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Polyakov Loops and Finite-Size Effects of Hadron Masses in Full Lattice QCD

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Abstract

Polyakov type loops are responsible for the difference between quenched and unquenched finite size effects on the QCD mass spectrum. With a numerical simulation, using appropriate **sea** quark spatial boundary conditions, we show that we can align the phases of spatial Polyakov loops in a predefined direction. Starting from these results, we propose a procedure to minimize fluctuations due to these effects in meson propagators.

1. The finite extension of the lattice is an important source of systematic errors in lattice QCD calculations. Theoretical and numerical investigations have addressed [1, 2, 3] recently the problem of finite size effects in full lattice QCD. The conclusions of these analyses are that in the range $La \sim 0.7-2$ fm (L^4 is the number of lattice points and a is the lattice spacing) in the hadronic lattice masses there are important extra power law corrections, besides the exponentially decaying asymptotic prefactor which is due to the emission of virtual pions from a point like hadron [4].

In the range $La \sim 0.7-2$ fm the first effect is dominant over the second one and we can effectively write for the lattice hadronic masses

$$m_L = m_\infty + cL^{-\nu}, \tag{1}$$

where $\nu = 1-2$ in the quenched case and $\nu = 2-3$ in full QCD.

The reason for this difference can be understood by looking, for example, at the **valence** quark hopping parameter expansion of the meson propagator that can be written in the form [2]:

$$G = \sum_C k_{val}^{l(C)} \langle W(C) \rangle + \sum_C k_{val}^{l(C)} \sigma_{val} \langle P(C) \rangle \tag{2}$$

where the sums extend over all possible closed paths (C) of length $l(C)$. $W(C)$ are standard Wilson loops completely contained into the lattice, while $P(C)$ are **valence** quark loops wrapping around the lattice in spatial directions (Polyakov type loops) and $\langle\cdot\rangle$ denotes gauge field average; the value of the index σ_{val} depends on the spatial boundary conditions on the **valence** quarks: $\sigma_{val} = +1$ for periodic and $\sigma_{val} = (-1)^n$ for antiperiodic boundary conditions, with n the number of windings around the lattice [1].

The averaged Polyakov loop $\langle P \rangle$ is different from zero in full QCD, while it is zero in the confined phase of quenched QCD. This means that the second term in eq.(2) is absent in the quenched case. This may explain the differences in the value of ν between quenched and full QCD.

To obtain comparable $L^{-\nu}$ finite size effects in the two cases one would like to remove or to reduce the Polyakov loop contributions in the unquenched case.

In this paper we want to show that this can be partially achieved by using suitable **sea** quarks spatial boundary conditions so as to force the

[1] In general $\sigma_{val} = \exp(in\phi)$ if we impose $\exp(i\phi)$ boundary conditions.

phase of the Polyakov loops to be one of the three elements of the center of the gauge group SU(3)[2]

$$Z_3 = \{z_0, z_1, z_2\}, \quad z_k = \exp(i\frac{2\pi k}{3}), \quad k = 0, 1, 2 \tag{3}$$

Fixing the phase of the Polyakov loops reduces the statistical fluctuations on the hadron propagator and, hence, on the computed hadron masses.

Of course, another possibility to kill the contribution from the second term in eq.(2) (also in the unquenched case) is to follow the prescription of [5], that is to say to compute successively the **valence** quark propagator on the same gauge configuration using for the fermionic fields the boundary conditions dictated by the three phases of Z_3 and then taking the average. This procedure is rather time consuming and we will not discuss it any further.

2. On a finite lattice with periodic boundary conditions on the gauge fields there is a symmetry of the pure gauge sector consisting in multiplying all links stemming from the plane x_μ=const and orthogonal to it, by an element z_k of Z_3.

Under this operation the Polyakov loops in the μ direction are not invariant, but they transform as

$$P \rightarrow z_k P \tag{4}$$

In full QCD the action consists of the gauge and the fermionic part. In the fermionic action

$$\begin{aligned} S_{Wilson} &= -k \sum_{x,\mu} \Big(\bar{\psi}(x)(1-\gamma_\mu)U_\mu(x)\psi(x+\mu) \\ &\quad + \bar{\psi}(x)(1+\gamma_\mu)U^\dagger_\mu(x-\mu)\psi(x-\mu) \Big) \\ &\quad + \sum_x \bar{\psi}(x)\psi(x) \end{aligned} \tag{5}$$

the kinetic part is not invariant under the previous transformation. Thus the symmetry, that in the quenched confined case guarantees $\langle P \rangle = 0$, is

[2]In the following for short we will refer to these Polyakov loops as polarized (or aligned) Polyakov loops.

explicitly broken by the kinetic part of the fermionic action. Since the non-invariant term is proportional to k, this violation is more important for light **sea** quarks.

It is possible to understand what happens on the plane x_μ=const with a simple model. If we make a double expansion of full QCD, both in $\beta = 6/g^2$ and in the hopping parameter, we obtain the 3–d Potts Model in an external magnetic field. The presence of the fermionic part of the QCD action is analogous to the existence of a magnetic field h which breaks the Z_3 symmetry. In the model the spin, Π, can take the three possible values:

$$\Pi_0 = 1, \quad \Pi_1 = e^{i2\pi/3}, \quad \Pi_2 = e^{-i2\pi/3} \tag{6}$$

and it is coupled to the external magnetic field via the Hamiltonian

$$H_h = h\Pi + h^\dagger \Pi^\dagger \tag{7}$$

which is not Z_3 invariant. The possible values taken by Π are in correspondence with the expected phases of Polyakov loops, while the values of h with the chosen **sea** quarks boundary conditions.

We summarize the relevant features of the lowest part of the energy spectrum for the interesting choices of h in figs. 1a-1e. We see that with $h = +|h|$ (periodic boundary conditions on **sea** quarks) the two states with $\Pi = \Pi_1$ and $\Pi = \Pi_2$ have the lowest energy and are degenerate, while with $h = -|h|$ (antiperiodic boundary conditions on **sea** quarks) the lowest energy state is the state $\Pi = \Pi_0$. Moreover (figs 1.d and 1.e) with the choices $h = -e^{-i2\pi/3}$ and $h = -e^{i2\pi/3}$, the states Π_1 and Π_2 respectively turn out to be the lowest lying energy states.

With an eye to the patterns of fig. 1, we thus expect that with periodic boundary conditions on **sea** quarks the $e^{i2\pi/3}$ and the $e^{-i2\pi/3}$ phases of the Polyakov loops will be present with equal probability and that with antiperiodic boundary conditions Polyakov loops are likely to be polarized in the Π_0 direction. Similarly we expect to be able to align the Polyakov loops along the $e^{i2\pi/3}$ (or $e^{-i2\pi/3}$) in the Z_3 space, if we choose $-e^{-i2\pi/3}$ (or $-e^{i2\pi/3}$ respectively) boundary conditions on the **sea** quarks.

To check the foregoing suggestions we performed on APE100 a full simulation of 2 flavors lattice QCD with Wilson fermions at $\beta = 5.3$ on a $8^3 \times 32$ lattice with $k_{sea} = 0.1670$. We carried out two different runs, one with fully periodic boundary conditions on the **sea** quarks and the other

	$< P_x >$	$< P_y >$	$< P_z >$
P	-0.0011(2)+i0.0003(2)	-0.0010(2)-i0.0001(4)	-0.0011(2)-i0.0007(2)
AP	0.0017(1)-i0.00006(11)	0.0019(2)+i 0.0001(2)	0.0015(3)-i0.000004(200)

Table 1: The three spatial components of the Polyakov loop (smearing zero) for the simulation at $\beta = 5.3$ on a $8^3 \times 32$ lattice with $k_{sea} = 0.1670$. Data are from trajectory 440 to trajectory 1790. In the first row there are the results for the simulation with periodic (P) spatial boundary conditions on the **sea** quarks and in the second row the results with antiperiodic (AP) conditions.

one with antiperiodic boundary conditions in the spatial directions and periodic in the temporal one. Gauge configurations have been produced with APE100 with the Hybrid Monte Carlo Algorithm (HMCA) described in reference [6]. After a thermalization of 440 trajectories of HMCA we have created a set of 1350 thermalized trajectories. On these we have performed the measurement of the spatial loops, P_x, P_y and P_z, taking only one every 5 consecutive trajectories. To reduce the fluctuations on the expectation value of the Polyakov loops, we used the smearing procedure of ref. [7].

The results for the phases of the spatial Polyakov loops P_x are reported in figs. 2 and 3. With antiperiodic spatial boundary condition, fig. 2, the values of the phase are close to zero, while with periodic boundary conditions, fig. 3, the phases are concentrated in two regions near $e^{i2\pi/3}$ and $e^{-i2\pi/3}$.

We have also verified in a quick simulation on a $4^3 \times 6$ lattice with $\beta = 3.0$ and $k_{sea} = 0.1670$ that, if we impose on **sea** quarks the spatial boundary conditions $-e^{i2\pi/3}$ (or $-e^{-i2\pi/3}$), Polyakov loops have, as expected, phases near $e^{-i2\pi/3}$ (or $e^{i2\pi/3}$ respectively), see figs. 4c-4d.

3. A study similar to the one presented above, concerning **valence** quarks, has been performed in ref. [5] in the case of quenched QCD. There, the authors had insufficient statistics and, hence, found that the mean value of the Polyakov loop was nonzero with the three possible values of the phases all present with non zero but different probabilities. As a consequence their estimate of the meson masses had a large dispersion, greater than 50%.

Also in the unquenched case with periodic boundary conditions on **sea** quarks we expect similar fluctuations because Polyakov loops are not vanishing and "unpolarized". However by choosing antiperiodic (or $-e^{i2\pi/3}$ or $-e^{-i2\pi/3}$) spatial boundary conditions, we may at least fix correspondingly the phases of the Polyakov loops and reduce statistical fluctuations on masses.

For instance in the simulation at $\beta = 5.3$ on a $8^3 \times 32$ lattice with $k_{sea} = 0.1670$ we obtain the results reported in Table 1 for the x, y and z components of the Polyakov loop, $< P_i >, i = x, y, z$, for both periodic and antiperiodic **sea** quarks spatial boundary conditions.

Statistical errors have been computed, separately for each spatial direction, by grouping the 270 measures in 10 bins of 27 numbers each. In the antiperiodic case the imaginary parts of P_x, P_y and P_z are compatible with zero, as expected, and the real parts are equal within errors. Also in the periodic case the real parts are equal within errors but the relative errors are about twice as large as before. Furthermore the imaginary parts are not compatible with zero. This fact is due to the *flip-flop*'s of the Polyakov loop phases between the two values $e^{i2\pi/3}$, $e^{-i2\pi/3}$.

In simulations using periodic boundary conditions on **sea** quarks, this kind of fluctuation could always be reduced by selecting a posteriori only the configurations in which the phases of P_x, P_y and P_z all lie close to a given Z_3 element. One should observe that this procedure, besides reducing the statistics by a factor of 8, may introduce unnecessary biases. In our opinion the best way is to start *ab initio* with one well specify spatial boundary condition that aligns the Polyakov loops in a given Z_3 direction.

The numerical simulations of this work have been performed using 2 months of CPU time on a 128 nodes APE100 machine.

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FIGURE CAPTIONS

Figure 1. The lowest lying energy levels of the model of eq.(7) for different values of h. The notation for the states is that of eq.(6).

Figure 2. Histogram of the phase of the x component of the Polyakov loop for antiperiodic spatial boundary condition on **sea** quarks. Data are from trajectory 440 to trajectory 1790. The lattice volume is $8^3 \times 32$.

Figure 3. Same of fig. 2 but for periodic boundary conditions on **sea** quarks.

Figure 4. Behavior of the phase of the average of the three spatial Polyakov loops as a function of the HMCA trajectory. Data are from trajectory 205 to trajectory 600. The lattice is $4^3 \times 6$. In fig. 4a we report the results for **sea** quarks periodic boundary conditions; in fig. 4b for antiperiodic spatial boundary conditions; in fig. 4c for spatial boundary conditions $-e^{-i2\pi/3}$ and in fig. 4d for spatial boundary conditions $-e^{i2\pi/3}$.

References

[1] M. Fukugita, H. Mino, M. Okawa, G. Parisi, A. Ukawa Phys. Lett. **B 294** (1992) 380.

[2] S. Aoki et al. Nucl. Phys. **B** (Proc. Suppl.) **34** (1994) 363.

[3] J. Kripfganz, C. Michael, Nucl. Phys. **B 314** (1989) 25.

[4] M. Lusher, Commun. Math. Phys. **104**, 177 (1986).

[5] G. Martinelli, G. Parisi, R. Petronzio, F. Rapuano, Phys. Lett. **B 122** (1983) 283.

[6] S. Antonelli, M. Bellacci, A. Donini, R. Sarno "Full QCD on APE100 Machines" Preprint n.972/93 Dep. of Phys. Universitá di Roma "La Sapienza"; To appear in Int. Jour. of Mod. Phys. C.

[7] M.Albanese *et al.* Phys. Lett **B 192**(1987)163.