Fixed boundary conditions and phase transitions in pure gauge compact QED

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Abstract

We have simulated the pure gauge compact QED with fixed boundary conditions, on lattices from $6^4$ to $16^4$. We argue that a lattice with this fixed boundary imposition corresponds actually to a lattice with spherical topology. We have found the presence of a phase transition without any trace of discontinuity. Moreover, the specific heat and the Binder cumulant are qualitatively consistent with a second order phase transition. The implications of this observation on the nature of the compact lattice QED are discussed.
Numerical simulations of lattice gauge theories are actually performed in a finite space-time box. The computer limitations imply severe restrictions on the lattice size of this box. For example, the largest lattices used today to simulate lattice QED are of the order of $22^4$. To avoid the border “effects” generated by such a box, periodic boundary conditions are usually adopted. From a geometrical point of view, this fact implies that the system is actually simulated on an hypertorus. In most cases this geometrical effect is not relevant, but in some other cases the association of a finite-box with periodic boundary conditions may originate unphysical effects.

Pure gauge lattice QED constitutes one of these special cases. The initial measures\cite{1} in small lattices suggested the presence of a second order phase transition but this transition became a first order one when the simulations were performed on larger lattices\cite{2}\cite{3}. In order to explain this fact one has to look at the confining mechanism in lattice QED.

Some time ago Poliakov\cite{4} and Banks, Myerson and Kogut\cite{5} showed that in the lattice (compact) QED monopole excitations appear naturally. Furthermore, the monopoles play a central role in the explanation of the phase-structure. In fact, they produce the “disorder” and give raise to the confinement. In $D = 3$ monopoles are 0-dimensional pointlike excitations whilst in $D = 4$ they become 1-dimensional, and, due to the magnetic flux conservation, they form closed loops. The density of monopole loops in four dimensions was measured as a function of the coupling $\beta$ and they observed a fall-off of the density over the phase transition.

A possible explanation for the discontinuity in the internal energy relies on the fact that a lattice with periodic boundary conditions is a hypertorus, so topologically nontrivial loops which wrap around the lattice are permitted. This wrapped loops are present only in the the confining side \cite{3}\cite{4} and clearly they have a fairly large action associated with them. So a jump is observed when they disappear at deconfining transition. This jump no longer survives in the infinite volume limit. In other words, the first order behaviour seems to be a spurious topological effect occurring in finite lattices with periodic boundary conditions \cite{3}\cite{5}.\[\]

This idea is supported by the recent simulations of the Wilson action on “closed topology” lattices by Lang and Neuhaus \cite{9}. These simulations, being performed on the four-dimensional boundary of a five-dimensional hy-
percure, found no metastability signal at the phase transition point. They suggest that, contrarily to the studies of compact QED on hypercubic lattices with periodic boundary conditions, the phase transition of pure gauge QED becomes of second order when simulated on lattices with the topology of a sphere. However, as pointed out recently in [10], these simulations still have some technical difficulties that can spoil the asymptotic scaling regime.

This letter is intended to contribute to the clarification of the real nature of the U(1) (compact) phase transition studying a different implementation of the spherical topology.

**Fixed boundary conditions**

Our starting point is the old observation [11] that in any local gauge theory the Wilson loop average in an infinite lattice can be bounded from above and below by the corresponding expectation value in a finite lattice with appropriate boundary conditions. In fact, the lower bound is reached with free boundary conditions and the upper bound can be obtained with fixed boundary values (i.e. all the gauge factors U(l) = 1 for l belonging to the boundary). This two bounds coincide outside the transition region and if one imposes the standard periodic boundary conditions the average of the Wilson loop interpolates between the two bounds exhibiting a kind of jump.

Looking carefully at the figures of [11] (obtained actually from rather small lattices), the behaviour of the fixed boundary run of the pure gauge compact QED shows a clear change of slope near the phase transition point. This curve seems to represent more a true transition than to be a simple bound of the internal energy. The main point is that a simulation performed with a system with fixed boundary conditions may corresponds actually to a system simulated on a lattice with spherical topology.

A simple geometrical argument may clarify this point. Fig 1 shows a two dimensional square lattice $L \times L$. Imagine that all links over the boundary are put and fixed to unity (dashed and dotted lines of Fig 1). All plaquettes containing one of these links will have a contribution to the action as a product of only three independent elements of U(1), representing a loop as a triangle, instead of an elementary square. This can be imagined, from a 3-d world point of view, as collapsing to a single point all the square lines of the border, i.e. obtaining a sphere instead of a torus.
Numerical simulations

To check this scenario we have performed a numerical simulation of the compact pure gauge U(1) theory on a lattice with fixed boundary conditions, studying the behaviour of the thermodynamical quantities (internal energy, specific heat, and Binder cumulant). To understand how we implemented these boundary conditions, let us to consider again the two dimensional square lattice of Fig. 1. We denote the points and links by

\[ n(i, j), \quad i, j = 1, L, \]

and

\[ l_\mu(i, j), \quad \mu = 1, 2, \]

respectively.

To “close” the lattices one has to assign values for the “extra” links

\[ l_2(L + 1, j), \quad j = 1, L, \]

and

\[ l_1(i, L + 1), \quad i = 1, L, \]

i.e. the dotted links of Fig. 1. If one imposes periodic boundary conditions, this assignment is performed repeating the values of the links belonging to the border

\[ l_2(1, j), \quad j = 1, L, \]

and

\[ l_1(i, 1), \quad i = 1, L, \]

i.e. the dashed links of Fig. 1.

Our implementation of the fixed boundary conditions takes into account this fact. We fix all dashed links to unity. Periodic boundary conditions fix also all remaining border links (dotted) to unity obtaining, actually, a lattice with spherical topology. Finally, one has only to avoid the Monte Carlo updating of these links during the simulation.

Our simulation has been performed in four dimensions. The border of a square domain in 4-d is a set of eight 3-d cubes. All plaquettes contained in these cubes are put to unity. Note that some plaquettes will have all their links fixed to unity. Those plaquettes will remain unchanged along the
simulation. The effect of these plaquettes is merely to add a constant factor
to the lattice action and, hence, they have no physical meaning.

The number of free plaquettes (i.e. rejecting those duplicated by the
periodic boundary conditions) in a simulation is just

\[ N^t_p = 6L^4, \]

but the number of free plaquettes (without counting those that are fixed to
unity) is just

\[ N^f_p = 6L^4 - 12L^3 + 6L^2. \]

This number comes from the fact that one has to subtract the plaquettes
belonging to the eight cubes of the boundary, taking into account that some
faces of these cubes are shared by them. The knowledge of this factor is
necessary to normalize the average internal energy density taking into ac-
count only the non-fixed plaquettes, but including all plaquettes with some
link variables (i.e. the "triangles" of the 2-d example). This differs from the
usual way of considering only the innermost four dimensional cubes of the
lattice[11].

Note that with these fixed boundary conditions just one point of the
lattice has a special connectivity with his neighbours. The consistence of our
results seems to point out that the effect of this point is not fundamental in
the phase structure of the theory.

Results

Since we have only changed the implementation of the boundary condi-
tions, our lattice action is the usual compact U(1) action

\[ S = \beta \sum_p (1 - \cos \theta_p), \]  

(1)

where \( \theta_p \) stands for the circulation of the gauge field around a plaquette
and \( \beta = 1/e^2 \) is the gauge coupling. We have measured the internal energy
density

\[ < E > = \frac{1}{N^f_p} \sum_p (1 - \cos \theta_p), \]  

(2)

the specific heat, through the energy fluctuations,

\[ C = N^f_p (< E^2 > - < E >^2), \]  

(3)

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and, finally, the Binder cumulant

$$B = 1 - \frac{<E^4>}{3 <E^2>^2}.$$  

(4)

To perform the numerical simulations we have chosen a standard heat bath simulation algorithm adapting an existing and well tested program to the new boundary conditions.

A detailed finite size analysis of this model is out of the scope of this letter and it will require a considerable numerical effort. Indeed, to fix the links of the 3-d border to unity implies that a significant fraction of the links is not changed and, hence, we have to go to larger lattices. The numerical results presented here come from some thermal cycles performed for lattice sizes $6^4, 8^4, 10^4, 12^4, 14^4$ and $16^4$. The statistics has been of 10,000 iterations per each $\beta$ value.

In Fig.2 we show the internal energy for different lattice sizes. No sign of discontinuity is observed. Moreover, a cross-over point seems to appear as $L$ increases, just approaching $\beta = 1$. This may be compatible with the presence of a continuous phase transition.

In Fig.3 we plot the specific heat $C$. The emergence of a peak which grows with $L$ and moves towards $\beta = 1$ can be clearly observed. Also the growing of that peak seems slow enough to ensure the absence of a weak first order transition.

The Binder cumulant is plotted in Fig.4. It shows a clear convergence to the expected value of $2/3$ characteristic of a second order transition. Furthermore, one can see that the value of $\beta$ for the minimum of the Binder cumulant and that for the maximum of $c$, being different for small lattice sizes, they coincide for $L \geq 14$.

Conclusions

These results, although being basically qualitative, point out the continuous character of the U(1) phase transition when periodic boundary conditions and the spurious effects they bear with are avoided. The next step would be a more detailed study (with much bigger statistics) in order to extract the critical exponents and check if they verify the hyperscaling relations. This will require a great computational effort since it would be necessary to simulate much large lattices.
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Figure captions

1. Sketch of a two-dimensional square lattice. Dotted links are the replica of the dashed ones generated through periodic boundary conditions. When imposing the fixed boundary conditions all these links are fixed to unity giving an “effective” spherical topology.

2. Internal energy measurement on lattice sizes from $6^4$ to $16^4$ with fixed boundary conditions. Results come from a thermal cycle with 10,000 measuring iterations per point.

3. Specific heat measurement on lattice sizes from $6^4$ to $16^4$ with fixed boundary conditions.

4. Binder cumulant measurement on lattice sizes from $6^4$ to $16^4$ with fixed boundary conditions. Dashed line represents the value $2/3$. 
