Order parameters and boundary effects in U(1) lattice gauge theory

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Abstract

We show that, independently of the boundary conditions, the two phases of the 4-dimensional compact U(1) lattice gauge theory can be characterized by the presence or absence of an “infinite” current network, with an appropriate definition of “infinite” for the various types of boundary conditions imposed on the finite lattice. The probability for the occurrence of an “infinite” network takes values 0 or 1 in the cold and hot phase, respectively. It thus constitutes a very efficient order parameter, which allows one to determine the transition region at low computational cost. In addition, for open and fixed boundary conditions we address the question of the impact of inhomogeneities and give examples of the reappearance of an energy gap already at moderate lattice sizes.
1. Introduction

Recently, using periodic boundary conditions, we have shown [1] that the phases of the 4-dimensional compact U(1) lattice gauge theory are unambiguously characterized by the topological properties of monopole current lines as well as by those of minimal Dirac sheets. Our topological analysis, based on mappings preserving homotopy, relied heavily on the chosen type of boundary conditions. Nevertheless we conjectured that the phases are more generally characterized by the presence or absence of an infinite structure, where a suitable definition, dependent on the boundary conditions, must be given for the meaning of “infinite” in presence of a finite lattice.

A major motivation for this work has been the verification of this conjecture. For this purpose we have studied systems with periodic, open and fixed boundary conditions. For periodic boundary conditions our results establish that the topological criterion is a much better estimator of the phases than the extension of the largest monopole network, which has also been proposed as an order parameter. For open and fixed boundary conditions we give an appropriate definition of “infinite” network and demonstrate that the phases are again determined by the presence or absence of an infinite network.

A second motivation for the present work is related to the fact that the widely accepted first order nature of the phase transition has recently been put into question. Indeed the authors of Ref. [2], modeling the U(1) system on the surface of a 5-dimensional cube rather than on the usual 4-dimensional torus, found no evidence of an energy gap and suggested that on a manifold with trivial homotopy group the energy gap disappears. This has initiated other investigations where fixed boundary conditions [3], suppression of monopoles at the boundaries [4] and open boundary conditions [5] have been used to study the effects of the boundary conditions.

In order to draw conclusions on such issues it is crucial to gain a proper understanding of the effects of the inhomogeneity in the Euclidean space distribution determined by the choice of non-periodic boundary conditions. Therefore, for the
cases of open and fixed boundary conditions we address this question as well. By suitable examples we show that the gap reappears already on lattices of moderate sizes so that its disappearance for certain types of boundary conditions is not absolute.

It has been known for some time \([5, 6]\) that for fixed and open boundary conditions the Wilson loop averages provide upper and lower bounds, respectively, on those obtained with periodic boundary conditions. Here we consider the effects of the inhomogeneities on the energy distribution: we will show that if one measures the energy distribution within shells at fixed distance from the boundary, large shifts of the peaks occur when one moves from shell to shell.

2. Order parameters

In this section we show that for periodic, open and fixed boundary conditions the presence or absence of an infinite network of monopole currents can indeed be taken as a criterion to distinguish between the phases, validating our generalized conjecture. We will give, of course, the appropriate definitions of “infinite” for the three types of boundary conditions. It will be seen that this criterion provides an order parameter which has the virtue of taking the values 1 and 0 in the hot and cold phases, respectively, and is thus superior to the one \([7]\) based on the relative size of the largest network \(n_{\text{max}}/n_{\text{tot}}\). Our order parameter allows one to determine the transition region at very low computational cost because the analysis of a single equilibrated configuration is already sufficient. One should keep in mind that the characterization of phases discussed here and the question of the order of the transition are distinct issues.

For periodic boundary conditions, which give the lattice the connectivity of a torus \(T^4\), we define “infinite” by “topologically nontrivial in all directions”. While for individual loops the topological characterization is straightforward, for the dense networks of monopole currents which occur in reality it requires the more sophisticated analysis which we developed and described in Refs. \([8, 9]\). Figure 1 gives our
results for $P_{\text{net}}$, i.e. the probability for the occurrence of a network which is nontrivial in all directions, as a function of $\beta$. It is obvious that this is an order parameter which takes values exactly equal to 0 and 1 for the cold and hot phase, respectively, and provides a better distinction between the phases than the ratio of the size of the largest monopole network to the total number of monopoles, $n_{\text{max}}/n_{\text{tot}}$.

In view of various suggestions which have been formulated in the past, we observe that a criterion based simply on the extension of the largest network, rather than on the topological characterization we mentioned above, is not adequate for periodic boundary conditions. The meaning of “infinite” in this case would be that for each direction the one-dimensional projection of the network covers the full extension of the lattice. In a test performed at the phase transition point on a $16^4$ lattice, where the peaks of the energy distribution are well separated, in the cold phase we have obtained the value 0.069(16) for this order parameter (i.e. the probability that the projection of the current network over all four axes spans the whole lattice extent), as opposed to 0.000 for $P_{\text{net}}$ considered above. Thus it is indeed neither extension nor size but rather the topology inherent in our criterion which is relevant in the case of periodic boundary conditions.

For open boundary conditions the lattice is no longer self-dual. On the dual lattice the current lines, i.e. the lines formed by the links carrying nonzero current, may end at the boundaries. In this case we define “infinite” as “touching the boundaries in all directions”. Figure 1 shows that the probability $P_{\text{net}}$ of getting the “infinite” network thus defined provides again an order parameter which takes values 0 and 1 in the cold and hot phase, respectively, and compares favorably with $n_{\text{max}}/n_{\text{tot}}$.

Fixed boundary conditions are obtained by setting all gauge variables $U$ to 1 at the boundary. The surface of the lattice is then made of 3-dimensional cubes with all their link variables equal to 1. On the dual lattice these cubes correspond to links with vanishing monopole current. Therefore, the subset on the dual lattice accessible to current lines is a lattice with open boundary conditions (while the original lattice with fixed boundary conditions is homeomorphic to the sphere $S^4$). Now we define “infinite” as “reaching the boundaries in all directions”. As can
be seen from Figure 1 the corresponding probability $P_{\text{net}}$ takes again values 0 and 1 in the two phases, and provides a much sharper distinction between them than $n_{\text{max}}/n_{\text{tot}}$.

We have checked for all the boundary conditions considered that our characterization of the phases by current networks not only works with Wilson’s action but also with the extension obtained by adding a monopole term with positive or negative coupling, i.e. with the action \[ S = \beta \sum_{\mu > \nu, x} (1 - \cos \Theta_{\mu \nu, x}) + \lambda \sum_{\rho, x} |M_{\rho, x}|, \tag{2.1} \]
where $M_{\rho, x} = \epsilon_{\rho \sigma \mu \nu} (\bar{\Theta}_{\mu \nu, x + \sigma} - \bar{\Theta}_{\mu \nu, x})/4\pi$ and the physical flux $\bar{\Theta}_{\mu \nu, x} \in [-\pi, \pi)$ is given by $\Theta_{\mu \nu, x} = \bar{\Theta}_{\mu \nu, x} + 2\pi n_{\mu \nu, x}$ \[10\]. We have verified that our criterion gives good results irrespective of lattice size (within the range of sizes available to us): in particular, it works with a $16^4$ lattice as well as with an $8^4$ lattice.

Comparing the results for different boundary conditions presented in Figure 1 it is apparent that for open and fixed boundary conditions the transition region is much larger than for periodic boundary conditions. The observed enlargement of the transition region reflects the considerably larger finite-size effects present for open and fixed boundary conditions.

In Ref. \[1\] we have shown that for periodic boundary conditions, instead of considering current networks, the phases can be characterized equally well by the topological properties of minimal Dirac sheets (obtained by minimizing the the number of Dirac plaquettes by a simulated-annealing gauge-fixing procedure). We found there that this holds true not only for the Wilson action but also if we add to it a monopole term with positive or negative coupling.

In this study we have performed a Dirac-sheet analysis for fixed boundary conditions, too. For the Wilson action it turned out that the characterization by minimal Dirac sheets works again, though with a transition region somewhat more extended than the one obtained with the network criterion. With a monopole term, however, and for very large negative couplings (e.g. $\lambda = -2.0$), corresponding to large monopole density, infinite Dirac sheets no longer form. Thus the criterion based
current networks remains the only available criterion for the characterization of the phases.

3. Energy distributions

In our simulations we have determined the plaquette energy distributions $P(E)$ (where $E = (1/6L^4) \sum_{\mu>\nu,x}(1 - \cos \Theta_{\mu\nu,x})$) as well as the monopole density distributions. In the following we illustrate only our results for $P(E)$ because the corresponding results for the monopole density are very similar. We present data taken at the phase transition, i.e. at the value $\beta = \beta_c$ where the specific heat is at a maximum, or very close to it. We reproduce in Table 1 the values which we have obtained for $\beta_c$ in correspondence to the various lattice sizes and boundary conditions which we have used.

Figure 2 shows $P(E)$ obtained on a $16^4$ lattice. For periodic boundary conditions the distribution exhibits a gap with well separated peaks, while for open and fixed boundary conditions there is no gap. The shifts of the averages are in agreement with the bounds given in Ref. [5] (in the comparison of the two sets of results one should remember that plaquette energy and Wilson loop factors are defined with opposite signs).

It should be mentioned here that although on a $16^4$ lattice with periodic boundary conditions the two peaks of the energy distribution are separated by a substantial gap, the algorithm we introduced in Ref. [11] makes it still possible to perform simulations that span both peaks.

With periodic boundary conditions no energy gap, indicative of a first order transition, is seen on a $4^4$ lattice, which is clearly a consequence of finite-size effects. One begins to observe a gap on an $8^4$ lattice, with some overlap between the peaks, while the gap becomes quite pronounced on a $16^4$ lattice, with large separation between the peaks. With the generalized action (2.1), for negative $\lambda$, where the phase transition gets stronger, a gap occurs also on the $4^4$ lattice (it is visible for $\lambda = -1.0$ and the peaks are well separated for $\lambda = -2.0$).
With open and fixed boundary conditions, there is no sign of a gap even with a $16^4$ lattice, as is apparent from Figure 2. The widths of the peaks nevertheless remain relatively small which suggests that a more complicated mechanism than simple smearing is at work. The numerical investigation of larger lattices is extremely demanding from the computational point of view. Thus the study of lattices large enough that the effects of the finite size and of the inhomogeneity are no longer important appears hardly feasible.

We have nevertheless been able to derive some information on whether the disappearance of the gap is absolute or depends on the size and/or other parameters of the system. In the following we demonstrate in two separate cases that even with a system made inhomogeneous by the choice of boundary conditions the gap can, in fact, be made to reappear.

In the first example we use fixed boundary conditions and the action (2.1). From Figure 3 we see that with an $8^4$ lattice for sufficiently large monopole density, i.e. negative $\lambda$, a gap emerges again. With open boundary conditions one finds very similar results. This shows that the effects of the inhomogeneity can be overcome by making the transition stronger (which is quite analogous to the way in which finite-size effects are overcome on the $4^4$ lattice with periodic boundary conditions in the example mentioned above).

In the second example we use mixed boundary conditions, i.e. fixed boundary conditions only in direction 0 and periodic boundary conditions in the other three directions. With these boundary conditions we observed that there is no gap on a $8^4$ lattice. In Figure 4 we show what happens if one considers a lattice of size $L_0 \times 8^3$. While for $L_0 = 8$, as mentioned above, there is no gap, for $L_0 = 16$ a gap is seen to occur again. Thus this simplified system demonstrates that the gap in the energy distribution reappears even with non-periodic boundary conditions when the system’s size becomes sufficiently large.

In order to study the effects of inhomogeneities in detail we considered shells (3-dimensional subsets) within the lattice and measured the plaquette energy distribution on each of the shells separately. We number the shells by $s = 1, \ldots, L/2,$
where $L$ is the lattice extension and $s = 1$ corresponds to the outmost shell. A shell consists of all lattice points where one of the coordinate is equal to $s - 1$ or to $L - s$.

Figure 5 shows the results obtained for each of the shells, separately, in the same simulations as illustrated in Figure 2. It is manifest that for open and fixed boundary conditions the distributions change dramatically from shell to shell. We should note here that the $P(E)$ in Figure 5 are normalized to the same constant for each individual shell. Because of their larger weights, the outer shells are dominant in the sum over the whole lattice.

In view of the large shifts apparent in Figure 5 one can hardly consider results about the presence or absence of a gap to be reliable with these types of boundary conditions unless one goes to much larger lattices where the impact of boundaries decreases.

The directions of the shifts for open and fixed boundary conditions in Figure 5 are in accordance with the lattice getting hotter and colder, respectively, for outer shells. The case of fixed boundary conditions may be described in terms of a picture [6] whereby, outside of the lattice volume, all the dynamical degrees of freedom are frozen. Similarly for open boundary conditions the finite lattice can be considered as embedded into a “hot environment”. It is conceivable that this strong “outside coupling” is what prevents the occurrence of a gap without affecting the widths of the peaks.

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Table 1

Phase transition points $\beta_c$

| boundaries | lattice | $\beta_c$   |
|------------|---------|-------------|
| open       | $8^4$   | 1.04(2)     |
|            | $16^4$  | 1.023(3)    |
| fixed      | $8^4$   | 0.91(3)     |
|            | $16^4$  | 0.981(3)    |
| periodic   | $8^4$   | 1.0075(1)   |
|            | $16^4$  | 1.01084(5)  |
| mixed      | $8 \times 8^3$ | 0.9901(3) |
|            | $16 \times 8^3$ | 1.0051(3) |
Figure captions

Fig. 1. Order parameters $P_{net}$ and $n_{max}/n_{tot}$ as functions of $\beta$ on $8^4$ lattices with periodic, open and fixed boundary conditions.

Fig. 2. Probability distributions $P(E)$ on $16^4$ lattices with periodic, open and fixed boundary conditions at $\beta = \beta_c$.

Fig. 3. Probability distributions $P(E)$ on the $8^4$ lattice with fixed boundary conditions and $\lambda = -1.5$, -1.8, -2.0 at $\beta = 1.84$, 2.046, 2.22, respectively.

Fig. 4. Probability distributions $P(E)$ on $8 \times 8^3$ and $16 \times 8^3$ lattices with mixed boundary conditions at $\beta = \beta_c$.

Fig. 5. Probability distributions $P(E)$ for shells on $16^4$ lattices with periodic, fixed and open boundary conditions at $\beta = \beta_c$. 
Figure 3:

\[ \lambda = -1.5 \]

\[ \lambda = -1.8 \]

\[ \lambda = -2.0 \]

Figure 4:

\[ 8^3 \]

\[ 16^3 \]
Figure 5: