QCD simulations with light Wilson-quarks

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Introduction

Monte Carlo simulations of QCD with dynamical quarks are done in most cases at relatively large quark masses (typically two quark flavours with $m_{ud} \geq m_s/2$.)
This makes the extrapolation to the physical point $m_{ud} \simeq m_s/20$ rather uncertain.

The extrapolation is done by using (PQ-)ChPT – typically to NLO (1-loop) order.
Estimates (see Sharpe-Shoresh, ...) show that one should perform simulations in the range $m_{ud} < m_s/5$.

For controlling higher orders (NNLO, NNNLO, resonance contributions, ...) models à la Adelaide (Leinweber et al.) could be very useful.

Unquenched numerical simulations at smaller quark masses represent a great challenge for computations.
The problem is the singularity of the effective gauge action ($\log\det Q$) at zero fermion mass. This implies, for instance, the divergence of the fermionic force near zero fermion mass.

Cost estimate for simulation of light quarks

Going to light quark masses in unquenched QCD simulations is a great challenge for computations because known algorithms have a substantial slowing down towards small quark masses.
The computational cost of a simulation with two light quarks can be parametrized as

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

Here r_0 is a physical length, for instance the Sommer scale parameter, m_π the pion mass, L the lattice extension and a the lattice spacing.

The value of the constant factor F depends on the precise definition of "cost". For instance, one can consider the number of floating point operations in one autocorrelation length of some important quantity, or the number of fermion-matrix-vector-multiplications necessary for achieving a given error of a quantity.
The cost also depends on the particular choice of the lattice action and of the dynamical fermion algorithm, which should be optimized.

qq+q Collaboration:

F. Farchioni, C. Gebert, I.M., E. Scholz, L. Scorzato

Using the TSMB algorithm for $N_f = 2$ simulations on $8^3 \cdot 16$ lattices at $a \simeq 0.27\,\mathrm{fm}$ and going down to small quark masses $m_q < m_s/5 \simeq 20\,\mathrm{MeV}$.

Integrated autocorrelations:

For the quark mass dependence of τ_{int}^{plaq} we obtain the power $z_\pi = 4$ with $F = 0.77 \cdot 10^9 \mathrm{flop}$.

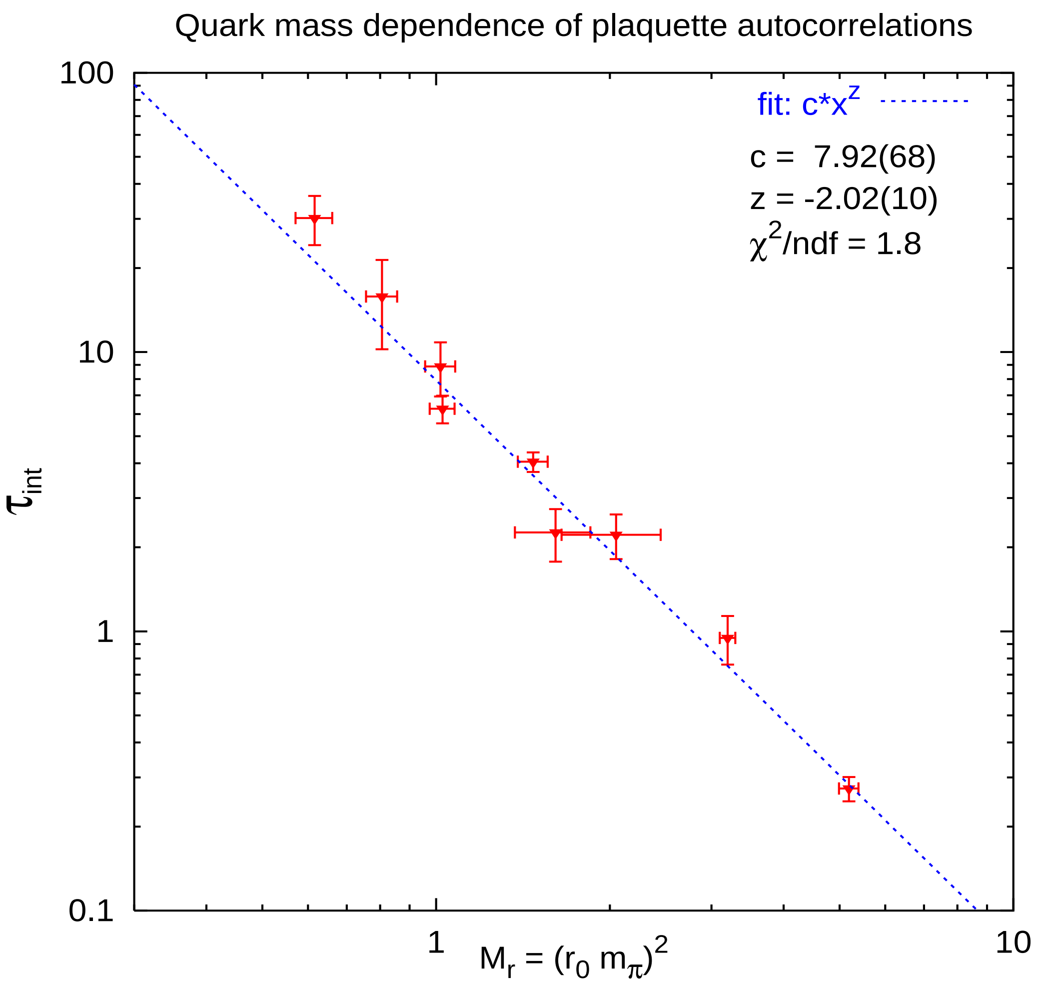

Figure 1: Power fit of the plaquette autocorrelation given in 10^6 MVM $\simeq 1.1 \cdot 10^{13}$ flop as a function of the dimensionless quark mass parameter $M_r = (r_0 m_\pi)^2$.

Autocorrelation of the pion mass: $\tau_{int}^{m_\pi}$

is in most cases substantially shorter than that of the average plaquette.

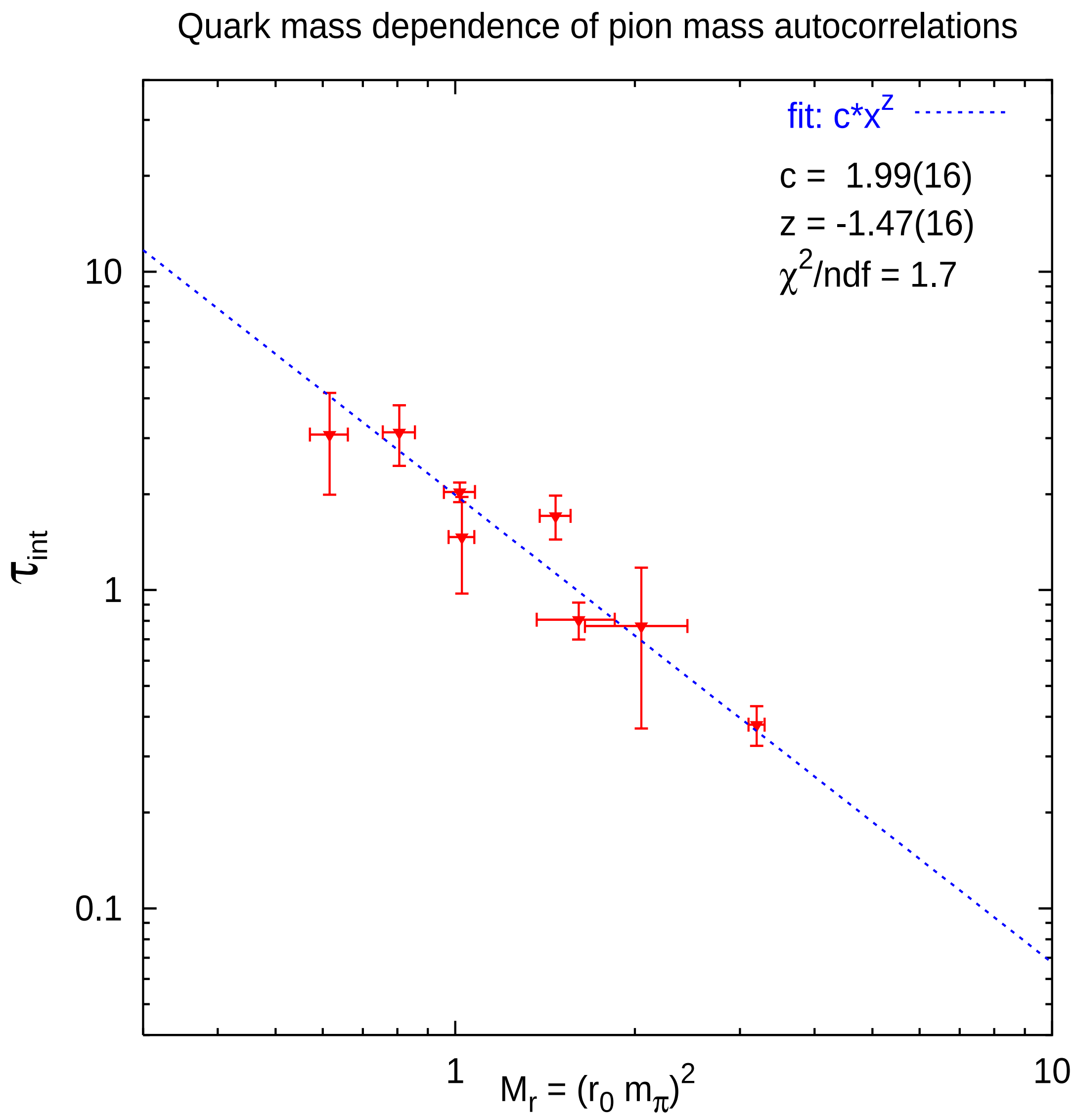

Figure 2: Power fit of the pion mass autocorrelation given in 10^6 MVM $\simeq 1.1 \cdot 10^{13}$ flop as a function of the dimensionless quark mass parameter $M_r = (r_0 m_\pi)^2$.

The integrated autocorrelation of the pion coupling is even shorter: $\tau_{int}^{f_\pi} < \tau_{int}^{m_\pi}$.

Volume dependence

Autocorrelations on larger lattices:
Example: 16^4 lattices in the same points as some of the $8^3 \cdot 16$ lattices. The physical volume is large:
$L \simeq 4 - 5\,\mathrm{fm}$, $L^4 \simeq 400 - 500\,\mathrm{fm}^4$.

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	$2.1(4) \cdot 10^{14}$

The quark masses are, respectively:
$m_{ud} \simeq 0.45\, m_s$ and $m_{ud} \simeq 0.25\, m_s$.
The cost increase with lattice volume is close to the trivial volume factor.
In case of the autocorrelation of the pion mass the observed increase turns out to be even smaller.

Smaller lattice spacings: the run (E16) shows a favourable behaviour, which is presumably due to the way the small eigenvalues are dealt with ($M_r \simeq 1.4$ as for (e16)).

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Eigelvalues of the fermion matrix: The effect of the quark determinant suppresses the density of eigenvalues of the quark matrix near zero.
The statistical weight of gauge configurations with negative fermion determinant of a single quark flavour is negligible.

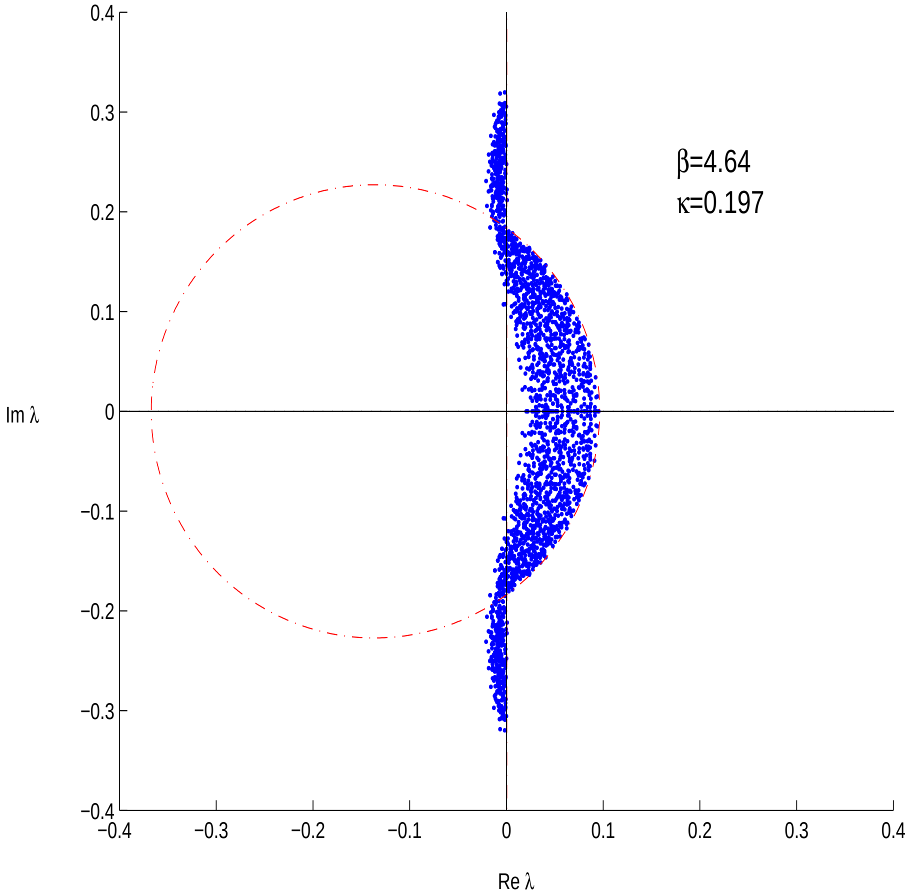


Figure 3: Low-lying eigenvalues from a set of O(10) configurations at $\beta = 4.64$ and $\kappa = 0.197$ on $8^3 \cdot 16$ lattice. The eigenvalues are determined inside the closed curve and to the left of the vertical line with the Arnoldi algorithm.

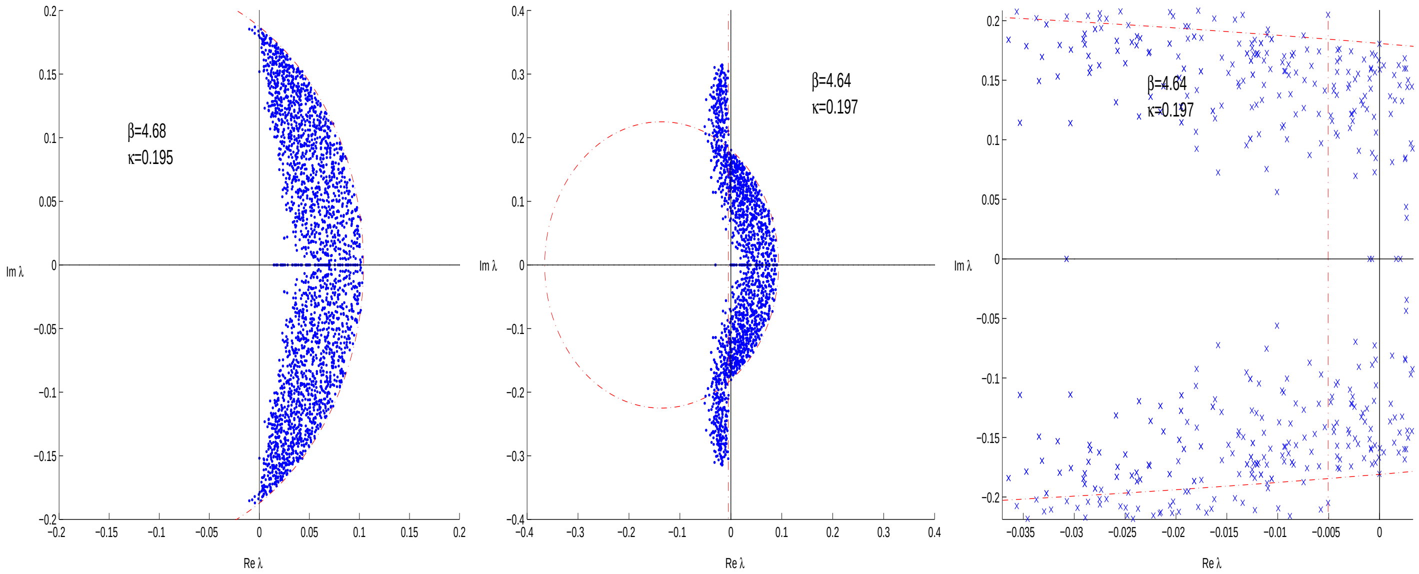


Figure 1. Low-lying eigenvalues for a set of 10 configurations with exceptionally small eigenvalues, at $\beta = 4.68$ and $\kappa = 0.195$ (left panel), $\beta = 4.64$ and $\kappa = 0.197$ (middle panel), detail (right panel).

Chiral logs?

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 previous data.

The one-loop ChPT formulas for m_π^2:

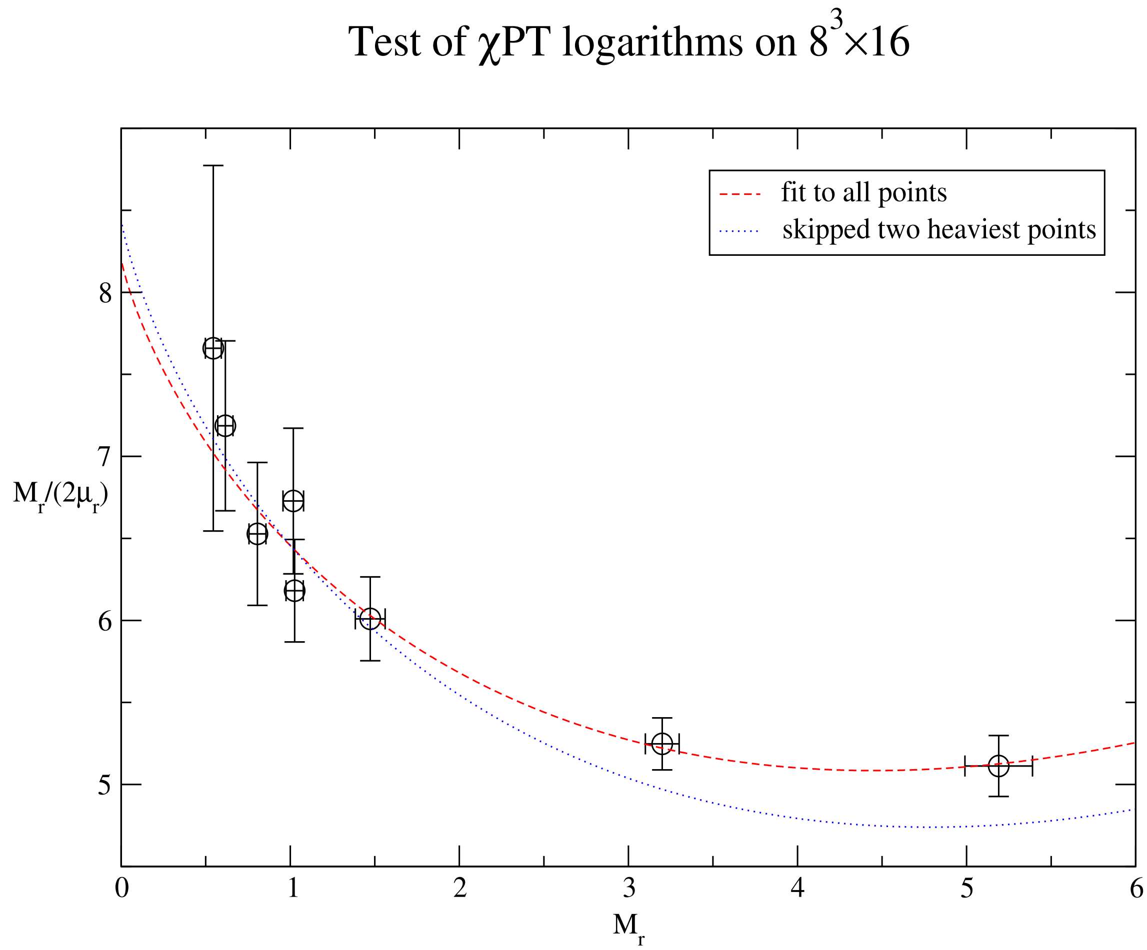
$$\frac{M_r}{2\mu_r} = Br_0 - \frac{M_r Br_0}{16\pi^2 (fr_0)^2} \log \frac{(\Lambda_3 r_0)^2}{M_r} + \mathcal{O}(M_r^2)$$

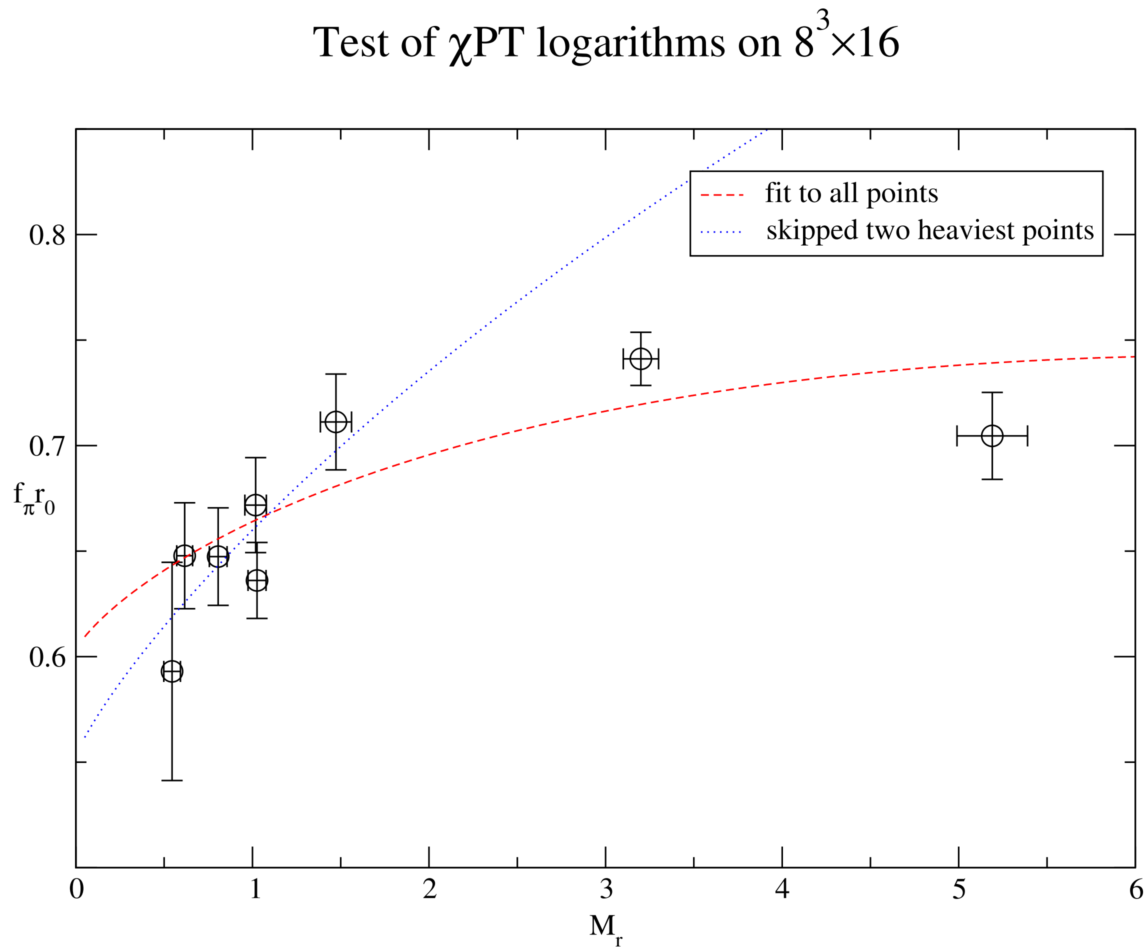
and for f_π:

$$f_\pi r_0 = fr_0 + \frac{M_r}{8\pi^2 fr_0} \log \frac{(\Lambda_4 r_0)^2}{M_r} + \mathcal{O}(M_r^2)$$

Notations: $M_r \equiv (r_0 m_\pi)^2$ and $\mu_r \equiv m_q^{PCAC} r_0$.

The fits with all points correspond to the parameters:
$Br_0 = 8.2,\ fr_0 = 0.27,\ \Lambda_3 r_0 = 3.5$ in the formula for m_π^2 and $fr_0 = 0.60,\ \Lambda_4 r_0 = 4.3$ in the formula for f_π.


Test of χPT logarithms on 8^3×16
fit to all points
skipped two heaviest points
$M_r/(2\mu_r)$
M_r
0
1
2
3
4
5
6
5
6
7
8


Test of χPT logarithms on 8^3×16
fit to all points
skipped two heaviest points
$f_\pi r_0$
M_r
0
1
2
3
4
5
6
0.6
0.7
0.8

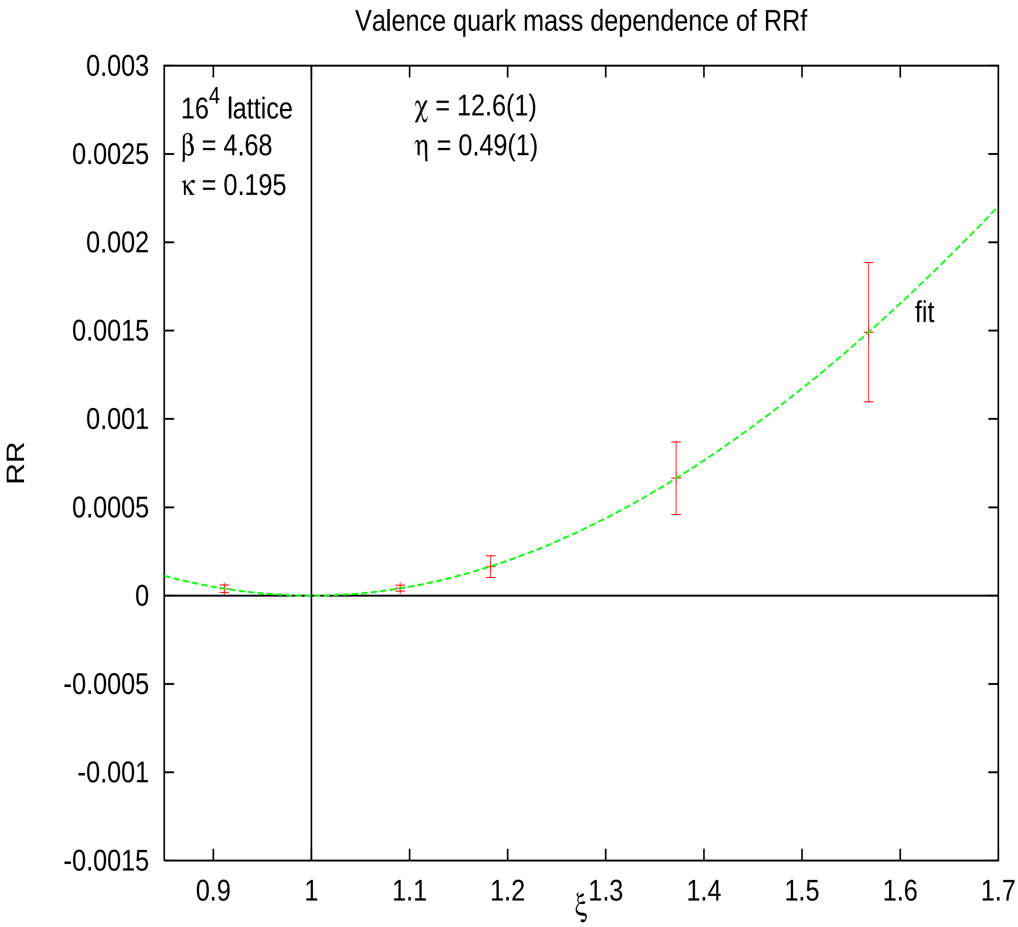
Valence quark mass dependence

PQChPT: (Sharpe-Shoresh, Rupak-Shoresh, ...)
Chiral logarithms also appear, for instance, in

$$RRf \equiv \frac{f_{VS}^2}{f_{VV} f_{SS}} = 1 + \frac{\chi_S}{64\pi^2} [\xi - 1 - \log(\xi)] + \cdots$$

where

$$\chi_S \equiv \frac{2B_0 m_q}{f_0^2} , \qquad \xi \equiv \frac{m_{Vq}}{m_{Sq}}$$



The PRELIMINARY value of the coefficient is close to the expectation: $\chi_S = 10(2)$.

Conclusion

- TSMB works fine for $m_{ud} \leq \frac{1}{5}m_s - \frac{1}{4}m_s$.

- The qualitative behaviour of chiral logarithms can be seen in the quark mass dependence of m_π^2 and f_π.

- The valence quark mass dependence also shows the chiral logarithms with the expected coefficients.

- For the quantitative determination of the Gasser-Leutwyler coefficients of ChPT one has to perform the limits $a \to 0$ and $\chi_S \to 0$.