Lattice QCD with a chiral twist (II)

Stefan Sint

UNIVERSIDAD AUTONOMA DE MADRID

Topics:

* B_K determination
* O(a) improvement
* Flavour breaking and its consequences
* Non-degenerate quarks, adding flavours

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Work done by a subset of the ALPHA Collaboration

- Petros Dimopoulos (University of Cyprus)
- Jochen Heitger (Universität Münster, Germany)
- Filippo Palombi (DESY Hamburg, Germany)
- Carlos Pena (CERN, Switzerland)
- Stefan Sint (Unversidad Autónoma de Madrid, Spain)
- Anastassios Vladikas (INFN Rome “Tor Vergata”, Italy)

The numerical simulations were (mostly) carried out on APE-1000 machines at DESY Zeuthen, Germany

An application to the computation of B_K

The B_K parameter is defined in QCD with dynamical u, d, s quarks:

$$\langle \bar{K}^0 | O^{\Delta S=2}_{(\mathrm{V-A})(\mathrm{V-A})} | K^0 \rangle = \tfrac{8}{3} F_K^2 m_K^2 B_K$$

The local operator

$$O^{\Delta S=2}_{(\mathrm{V-A})(\mathrm{V-A})} = \sum_{\mu} \left[\bar{s}\gamma_\mu (1-\gamma_5) d \right]^2$$

is the effective local interaction induced by integrating out the massive gauge bosons and t, b, c quarks in the Standard Model.

- only the parity-even part contributes to B_K

$$O_{(\mathrm{V-A})(\mathrm{V-A})} = \underbrace{O_{\mathrm{VV+AA}}}_{\mathrm{parity-even}} - \underbrace{O_{\mathrm{VA+AV}}}_{\mathrm{parity-odd}}$$

- Operator mixing problem with Wilson type quarks:

$$
\begin{aligned}
[O_{\mathrm{VV+AA}}]_{\mathrm{R}} &= Z_{\mathrm{VV+AA}}\Big\{O_{\mathrm{VV+AA}} + \sum_{i=1}^{4} z_i\ O_i^{d=6}\Big\} \\
[O_{\mathrm{VA+AV}}]_{\mathrm{R}} &= Z_{\mathrm{VA+AV}} O_{\mathrm{VA+AV}}
\end{aligned}
$$

$\Rightarrow$ parity-odd component renormalizes multiplicatively!

Question: Can we avoid the mixing problem by using the multiplicatively renormalized operator $O_{\mathrm{VA+AV}}$ to compute B_K?

- consider continuum theory for a light quark doublet ψ and the s-quark:

$$
\begin{aligned}
\mathcal{L}_f &= \bar{\psi}\left(D\!\!\!/ + m + i\mu_q\gamma_5\tau^3\right)\psi + \bar{s}\left(D\!\!\!/ + m_{\mathrm{s}}\right)s \\
\Rightarrow \quad O'_{\mathrm{VV+AA}} &= \cos(\alpha)O_{\mathrm{VV+AA}} - i\sin(\alpha)O_{\mathrm{VA+AV}} \\
&= -iO_{\mathrm{VA+AV}} \quad (\alpha = \pi/2)
\end{aligned}
$$

Maximally twisted light doublet ($\pi/2$ szenario)

- The operators are mapped to each other at “maximal twist” $\alpha = \pi/2 \Leftrightarrow m = 0$
- use Wilson quarks with a maximally twisted doublet and a standard s-quark

$$S_\mathrm{f} = a^4 \sum_x \{\bar{\psi}(x)(D_W + m_0 + i\mu_\mathrm{q}\gamma_5\tau^3)\psi(x) + \bar{s}(x)(D_W + m_{0,s})s(x)\}$$

$\Rightarrow$ simulations can get close to physical situation: mass degenerate u, d-quarks and a heavier s-quark

- HOWEVER:
  - benchmark results in lattice QCD usually performed for $m_s = m_d$
    $\Rightarrow$ zero mode problem is back for the s-quark
  - quenched approximation: quenched chiral log for $m_s \neq m_d$ (Sharpe ’95)

Mass degenerate (d, s) doublet ($\pi/4$ scenario)

Exchange the roles of s and u quarks, i.e. $\psi = (s, d)^T$:

- after the chiral rotation one then finds

$$\begin{aligned} O'_{\mathrm{VV+AA}} &= \cos(2\alpha) O_{\mathrm{VV+AA}} - i \sin(2\alpha) O_{\mathrm{VA+AV}} \\ &= -i O_{\mathrm{VA+AV}} \quad (\alpha = \pi/4) \end{aligned}$$

$\Rightarrow$ again the operators are mapped to each other provided $\alpha = \pi/4 \Leftrightarrow m = \mu_{\mathrm{q}}$

- can push down simultaneously d and s quark masses
- no zero modes (exceptional configurations): the u quark does not participate in correlation functions
- we know all finite renormalization constants and O(a) improvement coefficients which are necessary for the parameter tuning.

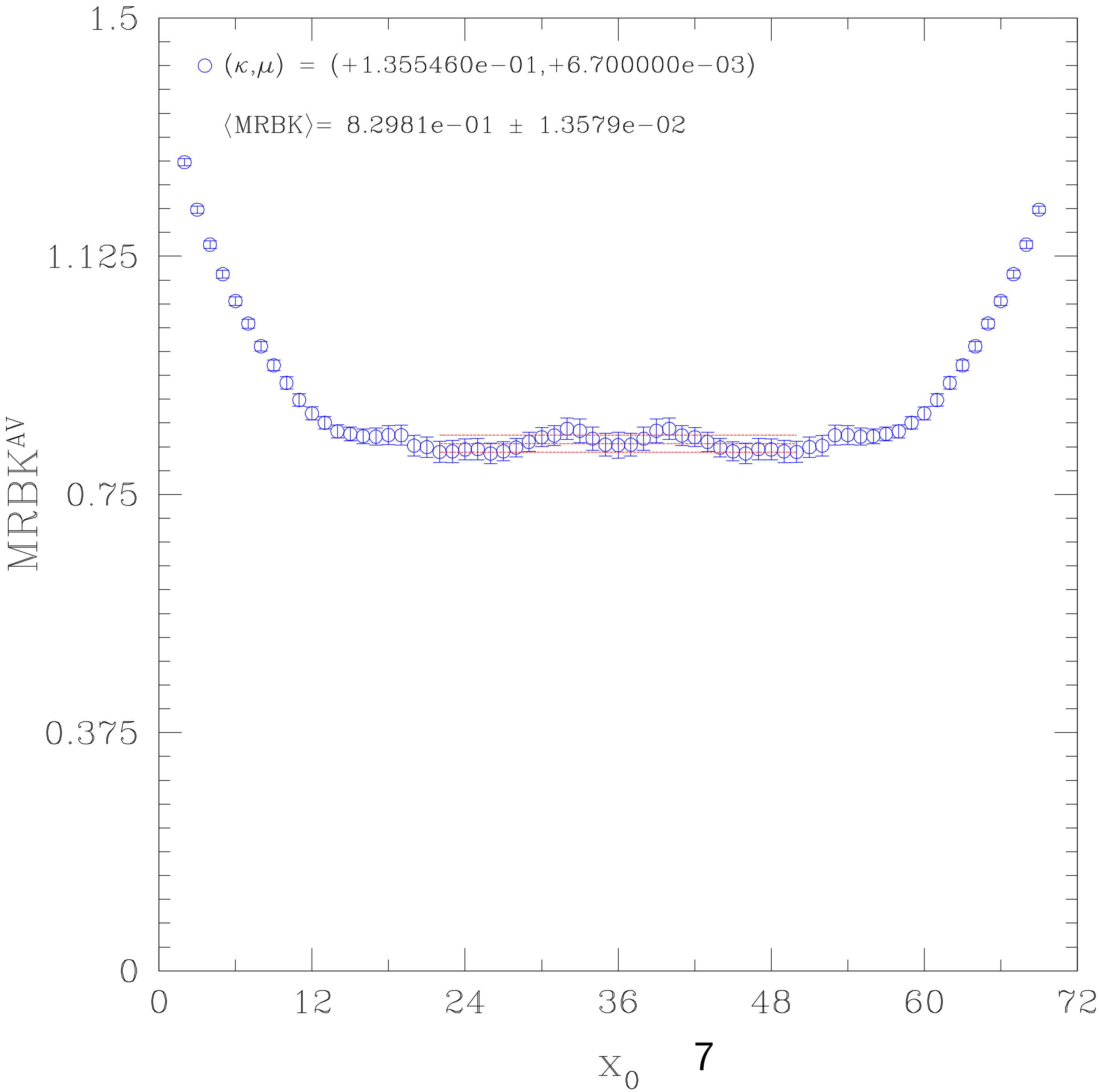
$\Rightarrow$ need to determine the multiplicative renormalization constant

A few simulation details

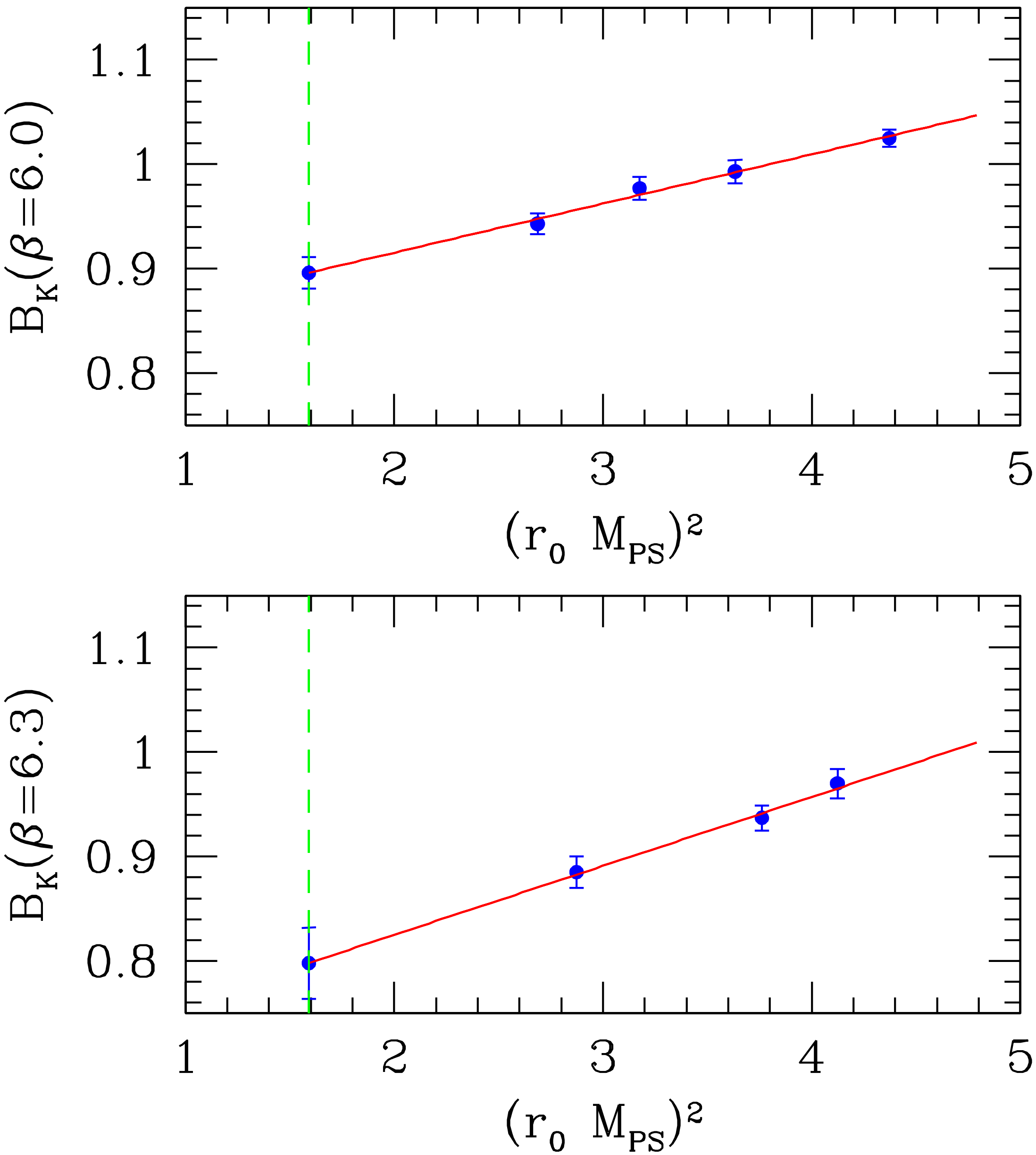
Use O(a) improved Wilson quarks with twisted mass term, standard Wilson plaquette action:

- 4-5 β-values $\in [6.0 - 6.45]$, corresponding to lattice spacings $a = 0.05 - 0.1$ fm (scale from $r_0 = 0.5$ fm)
- lattice volumes range from $16^3 \times 48$ to $32^3 \times 72$
- quark masses tuned to achieve $\alpha = \pi/2$ or $\alpha = \pi/4$ and pseudoscalar masses above or around m_K
- finite volume effects below statistical errors (checked at $\beta = 6.0$); At $\beta = 6.45$ the 32^3-lattice is too small $\Rightarrow$ small chiral extrapolation required even in $\pi/4$ case

Extract B_K directly from suitable ratios of correlation functions:

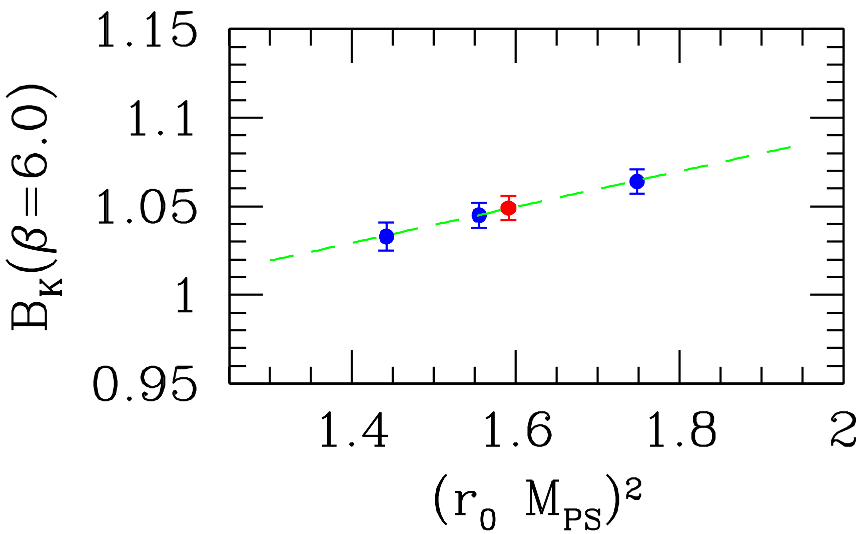


• $\pi/2$ case:

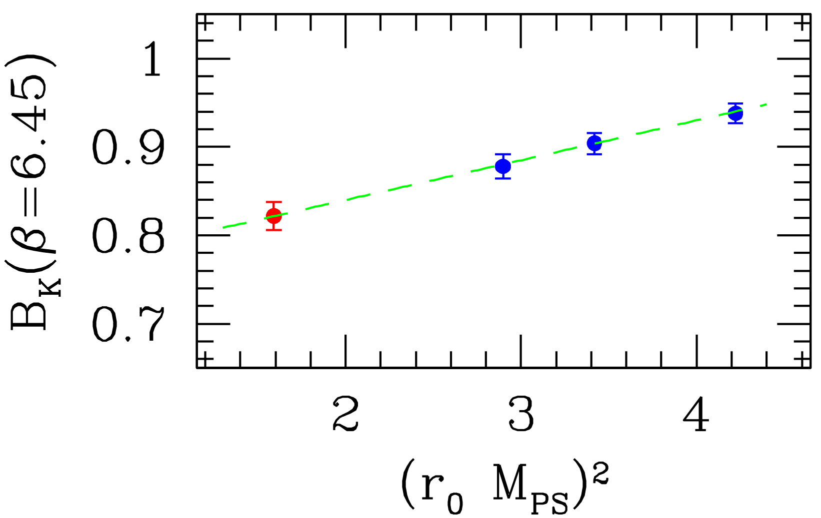


1.1
1
0.9
0.8
$B_K(\beta=6.0)$
1
2
3
4
5
$(r_0\ M_{PS})^2$
1.1
1
0.9
0.8
$B_K(\beta=6.3)$
1
2
3
4
5
$(r_0\ M_{PS})^2$

- $\pi/4$ case:

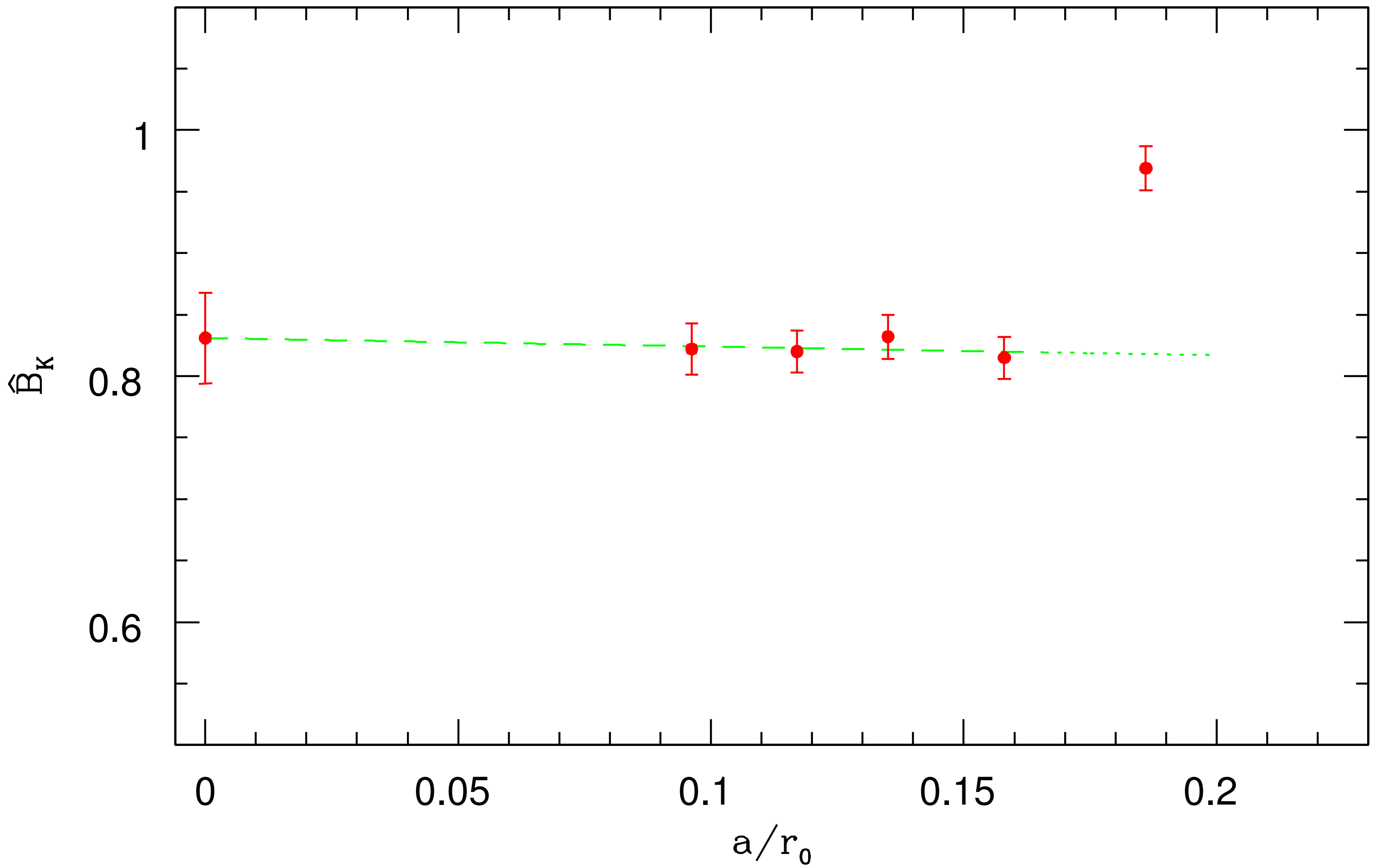


1.15
1.1
1.05
1
0.95
$B_K(\beta=6.0)$
1.4
1.6
1.8
2
$(r_0\ M_{PS})^2$

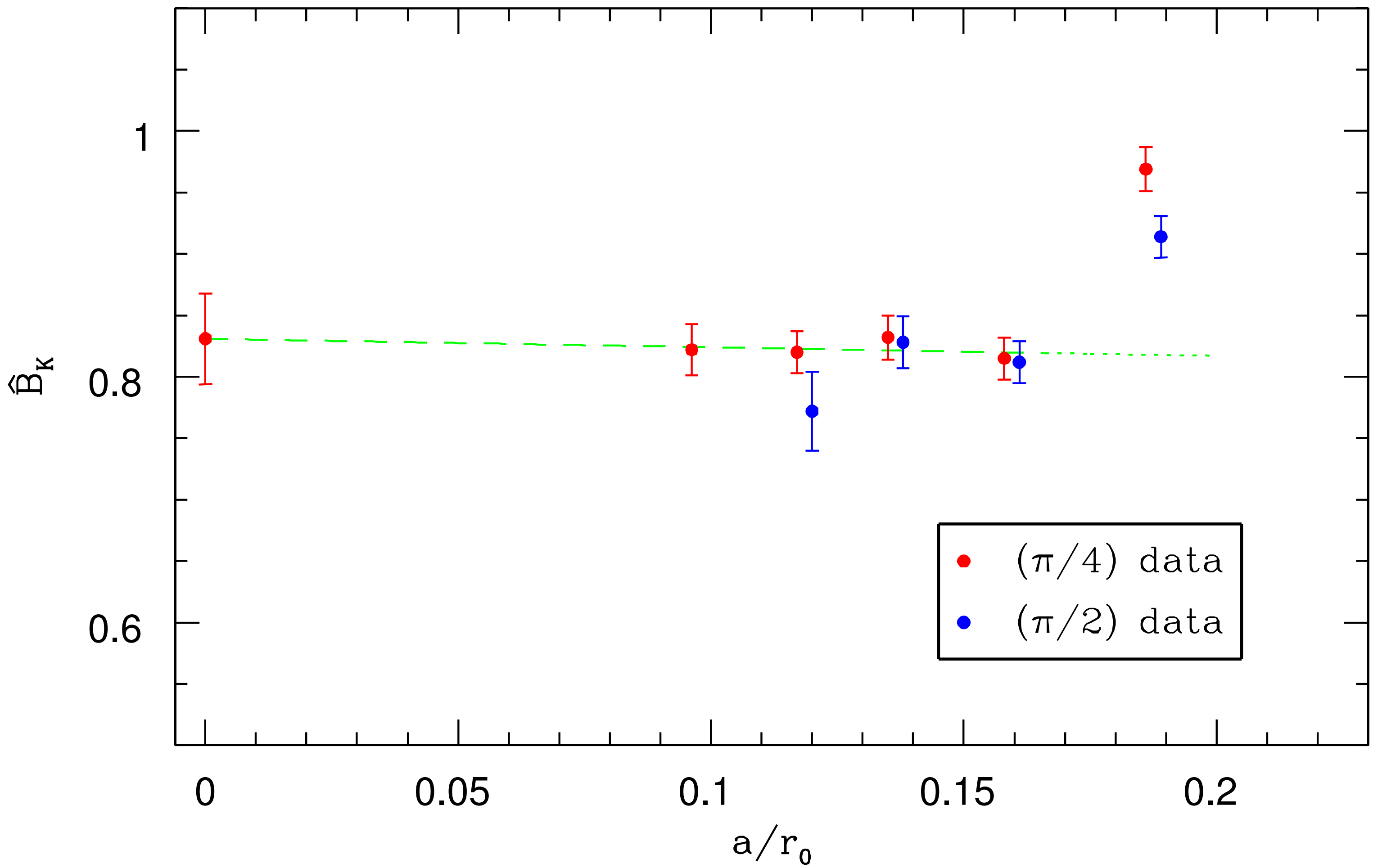


1
0.9
0.8
0.7
$B_K(\beta=6.45)$
2
3
4
$(r_0\ M_{PS})^2$

Continuum extrapolation of B_K ($\pi/4$ data):



(Preliminary) result: $\hat{B}_K = 0.834(37) \quad \Leftrightarrow \quad B_K^{\overline{\rm MS}}(2\,{\rm GeV}) = 0.604(27)$



Conclusions B_K

- We have performed a benchmark calculation of B_K in quenched model for QCD with controlled systematic errors:
  - finite size effects
  - excited states contributions (more complicated in tmQCD)
  - chiral interpolations/(small) extrapolations
  - non-perturbative renormalization
  - continuum extrapolation using 2 alternative formulations
  - SU(3) breaking: no dependence up to $(M_s - M_d)/(M_s + M_d) \approx 0.5$
- the (preliminary) total error meets the requirement (< 5 percent)
- compatible with results using other lattice regularisations (usually less controlled)
- Further progress requires dynamical quarks;

O(a) improvement

Recent interest in tmQCD mainly triggered by the observation of automatic O(a) improvement at maximal twist, $\alpha = \pi/2$ (Frezzotti & Rossi '03).

The argument only relies on Symanziks effective continuum theory:

- assume that we have tuned $m_{\rm PCAC} = 0$ i.e. the renormalized standard mass vanishes (up to O(a) effects)

- Symanziks effective continuum action is then given by

$$S_{\rm eff} = S_0 + aS_1 + O(a^2), \qquad S_0 = \int {\rm d}^4x \; \bar{\psi}(x) \left(\not{D} + i\mu_{\rm q}\gamma_5\tau^3 \right) \psi(x)$$

where S_0 is supposed to be regularised e.g. with Ginsparg-Wilson quarks on a much finer lattice, and S_1 is given by (afer using equations of motion)

$$S_1 = \int {\rm d}^4x \left\{ c\,\bar{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi + b_\mu\,\mu^2\bar{\psi}\psi \right\}$$

- cutoff dependence of lattice correlation function:

$$\langle O \rangle = \langle O \rangle^{\rm cont} - a\langle S_1 O \rangle^{\rm cont} + a\langle \delta O \rangle^{\rm cont} + O(a^2).$$

Here δO are the O(a) counterterms to the composite fields in O. Example:

$$O = V_\mu^1(x) P^2(y) \qquad \Rightarrow \quad \delta O = \left\{ c_{\rm v}\, i\partial_\nu T_{\mu\nu}^1(x) + b_{\rm v}\, \mu A_\mu^2(x) \right\} P^2(y)$$

- Introduce a $\gamma_5\tau^1$-transformation:

$$\psi \rightarrow i\gamma_5\tau^1\psi, \qquad \bar\psi \rightarrow \bar\psi\, i\gamma_5\tau^1$$

Under this transformation one has

$$\begin{array}{rcl} S_0 & \rightarrow & S_0 \\ S_1 & \rightarrow & -S_1 \\ O & \rightarrow & \pm O \quad \Rightarrow \quad \delta O \rightarrow \mp \delta O \end{array}$$

- Hence for $\gamma_5\tau^1$-even O one finds

$$\begin{aligned} \langle OS_1\rangle^{\rm cont} &= -\langle OS_1\rangle^{\rm cont} = 0 \\ \langle \delta O\rangle^{\rm cont} &= -\langle \delta O\rangle^{\rm cont} = 0 \\ \Rightarrow \quad \langle O\rangle &= \langle O\rangle^{\rm cont} + O(a^2) \end{aligned}$$

- while for $\gamma_5\tau^1$-odd O one gets

$$\begin{aligned} \langle O\rangle^{\rm cont} &= -\langle O\rangle^{\rm cont} = 0 \\ \langle OS_1\rangle^{\rm cont} &= \langle OS_1\rangle^{\rm cont} \\ \langle \delta O\rangle^{\rm cont} &= \langle \delta O\rangle^{\rm cont} = 0 \\ \Rightarrow \quad \langle O\rangle &= -a\langle OS_1\rangle^{\rm cont} + a\langle \delta O\rangle^{\rm cont} + O(a^2) \end{aligned}$$

$\Rightarrow$ $\gamma_5\tau^1$-even observables are automatically O(a) improved, while $\gamma_5\tau^1$-odd observables vanish up to O(a) terms.

Remarks:

- The $\gamma_5\tau^1$-symmetry corresponds to the physical flavour symmetry:

$$\psi' \to -i\tau^2\,\psi', \qquad \bar{\psi}' \to \bar{\psi}'\,i\tau^2.$$

  A similar argument based on parity has been given by Shindler

- A^a_μ and P^a have opposite $\gamma_5\tau^1$-parity!

$$\Rightarrow \qquad \langle \partial_\mu A^1_\mu(x) O_{\mathrm{even}} \rangle = 2\,\underbrace{m_{\mathrm{PCAC}}}_{\mathrm{O}(a)}\,\underbrace{\langle P^1(x) O_{\mathrm{even}} \rangle}_{\mathrm{O}(a)} = O(a^2)$$

  i.e. the critical mass is only defined up to O(a)

- in the O(a) improved theory one can determine m_{cr} up to an O(a^2) ambiguity but this requires a mixed source, and it depends on c_{A}.

- The O(a) ambiguity in $m_{\rm cr}$ does not spoil O(a) improvement: a shift in $m_c r$ by $a\Lambda^2$ corresponds to an insertion of the $\gamma_5\tau^1$-odd operator $\bar\psi\psi \Rightarrow$ O(a^2) effect in $\gamma_5\tau^1$-even correlators

- finite space time volume: there is no phase transition, no spontaneous symmetry breaking and analyticity in the quark mass parameters

$\Rightarrow$ massless Wilson quarks in a finite volume are automatically O(a) improved!

- infinite volume: the twisted mass $\mu_{\rm q}$ drives spontaneous chiral symmetry breaking. If it becomes too small, this is not true any more and the system realigns the vacuum state $\Rightarrow$ χPT (cf. S. Sharpe's lecture). This is beyond the scope of the Symanzik expansion, where the form of S_0 determines the symmetry breaking

- At small μ cutoff effects may formally still be O(a^2) but can be large ("bending phenomenon"), depending on the chosen definition of $m_{\rm cr}$: (Aoki & Bär, Sharpe & Wu, Sharpe, Frezzotti et al.)

- Use χPT and a "good" definition of $m_{\rm cr}$ (from pion physics) to control chiral extrapolations (Aoki & Bär, Sharpe & Wu, Sharpe) O(a) improvement of the action may also help

A few figures taken from A. Shindler's review at Lattice 2005

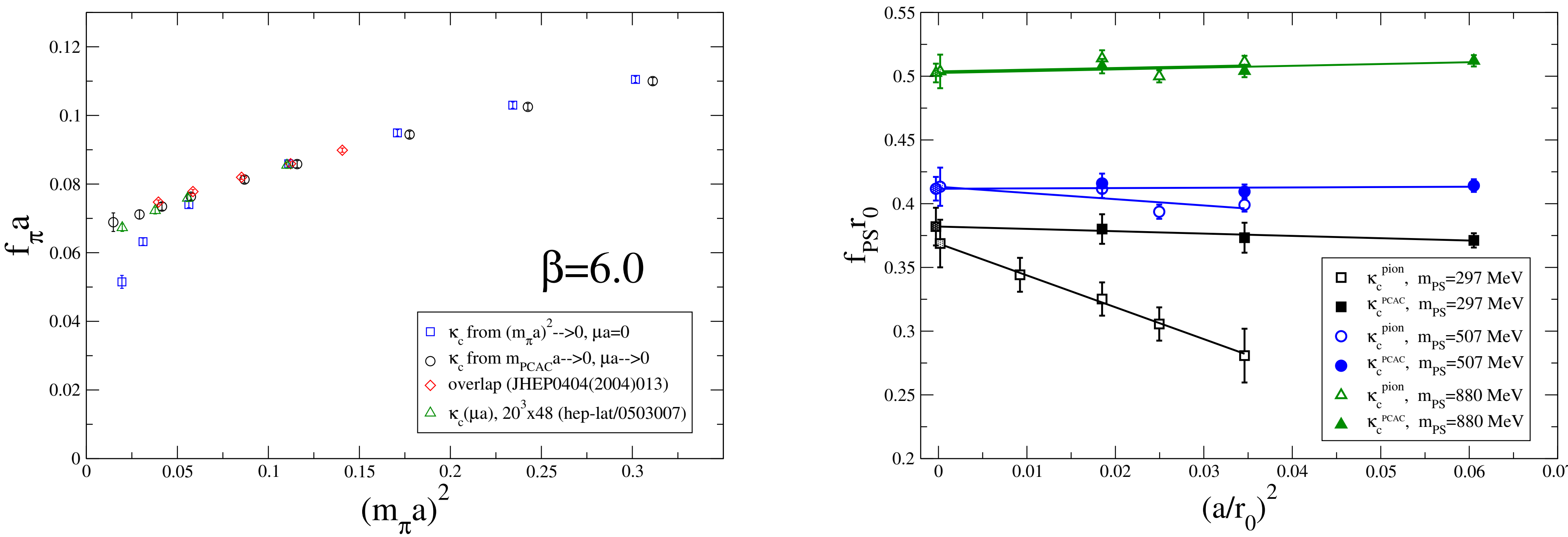


Figure 1: Left figure: comparison of the chiral behaviour at fixed lattice spacing ($\beta = 6.0$) of the pseudoscalar decay constant computed using method **A**, **B**, **C** and with results obtained with overlap fermions. Right panel: unconstrained continuum limit, for several values of fixed charge pion masses, of $r_0 f_{\rm PS}$ performed using method **A** and **C** to determine the critical mass.

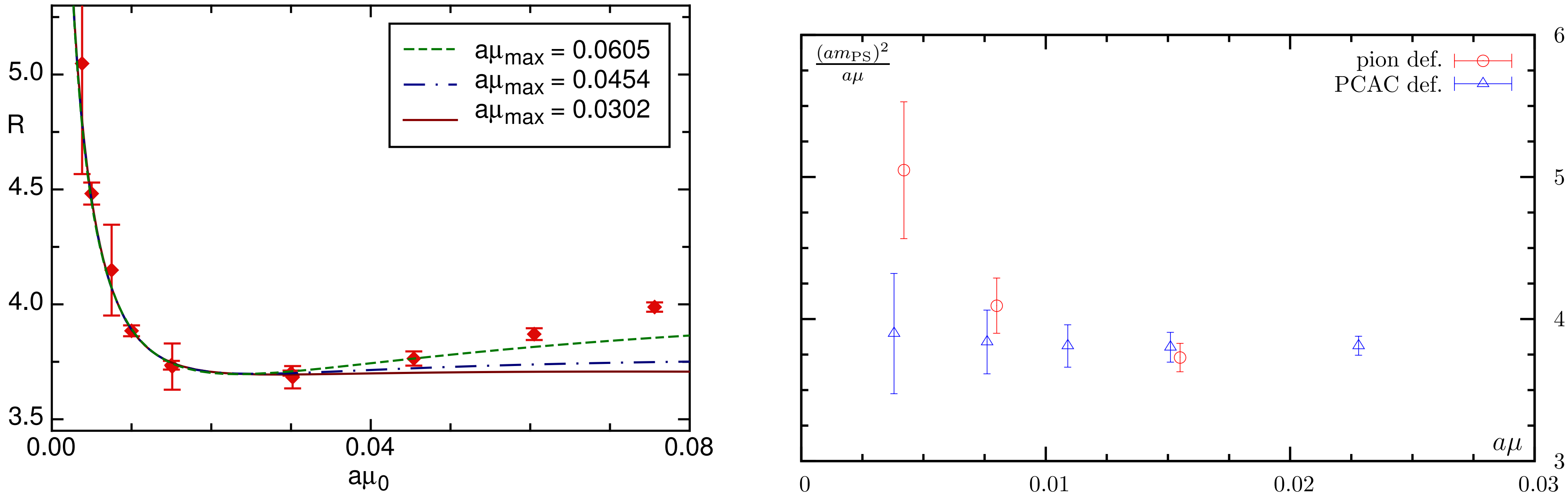


Figure 2: Left panel: bending phenomenon at β=6.0 on the ratio $R = \frac{a^2 m_{\rm PS}^2}{a\mu}$ and its description with χPT. Right panel: comparison of the ration R using method **A** and **C** to determine the critical mass.

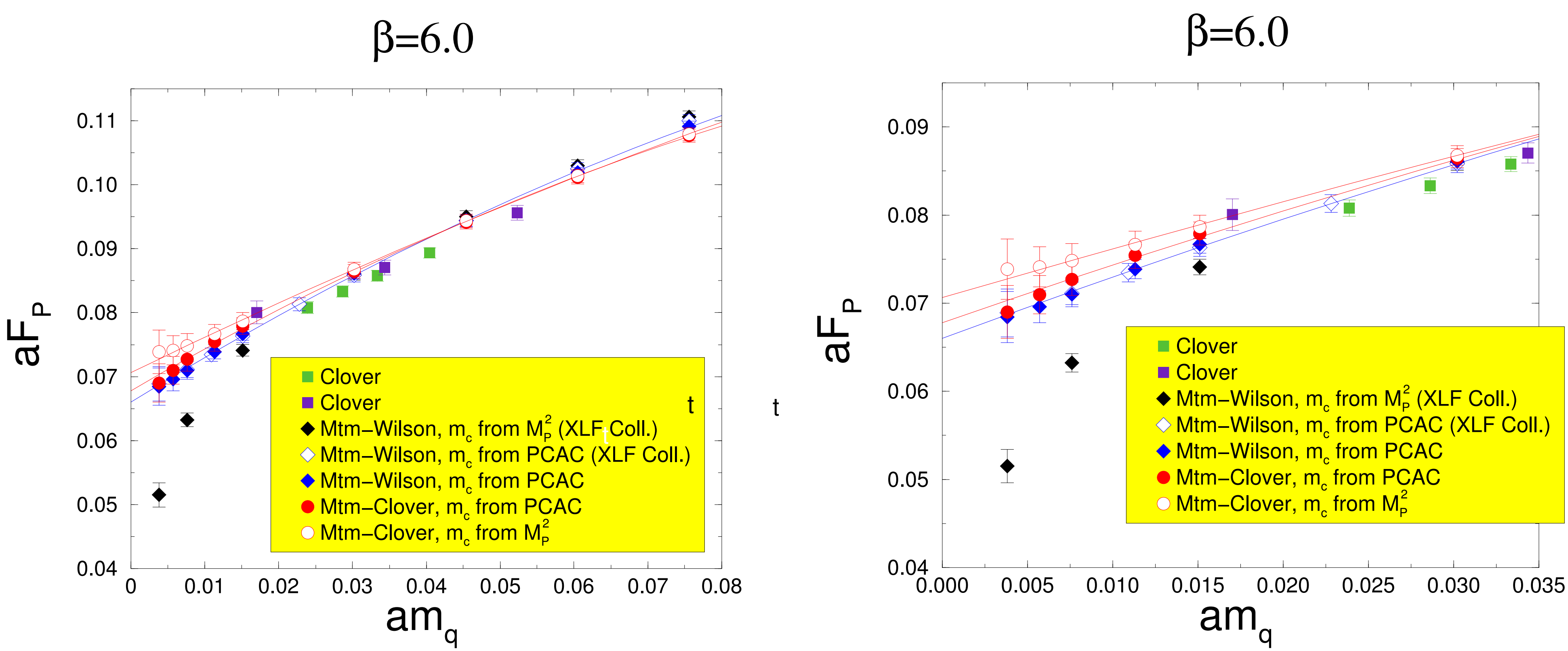


Figure 3: Comparison of the chiral behaviour at fixed lattice spacing ($\beta = 6.0$) of the pseudoscalar decay constant computed using method **A** and **C** for both tmQCD and non-perturbatively improved tmQCD.

Parity and flavour breaking

- mass splitting of flavour multiplets

- excited states analysis at fixed a must deal with all states of given *lattice quantum numbers*:

  - isosinglet scalar states in the neutral pion channel
  - can add a zero momentum neutral pion to any state without changing the lattice quantum numbers
  - not a problem if we are interested in pion states; possibly reduces the gap to the next excited states

  $\Rightarrow$ make your lattice a bit longer in the time direction

  - more difficult are states with *smaller* energy/mass than the state of interest

  $\Rightarrow$ requires multi state analysis (to disentangle e.g. isoscalar glueball from neutral pion state etc.)

- Flavour-parity breaking requires the computation of disconnected diagrams in some flavour non-singlet channels, in particular for the neutral pion (signal?)

Pion mass splitting

- maximal twist: only charged pions are Goldstone particles; expect a splitting

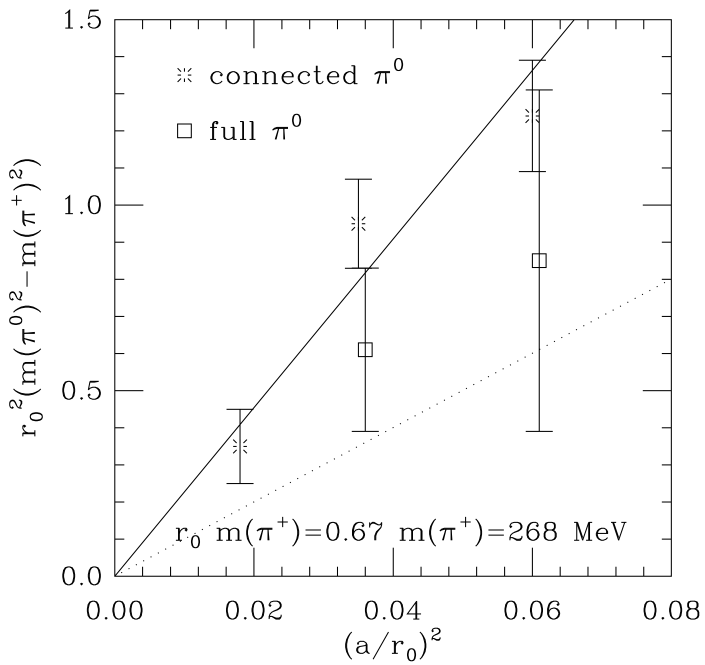
- technical complication: disconnected diagrams in neutral pion correlation function (recall that $P'^3 = i\frac{1}{2}S^0$ at $\alpha = \pi/2$)

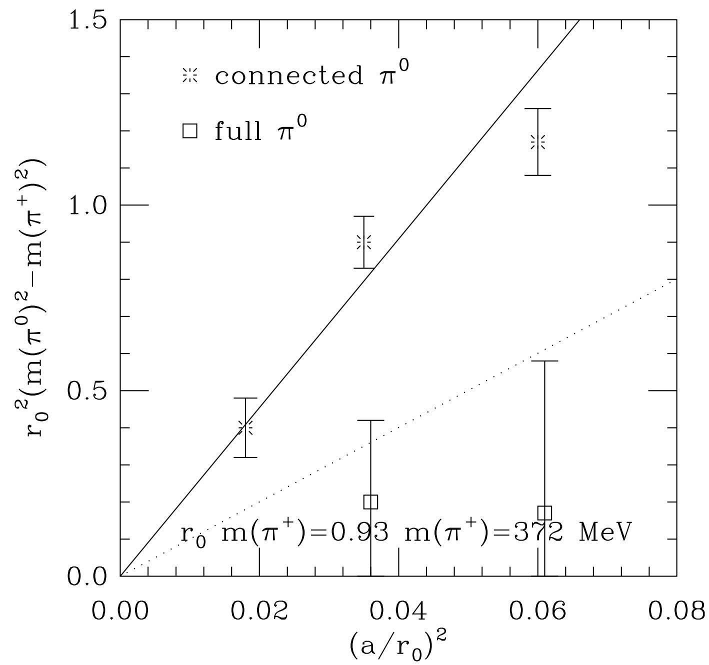
$$\begin{aligned} G_{\pi^0}(x-y) &= \langle S^0(x) S^0(y) \rangle \\ &= \langle -\mathrm{tr}\{S(x,y)S(y,x)\} + \mathrm{tr}\{S(x,x)\}\,\mathrm{tr}\{S(y,y)\}\rangle_G \end{aligned}$$

- quenched study by Jansen et al. (XLF collaboration) ,`hep-lat/0507032`;

  determine the masses for

  - the complete correlation function
  - only the connected part (with interpretation as "Osterwalder-Seiler" regularization of two-flavour QCD.





Re-interpretation

- introduce a second quark doublet χ with the same mass parameters as ψ

$\Rightarrow$ expect $N_{\rm f} = 4$ mass degenerate quark flavours in the continuum limit

- at maximal twist and at finite a there are
  - 8 conserved axial currents $\Rightarrow$ 8 Goldstone particles
  - 7 neutral pions are only approximate Goldstone particles, 3 of which are degenerate with the neutral pion of the first doublet, and 4 are obtained with connected diagrams only!

- splittings are found to be quite large in quenched approximation; parameterising

$$r_0^2(m_{\pi^0}^2 - m_{\pi^\pm}^2) \simeq c(a/r_0)^2$$

  one finds $c \approx 10$ (total propagator) and $c \approx 23$ (connected parts only)

- situation is comparable to staggered fermions: $c \approx 40$ for naive staggered fermions (Wilson gauge action) (Ishizuka et al.'94) and $c \approx 10$ for improved staggered fermions (Aubin et al '04);

  however, there is much more chiral symmetry!

Kaon mass splittings

- R. Lewis reported at Lattice 2005 on results for the kaon splitting `hep-lat/0509056`

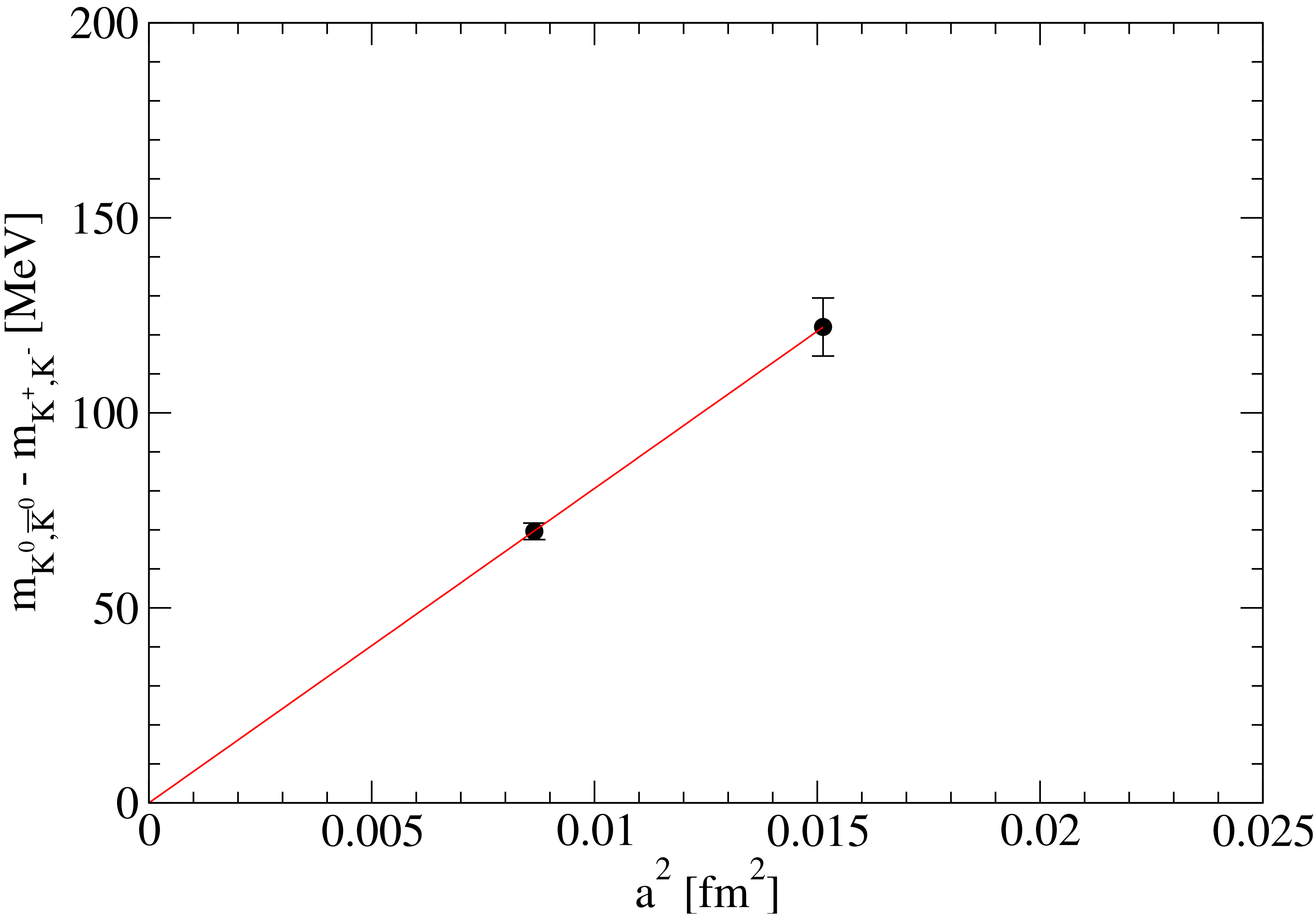
⇒ should be directly comparable to connected contributions discussed for the pions (just call members of second doublet strange and charm)

- at $a = 0.1\,\mathrm{fm}$ the neutral kaon is about $80MeV$ heavier than the charged kaons

- Within B_K project, $\pi/2$ scenario (O(a) improved action, standard O(a) improved s-quark, O(a) improved mass parameters tuned to achieve $s-d$ degeneracy up to O(a^2):

⇒ find smaller splittings 10-20 MeV, e.g.

$$\beta = 6.0: \qquad aM_{\mathrm{PS}}^{ss} = 0.3015(12), \quad aM_{\mathrm{PS}}^{sl} = 0.3053(11), \quad aM_{\mathrm{PS}}^{ll} = 0.2976(11)$$



200
150
100
50
0
0
0.005
0.01
0.015
0.02
0.025
a^2 [fm^2]
m_{K^0,\bar{K}^0} - m_{K^+,K^-} [MeV]

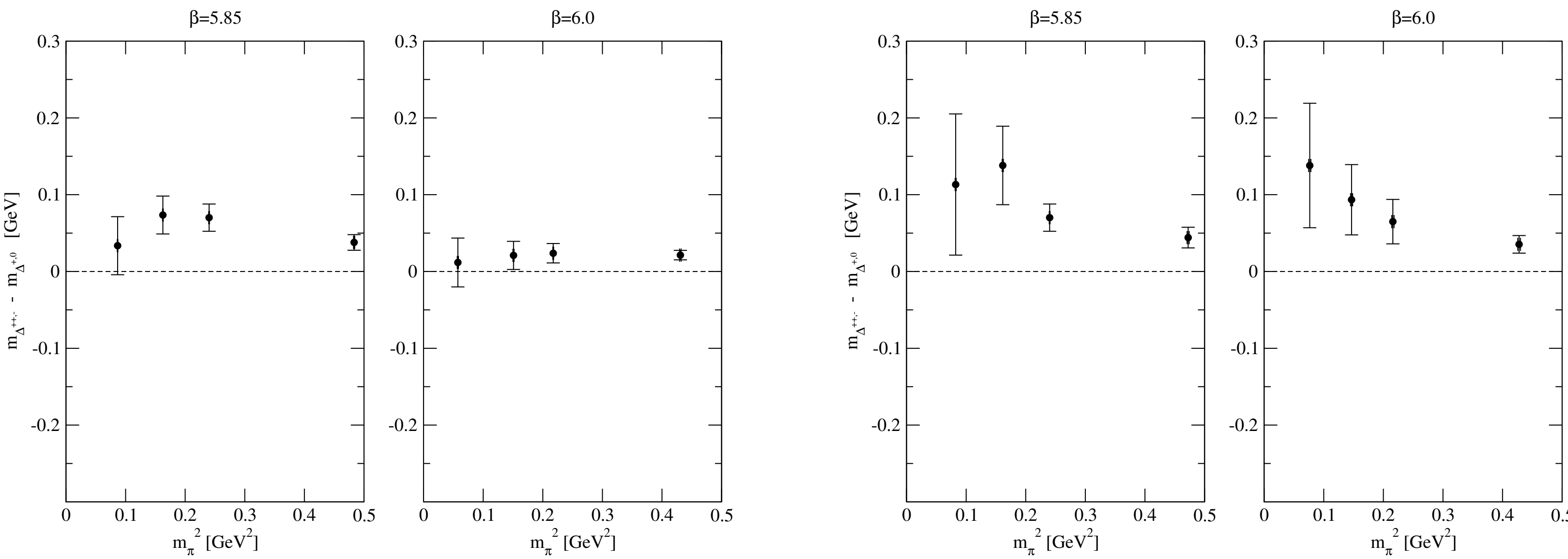
Mass splitting within the nucleon Δ-resonances

- Quenched study by Abdel-Rehim, Lewis, Woloshin `hep-lat/0503007`;
  advantage: no disconnected diagrams

- Recall from particle data book:

$$\Delta^{++} = uuu, \quad \Delta^{+} = uud, \quad \Delta^{0} = udd, \quad \Delta^{-} = ddd,$$

  is a $S = 0, I = 3/2$ isospin quadruplet, e.g. the $\Delta(1232)$ with spin/parity $3/2^{+}$



left two figures: m_{cr} from the pion

right two figures: m_{cr} from parity restoration

- I think errors are still too large to draw conclusions

Non-degenerate quarks and additional flavours

- twisted mass QCD is formulated for 2 mass degenerate quarks; good approximation for up and down
- is it possible to make the doublet non-degenerate?
- how can be introduce the strange and charm quarks?
- Consider (Frezzotti,Rossi '04))

$$\mathcal{L}_f = \bar{\psi}\left(\not{D} + m + i\mu_{\rm q}\gamma_5\tau^3 + \Delta m\tau^1\right)\psi$$

$\Rightarrow$ physical quark masses are

$$M_{\pm} = \sqrt{m^2 + \mu_{\rm q}^2} \pm \Delta m$$

- no zero modes:

$$\begin{aligned} & \det\left(D_W + m_0 + i\mu_{\rm q}\gamma_5\tau^3 + \Delta m\tau^1\right) \\ = \quad & \det\left(Q^2 + \Delta m(D_W - D_W^\dagger) + \mu_{\rm q}^2 - \Delta m^2\right) \neq 0 \quad \text{if } \mu_{\rm q}^2 > \Delta m^2 \end{aligned}$$

- renormalized mass parameters:

$$\Delta m_{\rm R} \quad = \quad Z_{\rm S}^{-1}\Delta m, \qquad \mu_{\rm R} = Z_{\rm P}^{-1}\mu_{\rm q} \Rightarrow |\Delta m_{\rm R}| < (Z_{\rm P}/Z_{\rm S})\mu_{\rm R}$$

$\Rightarrow$ probably a weak restriction at maximal twist (value of Z_P/Z_S depends on details of the regularisation, $\rightarrow 1$ at weak coupling)

- observations:

1. $\gamma_5\tau^1\left(D_W + m_0 + i\mu_{\rm q}\gamma_5\tau^3 + \Delta m\tau^1\right)$ is hermitian, i.e. the determinant is real

2. at $\Delta m = 0$ the determinant is positive; by continuity it remains positive for $\Delta m \neq 0$.

$\Rightarrow$ HMC simulations possible with $N_{\rm f} = 2$ mass-nondegenerate light quarks!

- propagator computation has to deal with 2×2 flavour structure explicitly

First simulations are being carried out (K. Jansen, I. Montvay et al.) for $N_{\rm f} = 2 + 1 + 1$, i.e. a degenerate light doublet and a non-degenerate strange-charm doublet

Warnings:

- O(a^2) splittings between pions in the 4-flavour case are large!

- for the strange-charm doublet one needs some fine tuning for the strange quark: $m_s = 100\,\mathrm{MeV}, \quad m_c = 1300\,\mathrm{MeV}$ is obtained as

$$m_s = (700 - 600)\,\mathrm{MeV}, \qquad m_c = (700 + 600)\,\mathrm{MeV}$$

- One needs to be careful not to count the charm degree of freedom twice ($\rightarrow B_K$)

Conclusions

- Cutoff effects are found to be small in B_K quenched, despite incomplete O(a) improvement

$\Rightarrow$ precision result for B_K in quenched QCD

- $N_\mathrm{f} = 2$ twisted mass QCD at maximal twist is O(a) improved.

- O(a^2) effects may become large as the twisted mass decreases due to competition of cutoff effects with the mass term

$\Rightarrow$ can be controlled by chiral perturbation theory (perfectly suited for this task)

- O(a^2) flavour symmetry violations can be large, especially in the 4-flavour set-up.

- Adding a standard O(a) improved Wilson s-quark to an O(a) improved twisted mass doublet, the kaon mass splittings seem much smaller!

$\Rightarrow$ Question: Does the O(a) improved action reduce some of these a^2 errors?