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Preparing for $N_f = 2$ simulations at small lattice spacings

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We discuss some large effects of dynamical fermions. One is a cutoff effect, others concern the contribution of multi-pion states to correlation functions and are expected to survive the continuum limit. We then turn to the preparation for simulations at small lattice spacings which we are planning down to around $a = 0.04$ fm in order to understand the size of $\mathrm{O}(a^2)$-effects of the standard $\mathrm{O}(a)$-improved theory. The dependence of the lattice spacing on the bare coupling is determined through the Schrödinger functional renormalized coupling.

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1. Introduction

The ALPHA collaboration has worked over the years on a determination of the QCD Λ-parameter starting from experimental low energy hadronic input and using perturbation theory in a renormalized coupling at sufficiently high energy scales. At these scales it was demonstrated that perturbation theory is very accurate. The quoted results for the $\overline{\mathrm{MS}}$ Λ-parameter are $\Lambda^{(0)}_{\overline{\mathrm{MS}}} r_0 = 0.60(5)$ [1] in the quenched approximation and $\Lambda^{(2)}_{\overline{\mathrm{MS}}} r_0 = 0.62(4)(4)$ [2] with $N_\mathrm{f} = 2$ dynamical quarks. On the other hand the $N_\mathrm{f} = 5$ value extracted by matching various experimental data to perturbation theory in the (not always very) high energy region translates into $\Lambda^{(5)}_{\overline{\mathrm{MS}}} r_0 \approx 0.55$ [3], when $r_0 = 0.5\,\mathrm{fm}$ [4] is used. Superficially this suggests a nice agreement, but the perturbative matching across the quark thresholds [5] yields $\Lambda^{(4)}_{\overline{\mathrm{MS}}}/\Lambda^{(5)}_{\overline{\mathrm{MS}}} \approx 1.4$ which does not connect smoothly to the $N_\mathrm{f} = 0, 2$ numbers. In order to say more about this comparison, the low energy scale r_0 should be replaced by an experimental observable and the continuum limit should be evaluated with a better confidence than it was possible in [2]. Significant progress in the understanding of the continuum limit requires to simulate smaller lattice spacings with good accuracy. We will motivate this further in Sect. 2. The difficult simulations are the ones in large volume where for example the Kaon decay constant is to be determined to set the energy scale in GeV. We will briefly explain in Sect. 3 that our previous approach of using Schrödinger functional boundary conditions in that part of the calculation meets somewhat unexpected (practical) difficulties. Since these are related to true dynamical fermion effects, they are theoretically interesting, but it appears to be better to switch to (anti)-periodic boundary conditions in this part of the calculation. In Sect. 4 we will finally discuss a determination of the dependence of the lattice spacing on the bare coupling. This represents a useful piece of information for fixing the parameters of the large volume simulations.

Before entering our discussion we add a comment on the motivation. One might object to the whole project of a determination of the Λ-prameter that very precise lattice determinations for $\alpha_{\overline{\mathrm{MS}}}(M_\mathrm{Z})$ have already been published [6]. However, apart from the use of rooted staggered fermions, in these determinations perturbation theory has been used at rather low renormalization scales and for non-universal quantities (small Wilson loops). These are defined at the scale of the (lattice)-cutoff. It is apparent from the discussion in [6] that the use of perturbation theory is problematic. The known terms in the expansion either have large coefficients or, if one resums by choosing a different scheme, the renormalization scale becomes even smaller and the expansion parameter larger. In order to describe the data several higher order terms in the expansion are fitted. Thus it appears that a computation following the ALPHA-strategy, where the continuum limit is taken and perturbation theory is verified to apply for the considered *renormalized* coupling, remains very well motivated. We do not see any alternative to this strategy if a full control of all systematics is desired.

In the following considerations we use the standard O(a)-improved theory with Wilson's gauge action and the non-perturbatively determined [7] coefficient c_sw of the Sheikholeslami-Wohlert term [8].

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2. Cutoff effects in Z_A

In [9] we have presented evidence that cutoff effects tend to be larger in full QCD than they are in the quenched approximation. Here we would like to draw the reader's attention to the non-perturbative determination of Z_A presented in [10]. It uses a Ward identity in the Schrödinger functional in an $L^3 \times 9/4L$ geometry with $L \approx 0.8\,\mathrm{fm}$ as in the quenched approximation [11]. It can be shown that the quark-propagator disconnected diagrams which enter the Ward idenity vanish in the continuum limit. They are of $\mathrm{O}(a^2)$ at a finite lattice spacing. In contrast to the quenched approximation where already at $a = 0.1\,\mathrm{fm}$ they were insignificant (in comparison to the numerical precision), for $N_\mathrm{f} = 2$ they contribute an about 15% effect in Z_A at such a lattice spacing. Even if this effect disappears very quickly at smaller a, it is unpleasantly large at the lattice spacings one typically would like to include in a continuum extrapolation.

In the mean time we have investigated the problem further, finding that qualitatively this effect persists if one changes the angle θ in the spatial fermion boundary condition. Alternatively we considered the Ward identity between static-light states in such a way that disconnected diagrams are absent. Unfortunately, even when using HYP discretizations for static quarks [12] the statistical errors in Z_A become relatively large at the smaller lattice spacings. Still, we confirmed that Z_A defined in this way is rather close to the definition with light-light states but disconnected diagrams dropped.

In general, cutoff effects are expected to be more prominent in correlation functions (and for time separations) where excited state contributions are very important. We therefore investigate at present whether the approximate ground state projection of [13] suppresses the disconnected contribution to Z_A thus accelerating the continuum limit. Whether this attempt is successfull or not, these difficulties suggest that one most likely needs smaller a with dynamical fermions than in the quenched approximation. We now turn to another strong effect of dynamical fermions – one that is expected to persist in the continuum limit.

3. The large-volume Schrödinger functional

Apart from the non-perturbative evaluation of renormalization constants, the Schrödinger functional also proved to be advantageous for the computation of hadron masses and matrix elements such as F_K in the quenched approximation [14]. A time extent of $T = 3\,\mathrm{fm}$ allowed to clearly isolate ground state contributions. We have then attempted to compute the pseudoscalar masses and decay constants for $N_\mathrm{f} = 2$ with an $L^3 \times T$ Schrödinger functional, keeping $L \geq 2\,\mathrm{fm}$ and $T \approx 2.5\,\mathrm{fm}$. Indeed, at a quark mass around the physical strange quark mass ($\kappa = 0.1355$), the effective mass of the pseudoscalar correlation functions $f_\mathrm{A}, f_\mathrm{P}$ (see e.g. [15] for their definition) exhibit short plateaux. An example is shown in the upper part of Fig. 1.

However, the plateaux disappear quickly when the quark mass is lowered. For a quark mass of about half the strange quark mass ($\kappa = 0.13605$), excited state contaminations are strongly present in both the vacuum channel and in the pion channel. The former yield contributions $\propto \exp(-(T - x_0)\,E_1^{\mathrm{vac}})$ and the latter $\propto \exp(-x_0\,(E_1^{\pi} - m_\pi))$. Once these two leading contaminations are included, fits to the correlation functions are still reasonable. We show a fit where we have fixed $E_1^{\mathrm{vac}} = 2m_\pi$, $E_1^{\pi} = 3m_\pi$. These are the energies of the multi pion states with the correct

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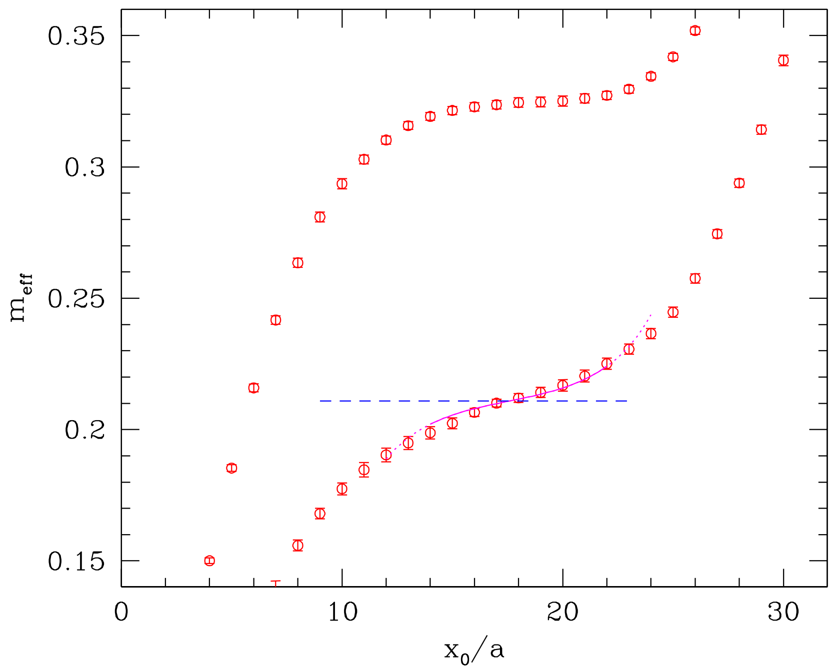

Figure 1: The effective mass for the Schrödinger functional correlation function f_P at $\beta = 5.3$ on a $24^3 \times 32$ lattice for $\kappa = 0.1355$ and $\kappa = 0.13605$. The fit described in the text is extended outside the fit-range as a dotted curve. The dashed line indicates the fitted pion mass.

quantum numbers, when the interaction of the pions is neglected. At sufficiently large L this is a good approximation.

We may conclude that *multi-pion states are observed*, as expected in the full theory. Their amplitude appears to be significantly stronger than with (point-to-point correlators and) periodic boundary conditions [16]. The standard Schrödinger functional boundary operators have a strong overlap with these states. Even though it is interesting to observe these *strong effects of dynamical fermions* and a consistent description over a significant range of x_0 can be achieved in the form of a fit, their presence hampers a reliable estimation of the systematic errors. We have hence decided to switch to periodic boundary conditions for the purpose of computing large volume matrix elements.

4. The lattice spacing as a function of the bare coupling

As a first step towards such computations we now compute, in a massless renormalization scheme, the dependence $a(g_0)$ of the lattice spacing on the bare coupling g_0 for $0.04\,\mathrm{fm} \lesssim a \lesssim 0.1\,\mathrm{fm}$. Of course the function $a(g_0)$ is not unique, but only defined up to cutoff effects, which depend on the renormalized quantity that is held fixed. We employ a renormalization condition which is relatively easily evaluated and which does not introduce artificially large a-effects. This has proven to be the case for the standard Schrödinger functional coupling $\bar{g}^2(L)$, defined in [17, 18], at vanishing quark mass.

We further specify a scale L^* by

$$\bar{g}^2(L^*) = 5.5\,, \tag{4.1}$$

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L/a	β	κ	$\bar{g}^2(L)$	am	
8	5.3	0.136197	5.65(5)	0	
8	5.3574	0.13564	5.59(5)	0.024(1)	
8	5.3574	0.1367	4.98(13)	−0.011(1)	[2]
8	5.3574	0.136365	5.26(6)	0	interpolated
10	5.5	0.136712	5.11(8)	−0.0008(2)	
12	5.6215	0.136665	5.62(9)	0.0019(2)	
16	5.8097	0.1366077	5.48(12)	0	[2]

Table 1: Raw simulation results and interpolated values. Values of $am = 0$ indicate that $|z| = |Lm|$ is estimated to be at most 5×10^{-3}.

which is known to lead to $L^*/a \gtrsim 8$ for the planned range of a. For such a choice, table 7 of [2] shows a change of $\bar{g}^2$ by about $\Delta\bar{g}^2 = 0.3$ when the boundary $\mathrm{O}(a)$ improvement coefficient c_t is changed from its 1-loop to its 2-loop approximation. Using the non-perturbative beta-function of [2],

$$L\frac{\mathrm{d}}{\mathrm{d}L}\bar{g}^2 = -2\,\bar{g}\,\beta(\bar{g}) = 0.21(1)\,\bar{g}^4 \;\text{ at } \bar{g}^2 \approx 5.5\,, \tag{4.2}$$

a value $\Delta\bar{g}^2 = 0.3$ translates into a 5% change in L^* and thus a. The definition eq. (4.1) is completed by an exact definition of the massless point. We choose the PCAC mass m (with non-perturbative c_A [13]) with Schrödinger functional boundary conditions, with $T = L = L^*$, $\theta = 0.5$ and a vanishing background field.

Good guesses for the bare parameters g_0, κ at a prescribed L/a are easily made starting from table 11 of [2]. When the result of a determination of $\bar{g}^2(L)$ is close to the target eq. (4.1) and m is close to zero, we may correct by a first order Taylor expansion with derivatives eq. (4.2) and an estimate of

$$s = \frac{1}{L}\frac{\partial}{\partial m}\bar{g}^2|_L\,. \tag{4.3}$$

From the results at two different values of m and fixed $\beta = 6/g_0^2 = 5.3574$ in Table 1 we extract

$$s = 2.2(5) \;\text{ at } \bar{g}^2(L) \approx 5.5\,. \tag{4.4}$$

The rest of the simulation results of that table are then corrected to match the target with this value of s (including its error) and with eq. (4.2). We arrive at Table 2 where a precision between 0.8% and 1.9% is seen. These numerical values are very well described by the simple linear interpolation formula

$$\log(L^*/a) = 2.3338 + 1.4025\,(\beta - 5.5) \tag{4.5}$$

as seen in Fig. 2 where a ± 0.02 “error band” is shown.

β	$\log(L^*/a)$
5.3000	2.056(08)
5.3574	2.120(11)
5.5000	2.368(14)
5.6215	2.474(14)
5.8097	2.776(19)

Table 2: Results for L^*/a.

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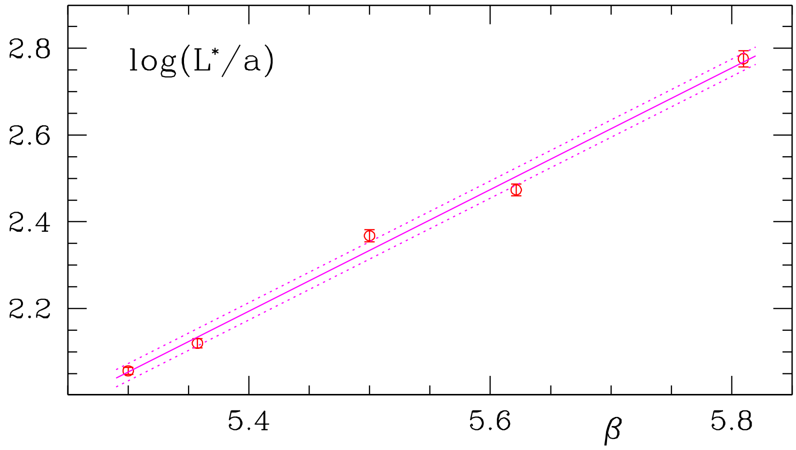

Figure 2: The results for L^*/a as a function of β.

5. Outlook

Using the estimate $a \approx 0.08\,\mathrm{fm}$ at $\beta = 5.3$ [16], we have estimated the pairs $(\beta, L/a) = (5.5, 32)$ and $(5.7, 48)$ in order to remain in the large volume region $L \geq 1.9\,\mathrm{fm}$. We are currently carrying out first simulations at these parameters. Quark masses on the $L/a = 48$ lattice are initially designed to be only slightly below the mass of the strange quark. The reason is that our first goal is to carry out a precise scaling test, which is best done at not too small quark mass. Combining with the results of [16, 19] a significant range of a close to the continuum can be covered.

The simulations are currently being done with the DD-HMC algorithm [20]. Release 1.0 of Martin Lüscher's software [21] has been adapted for the BlueGene/L and an efficiency around 30% has been achieved. The simulations do thus run at a sufficient speed to expect results from the BlueGene/L in Jülich rather soon. These efforts are part of coordinated lattice simulations (CLS) carried out together with other lattice groups at CERN, Madrid, Mainz, Rome (Tor Vergata) and Valencia.

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