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BOUNDARY EFFECTS AND HADRON MASSES IN LATTICE QCD

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A relevant contribution to the large fluctuations of hadron masses present in lattice calculations with periodic boundary conditions is due to unphysical quark paths which are absent in the infinite volume limit. We show that these contributions can be eliminated by averaging over possible rotations of the boundary links by the elements of the Z(3) subgroup. In this way the "effective" volume for these paths is triplicated.

In this paper we re-analyze the results obtained in ref. [1] in order to understand the origin of the large fluctuations of the values of hadron masses observed for different gauge field configurations depending on the presence of long range correlations (up to 300–400 Monte Carlo sweeps) between successive gauge field configurations. This point is illustrated in fig. 1 (taken from ref. [1]) which shows the value of the ρ squared mass computed from different gauge field configurations at $K = 0.1475$ (K is the Wilson hopping parameter [2]), as a function of the number of Monte Carlo sweeps. It is natural to think that the long range correlations originate from the freezing of the gauge fields in some state whose relaxation time for lattice with $V = 5^3 \times 10$ and $\beta = 6.0$ is about 300–400 sweeps. At this value of β, since we are considering a rather small lattice (with periodic boundary conditions), the tunnelling of link configurations

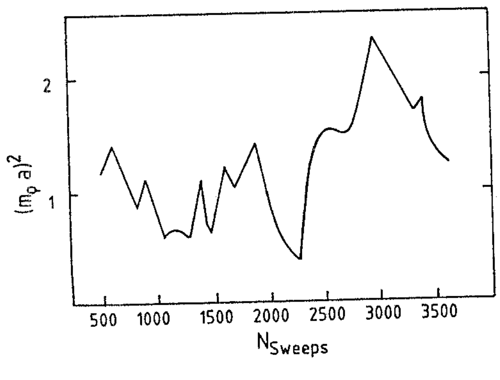

Fig. 1. The squared mass of the ρ meson times the lattice spacing a at $K = 0.1475$ as a function of the total number of Monte Carlo sweeps. Analogous curves can be drawn for the other hadrons.

from one state to another gives a large (and slow) variation of the masses. We identify the quantity which classifies the state that a certain configuration belongs to as the spatial loop defined in the following way:

$$\Pi_i = \left\langle \mathrm{Tr}\left(\prod_{n=1}^{L_i} U_i(x + n \cdot \hat{i}) \right) \right\rangle , \tag{1}$$

where $U_i(x)$ are the links in the spatial direction L_i. L_i is the size of the lattice in that direction and $\langle\ \rangle$ indicates the average of Π_i over the hyperplane orthogonal to the i direction.

At large β we expect that the value of Π_i averaged over gauge field configurations is different from zero and slowly varying with the number of Monte Carlo sweeps [3].

This ansatz has been confirmed in two ways. First we have studied the dependence of the masses on the spatial loop by multiplying the gauge fields on the boundary, for a certain configuration, by an element of Z(3), centre of the group. For example:

$R_x(U)$:

$U_\mu(x) \to U_\mu(x)$

but

$$U_x(L_x) \to \exp(2\pi \mathrm{i}/3) U_x(L_x) , \tag{2}$$

where L_x is the maximum value of the x coordinate on the lattice. The configuration obtained after this transformation still has the same action but it is characterized by different values of Π_i. We give below the value of the pion mass, for a typical configuration (at $K = 0.1475$), after the application of several transformations like that of eq. (2) in different directions as shown in table 1. The variation of the pion mass is comparable with the fluctuations observed among different uncorrelated configurations and shows that a variation in phase of the spatial loop can be responsible for these large fluctuations. As a second check we observed a strong correlation between the values of the phase of the spatial loop and the values of hadron masses: indeed variations of the values of the masses correspond to variations of the phase.

The masses depend on spatial loops because of "fake" diagrams in which a quark crosses the boundary as shown in fig. 2a. These diagrams disappear in the infinite volume limit and on a finite lattice they can be eliminated by hand in the hopping parameter expansion [5] [‡1].

A clear example of these large effects is given by the free field case: if one rotates the boundary conditions by a Z(3) transformation [$R_x R_y R_z$; cf. eq. (2)] the minimum momentum carried by a quark along the spatial directions is:

$$p^i_{\mathrm{MIN}} = 2\pi/(3L_i) , \tag{3}$$

which corresponds to a rather large variation in the determination of hadron masses. From eq. (3) in the present case ($\beta = 6.0$) we would expect a variation of the pion mass of about 100% at $K = 0.1475$: the dependence on Z(3) rotations in the interacting case [cf. table 1] seems to be even stronger. The variation of the masses corresponds to a shift in the complex plane of the critical K, K_c, defined as the value at which the pion becomes massless. The shift is of order $(1/L)^2$; for the real part it amounts to 5%. In order to minimize the effects of the spatial loops it is convenient, for a given gauge field configuration, to average the hadron propagator over Z(3) transformations on the boundary. This procedure eliminates diagrams like those of fig. 2a as illustrated in fig. 2b. The only diagrams which survive are those of the type shown in fig. 2c and 2d. The diagram of fig. 2c is a "good" diagram, in the sense that it exists also in the infinite volume limit. Diagrams like that in fig. 2d are "fake" diagrams. For these survival diagrams it is necessary for a quark to cross at least three times the boundary: we gain a factor three in the effective volume.

Table 1

M_π [a)]	Rotation
0.44	1
0.62	R_x
1.01	$R_x R_y$
1.45	$R_x R_y R_z$

a) The mass has been computed by fitting the pion propagator with one hyperbolic cosine (cf. refs. [1] and [4]).

‡1 At small β the rapid fluctuations of the spatial loop as function of the configuration number naturally average to zero the effects of those "fake" diagrams.

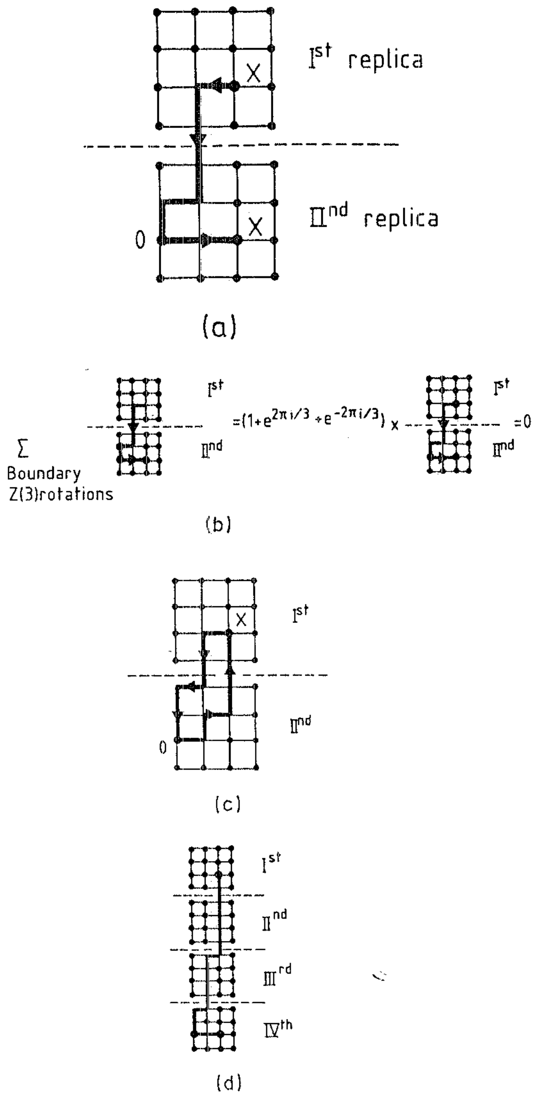

Fig. 2. (a) Example of a "fake" quark path contributing to a meson propagating between 0 and x. In the figure two replicas of the lattice are shown. One of the quarks crosses the boundary and arrives in x on a different replica of the lattice. (b) The diagram of (a) is removed by averaging over the boundary conditions with the transformation defined in eq. (2). (c) Example of a diagram which survives after the average, and which is present also in the infinite volume limit. (d) Example of a diagram which cannot be removed by the average because the phase accumulated by the propagator of the quark by crossing three times the boundary is a multiple of 2π.

In our Monte Carlo simulations [1] we generated 32 gauge field configurations to compute the hadron masses. We classify our configurations in the following way:

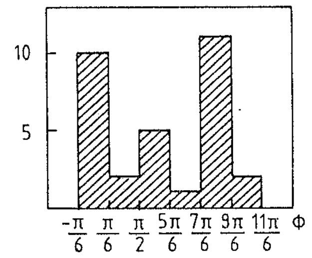

Fig. 3. Distribution of the configurations according to the phase of the spatial loop.

(i) We compute the phase ϕ_i of the spatial loop Π_i for each configuration and $i = x, y, z$.

(ii) We divide the total range of $\phi (0 < \phi < 2\pi)$ into six parts starting from $-\pi/6$, so that three of these sectors will be centered around 0, $2\pi/3$ and $-2\pi/3$ values respectively. The distribution of the configurations in ϕ (averaged in the three directions) is shown in fig. 3. There is a clear clustering around $0, 2\pi/3$ and $-2\pi/3$.

(iii) We assign a factor 1 if $-\pi/6 \leqslant \phi_i \leqslant \pi/6$ and a factor η if $\pi/2 \leqslant \phi_i \leqslant 5\pi/6$ or $7\pi/6 \leqslant \phi_i \leqslant 9\pi/6$ which correspond to the two non-trivial Z(3) rotations.

For example a configuration which has $-\pi/6 \leqslant \phi_{x,y,z} \leqslant \pi/6$ will be classified by 1, a configuration with $-\pi/6 \leqslant \phi_{x,y} \leqslant \pi/6$ and $\pi/2 \leqslant \phi_z \leqslant 5\pi/6$ by η and a configuration with $\pi/2 \leqslant \phi_x \leqslant 5\pi/6$ and $7\pi/6 \leqslant \phi_{y,z} \leqslant 9\pi/6$ by η^3. The configurations whose phases do not fall in the interesting intervals will not be considered in the following. With the definitions given above we can render quantitative our observations on the correlations between the values of the masses and the phases of the loops. In fact by dividing our configurations in four classes $(1, \eta, \eta^2, \eta^3)$ we find at $K = 0.1475$ the values of the pion mass and of the critical K listed in table 2. Moreover, the distribution of the

Table 2
The possible Z(3) classes of the configurations, their statistical weight and the mass of the pion computed for each class. Note the strong correlation between the mass and the class.

Class	Weight	m_π	K_c
1	1	0.63	0.1567
η	6	0.73	0.1558
η^2	12	0.83	0.1642
η^3	8	1.22	0.1976

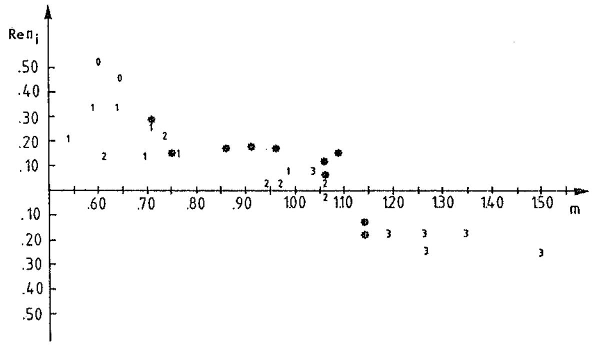

Fig. 4. The correlation of the pion mass at $K = 0.1475$ versus the real part of the spatial loop for configurations belonging to different classes (see text). The stars refer to unclassified configurations.

pion mass at $K = 0.1475$ is reported against the real part of the spatial loop in fig. 4. The numbers refer to the class that a certain configuration belongs to ($0 = \eta^0$; $1 = \eta^1$; $2 = \eta^2$; $3 = \eta^3$). Note the rather large dispersion within the same class.

From our previous discussion, it turns out that significant statistics are achieved when a set of configurations represent a good average over the different classes of Z(3) rotations with the correct statistical weight reported in table 2. To check this point we took the average propagator over each class of configurations and then we averaged the propagators over different classes with the correct statistical weight. From the propagators at different K's ($K = 0.145$, 0.1475, 0.150) we computed K_c and the lattice spacing a^{-1} in physical units by fixing the ρ mass at its experimental value. We found:

$$K = 0.160, \quad a^{-1} = 1.25 \text{ GeV}, \qquad (5)$$

which is in good agreement with the results of ref. [1] and confirms their statistical significance.

A good average over Z(3) rotations can be easily enforced in a Monte Carlo simulation: one rotates independently each of the spatial boundaries by a random Z(3) element every few Monte Carlo sweeps.

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