

Review of Boundary Effect on Observables in Lattice Gauge Theory

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Abstract: In this review paper we are going to address an issue in the simulation of lattice gauge theory, is that the distribution of gauge configurations over different topological sectors. These different topological regions are characterized by topological charge (Q). The distribution of Q becomes more and more difficult as the continuum limit (lattice spacing goes to zero) is approached. As a consequence, autocorrelation times of physical quantities like Q grows rapidly making the calculation of expectation values time consuming and it may sometime does not produce the expected results of the simulation. Without periodic an open boundary condition on the gauge field in the temporal direction has been recently proposed to overcome the spanning or distribution problem of Q. In this review paper, the interesting observables to study are Q and the topological susceptibility and lowest glueball (scalar) mass using open and periodic boundary conditions.

Key words: Lattice QCD, Periodic Boundary, Open Boundary, Topological Susceptibility, Glueball mass.

I. INTRODUCTION

Lattice QCD is a well-known non-perturbative approach to solving the QCD theory of quarks and gluons. It is a lattice gauge theory formulated on a grid or lattice of points in space and time. When the size of the lattice is taken infinitely large (infinite volume) and its sites infinitesimally close to each other (lattice spacing tends to zero), the continuum QCD is recovered [1].

In the numerical simulation of lattice QCD, the distribution of gauge configurations over different topological sectors becomes more and more difficult as the continuum limit (lattice spacing tends to zero) is approached. As a consequence, autocorrelation times of physical quantities grow rapidly making the calculation of expectation values time consuming and it may sometime even invalidate the results of simulation.

Open boundary condition (OBC) on the gauge field in the temporal direction has been recently proposed to overcome this problem [2, 3, 4]. Lattice gauge theory with such boundary conditions has no barriers between different topological sectors. The observables to study are the topological charge and the topological susceptibility in pure Yang-Mills theory which is related to the eta-prime particle mass. Recently few high precision calculations of the observables are done with periodic boundary condition (PBC) as well as open boundary condition (OBC). In this paper, we address the question whether an open boundary condition in the temporal direction can able to span Q and can yield the expected value of the topological susceptibility and glue ball mass in SU(3) Yang-Mills theory.

II. BOUNDARY CONDITIONS

Conventional lattice QCD simulations use periodic boundary conditions in all directions (i.e. four-dimensional torus), for the obvious reason that they minimize boundary effects.

The gauge and quark fields live on four-dimensional space-time manifold with Euclidean metric, time extent T and spatial extent L. Open boundary conditions in time does not wrap around in this direction, i.e. there are no terms in the action which couple the field variables at time $x_0 = 0$ to those at the largest time $x_0 = T - a$, while space is taken to be a three-dimensional torus, i.e. all the fields are required to satisfy periodic boundary conditions in the space directions. In the continuum theory, they amount to imposing boundary conditions,

$$G_{0k}(x)|_{x_0=0} = G_{0k}(x)|_{x_0=T} = 0, \quad k = 1,2,3 \quad (1)$$

on the gauge field where $G_{\alpha\beta}$ is the field tensor of the fundamental gauge field.

However, when choosing open instead of periodic boundary conditions in the physical time direction, the boundary between the topological sectors disappears, the space of the fields becomes connected and thus one expects to observe only moderately increasing autocorrelation times if the slowdown of the algorithm is indeed mainly caused by the separation of the sectors.

III. OBSERVABLES

The field theoretical definition of the topological charge density is

$$q(x) = \frac{1}{32\pi^2} \epsilon_{\alpha\beta\sigma\rho} \text{tr} \{ G_{\alpha\beta}(x) G_{\sigma\rho}(x) \} \quad (2)$$

using some discretization of the field strength tensor G . Then, the topological charge is

$$Q = \int d^4x q(x) \quad (3)$$

where d^4x is the four space-time volume and the topological susceptibility is

$$\chi = \frac{\langle Q^2 \rangle}{V} \quad (4)$$

Here V represents the four space-time volume and angular bracket denotes the configuration average. There is another observable is Glue Ball mass which is calculated from energy density (operator) two point correlators.

IV. SIMULATION DETAILS

We have generated gauge configurations [5] (using unimproved Wilson gauge action) in $SU(3)$ lattice gauge theory at different lattice volumes and gauge couplings using the openQCD program. Gauge configurations using periodic boundary conditions also have been generated for several of the same lattice parameters (necessary changes to implement periodic boundary condition in temporal direction were made in the openQCD package for pure Yang-Mills case). Details of the simulation parameters are summarized in table 1. In this table, O and P correspond to open and periodic boundary configurations respectively.

Table1. O and P refer open and periodic boundary condition ensembles.

Lattice	Volume	N _{cnfg}	Lattice spacing a in (fm)
O ₁	24 ³ × 48	3970	0.067
O ₂	32 ³ × 64	3028	0.050
O ₃	48 ³ × 96	2333	0.040
P ₁	24 ³ × 48	3500	0.067
P ₂	32 ³ × 64	1958	0.050

Configurations are generated through Hybrid Monte Carlo (HMC) algorithm. We employ the algebraic definition for the topological charge density and Wilson flow is used to smooth the gauge field. We have done simulation with periodic as well as open boundary condition.

V. RESULTS

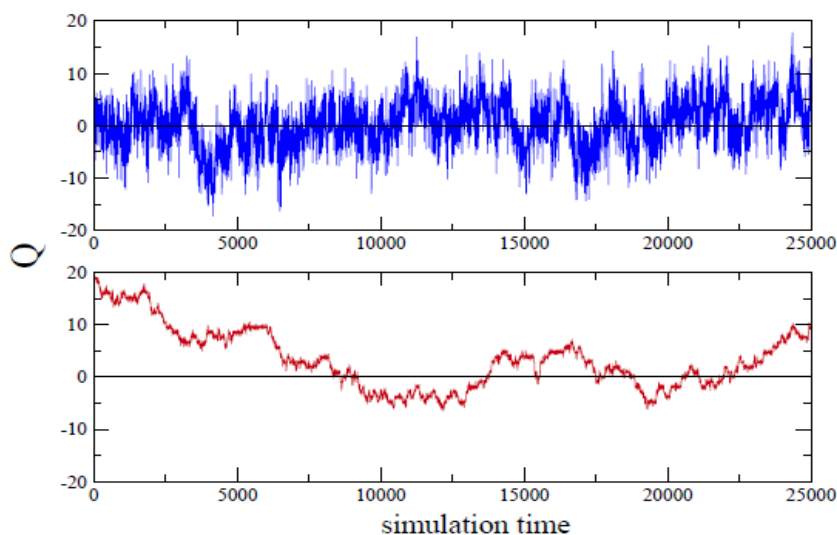


Figure 1: Trajectory history of topological charge (Q) versus simulation time at $a = 0.040$ fm and lattice volume $48^3 \times 96$ for OBC (top) and PBC (bottom) lattice

From the above figure, it is evident that successive configurations are correlated much more for PBC compared OBC lattice. The extracted values of Topological susceptibility and Glueball Mass are given in Table 2.

Table2. Extracted values of Topological susceptibility and Glueball Mass

Lattice	Volume	Lattice spacing a in (fm)	Topological Susceptibility (MeV)	Glueball Mass (MeV)
O ₁	24 ³ × 48	0.067	185.4 (2.3)	1683(204)
O ₂	32 ³ × 64	0.050	188.6 (3.5)	1653(225)
O ₃	48 ³ × 96	0.040	179.6 (3.4)	1605(191)
P ₁	24 ³ × 48	0.067	191.1 (3.0)	1538(62)
P ₂	32 ³ × 64	0.050	180.8 (5.9)	1512(51)

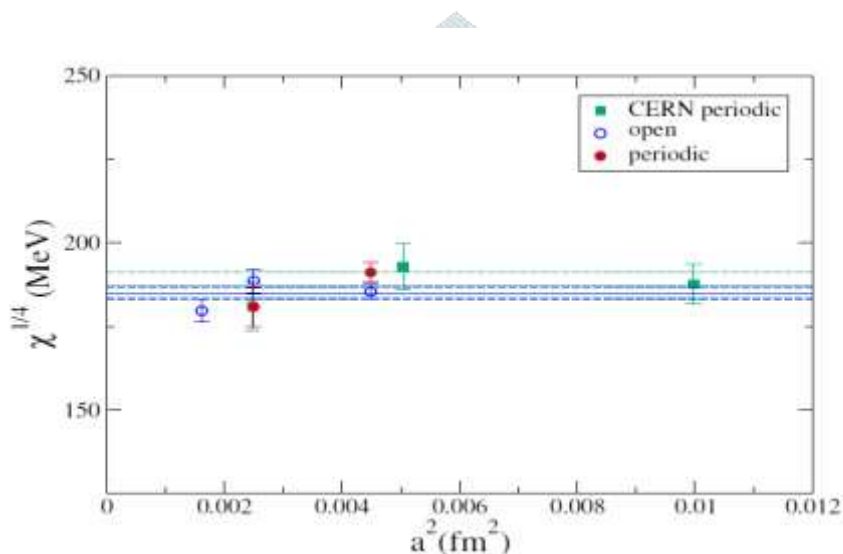


Figure 2: Topological susceptibility ($\chi^{1/4}$) in dimensionful unit plotted versus a^2 for both OBC and PBC lattice for different lattice spacing and for comparison data from CERN for PBC is also plotted.

From the figure 2, we find that the results for open and periodic lattices are very close to each other. The extracted value is 184.7 (1.7) MeV which compares well with the result 187.4 (3.9) MeV of CERN Data [6]. In the paper [7], the authors commented that to get precise result one has to do large volume lattice simulation to avoid the finite volume effect. In papers [8, 9], authors also cited the paper [5] and also said that to get the precise result one has to go smaller lattice spacing and has to do a detail study about the sampling of the gauge configurations. And from last column of Table 2, we have seen that Open and Periodic boundary conditions are producing the same value of lowest scalar glueball mass within error bar. More over any standard literature in recent time has fallen into the same ballpark.

VI. CONCLUSION

With open boundary condition in the temporal direction of the lattice, one can overcome, to a large extent, the problem of trapping and performed simulation. The open boundary condition can yield the expected value of the topological susceptibility and lowest glueball mass in lattice Yang-Mills theory. The results agree with numerical simulations employing periodic boundary condition with larger errorbar. In this review paper, we can say that to get the precise result about topological observables, we have to adopt open boundary conditions with smaller lattice spacing and larger lattice volume to make a confirm statement of their agreement.

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