DESY 03-003

arXiv:hep-lat/0301013 v1 14 Jan 2003

NUMERICAL SIMULATION WITH LIGHT WILSON-QUARKS

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The computational cost of numerical simulations of QCD with light dynamical Wilson-quarks is estimated by determining the autocorrelation of various quantities. In test runs the expected qualitative behaviour of the pion mass and coupling at small quark masses is observed.

1. Introduction

In Nature there exist three light quarks (u, d and s) which determine hadron physics at low energies. Numerical simulations on the lattice have to deal with them – which is not easy because the known simulation algorithms slow down substantially if light fermions are involved.

At present most dynamical ("unquenched") simulations are performed with relatively heavy quarks, in case of Wilson-type lattice fermions typically at masses above half of the strange quark mass, and then chiral perturbation theory (ChPT)[1] is used for extrapolating the results to the small u- and d-quark masses. This extrapolation is better under controle if the dynamical quarks are as light as possible.

In this talk I report on some recent work of the qq+q Collaboration concerning numerical simulations with light Wilson-quarks[2,3,4]. We used the two-step multi-boson (TSMB) algorithm[5] which turned out to be relatively efficient for light fermions in previous investigations of supersymmetric Yang-Mills theory. (For a review with references see ref.[6]).

2. Estimates of computational costs

In numerical Monte Carlo simulations the goal is to produce a sequence of statistically independent configurations which can be used for obtaining estimates of expectation values of different quantities. A measure of inde-

pendence is provided by the values of the *integrated autocorrelation lengths* in the configuration sequence, usually denoted by τ_{int}^{Q}. This depends on the quantity Q of interest and gives the distance of statistically independent configurations.

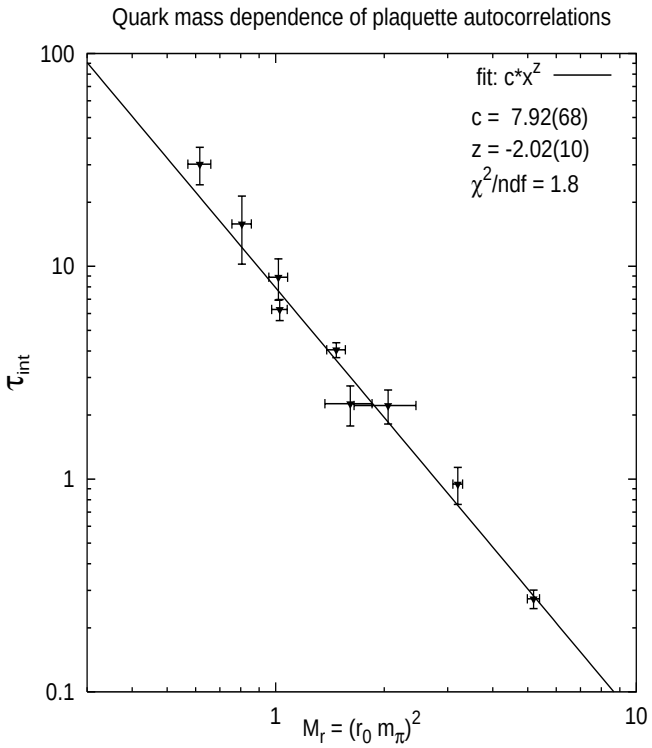

Figure 1. Power fit of the average plaquette autocorrelation given in units of $10^6 \cdot$MVM as a function of the dimensionless quark mass parameter M_r. The best fit of the form cM_r^z is at $c = 7.92(68)$, $z = -2.02(10)$.

The qq+q Collaboration has recently performed a series of test runs on $8^3 \cdot 16$, $12^3 \cdot 24$ and 16^4 lattices with $N_f = 2$ and $N_f = 2 + 1$ quark flavours. The quark masses were in the range $\frac{1}{6}m_s < m_q < 2m_s$ and the autocorrelations of several quantities as average plaquette, smallest eigenvalue of the fermion matrix, pion mass and coupling etc. have been determined. The error analysis and integrated autocorrelations in the runs have been obtained using the *linearization method* of the ALPHA collaboration[7].

The computational cost of obtaining a new, independent gauge configuration in an updating sequence with dynamical quarks can be parametrized,

for instance, as[2]

$$C = F\ (r_0 m_\pi)^{-z_\pi} \left(\frac{L}{a}\right)^{z_L} \left(\frac{r_0}{a}\right)^{z_a} \quad . \tag{1}$$

Here r_0 is the Sommer scale parameter, m_π the pion mass, L the lattice extension and a the lattice spacing. The powers $z_{\pi,L,a}$ and the overall constant F are empirically determined. The unit of "cost" can be, for instance, the number of necessary fermion-matrix-vector-multiplications (MVMs) or the number of floating point operations to be performed. For an example on the quark mass dependence of the cost see figure 1 which is taken from ref.[2]. This shows that the quark mass dependence in case of the average plaquette is characterized by a power $z_\pi \simeq 4$. For other quantities, as the smallest eigenvalue of the fermion matrix and the pion mass, a smaller power $z_\pi \simeq 3$ is observed.

Other tests on the lattice volume and lattice spacing dependence showed a surprisingly mild increase in both directions if compared to the data[2] on $8^3 \cdot 16$ lattice at $a \simeq 0.27\,\mathrm{fm}$. Some results on the volume dependence of the average plaquette autocorrelation τ_{int}^{plaq} are given in the first four lines of table 1. The runs with label (e16) and (E16) belong to almost the same

Table 1. Runs for comparing the simulations costs (given in numbers of floating point operations) at different volumes and lattice spacings.

label	lattice	β	κ	τ_{int}^{plaq} [flop]
(e)	$8^3 \cdot 16$	4.76	0.190	$4.59(37) \cdot 10^{13}$
(e16)	16^4	4.76	0.190	$7.5(1.3) \cdot 10^{14}$
(h)	$8^3 \cdot 16$	4.68	0.195	$1.7(6) \cdot 10^{14}$
(h16)	16^4	4.68	0.195	$1.10(17) \cdot 10^{15}$
(E16)	16^4	5.10	0.177	$2.1(4) \cdot 10^{14}$

quark mass ($M_r \simeq 1.4$) but have by a factor of about 1.5 different lattice spacing. A typical expectation for the power governing the lattice spacing dependence is $z_a = 2$ which would imply by a factor of 2.25 lager value for (E16) than for (e16). Compared to run (e) $z_L = 4$ and $z_a = 2$ would imply for (E16) an increase by a factor 36 instead of the actual factor $\simeq 4$. The observed relative gain is partly due to some improvements of the simulation algorithm (see ref.[3]) and is, of course, very welcome in future simulations.

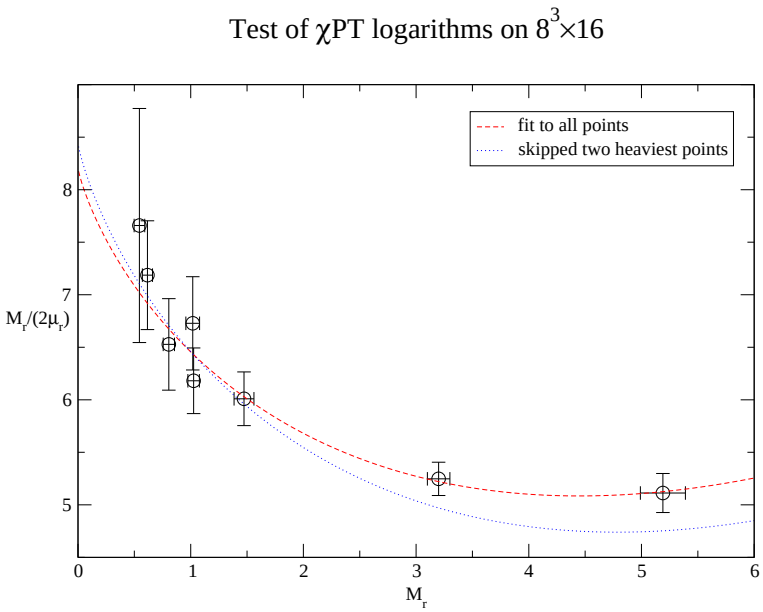

Figure 2. Fits of the pseudoscalar meson mass-squared with the one-loop ChPT formula.

3. Chiral logarithms?

The behaviour of physical quantities, as for instance the pseudoscalar meson ("pion") mass m_π or pseudoscalar decay constant f_π as a function of the quark mass are characterized by the appearance of *chiral logarithms*. These chiral logs, which are due to virtual pseudoscalar meson loops, have a non-analytic behaviour near zero quark mass of a generic form $m_q \log m_q$. They imply relatively fast changes of certain quantities near zero quark mass which are not seen in present data[8,9,10,11,12].

Although we have rather coarse lattices ($a \simeq 0.27\,\mathrm{fm}$) and, in addition, up to now we are working with unrenormalized quantities – without the Z-factors of multiplicative renormalization – it is interesting to see that the effects of chiral logs are qualitatively displayed by our data. Fits with the ChPT-formulas (see, for instance, ref.[13,14]) are shown in figures 2 and 3. These are taken from ref.[4,15] where the fit parameters are also quoted. To see the expected qualitative behaviour with chiral logarithms in numerical simulations at small quark masses is quite satisfactory but for a quantitative determination of the ChPT parameters one has to go to smaller lattice spacings.

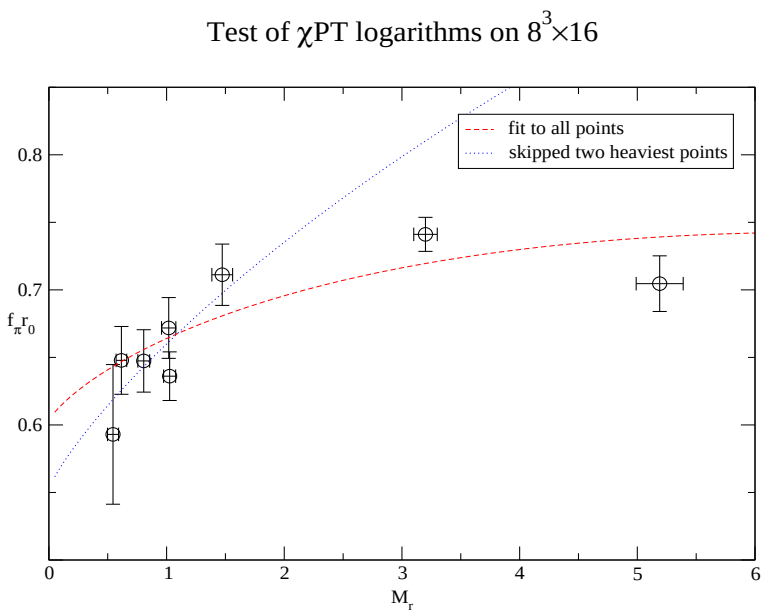

Figure 3. Fits of the pseudoscalar meson decay constant with the one-loop ChPT formula.

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