From 2-d models such as O(N) and CP(N-1) theories with θ-terms, 4-d SU(N) gauge theories with topological terms, all the way to full QCD with a vacuum angle, and we have started to prepare studies of these more challenging lattice field theories with θ-terms. On a more speculative side one might even consider treating axion models with the DoS techniques we propose here, which, however, clearly is an option that has to wait until more experience has been obtained with simpler systems.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

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