Results from Lattice QCD simulations with a twisted mass

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ECT* Workshop - 2nd October 2006

Increased reliability of lattice computations mainly due to the possibility of simulating light quark masses in realistic situations

Remaining dominant systematic uncertainties:

Cost ~ $(L/a)^5(am_q)^{-2}$

- 'Chiral' extrapolation:
  from m_π = 300 - 500 MeV to m_π^{phys}= 139 MeV, ($m_q \sim m_\pi^2$)

- Continuum extrapolation
  - see expected scaling behavior as the lattice spacing $a \to 0$,
  - different regularizations must agree.

- Lattice Perturbative calculations
(needed for matching with continuum)

Summary

1. $N_f = 2$ Lattice QCD simulations with light dynamical twisted mass quarks.

2. Chiral Perturbation Theory for the lattice (Finite Volume ChPT; Wilson-ChPT).

3. $N_f = 2 + 1 + 1$ simulations.

4. Mixed Actions: chiral fermions on a tmQCD sea.
   ⇒ talk by Oliver Bär.

Simulations with light dynamical quarks

Algorithmic improvements for Wilson fermions

1. Domain Decomposition + multiple time scales
[Lüscher Comput.Phys.Comm 165 (2005)]

2. Mass preconditionig (Hasenbusch trick)+ multiple time scales
[Urbach et al. Comput.Phys.Comm 174 (2006)]

3. RHMC + multiple pseudofermions
[Clark, Kennedy hep-lat/0608015]

Performances are comparable at the same simulation point (Wilson gauge + Wilson fermions β=5.6, V=24^3x32).

Great news if compared to the sad perspective after the Berlin Lattice conference (2001).

Still physical point is far:
other improvements are needed

Light dynamical quarks with Twisted Mass QCD

[Alpha JHEP0108:058,2001]

$$D_{\rm cont} = m_q + e^{i\gamma_5\tau_3\alpha}\ \gamma_\mu\nabla_\mu$$

$$D_{\rm lattice} = m_q + e^{i\gamma_5\tau_3\alpha}\left(\frac{1}{2}\gamma_\mu\left[\nabla_\mu^{\rm forw} + \nabla_\mu^{\rm back}\right] - a\frac{1}{2}\nabla_\mu^{\rm f}\nabla_\mu^{\rm b} + m_{\rm crit}\right)$$

$$D_{\rm tm} = m_0 + i\mu\tau_3\gamma_5 + \tfrac{1}{2}\gamma_\mu\left[\nabla_\mu^{\rm f} + \nabla_\mu^{\rm b}\right] - a\tfrac{1}{2}\nabla_\mu^{\rm f}\nabla_\mu^{\rm b}$$

- $\det[D_{tm}]=\det[D_w^2+\mu^2]$ => protection against small eigenvalues; affordable computational cost.
- $m_0 = m_{crit}$ => O(a) improvement for hadron masses, matrix elements, form factors, decay constants. [Frezzotti, Rossi 2004]
- Simplifies mixing problems for renormalization.

- New flavor breaking terms.
- O(a) Improvement requires a determination of m_{crit}

-> Big improvement over Wilson fermions adds on top of Algorithmic improvements

Lattice QCD simulations with dynamical quarks

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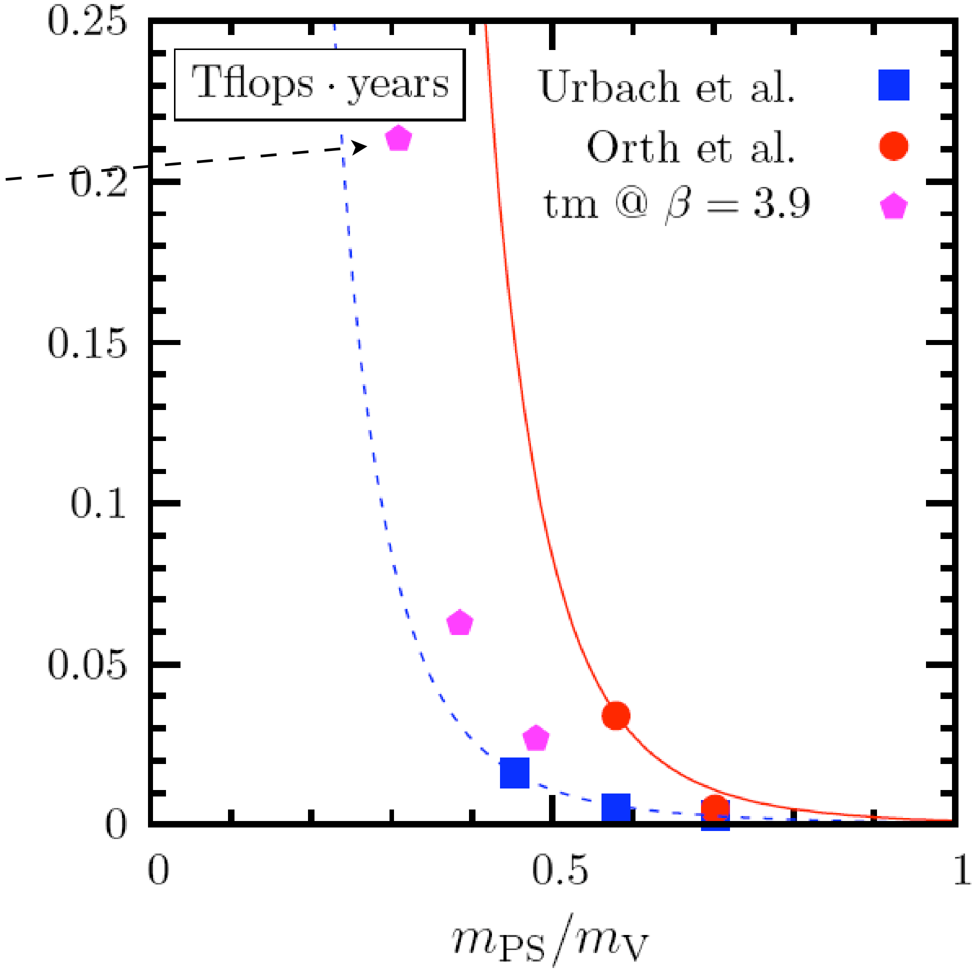
<u>Plan</u>:
- 3 lattice spacings (0.075 - 0.125 fm)
- Pion masses in range 250 - 500 MeV
- Lattice Volumes larger than 2 fm.

Recent simulation points (ETMC)

N_f=2

β	μ	L^3xT	a [fm]	m_π [MeV]	#meas
3.9	0.0040	24^3x48	~0.095	~280	1811
	0.0064	24^3x48		~350	1507
	0.0085	24^3x48		~400	1533
	0.0100	24^3x48		~440	1232
	0.0150	24^3x48		~535	1000
	0.0040	32^3x64		-	therm
4.05	0.0030	32^3x64	~0.075	~270	955
	0.0060	32^3x64		~380	104
	0.0080	32^3x64		-	therm
	0.0100	32^3x64		-	therm

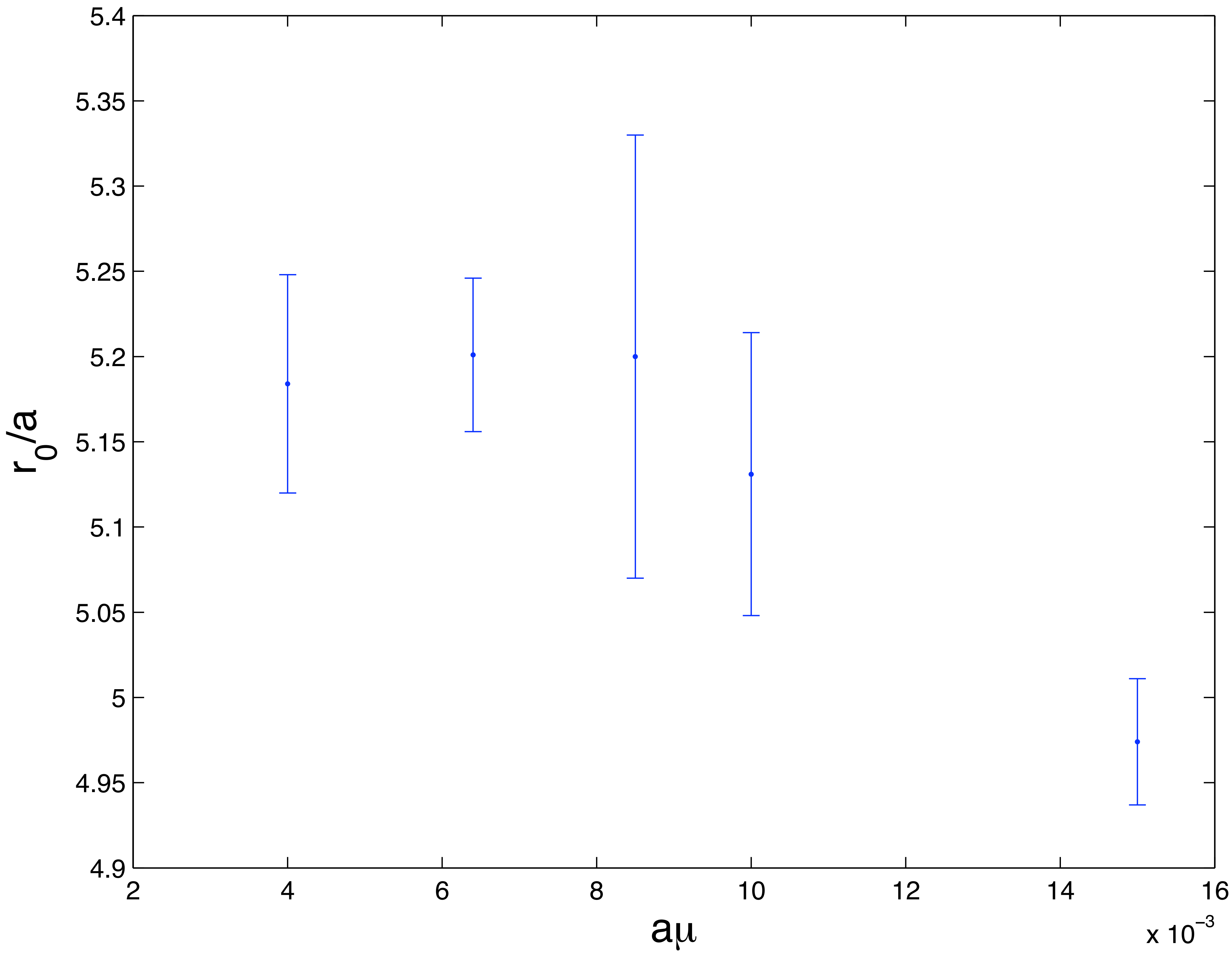


For how many years you need a Teraflop machine to produce 1000 independent gauge configurations at a given point

Scale set by r_0 (surprisely constant with μ)

Simulations performed in:
Jülich BGL; QCDOC; APENext Roma + Zeuthen; Münich Altix; MareNostrum

Setting the scale

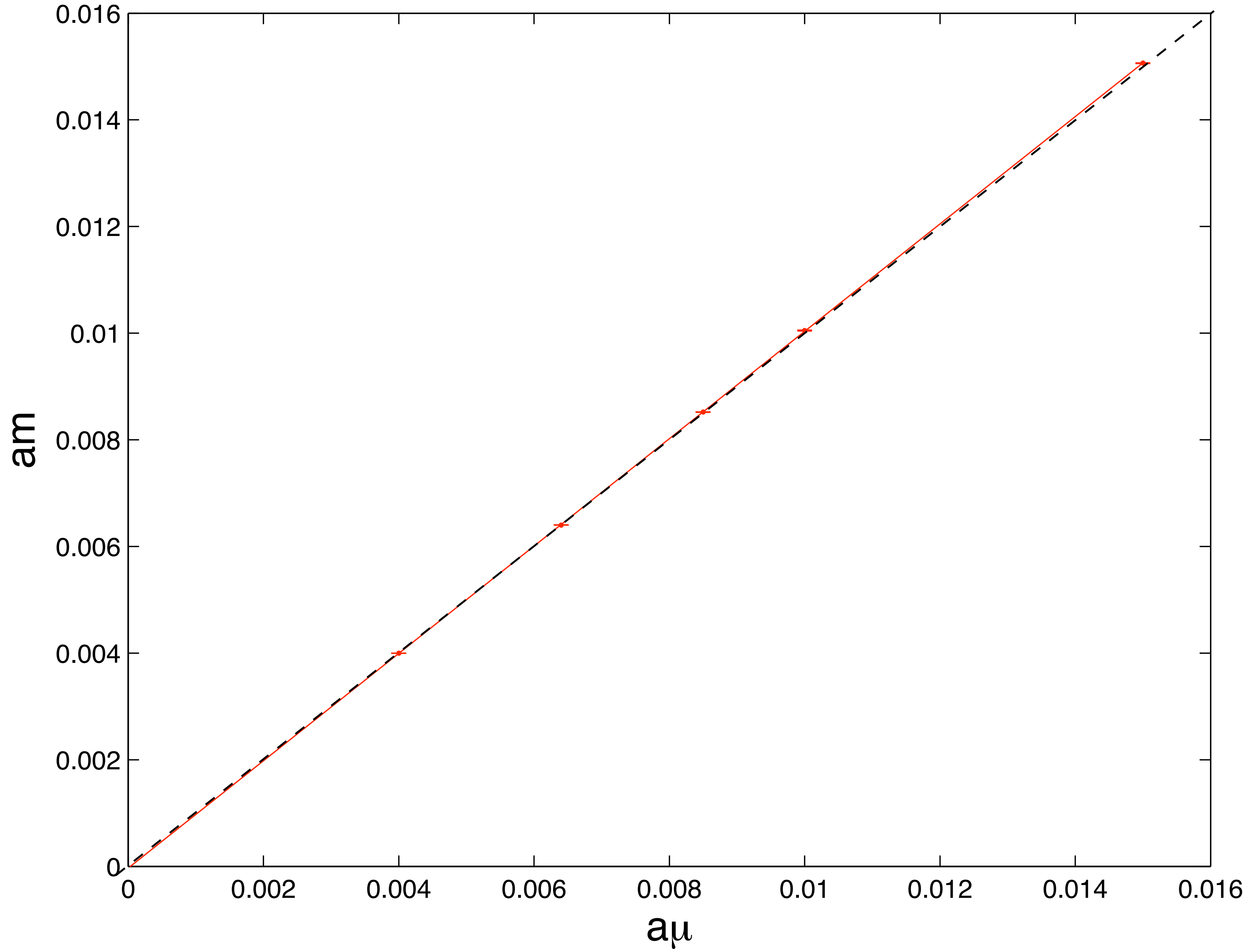


$\beta=3.9$
$V=24^3\times48$

r_0/a quite constant with μ (does not need to be)

Full twist

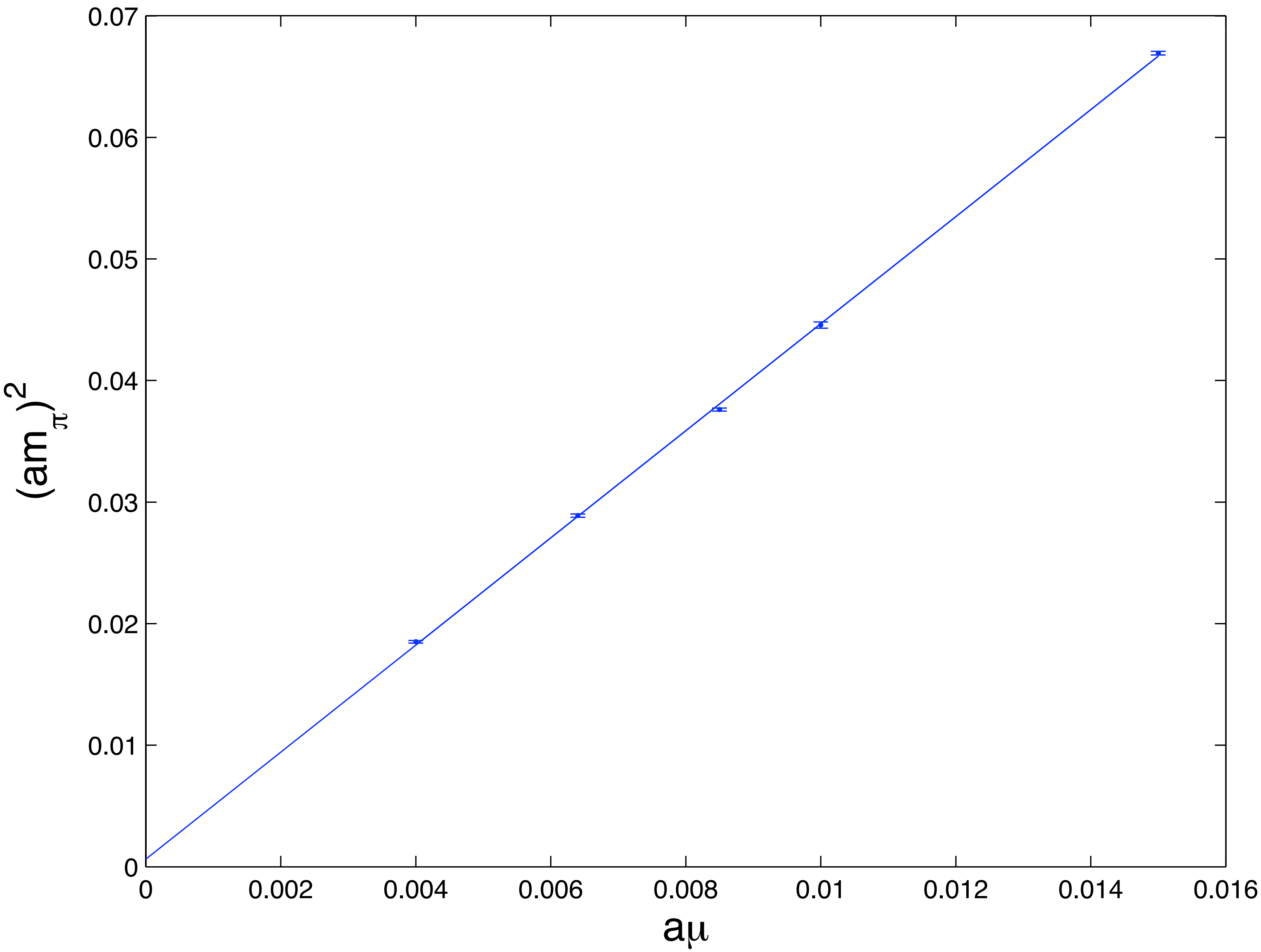
=> *O(a)* Improvement



β=3.9
V=24³x48

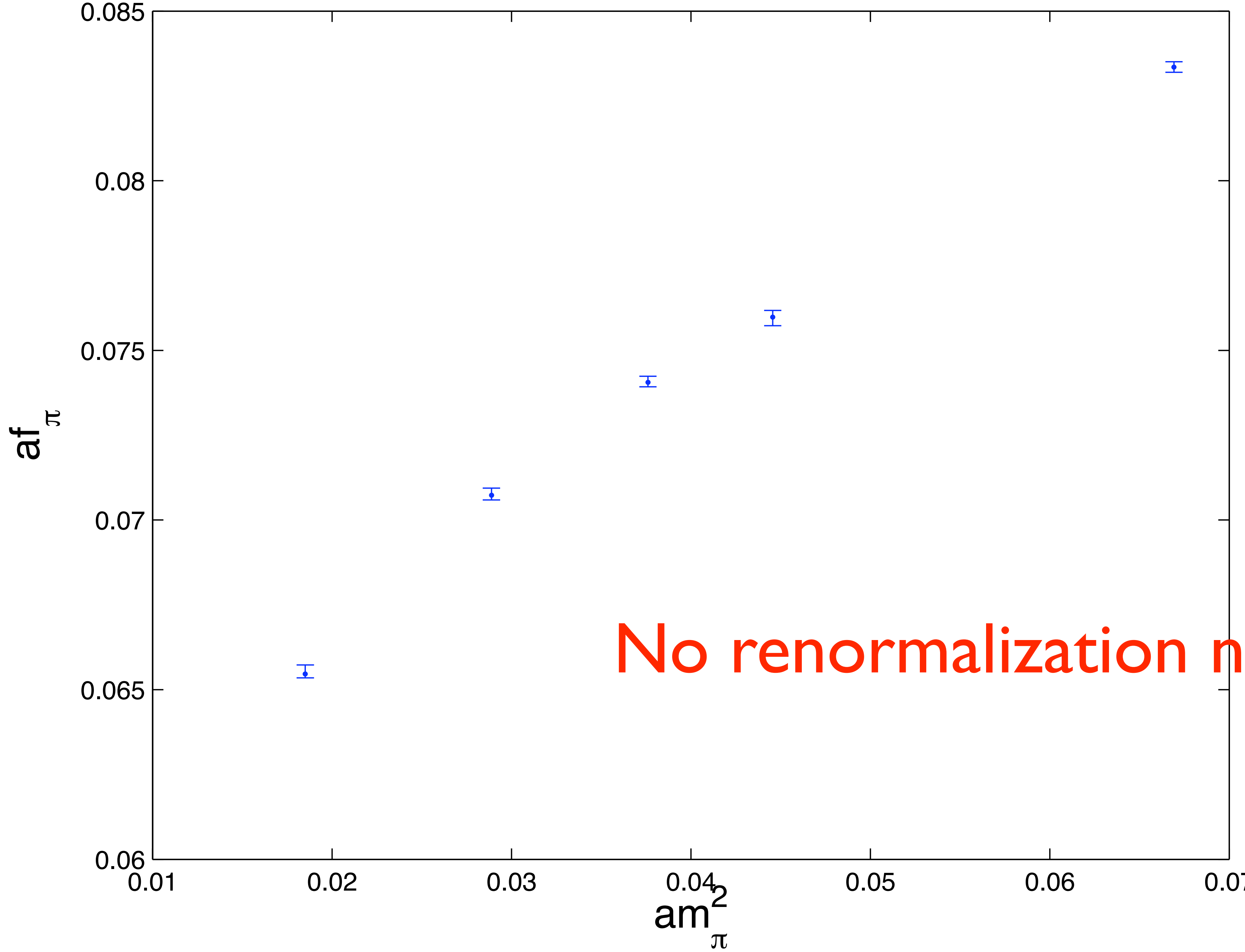
$$am = \sqrt{(Z_A\, am_{\mathrm{PCAC}}^{\mathrm{untwisted}})^2 + (a\mu)^2} \qquad (Z_A = 1)$$

Pion mass (aM_π) vs. quark mass $a\mu$



$\beta=3.9$
$V=24^3\times48$

Pion decay constant (aF_π) vs. Pion mass (aM_π)



β=3.9
V=24^3x48

No renormalization needed !!

Of course we need to set the scale and extrpolate to physical M_π => ChPT

Unquenched configurations are ready:

Many other physical results to come soon!!

Chiral Perturbation Theory

Chiral Perturbation Theory [Weinberg '79, Gasser-Leutwyler '84]

By Goldstone theorem: if $m_q=0$, the spectrum has a set of massless modes parametrized by the cosets manifold: $\Sigma \in [SU(N_f)_L \times SU(N_f)_R] / SU(N_f)_V$

If m_q, E, p << Λ_{QCD} ~ 1 GeV, Dynamics essentially given by the almost massless modes above.

- Write the most general lagrangian preserving the full symmetry (one unknown coefficient $\forall$ invariant term).

- Add symmetry breaking terms, which transform as the mass terms.

- Expand in powers of m_q and p. At LO:

$$\mathcal{L}_2 = \frac{F^2}{4} Tr(\partial_\mu \Sigma \partial^\mu \Sigma^\dagger) - \frac{F^2 B}{2} Tr(m\Sigma^\dagger + \Sigma m^\dagger)$$

- Very successful phenomenological approach.
- Lattice QCD can in principle predict the unknown coefficients (at LO F,B, at NLO L_i)
- ChPT provides analytical functions essential to fit lattice data.

Cutoff Chiral Perturbation Theory

Finite Volume ChPT (*IR cutoff*)

relevant for us p-regime: $M_\pi L >> 1$ (see also ϵ-regime: $M_\pi L < 1$)

2 approaches:

- Lüscher '86
- Gasser, Leutwyler '87

combining both approaches: Colangelo, Dürr, Haefeli Nucl.Phys.B721 (2005)

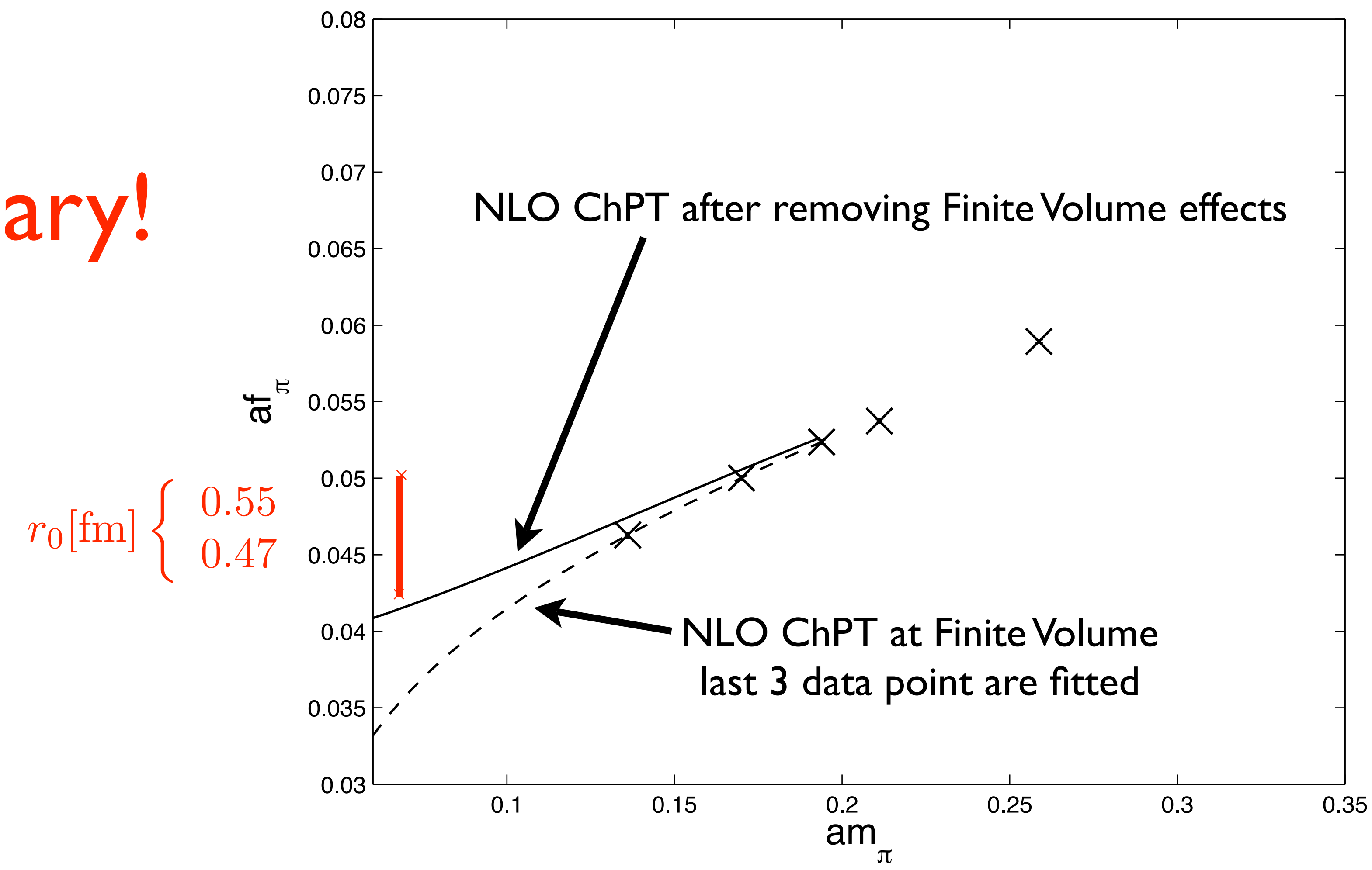
ChPT with lattice artifacts (*UV cutoff*) (Wilson-ChPT)

- introduced: Sharpe, Singleton '98
- developed: Rupak, Shoresh'02 and Bär'03, Aoki'03
- extended to tmQCD: Sharpe, Wu; L.S;Münster,Schmidt,Scholz;Aoki, Bär.'04
- extended to staggered: Sharpe, Lee '99; Bernard,Aubin,Wang
- recent review Sharpe hep-lat/0607016

ChPT with Finite Volume corrections

Corrections from ChPT [Gasser, Leutwyler '87]
NLO ChPT fit

Preliminary!



Caveat 1. Large error on the physical point due to r0 indetermination
Caveat 2. Better assessment of finite size effects. (Colangelo, Dürr, Haefeli Nucl.Phys.B721 (2005))
Caveat 3. No continuum extrapolation yet.
Caveat 4. Note: we assume here a=a(β).

ChPT with lattice artifacts (W-ChPT)

The problem: the path from the lattice to continuum ChPT is quite long...

$$\mathcal{L}^{\text{lattice}}_{\text{QCD}} = -\frac{1}{g_0^2}\mathrm{tr}U_P + \bar{\psi}_l(x)\left[\frac{1}{2}\overleftrightarrow{\nabla\!\!\!/} - r\frac{a}{2}\nabla^\star\cdot\nabla + m_0\right]\psi_l(x)$$

↓

$$\mathcal{L}^{\text{Symanzyk}}_{\text{QCD}} = -\frac{1}{2}\mathrm{tr}F^2_{\mu\nu} + \bar{\psi}(D\!\!\!\!/ + m)\psi + \underline{c_{\text{sw}}a\bar{\psi}i\sigma_{\mu\nu}F_{\mu\nu}\psi} + O(am, a^2)$$

↓

$$\mathcal{L}^{\text{continuum}}_{\text{QCD}} = -\frac{1}{2}\mathrm{tr}F^2_{\mu\nu} + \bar{\psi}(D\!\!\!\!/ + m)\psi \longrightarrow \mathcal{L}^{\text{continuum}}_{\text{ChPT}}$$

... but we can divide it into steps

$$\mathcal{L}^{\text{lattice}}_{\text{QCD}} = -\frac{1}{g_0^2}\mathrm{tr}U_P + \bar{\psi}_l(x)\left[\frac{1}{2}\overleftrightarrow{\nabla\!\!\!/} - r\frac{a}{2}\nabla^\star\cdot\nabla + m_0\right]\psi_l(x)$$

$\downarrow$

$$\mathcal{L}^{\text{Symanzyk}}_{\text{QCD}} = -\frac{1}{2}\mathrm{tr}F^2_{\mu\nu} + \bar{\psi}(D\!\!\!/ + m)\psi + \underline{c_{\text{sw}}a\bar{\psi}i\sigma_{\mu\nu}F_{\mu\nu}\psi} + O(am, a^2) \longrightarrow \mathcal{L}^{\text{lattice}}_{\text{ChPT}}$$

$\downarrow$

$$\mathcal{L}^{\text{continuum}}_{\text{QCD}} = -\frac{1}{2}\mathrm{tr}F^2_{\mu\nu} + \bar{\psi}(D\!\!\!/ + m)\psi \longrightarrow \mathcal{L}^{\text{continuum}}_{\text{ChPT}}$$

Lattice-Chiral Perturbation Theory [Sharpe and coll.'98]

Include lattice artifacts

- Leading Order $a\bar{q}\sigma_{\mu\nu}F^{\mu\nu}q$ which transforms like a mass term $m\bar{q}q$

Near the continuum: $a\Lambda_{QCD} << 1$

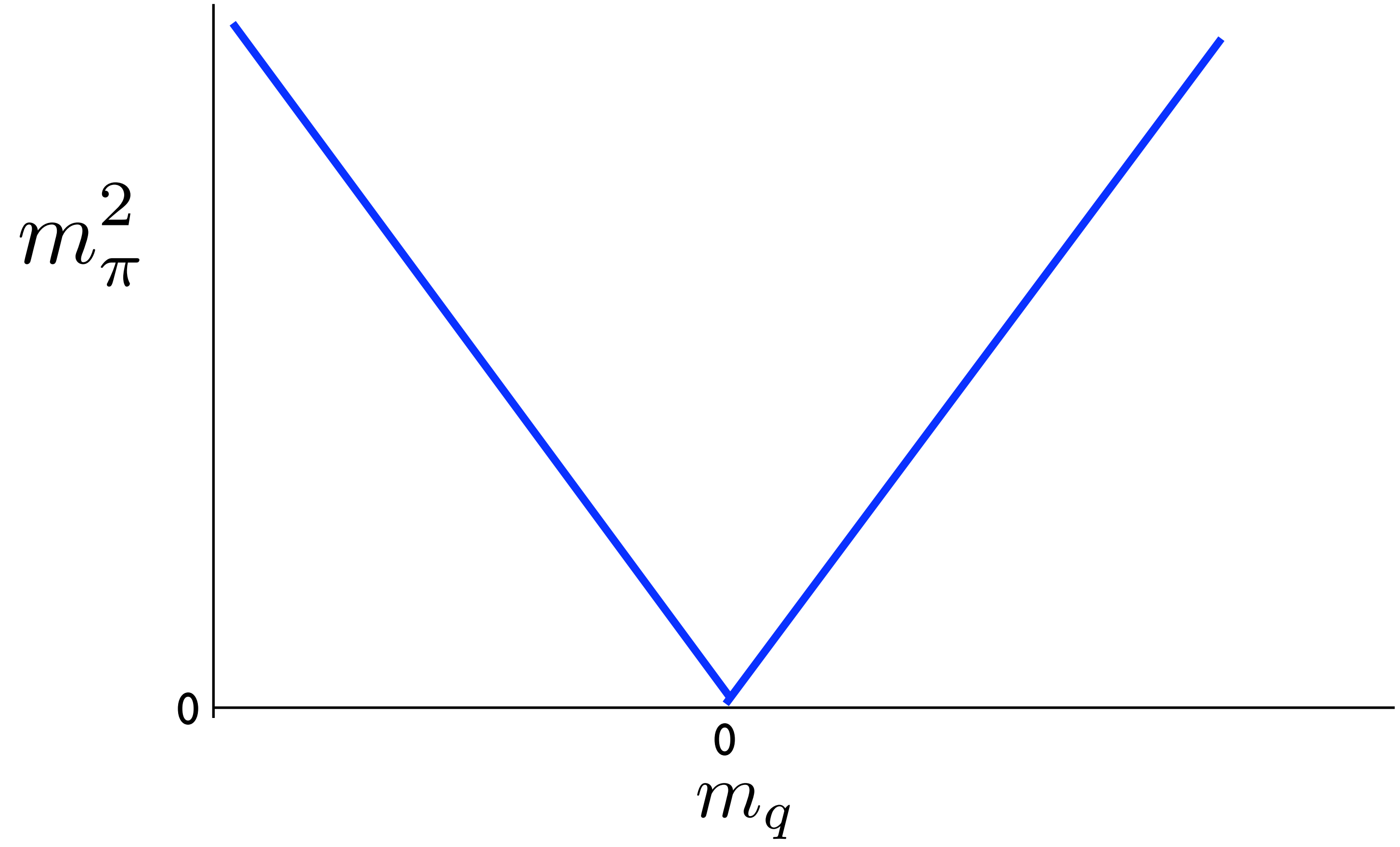
$$\mathcal{L}_2 = \frac{F^2}{4}Tr(\partial_\mu\Sigma\partial^\mu\Sigma^\dagger) - \frac{F^2 B}{2}Tr(m\Sigma^\dagger + \Sigma m^\dagger) - \frac{F^2 W}{2}Tr(a\Sigma^\dagger + \Sigma a^\dagger)$$

- Interesting part is actually a Next to Leading Order.
- At NLO, besides L_i 's, we must introduce also W_i 's.
- The W_i 's depend on the lattice action and on the definitions of the currents.

Is that useful?

Consider the relation between the mass of the *Goldstone modes* m_π and *quark* mass m_q <u>in the continuum.</u>

Gell-Mann Oakes Renner (LO ChPT): $$m_\pi^2 = 2B_0|m_q|$$

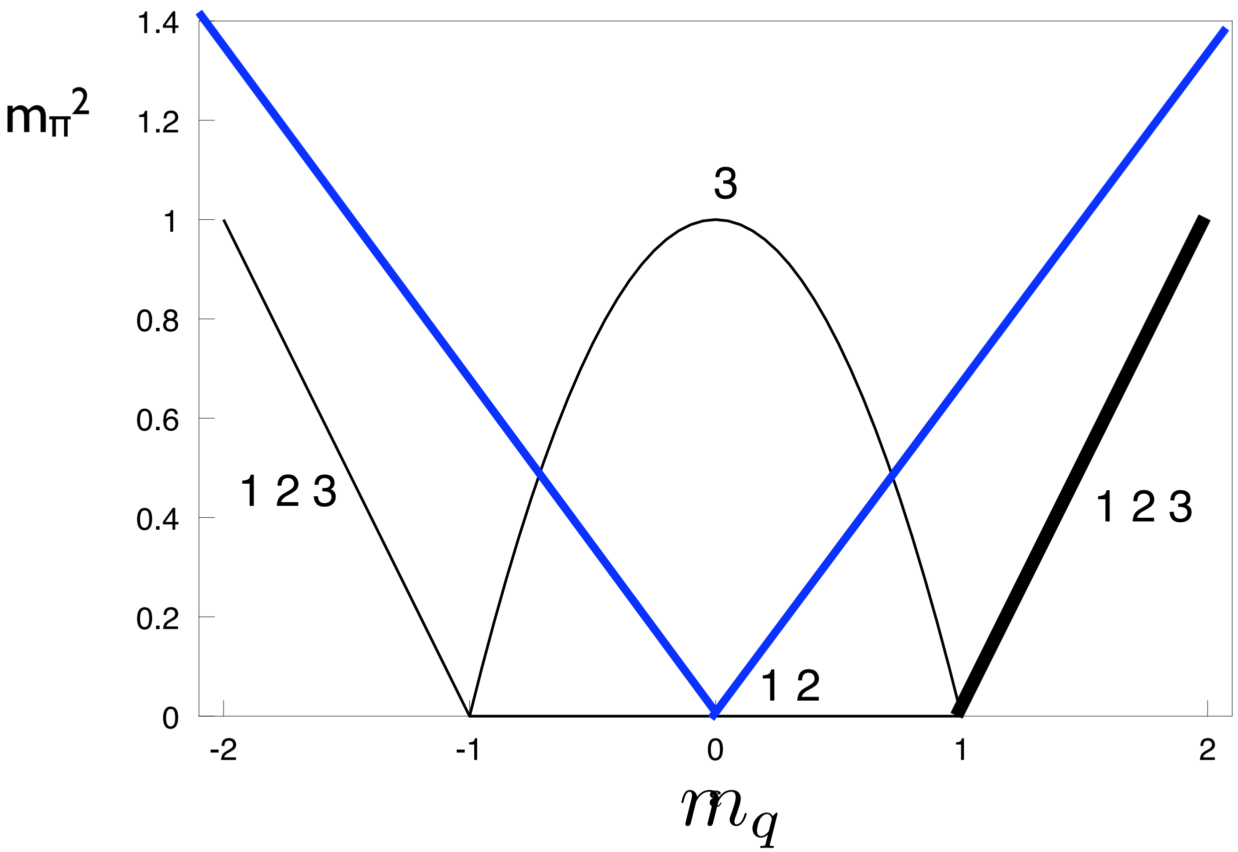


Is that useful?

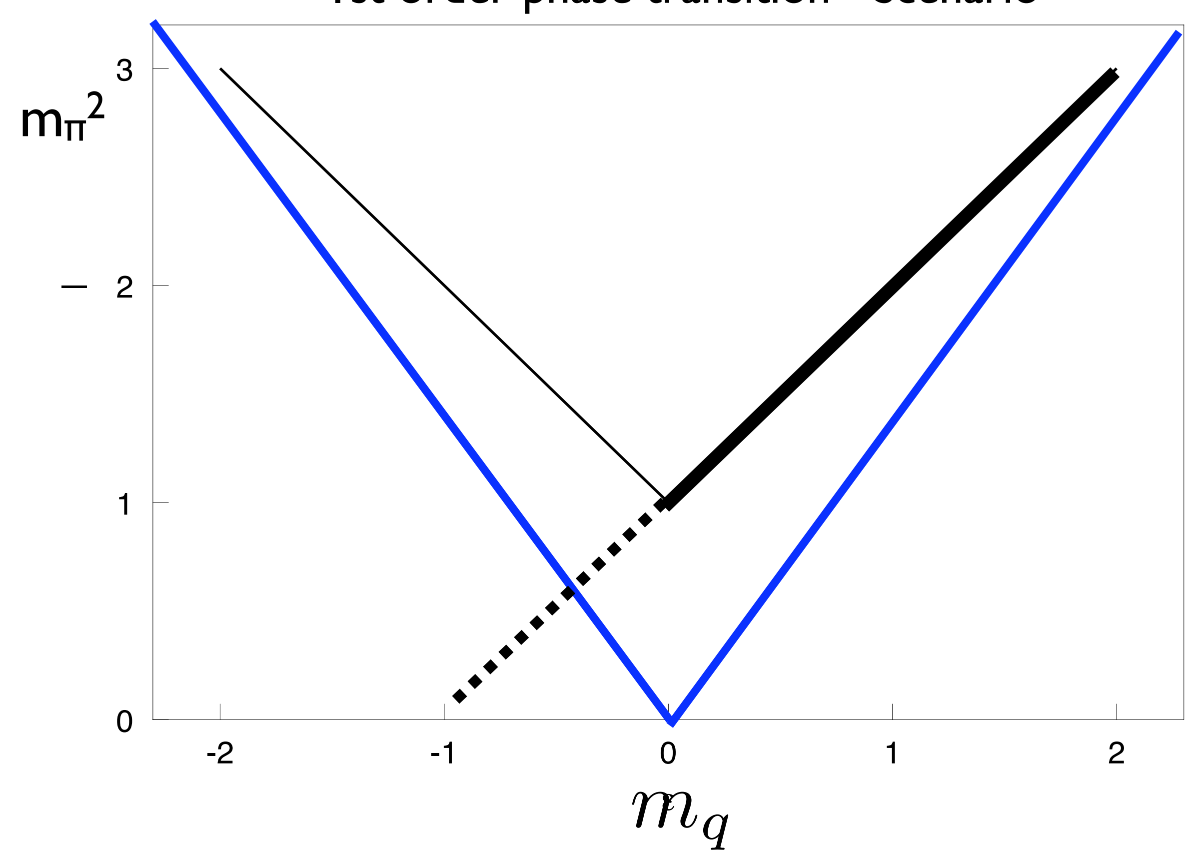
The <u>Phase structure</u> of QCD near m_q=0 is modified by lattice artifacts

Sharpe Singleton '98: Lattice modified Gell-Mann Oakes Renner: $m_\pi^2 = 2B_0|m_q|$

Aoki - Scenario

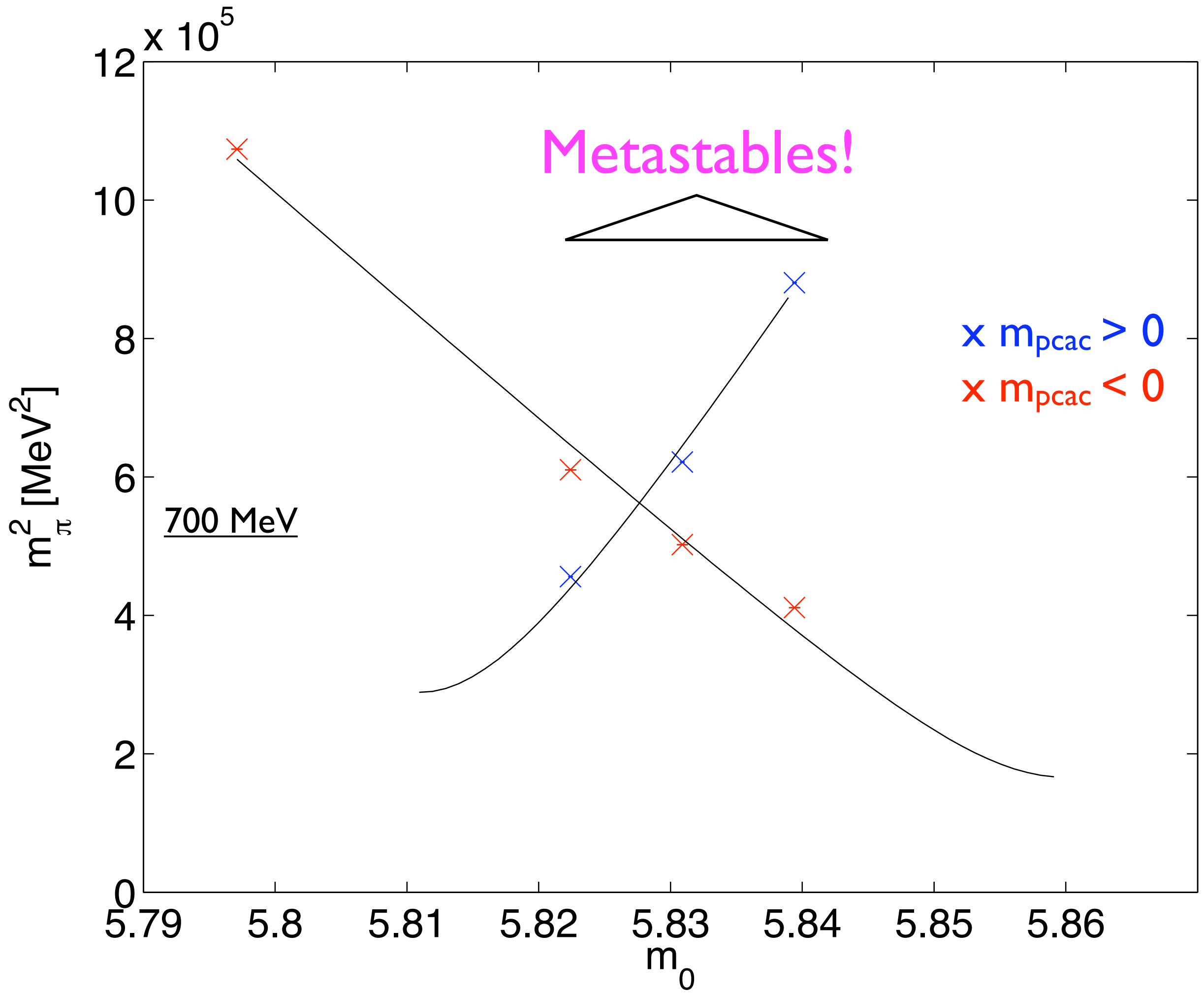


1st order phase transition - Scenario



Indeed simulations confirmed the 1st order phase transition scenario [XLF and qq+q]

As before: $m_\pi^2 \text{ vs. } m_q$



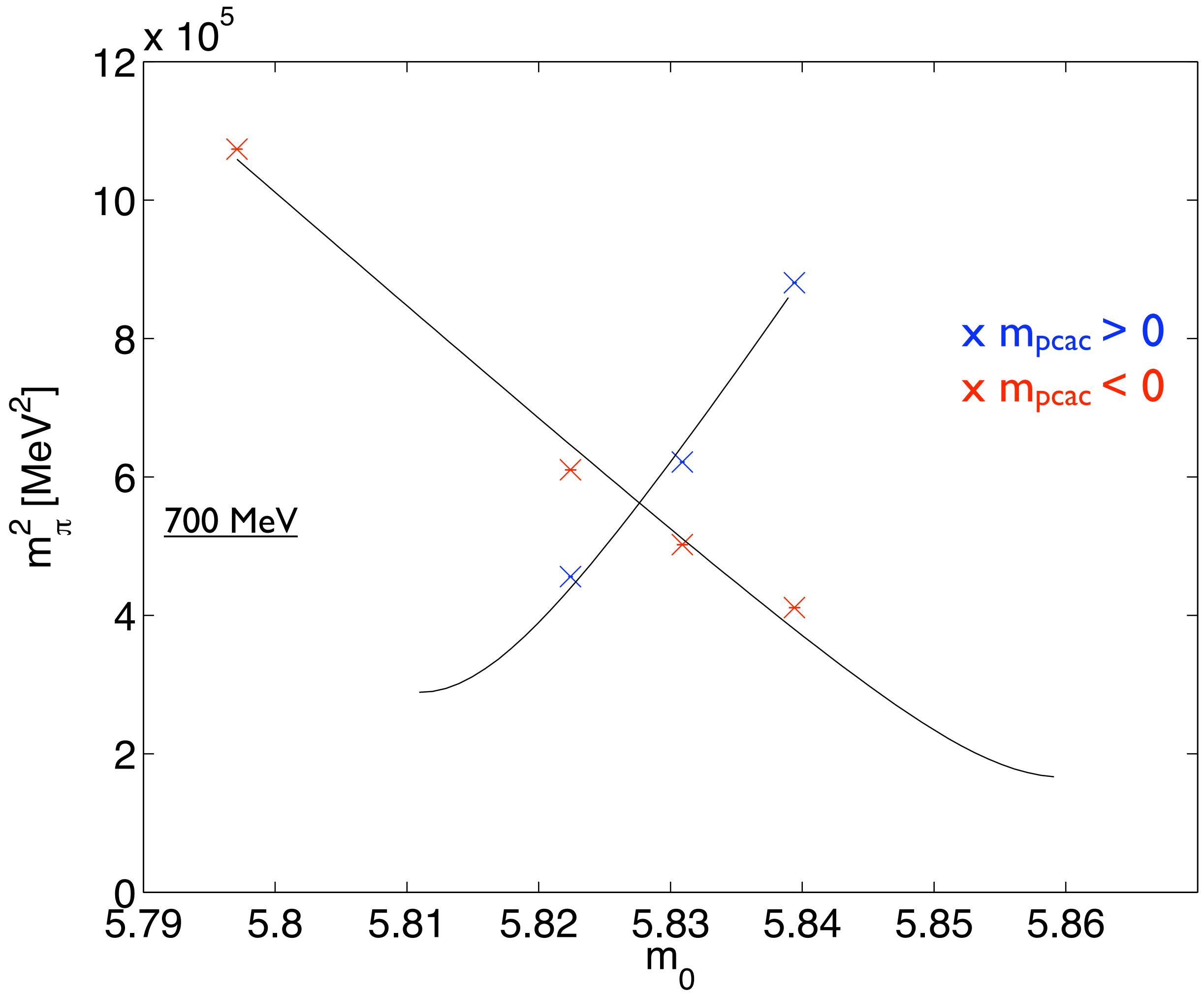
PLAQ gauge,
twisted mass: aμ=0.01,
a ~0.16 fm, β=5.2

- Sharpe Singleton (Lattice-ChPT) pattern confirmed.
- Metastabilities could make you overlook the problem!

Confirmed by simulations with both HMC and TSMB algorithm.
No numerical instabilities.

Indeed simulations confirmed the 1st order phase transition scenario [XLF and qq+q]

As before: m_π^2 vs. m_q



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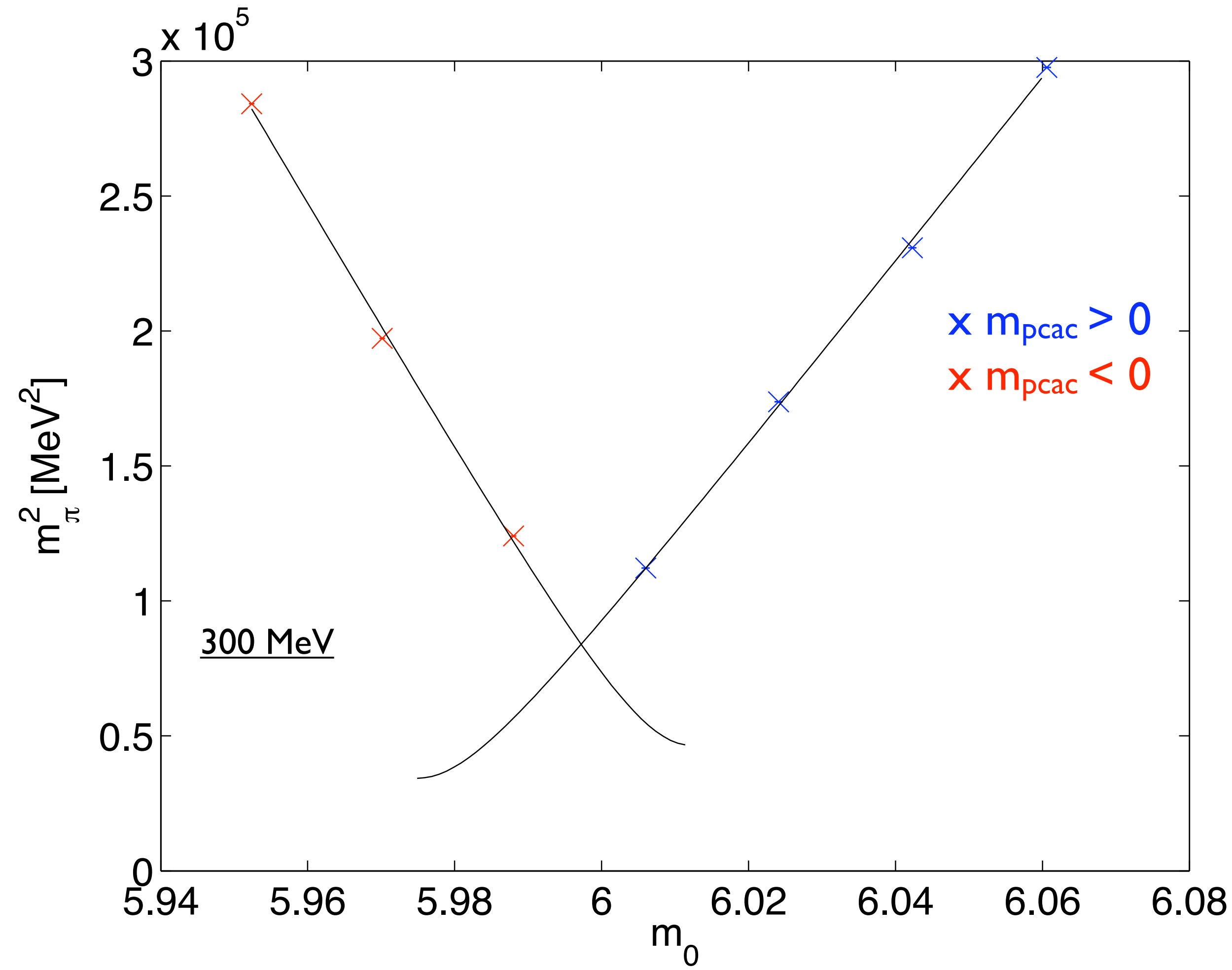


DBW2 gauge,
twisted mass: aμ=0.01,
a ~0.19 fm, β=0.67

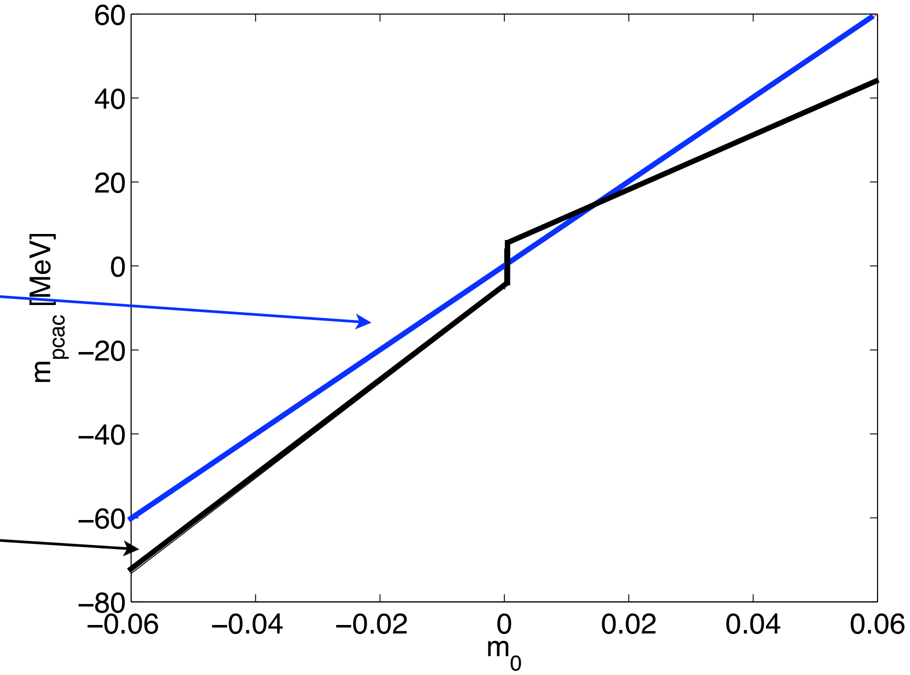
strong dependence on the Gauge Action

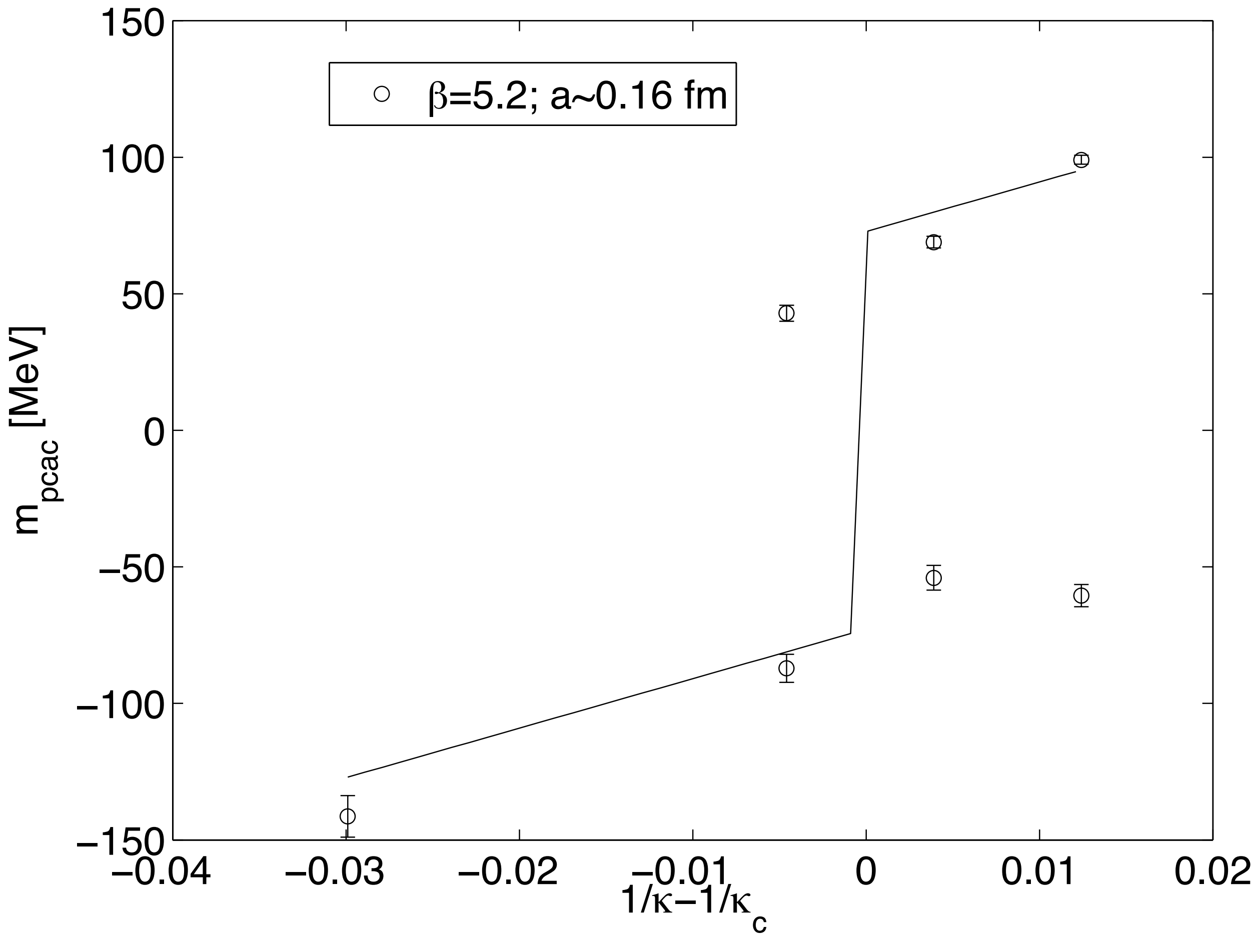
⇨ Bad problem but simple solution: different starting points, hysteresis loops

Consider also m_{pcac}

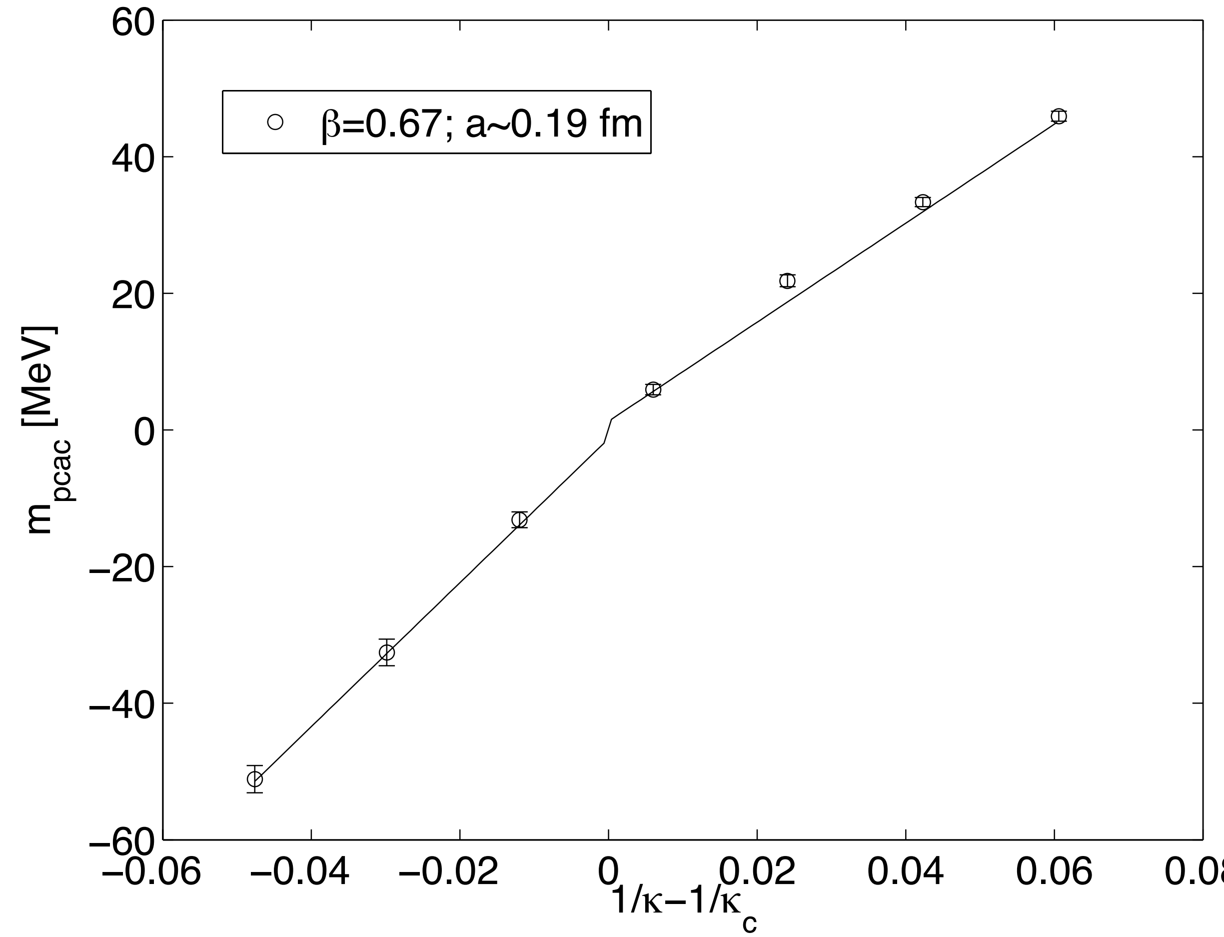
Continuum: $m_{pcac} = m_q$

Lattice modified relation m_{pcac} vs. m_q





PLAQ gauge,
twisted mass: aμ=0.01,
a ~0.16 fm



DBW2 gauge,
twisted mass: aμ=0.01,
a ~0.19 fm

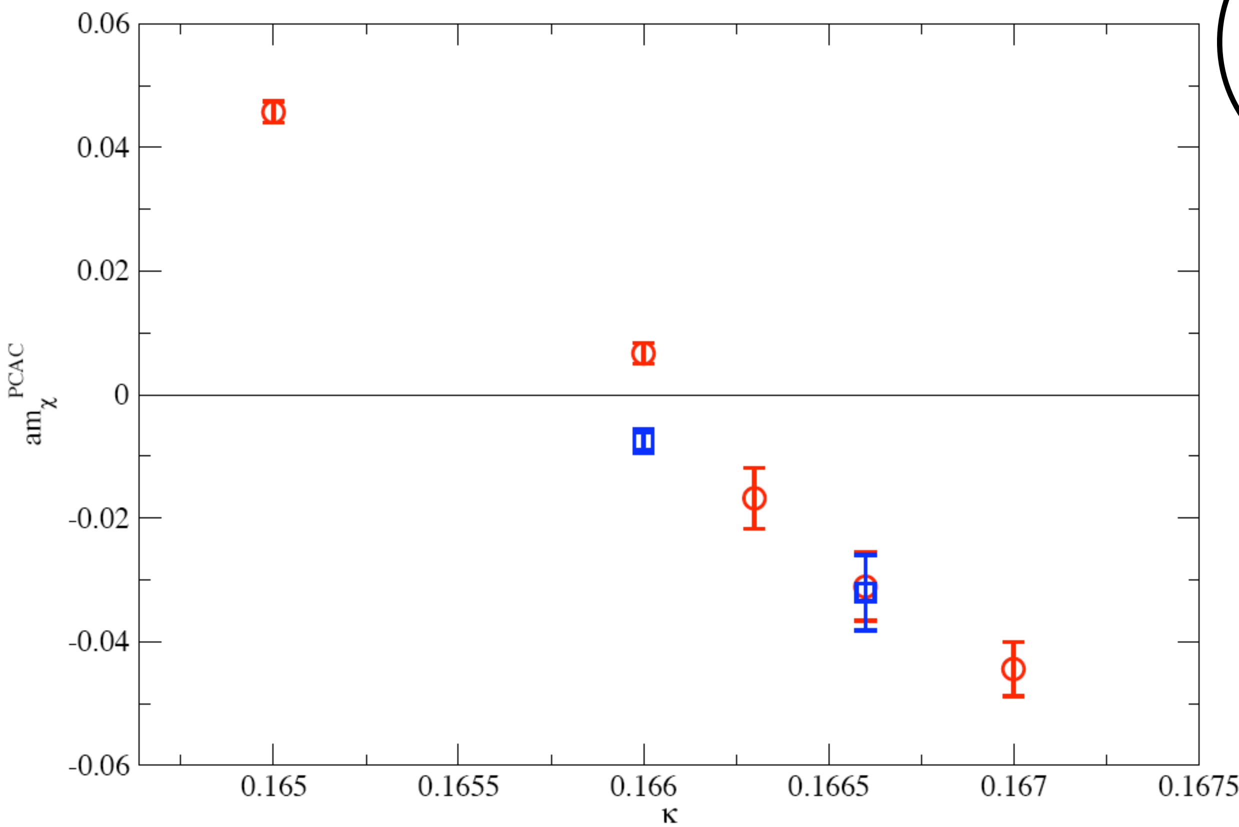
Choice: Tree Level Symanzik Improved Gauge Action

$$S_{\text{gauge}} = (1 - 8c_1)\,\mathrm{Tr}(\square) + c_1\,\mathrm{Tr}(\square\square) \begin{cases} c_1 = 0 & \text{PLAQ} \\ c_1 = -\frac{1}{12} & \text{TLSym} \\ c_1 = -0.331 & \text{Iwasaki} \\ c_1 = -1.4088 & \text{DBW2} \end{cases}$$

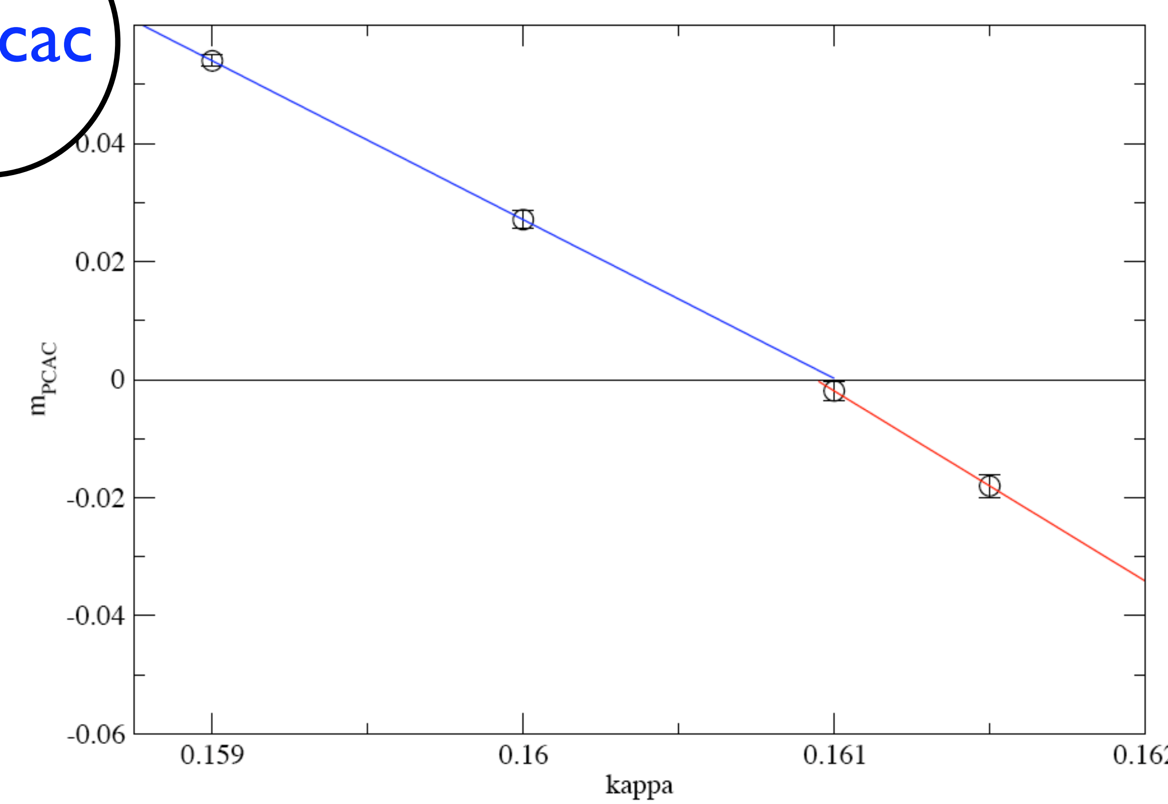
- TLSym: Tree Level in PT
- Iwasaki: RG non PT Imp.
- DBW2: RG non PT Imp.

Check that simulations from both starting point agree:

m_{pcac}



TLSym gauge,
twisted mass: $a\mu=0.005$,
Vol=12^3x24
a ~0.14 fm



TLSym gauge,
twisted mass: $a\mu=0.0075$,
Vol=16^3x32
a ~0.1 fm

Phase structure and algorithmic instabilities

Algorithmic instabilities in HMC with light quarks
(very general problem)

Nice identification of the problem: [Del Debbio et al. JHEP0602:011,2006]

σ = mean square deviation of the lowest eigenvalue of the hermit. lattice Dirac op. $|\gamma_5 D|$

$\overline{\mu}$ = average lowest eigenvalue of $|\gamma_5 D|$

Problems appear when $\overline{\mu} >> \sigma$ is not satisfied

$\overline{\mu}$ is proportional to the physical mass

One observe that $\sigma = \frac{a}{\sqrt{V}}$

Solution: $m_\pi L >> \sqrt{a(2B/Z)}$

Remark: in our case the Twisted Mass μ is already a rigid IR cutoff.

However, the phase structure is independent on the algorithm.

In fact the two "safety" conditions are independent

Safety from Algo. instabilities [Del Debbio et al. JHEP0602:011,2006]

$$m_\pi L >> \sqrt{a(2B/Z)}$$

Safety from 1st order ph.trans. [Sharpe,Singleton PRD58; Sharpe,Wu PRD71]

$$m_\pi >> a\sqrt{2B\Lambda^3}$$

See also Sharpe PRD74

Pion Mass Splitting

In tmQCD flavor symmetry is broken.
A good measure of it is the pion mass splitting.
To NLO in ChPT with lattice artifacts [L.S.'04, Sharpe,Wu'04]

$$m^2_{\pi\pm} - m^2_{\pi 3} = c\, a^2 \sin(\omega)^2$$

This is related to the phase structure because:

If c<0 => Aoki phase
If c>0 => 1st order phase trans. at finite m_π $\longrightarrow$ $m^2_{\pi \min} = c\, a^2$

[Sharpe,Singleton PRD58]

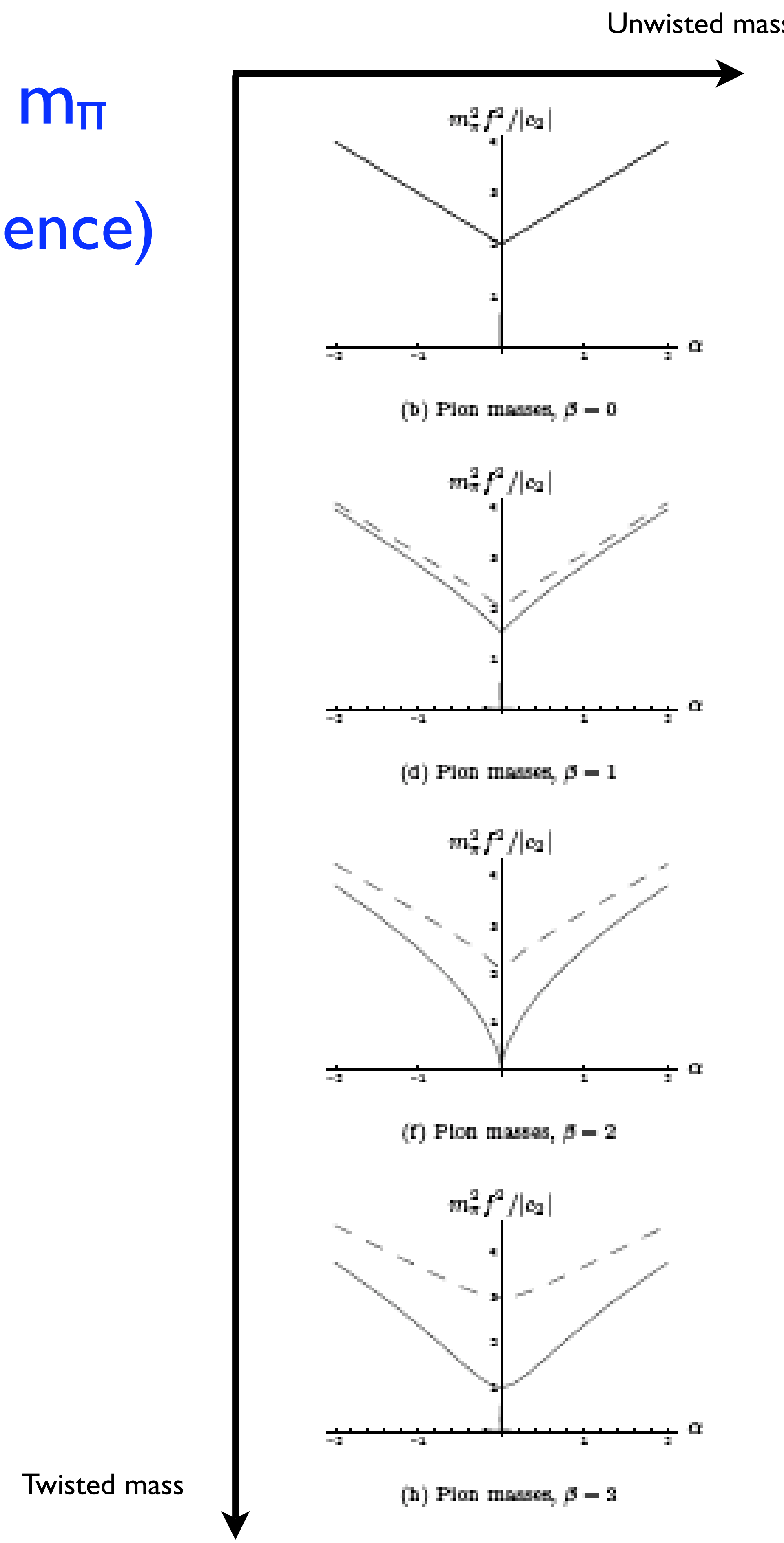
Picture for $m_{\pi 3}$ and m_{π}

(twisted/untwisted dependence)

[Sharpe,Wu '04]

$m_{\pi 3}$ goes below the minimum
at NON zero twisted mass.

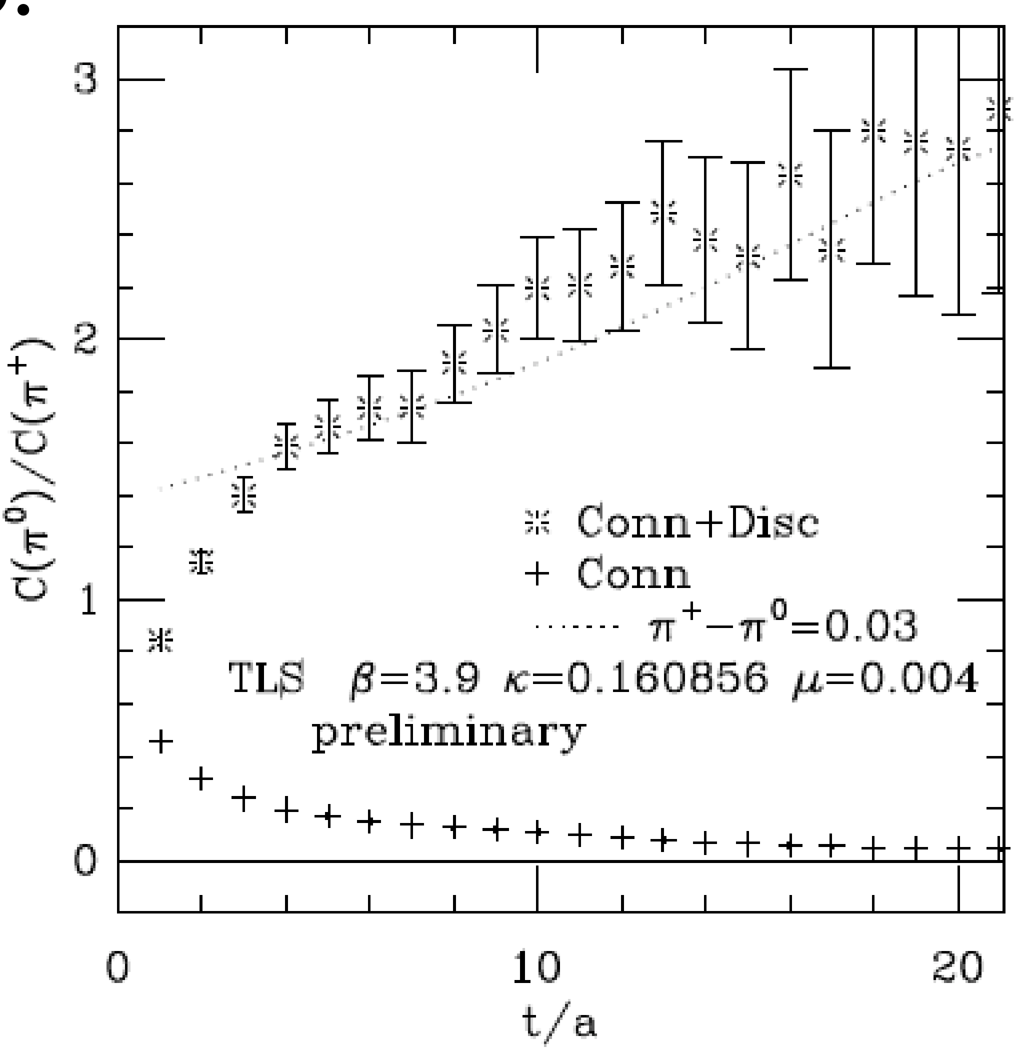
Large split attained in a small region
for small twisted mass values.



Preliminary Pion mass splitting

Thanks to the Liverpool group!

$$am_{\pi\pm} = 0.1369(5)$$
$$am_{\pi3} = 0.098(4)$$
$$am_{\pi\pm} - am_{\pi3} = 0.03(1)$$



$$m_{\pi\min} \simeq 198(8)(20)\ \mathrm{MeV}$$

From indetermination of r0

statistic

Definition of fixed *lattice spacing* at different masses

- Pion mass splitting is mass independent up to NNLO: $m^2_{\pi\pm} - m^2_{\pi 3} = c\, a^2 \sin(\omega)^2$

-This offers a probably impractical but theoretically clear definition of *lattice spacing a*, which is compatible whit ChPT

- In the physical point all definition of a' are ok, even if: $a' = a(1 + \lambda\, m/\Lambda_{\rm QCD})$
  (even $a=aF_\pi/(92\text{MeV})$)

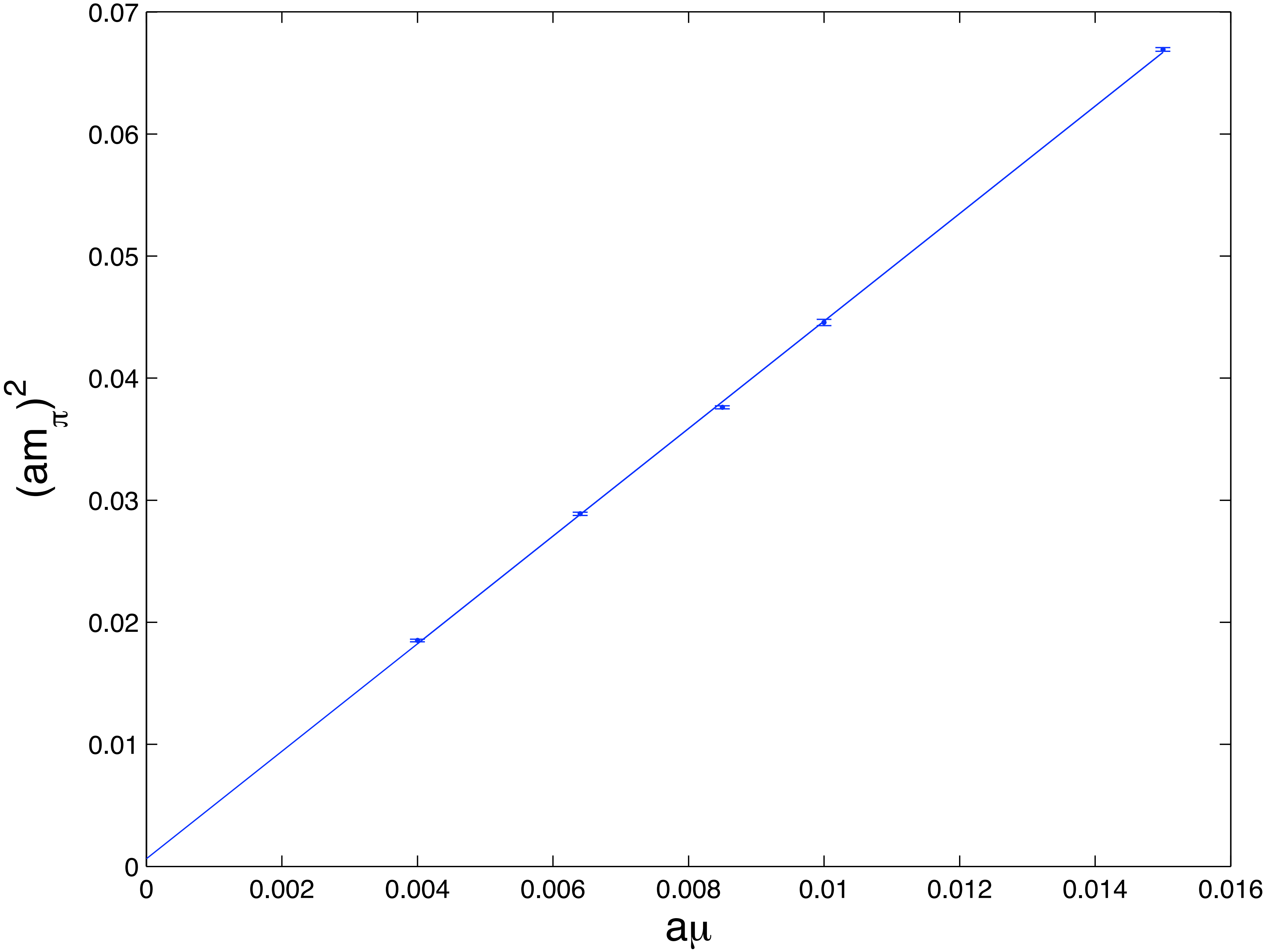
- However, to compare with ChPT, only those are good such that at least. Otherwise LEC's would be wrong in the continuum limit $a' = a(1 + \lambda\, a\, m)$

- No problems for ratios of quantities which have ChPT predictions (for example: F_π/M_π)
- But it is a problem when fitting for example: aF_π

Is it possible to prove that the usual definition $a=a(\beta)$ has a good relation with the natural one in ChPT ?

- The relation between the two definitions $a=a(\beta)$ and $a=a(r_0)$ has been discussed in [Aoki at Lattice2000, Sommer at Lattice 2003].

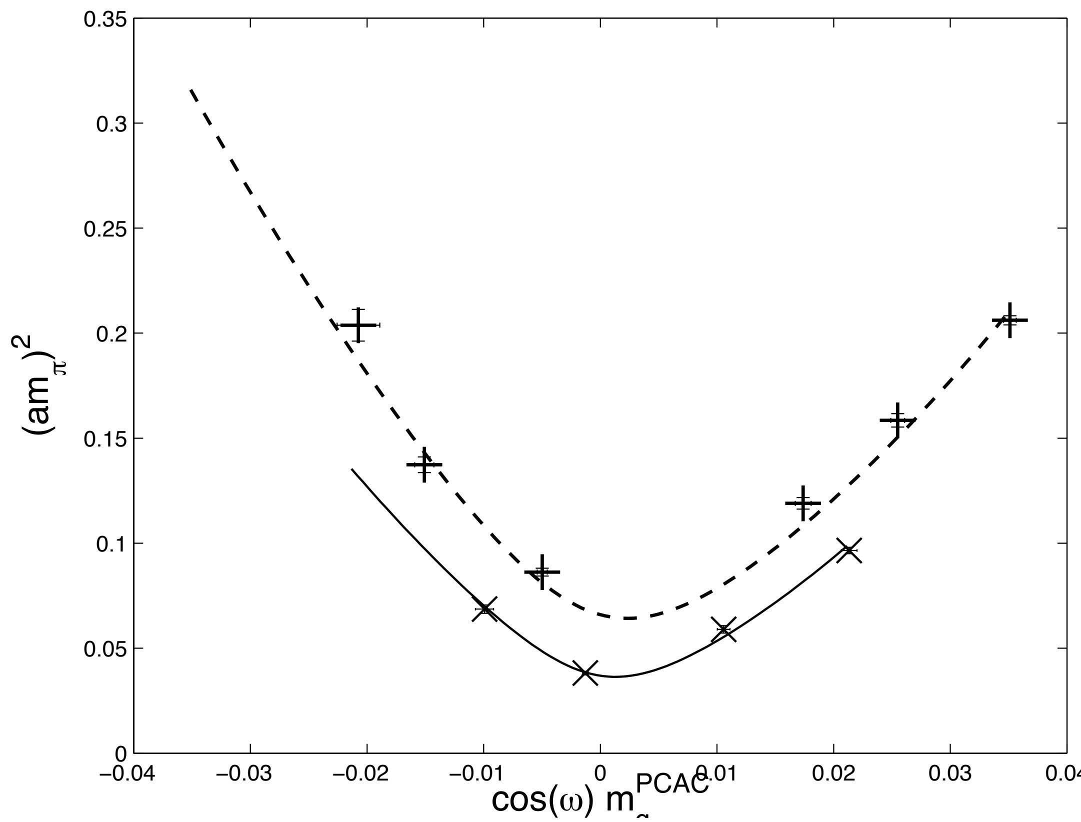
... which is probably the case for a large range of masses

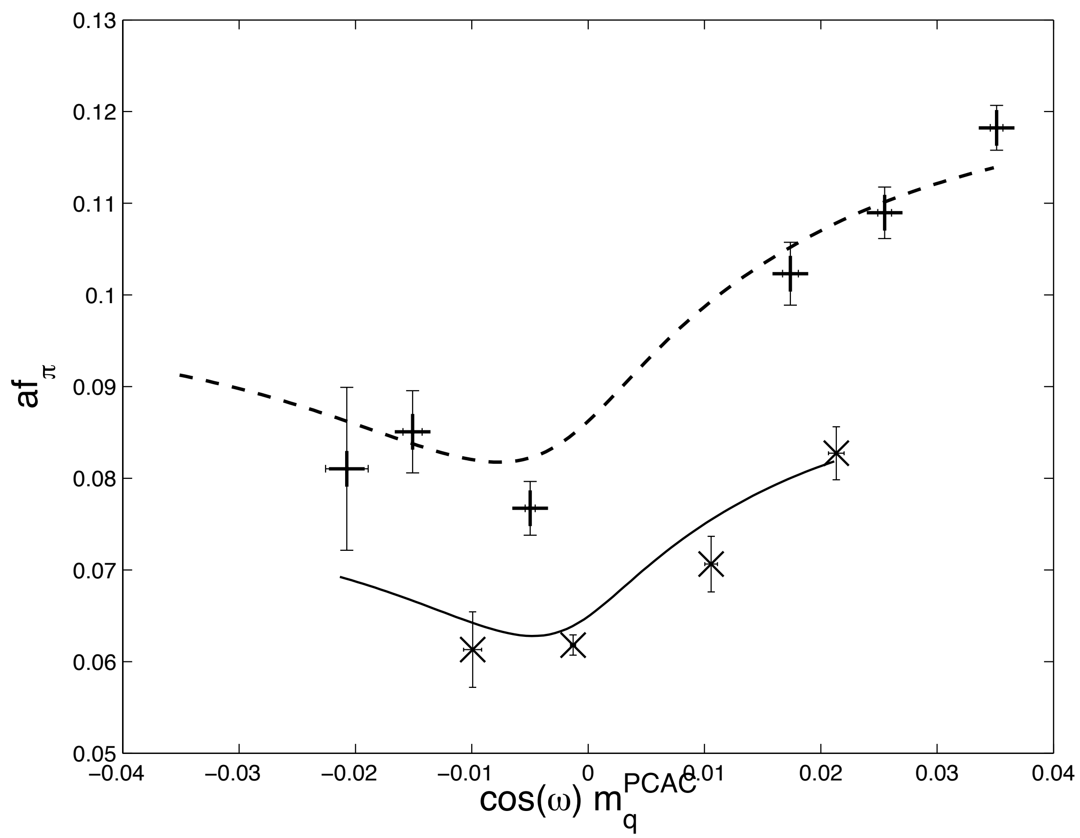


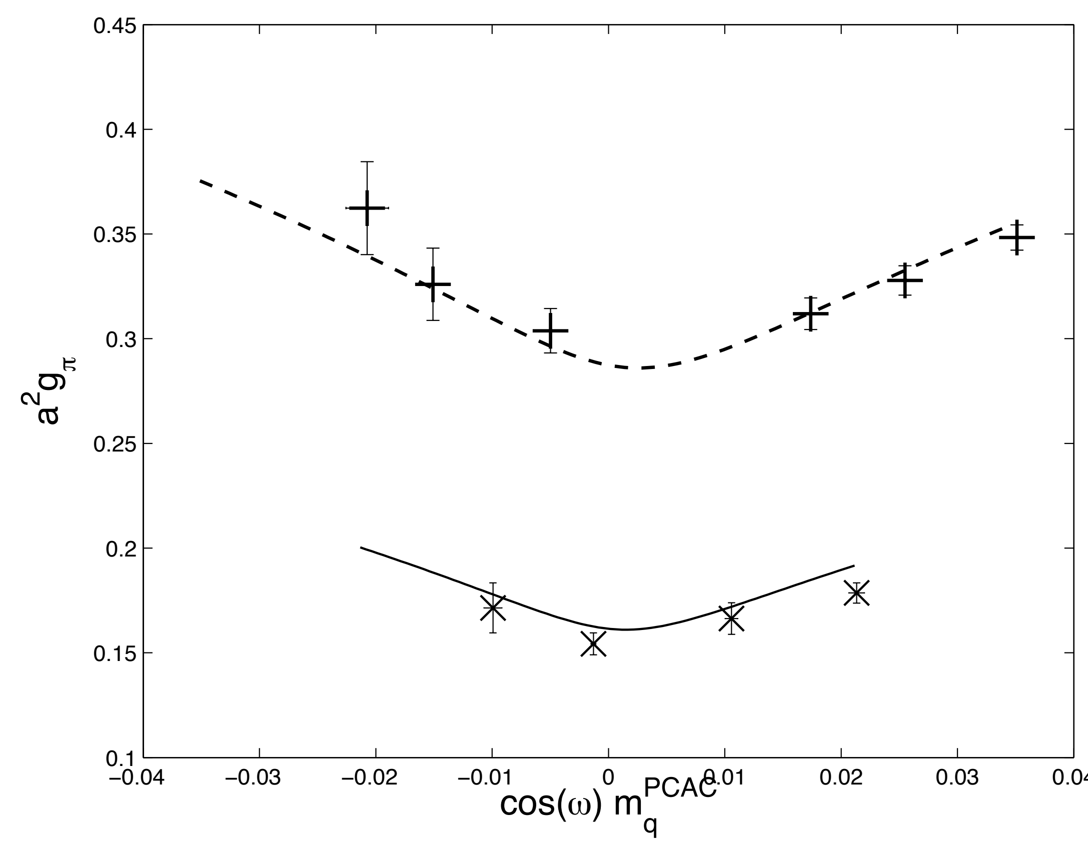
Other examples

Global fits of m_π, f_π, g_π
at different quark masses
at different lattice spacings

Many constraints, Compatible results!







Here the lattice spacing is quite large: a~0.15-0.20 fm

Scaling very good!

Nf = 2+1+1

-Realistic QCD simulations should include the dynamical strange

-No “single twisted fermion” possible.

-Obvious possibility: untwisted strange.

-Alternative: introduce both strange and charm a la
[Frezzotti Rossi ‘04] as mass split dublet.
(determinant remains positive).

Valid representation for the heavy doublet:

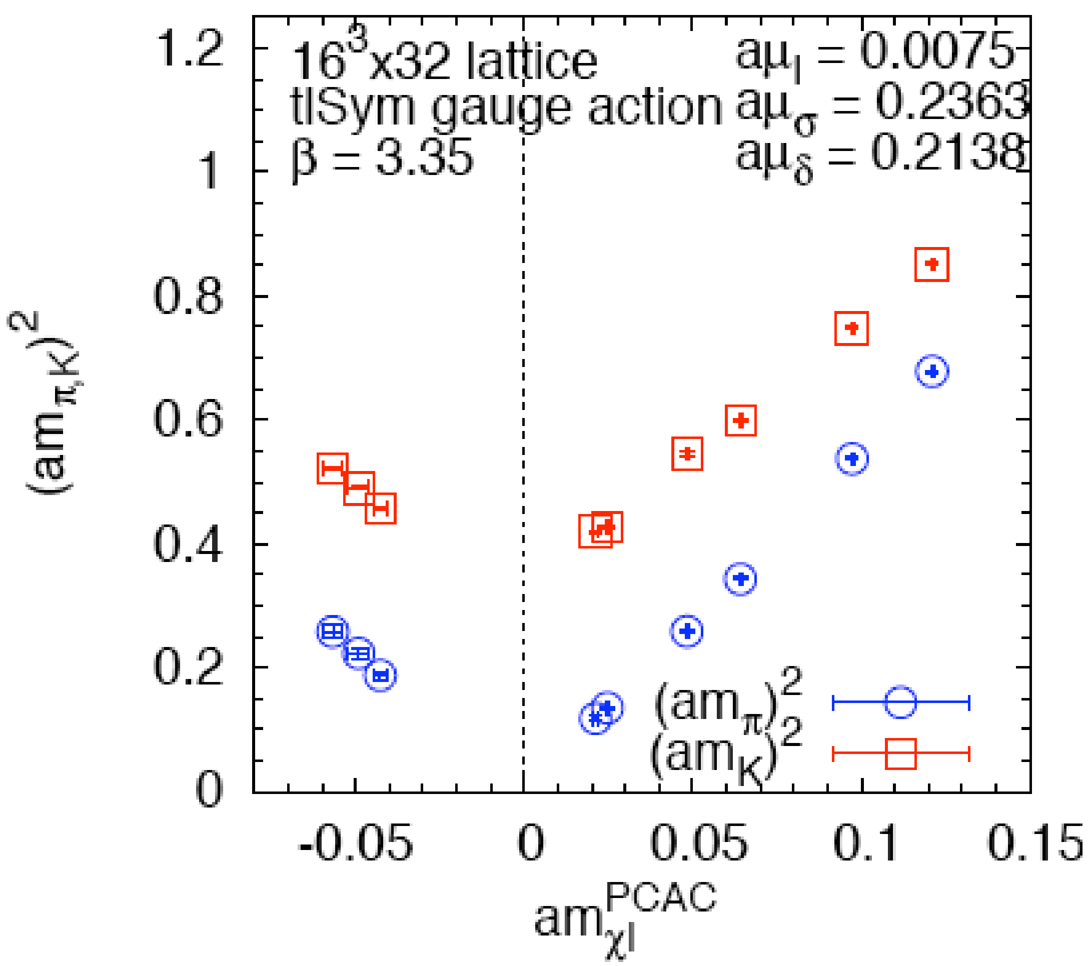
$$D_{\rm tm} = m_0 + i\mu_\sigma \tau_i \gamma_5 + \mu_\delta \tau_j + \frac{1}{2}\gamma_\mu \left[\nabla^{\rm f}_\mu + \nabla^{\rm b}_\mu\right] - a\frac{1}{2}\nabla^{\rm f}_\mu \nabla^{\rm b}_\mu$$

Two new parameters to tune, but no new critical mass.
(m_0 - which is the difficult one - is the same as for the light dublet).

A bit more algebra to work out the physical currents.
(but this needs to be done only once)

[Chiarappa et al. hep-lat/0606011]

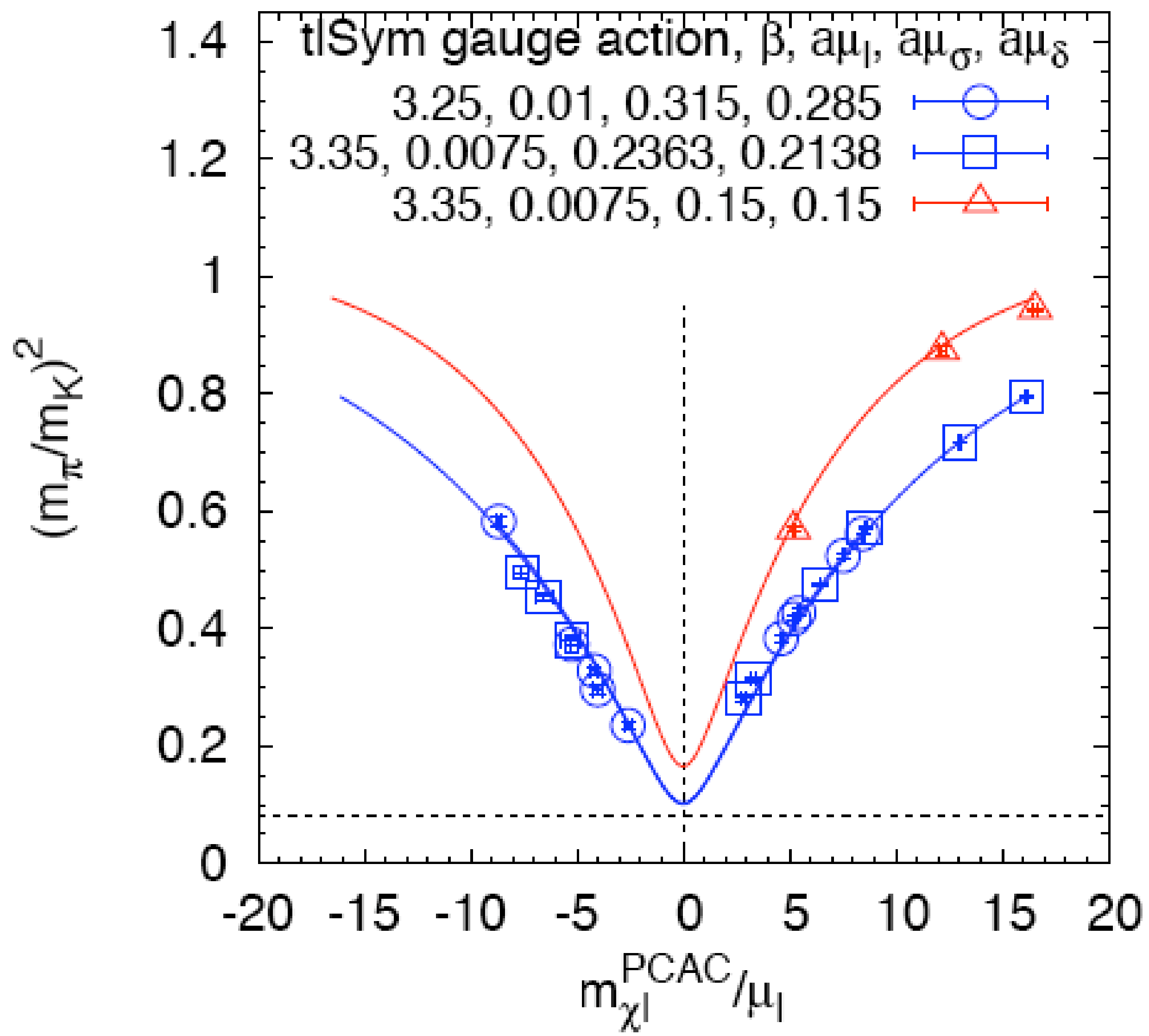
Some results of Pion and Meson masses



a~0.15fm

Algorithm: PHMC [Montvay, Scholz Phys.Lett.B623]

ChPT



$$\frac{m_\pi^2}{m_K^2} = \frac{2m_{ud}}{m_{ud}+m_s} \qquad \text{(LO ChPT)}$$

$$m_{ud} = \sqrt{(Z_A m_{\chi l}^{\text{PCAC}})^2 + \mu_l^2}$$

$$m_s = \sqrt{(Z_A m_{\chi h}^{\text{PCAC}})^2 + \mu_\sigma^2} - \frac{Z_P}{Z_S}\mu_\delta$$

fitted $Z_P/Z_S \simeq 0.45$

take Z_A as input

$m_{\chi l}^{\text{PCAC}} \approx m_{\chi h}^{\text{PCAC}}$

Conclusions

- tmQCD has entered the production phase: more physical quantities to come soon.
- Some preliminary analysis of Finite Size effects.
- Wilson-ChPT is very useful to asses consistency of effects of small lattice artifacts.
  Nice agreement between phase structure and pion mass splitting => associated $O(a^2)$ effects under control
- Nf=2+1+1 simulations are coming.
- Mixed Actions: see talk by Oliver Bär.