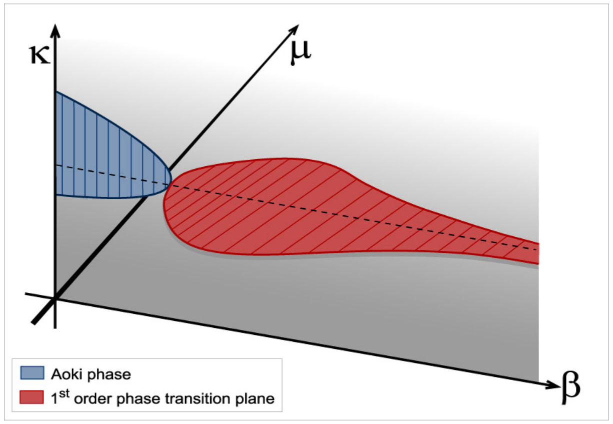
Towards realistic Simulations of Lattice-QCD: the Approach of Twisted Mass Fermions

Karl Jansen

- **Small quark masses and improved scaling quenched**
- **A surprise for dynamical quarks: the phase structure**



Twisted Mass Team

- **NIC, Zeuthen**
  K. Nagai, M. Papinutto, A. Shindler, C. Urbach, U. Wenger, I. Wetzorke, K.J.
- **DESY, Hamburg**
  I. Montvay, N. Ukita, E. Scholz
- **Münster University**
  F. Farchioni, P. Hoffmann, G. Münster
- **Humboldt University**
  L. Scorzato
- **University of Rome II**
  R. Frezzotti, G. Rossi

Publications (numerical simulations)

Quenched studies

- *Going chiral: Overlap versus twisted mass fermions*, hep-lat/0411001
- *Scaling test for Wilson twisted mass QCD*, hep-lat/0312013
- *Light quarks with twisted mass fermions*, hep-lat/0503031
- *Quenched scaling of Wilson twisted mass fermions*, hep-lat/0507010
- *Flavour breaking effects of Wilson twisted mass fermions*, hep-lat/0507032
- *Comparing iterative methods for overlap and twisted mass*, hep-lat/0409107

Dynamical Quarks

- *Exploring the phase structure of lattice QCD with twisted mass quarks*, hep-lat/0409098
- *Twisted mass quarks and the phase structure of lattice QCD*, hep-lat/0406039
- *The phase structure of lattice QCD with Wilson quarks and renormalization group improved gluons*, hep-lat/0410031
- *Lattice spacing dependence of the first order phase transition for dynamical twisted mass fermions*, hep-lat/0506025

Overview

- *Dynamical twisted mass fermions*, hep-lat/0509131
- *Plenary talk at Lattice2005, A. Shindler*

Wilson (Frezzotti, Rossi) twisted mass QCD (Frezzotti, Grassi, Sint, Weisz)

$$D_{\rm tm} = m_q + i\mu\tau_3\gamma_5 + \frac{1}{2}\gamma_\mu \left[\nabla_\mu + \nabla_\mu^*\right] - a\frac{1}{2}\nabla_\mu^*\nabla_\mu$$

quark mass parameter m_q , twisted mass parameter μ

- $m_q = m_{\rm crit} \rightarrow$ O(a) improvement for
  hadron masses, matrix elements, form factors, decay constants

- $\det[D_{\rm tm}] = \det[D^2_{\rm Wilson} + \mu^2]$
  $\Rightarrow$ protection against small eigenvalues

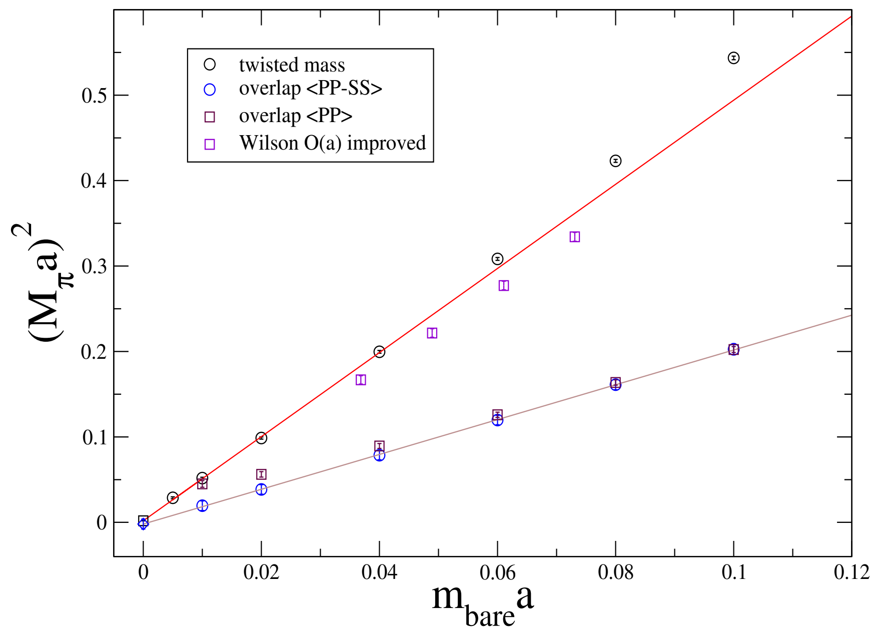
- computational cost comparable to staggered
  talk by C. Urbach

- simplifies mixing problems

twisted mass against overlap fermions: how chiral can we go?

Bietenholz, Capitani, Chiarappa, Hasenbusch, K.J., Nagai, Papinutto,
Scorzato, Shcheredin, Shindler, Urbach, Wenger, Wetzorke

$\beta = 5.85$ **only**



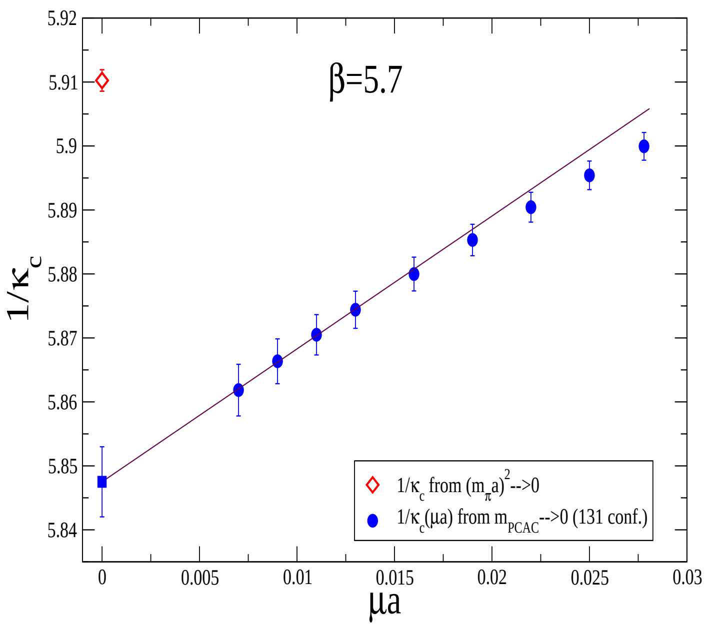
$\Rightarrow$ twisted mass simulations can reach quarks masses as small as overlap substantially smaller than O(a)-improved Wilson fermions

Choice of the critical quark mass

relation quark mass m_q and hopping parameter κ , $\kappa = 1/(2am_q + 8)$

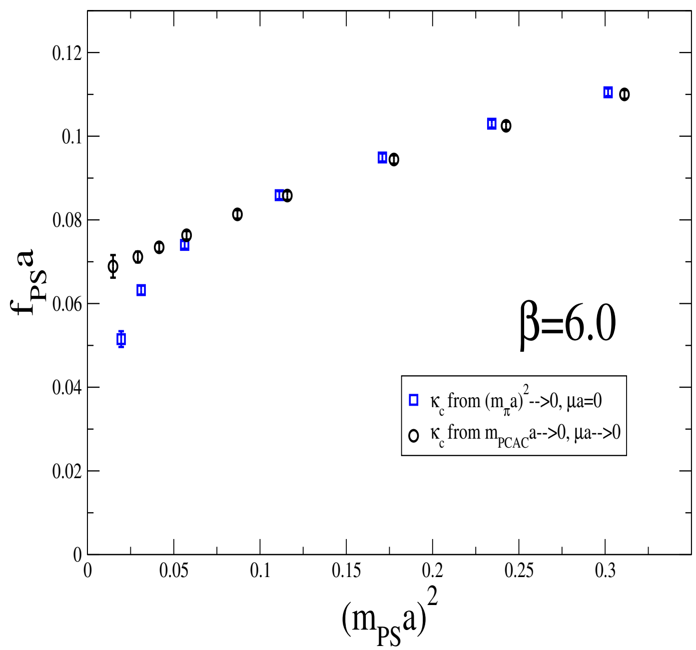
- κ_c $(m_{\rm crit})$ from vanishing of pion mass
- κ_c $(m_{\rm crit})$ from vanishing of PCAC quark mass

$\longrightarrow$ both lead to $O(a)$-improvement (Frezzotti-Rossi)
different but can have substantially $O(a^2)$-effects
(Frezzotti, Martinelli, Papinutto, Rossi)



The bending phenomenon

comparison of pion definition and PCAC definition of critical quark mass



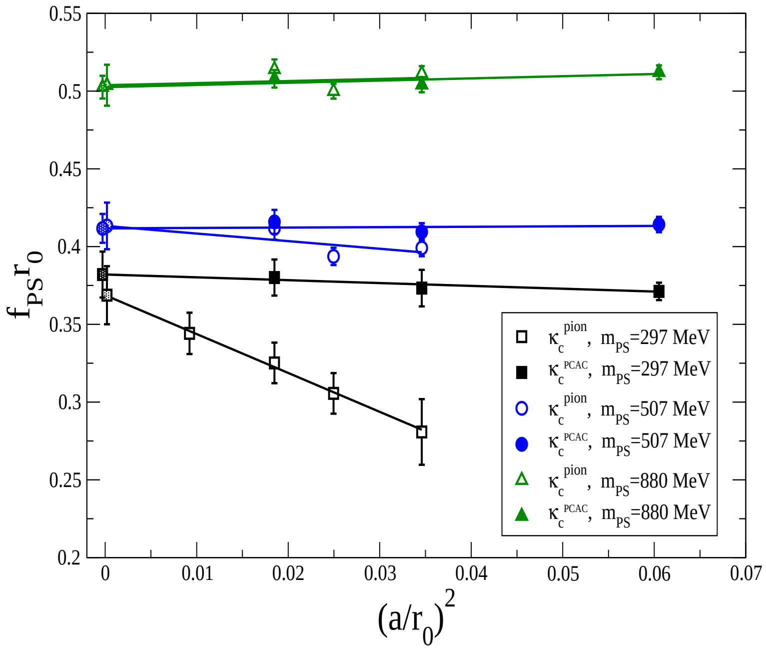
$\longrightarrow$ triggered quite some discussion

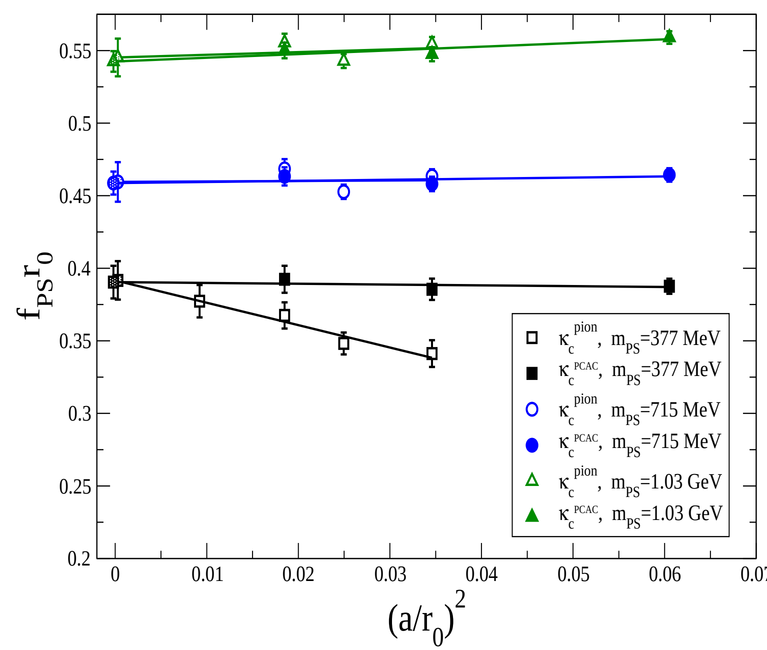
(Frezzotti-Rossi, Aoki-Bär, Sharpe-Wu, Sharpe, Frezzotti, Martinelli, Papinutto, Rossi)

$\longrightarrow$ explanation: pion definition leads to large O(a^2) cut-off effects $\propto a^2/m_\pi^4$

$\longrightarrow$ PCAC definition these infrared enhanced cut-off effects are eliminated O(a^2) cut-off effects $\propto a^2/m_\pi^4$

Scaling of F_{PS}

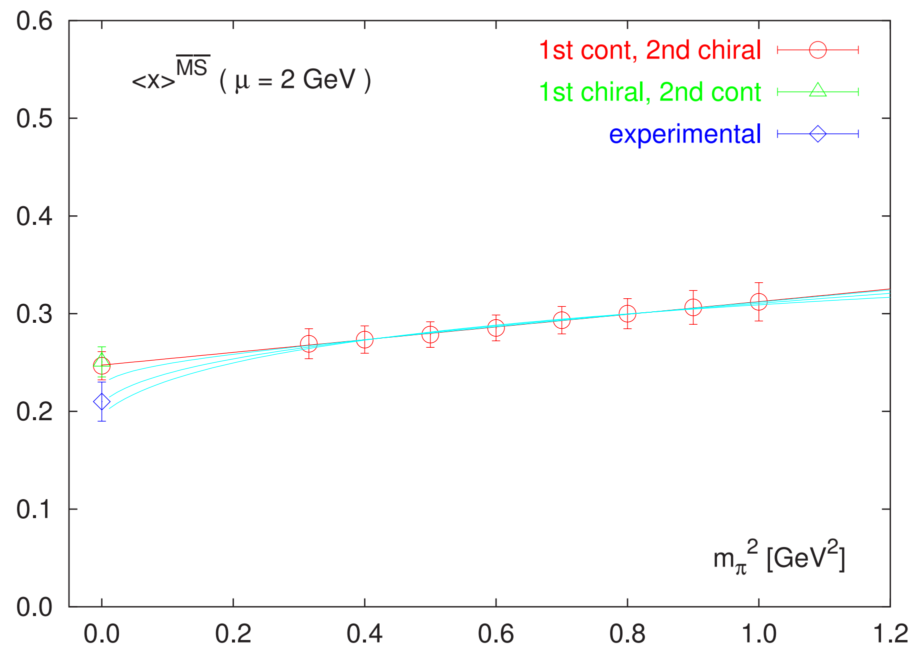




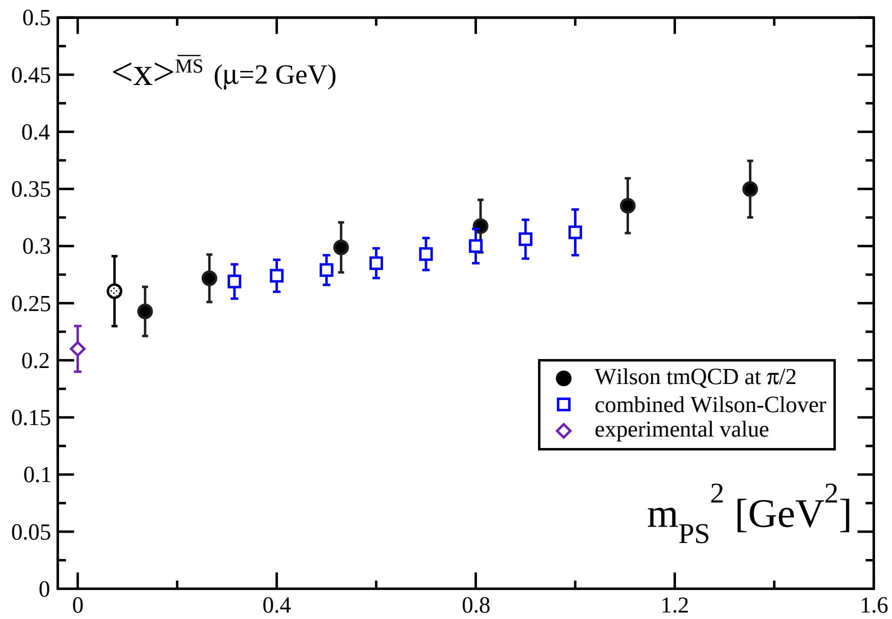
$\langle x \rangle$ in the pre-twisted mass era

Guagnelli, K.J., Palombi, Petronzio, Shindler, Wetzorke

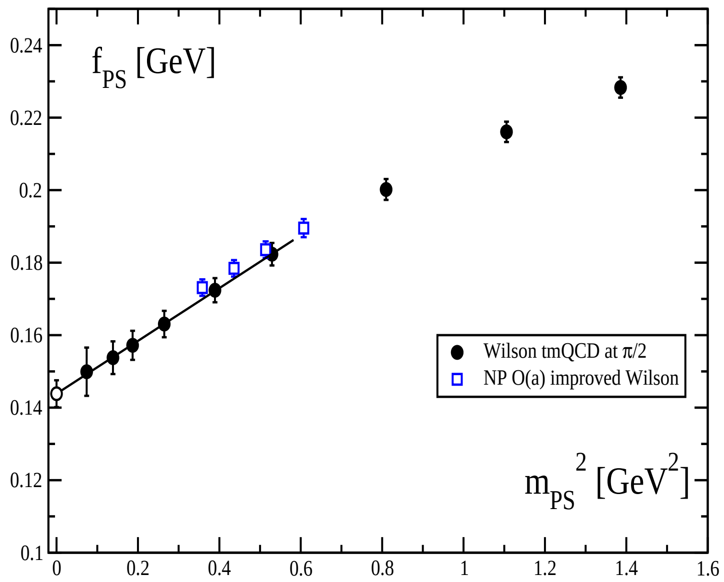
- Schrödinger Functional
- combined Wilson and $O(a)$-improved Wilson
- controlled
  - non-perturbative renormalization
  - continuum limit
  - finite volume effects
  - statisitical errors

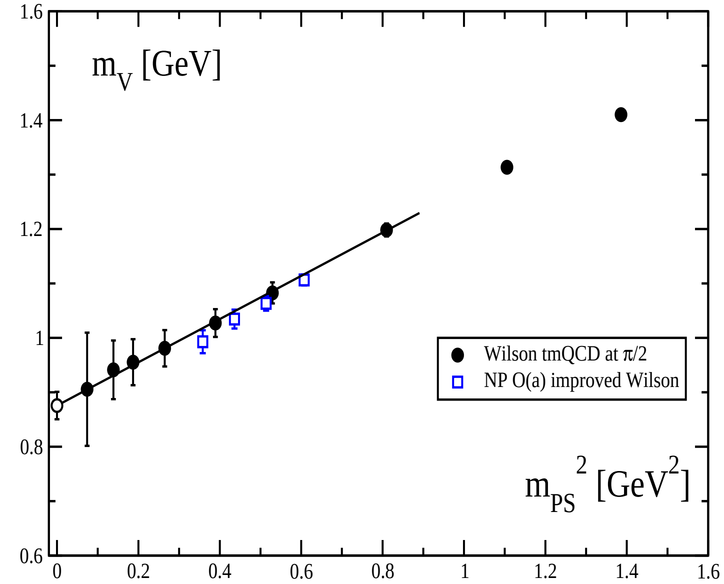


$\langle x \rangle$ with twisted mass

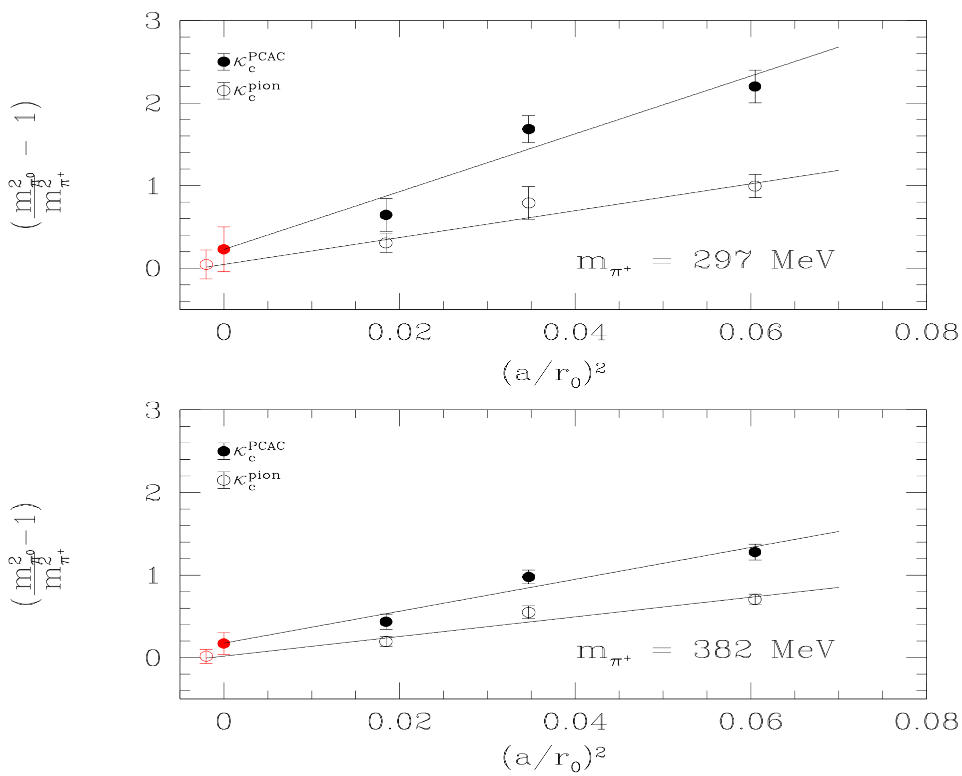


F_{PS} and m_ρ in the continuum





Flavour breaking effects



Summary of quenched situation for maximally twisted mass QCD

- O(a)-improvement verified
- with PCAC definition of critical quark mass: also $O(a^2)$ effects small
- pion masses of O(250)MeV perfectly possible
- flavour breaking effects are $O(a^2)$ size comparable with staggered fermions

With available improved dynamical algorithms

$\Rightarrow$ nothing between us and dynamical simulations of maximally twisted mass QCD

Dynamical Quarks:
The phase structure of lattice QCD

Farchioni, Frezzotti, Hofmann, K.J., Montvay, Münster,
Rossi, Scholz, Shindler, Ukita, Urbach, Wenger, Wetzorke

Let me describe a typical computer simulation:[...]
the first thing to do is to look for phase transitions (G. Parisi)

lattice simulations are done *under the assumption*
that the transition is continuum like

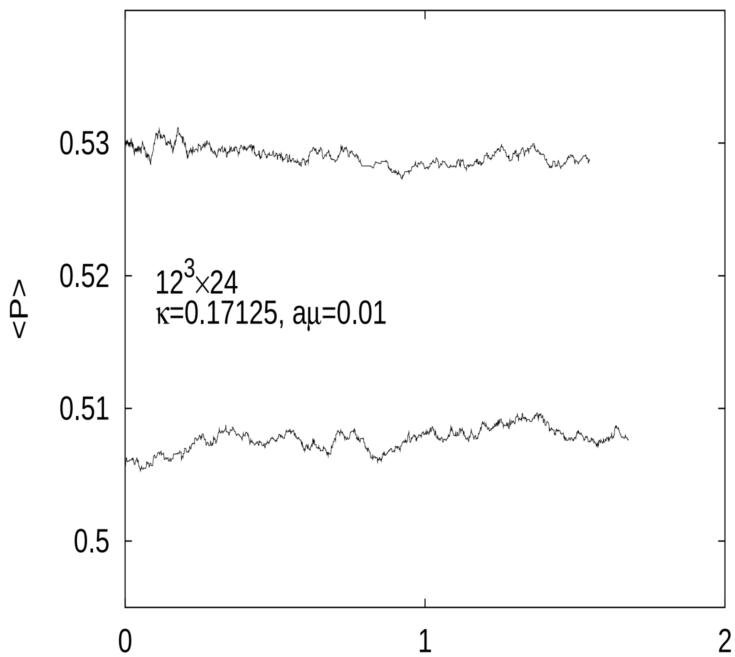
- first order, jump in $< \bar{\Psi}\Psi >$ when quark mass m changes sign

- pion mass vanishes at phase transition point

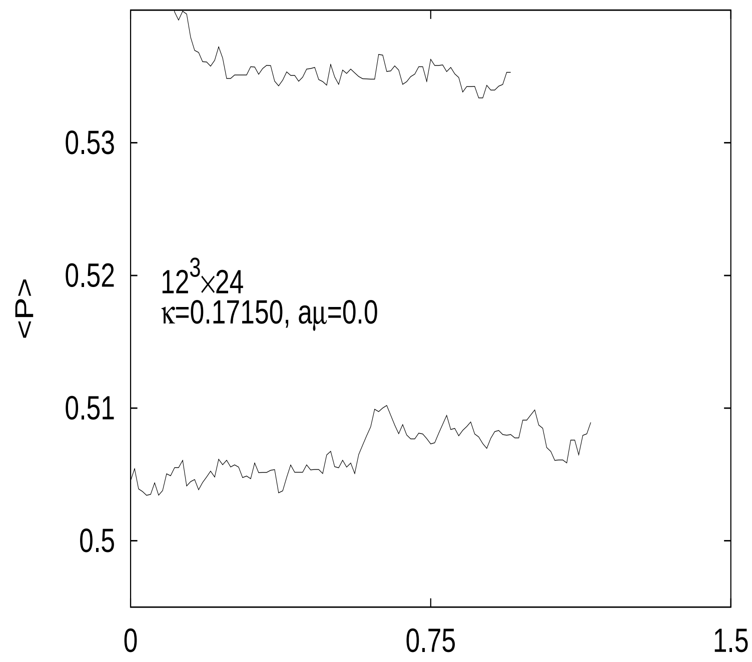
$\longrightarrow$ twisted mass fermions offer a tool to check this

Metastabilities in plaquette expectation value

cold (high plaquette) and hot (low plaquette) starts: long-living states

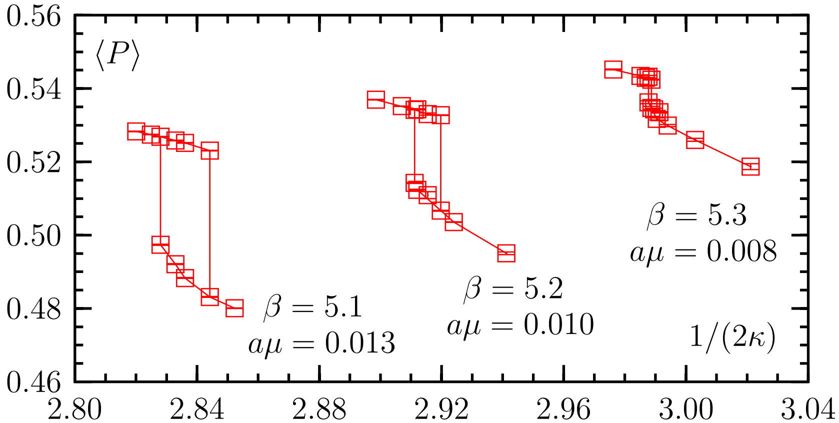


non-vanishing μ

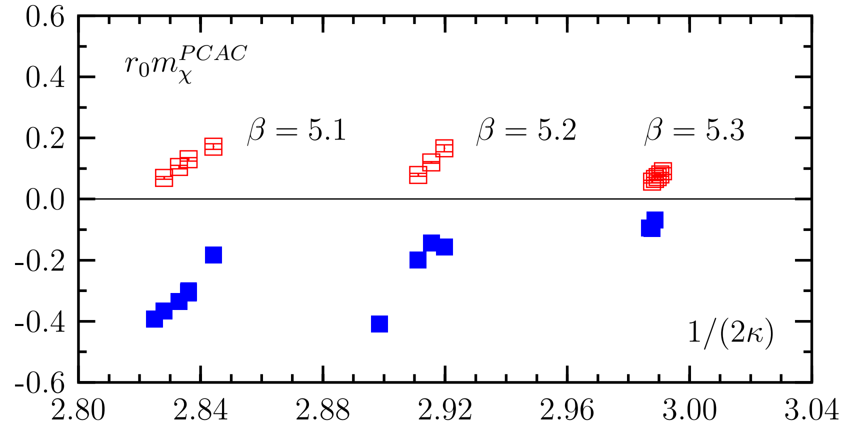


pure Wilson case

Lattice spacing dependence of the phase transition



Plaquette expectation value



PCAC quark mass

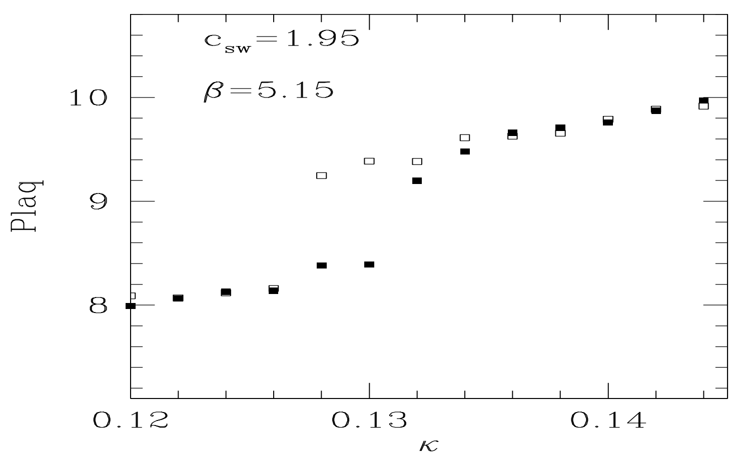
Earlier signs of phase diagram

- **Earlier signs of first order phase transitions**

  Blum, PRD 50 3377 ('94)

  CP-PACS collaboration, Nucl.Phys. (Proc.Suppl.) 106 (2002) 263, hep-lat/0409016

  my own little experiments



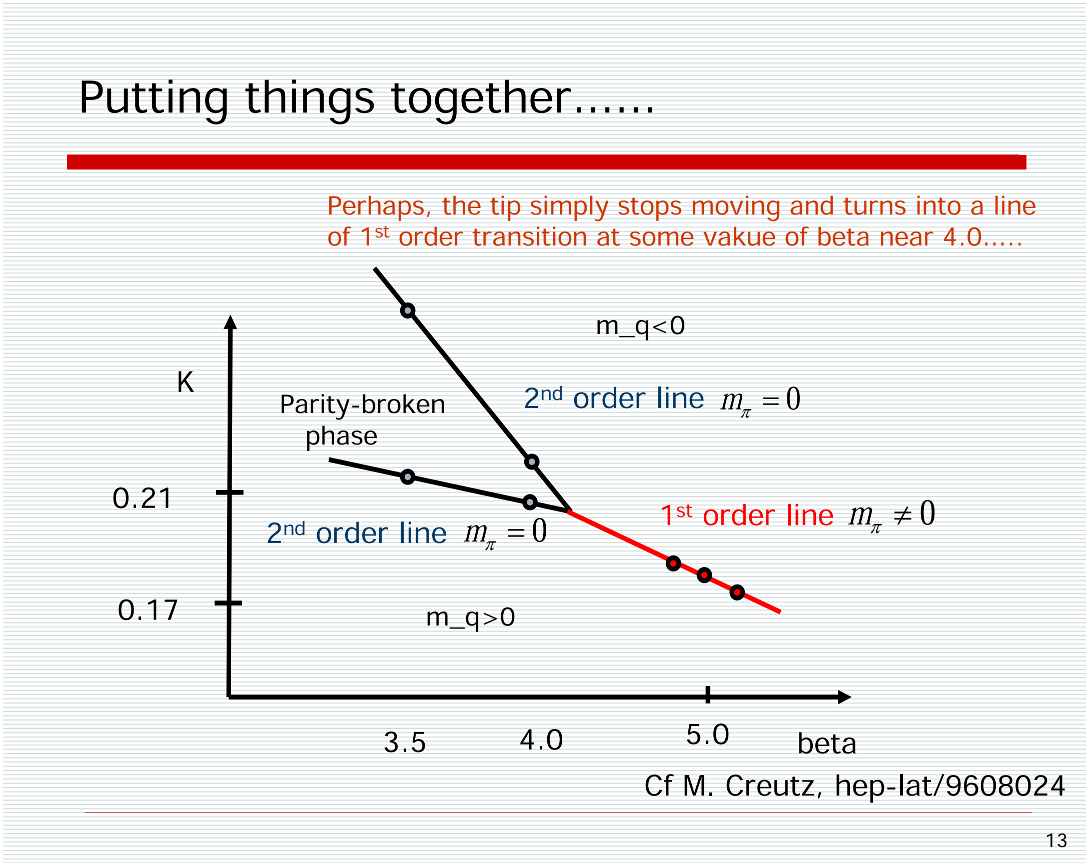
- **Aoki Phase**

  Bitar, hep-lat/9602027

  Sternbeck, Ilgenfritz, Kerler, Müller-Preussker, Stüben, hep-lat/0309059, hep-lat/0309057

Phase structure anticipated from M. Creutz

Taken from talk A. Ukawa, ILFTN workshop in Izu, Japan



Interpretation in the framework of chiral perturbation theory

Sharpe, Singleton; Münster; Sharpe, Wu: Scorzato

Chiral lagrangian uncluding O(a) lattice artefacts

$$\mathcal{L}_2 = \frac{F_0^2}{4}\,\mathrm{Tr}\left(\partial_\mu U^\dagger \partial_\mu U\right) - \frac{F_0^2}{4}\,\mathrm{Tr}\left(\chi U^\dagger + U\chi^\dagger\right) - \frac{F_0^2}{4}\,\mathrm{Tr}\left(\rho U^\dagger + U\rho^\dagger\right),$$

$$U(x) = \exp\left(\frac{i}{F_0}\pi_b(x)\tau_b\right), \quad \chi = 2B_0(\tilde{m}\,\mathbf{1} - i\mu\tau_3), \quad \rho = 2W_0 a\,\mathbf{1}$$

Writing $U = u_0\mathbf{1} + iu_a\tau_a, \qquad a = 1,2,3, \quad u \equiv (u_0, u_1, u_2, u_3), \quad u\cdot u = 1$

physical significance of u_0

$$\langle \bar{q}q\rangle = -2F_0^2 B_0 \langle u_0\rangle$$

effective potential (at $\mu = 0$)

$$V = -c_1\, u_0 + c_2\, u_0^2\,,$$

where

$$c_1 = 2F_0^2(B_0 m_q + W_0 a)$$

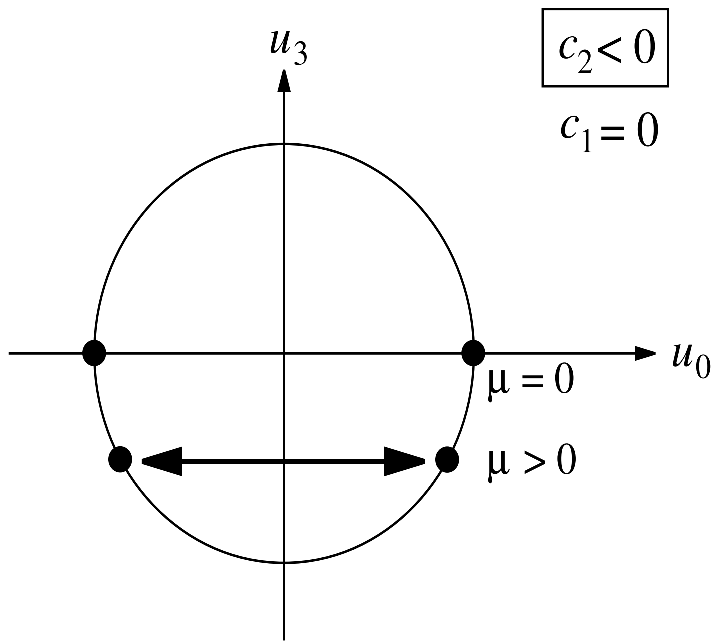
Including μ potential up to O(a^2)

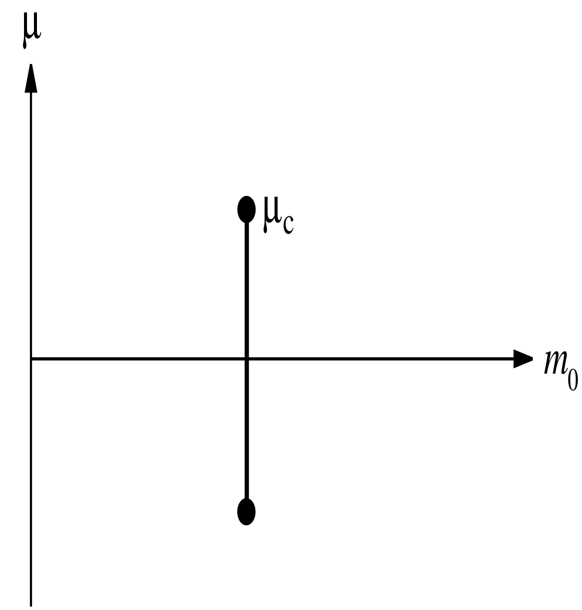
$$V = -c_1\, u_0 + c_2\, u_0^2 + c_3\, u_3\,,$$

$$c_3 = 2F_0^2 B_0\, \mu.$$

First order phase transition for $c_2 < 0$ (case $c_2 > 0$: Aoki phase)

$c_1 = 0 \Rightarrow$ first order phase transition, where u_0 changes sign discontinuously





u_0, u_3 plane

phase digram at fixed β

Properties of phase transition

endpoint of the transition μ_c

$$\mu_c = \frac{|c_2|}{F_0^2 B_0} \sim a^2$$

neutral pion mass

$$m_{\pi 3}^2 = \frac{1}{2F_0^2|c_2|}(4c_2^2 - c_3^2) \sim a^2$$

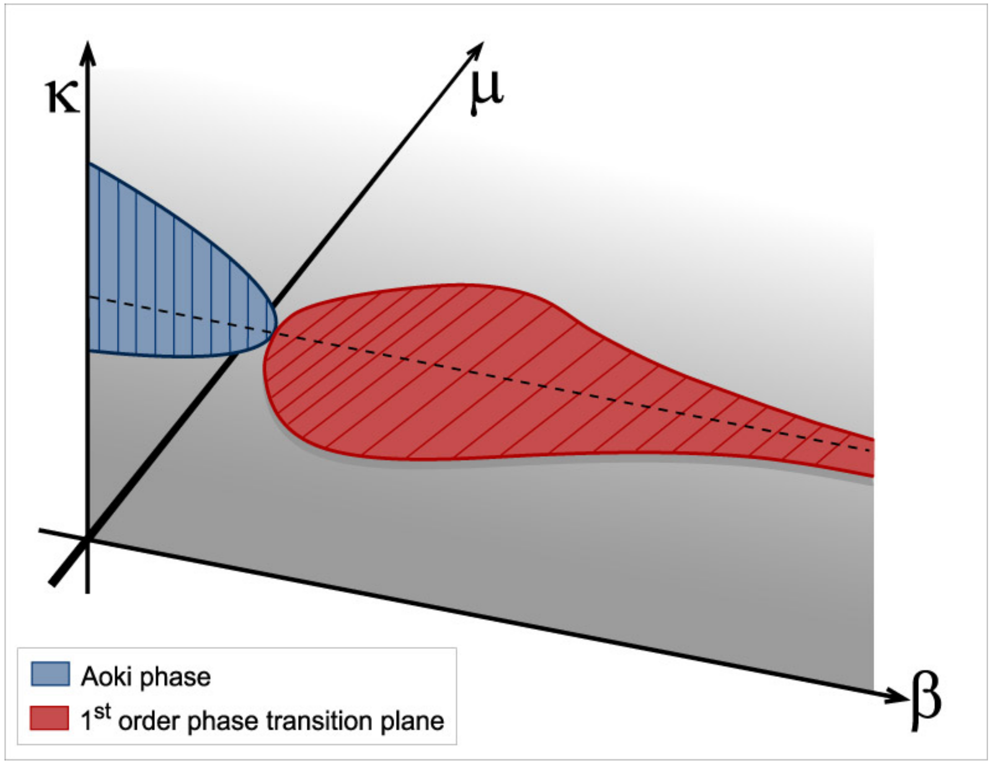
charged pion mass

$$m_{\pi 1}^2 = m_{\pi 2}^2 = \frac{2|c_2|}{F_0^2} \sim a^2.$$

condensate

$$\Delta < \bar{\chi}\chi >= -4F_0^2 B_0 \sqrt{1 - \frac{c_3^2}{4c_2^2}} = -\frac{4F_0^3 B_0}{\sqrt{2|c_2|}} m_{\pi 3}\,,$$

Revealing the generic phase structure of lattice QCD



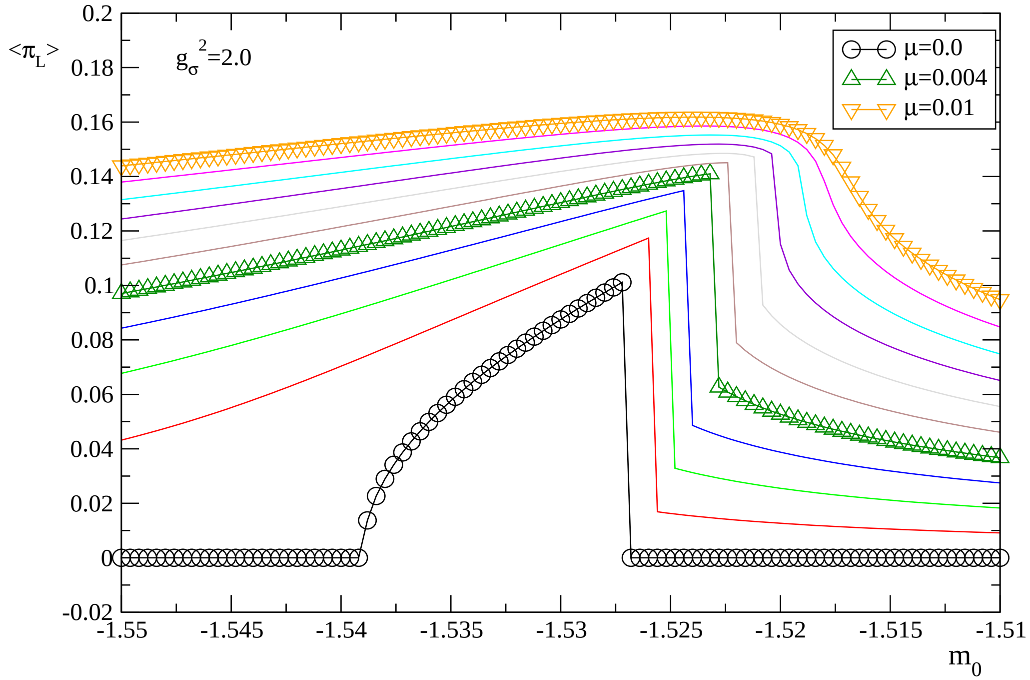
Phase structure of 2-dimensional Wilson twisted mass Gross-Neveu model in large-N

Kei-ichi Nagai, K.J.

extension to twisted mass of old work by

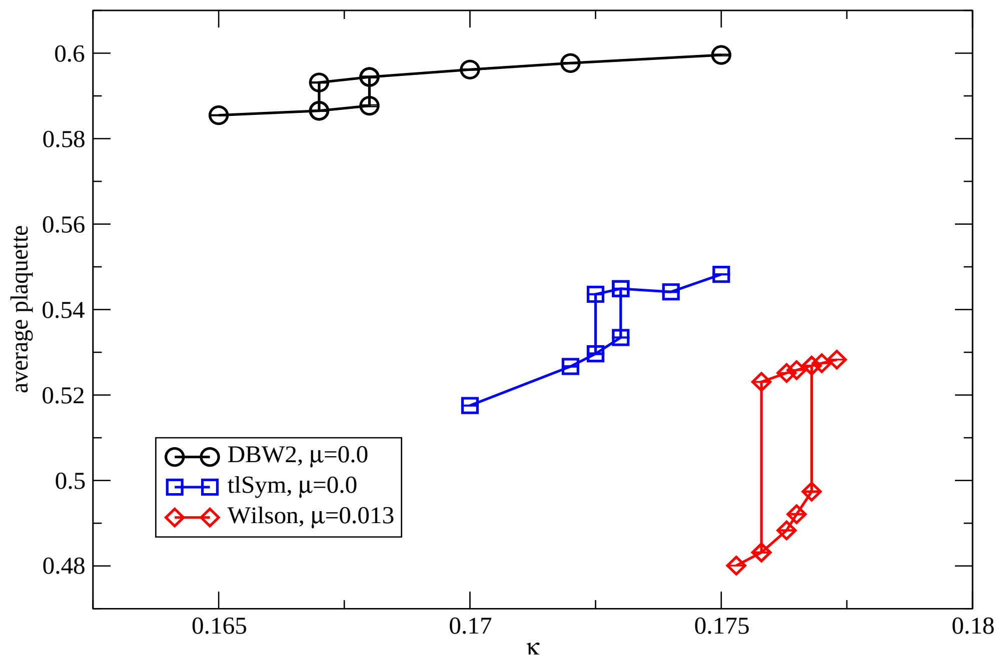
Aoki, PRD 30,2653 ('84), Aoki&Higashijima, Prog. Theor. Phys. 76 521 ('86),

Izubuchi,Noaki,Ukawa, hep-lat/9805019



Dependence of first transition on the gauge action

- plaquette gauge action
- add rectangular loop with coefficient
  - $c_2 = -1.4088$ DBW2 action
  - $c_2 = -1/12$ Tree level Symanzik improved action (tlSym)



Chiral perturbation theory for the phase transition

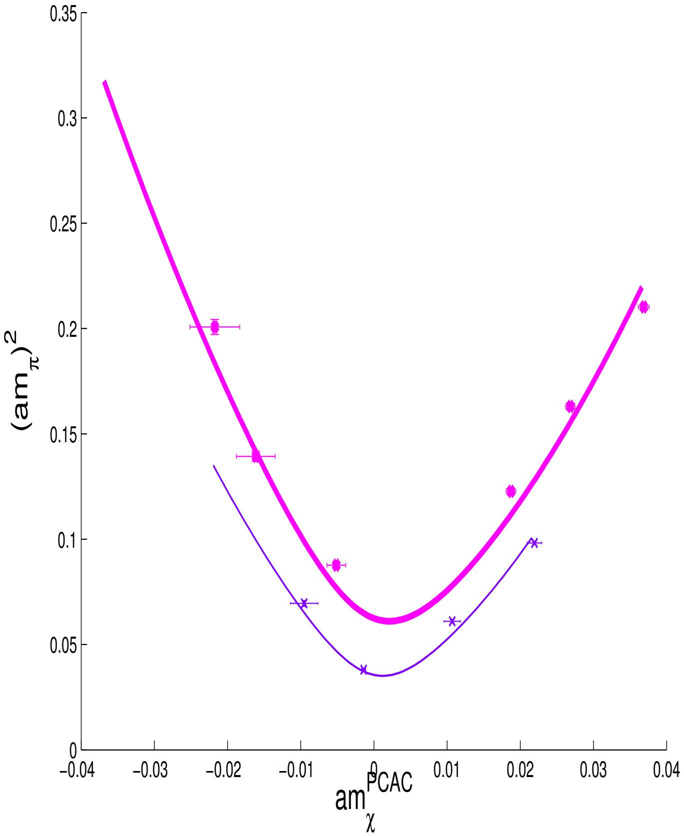
In the regime $m/\Lambda_{QCD} \gtrsim a\Lambda_{QCD}$

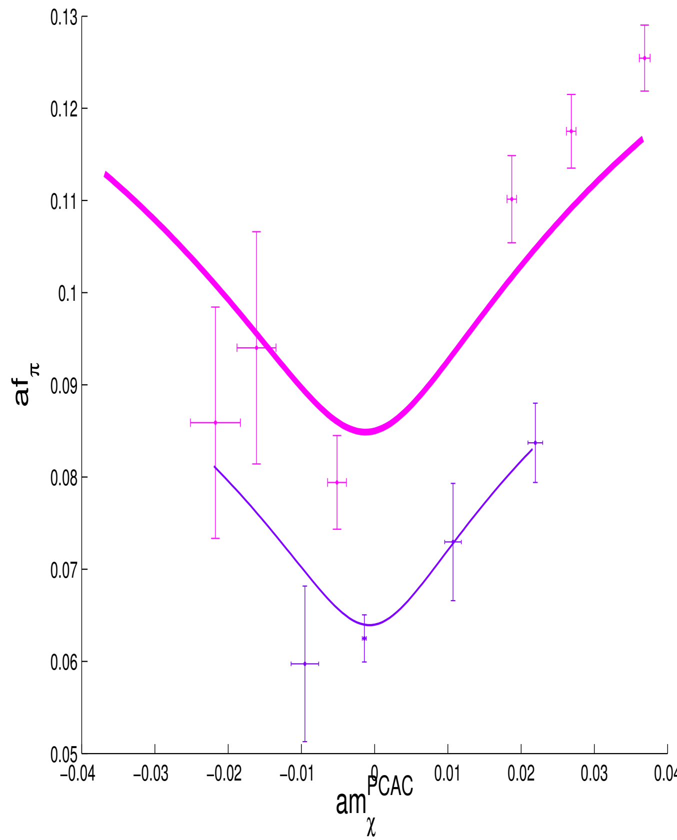
$$M = 2B_0/Z_P\sqrt{m^2_{PCAC,\chi} + \mu^2} \qquad \Lambda_R = 4\pi F_0 \qquad \cos\omega = \frac{m_{PCAC,\chi}}{\sqrt{m^2_{PCAC,\chi}+\mu^2}}$$

$$\begin{aligned}
m_\pi^2 &= M + \frac{8}{{F_0}^2}\left\{M^2(2L_{86} - L_{54}) + 4aM\cos\omega(w - \tilde{w})\right\} + \frac{M^2}{32F_0^2\pi^2}\log\left(\frac{M}{\Lambda_R^2}\right) \\
f_\pi &= F_0 + \frac{4}{F_0}\left\{ML_{54} + 4a\cos\omega\tilde{w}\right\} - \frac{M}{16F_0\pi^2}\log\left(\frac{M}{\Lambda_R^2}\right) \\
g_\pi &= B_0/Z_P\left[F_0 + \frac{4}{F_0}\left\{M(4L_{86} - L_{54}) + 4a\cos\omega(2w_s - \tilde{w})\right\} - \frac{M}{32F_0\pi^2}\log\left(\frac{M}{\Lambda_R^2}\right)\right]
\end{aligned}$$

parameters to fit: B_0/Z_P, F_0, L_{86}, L_{54}, w, $\tilde{w}$

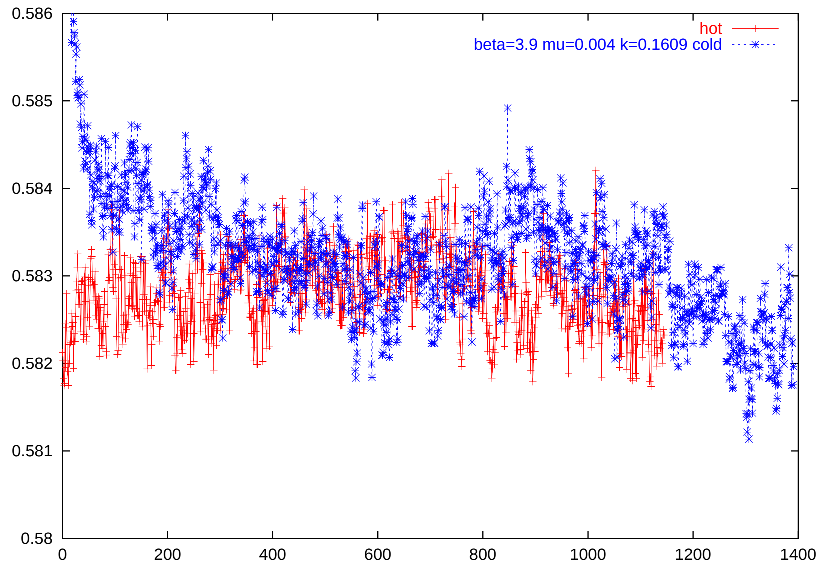
Confronting χPT with simulation data





Where we stand

- tlSym action:
  $\beta = 3.75 \ \ (a = 0.12\text{fm})$ minimal pion mass of $m_\pi^{\min} > 400\text{MeV}$
  difficult to run, large correlations in plaquette time history
  $\beta = 3.9 \ \ (a = 0.09\text{fm})$ minimal pion mass of $m_\pi^{\min} = 280\text{MeV}$ on $16^3 \cdot 32$
  smooth runs, no metastabilities



- $N_f = 2 + 1 + 1$
  - Algorithm (PHMC) is working fine
  - first results available
  - tuning not very difficult

Conclusion

★ Wilson twisted mass fermions at maximal twist

→ are O(a)-improved

→ with PCAC definition: also O(a^2) effects are small at small quark masses

→ pseudo scalar masses O(250)MeV can be reached, quenched and dynamical

→ with existing algorithmic improvements performance costs
are comparable to (in-exact) staggered fermion simulations

→ $N_f = 2 + 1 + 1$ simulations seem to go smooth (PHMC algorithm, tuning)

⇒ a combination of tlSym gauge and maximally twisted mass fermions
defines an action that is ready to go