Exploring the phase structure of lattice QCD with twisted mass quarks

Collaboration:

F. Farchioni[a] R. Frezzotti[b], K. Jansen[c], I. Montvay[d], G.C. Rossi[e], E. Scholz[d], A. Shindler[c], N. Ukita[d], C. Urbach[c,f], I. Wetzorke[c]

[a] Universität Münster
[b] INFN Milano and Università di Milano "Bicocca"
[c] NIC/DESY Zeuthen
[d] DESY Hamburg
[e] Universitá di Roma "Tor Vergata"
[f] Freie Universität Berlin

Outline

- Motivation and Notation
- Simulation Algorithms: TSMB and HMC
- Phase structure in the $\kappa - \mu$ plane: Metastabilities
- Results
- Interpretation
- Conclusion and Outlook

Motivation

Simulations with Wilson fermions at small quark masses have a severe problem:

Unphysical small eigenvalues of the Wilson Dirac operator drive simulations with small quark masses difficult if not impossible.

One way to cure this problem is the Wilson twisted mass formulation:

The twisted mass μ serves as an infrared cut-off
to avoid accidental small eigenvalues.

In addition: $\mathcal{O}(a)$ improvement without additional improvement terms at full twist for allmost all physical quantities [R. Frezzotti, G.C. Rossi, `hep-lat/0306014`].

Notation

The Wilson tmQCD lattice action in the twisted base (χ) reads:

$$S[\chi, \bar{\chi}, U] = \bar{\chi}(D[U] + m_0 + \mu i \gamma_5 \tau_3)\chi$$

Note: $\det\left[D[U] + m_0 + \mu i \gamma_5 \tau_3\right] = \det\left[(D[U] + m_0)^\dagger (D[U] + m_0) + \mu^2\right]$.

Rescale with

$$\chi \to \frac{\sqrt{2\kappa}}{a^{3/2}}\chi\,, \quad \bar{\chi} \to \frac{\sqrt{2\kappa}}{a^{3/2}}\bar{\chi}\,, \quad \kappa = (2am_0 + 8r)^{-1}\,, \quad \tilde{\mu} = 2\kappa\mu$$

to get the standard hopping parameter representation.

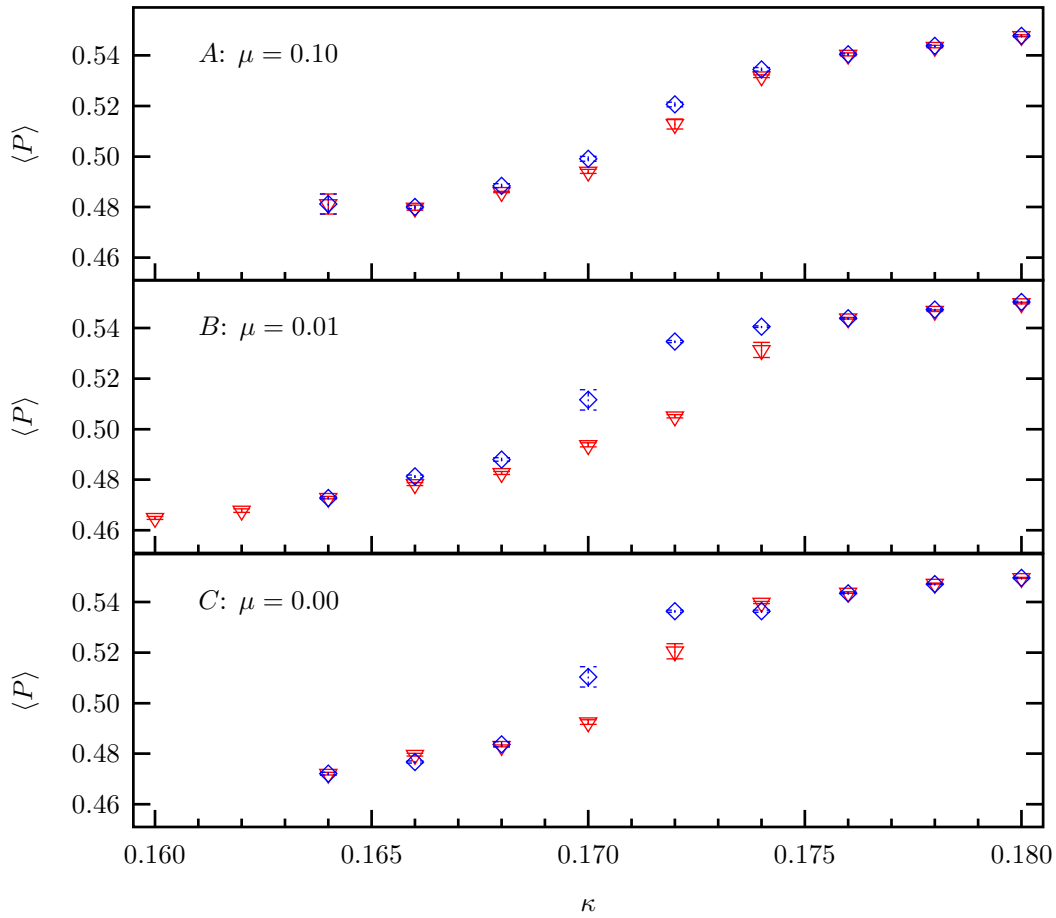
Simulation algorithms

We have two independent algorithms implemented, running and tested:

- Two Step Multi Boson (TSMB) algorithm with Even-Odd preconditioning.
- Hybrid Monte Carlo (HMC) algorithm with Even-Odd preconditioning and Hasenbusch trick.

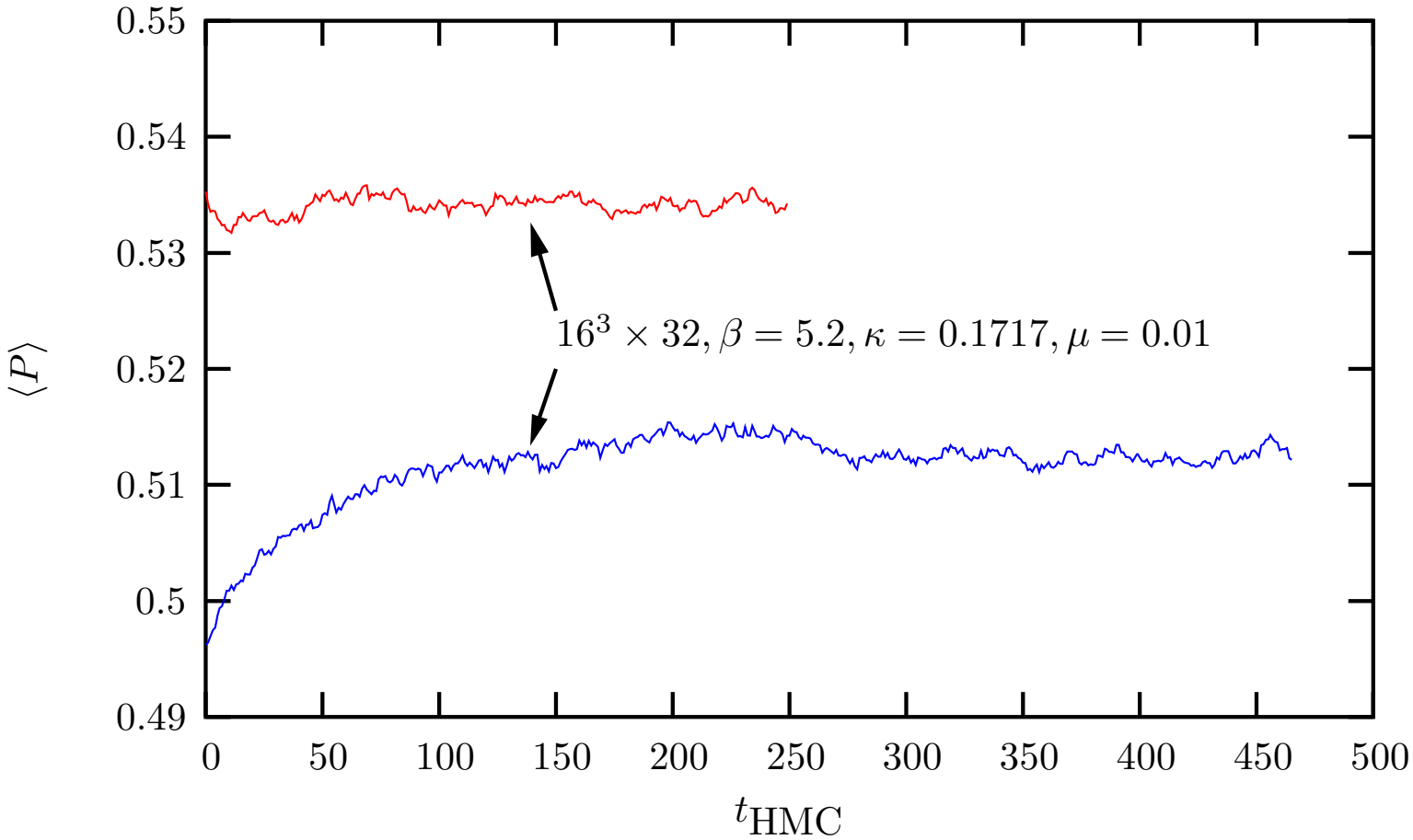
Simulation points: $\beta = 5.2$, various lattice sizes, different values for κ and μ.

Thermal cycles

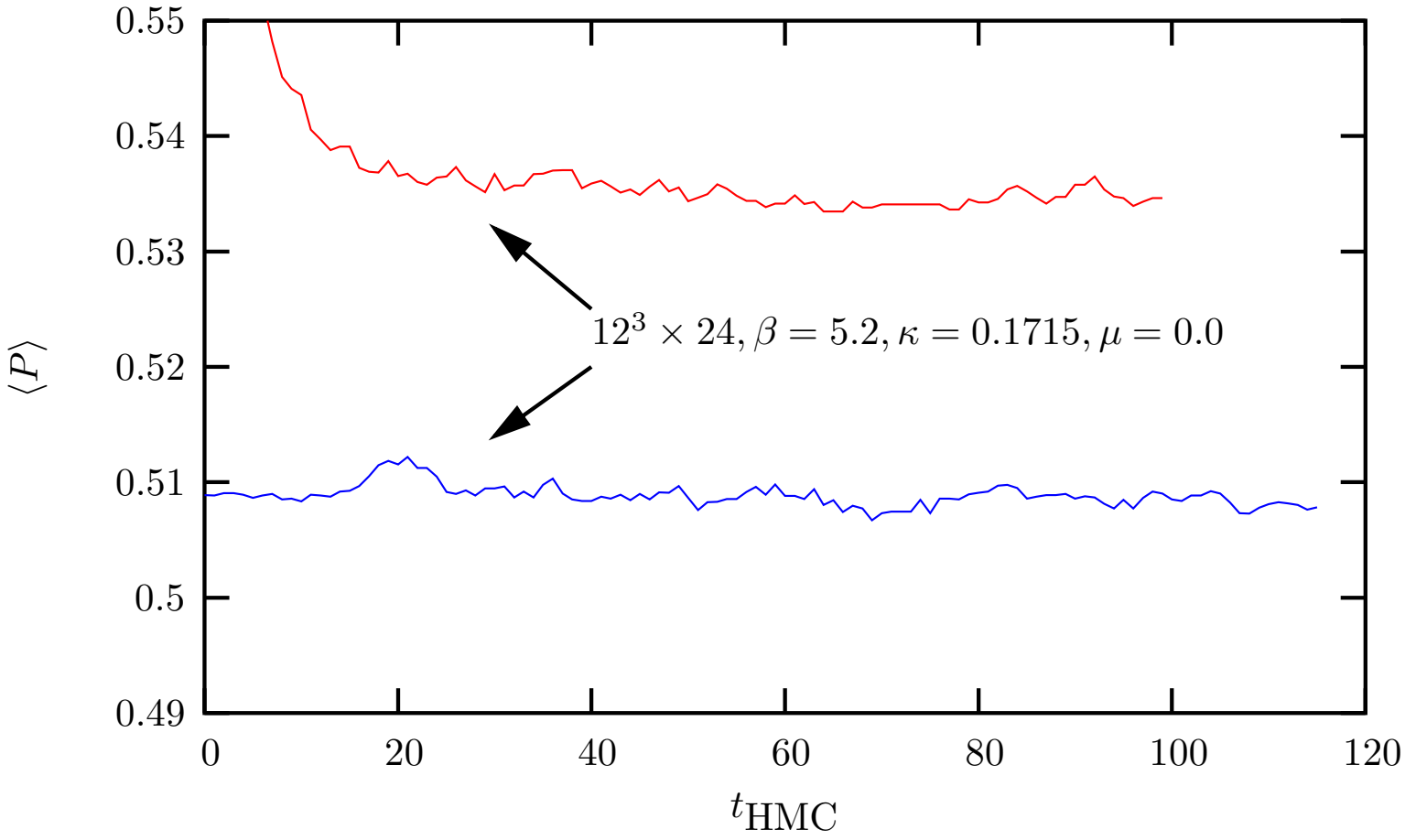


$8^3 \times 16$ lattice,
150 measurements
per value of κ
Forward direction
Backward direction

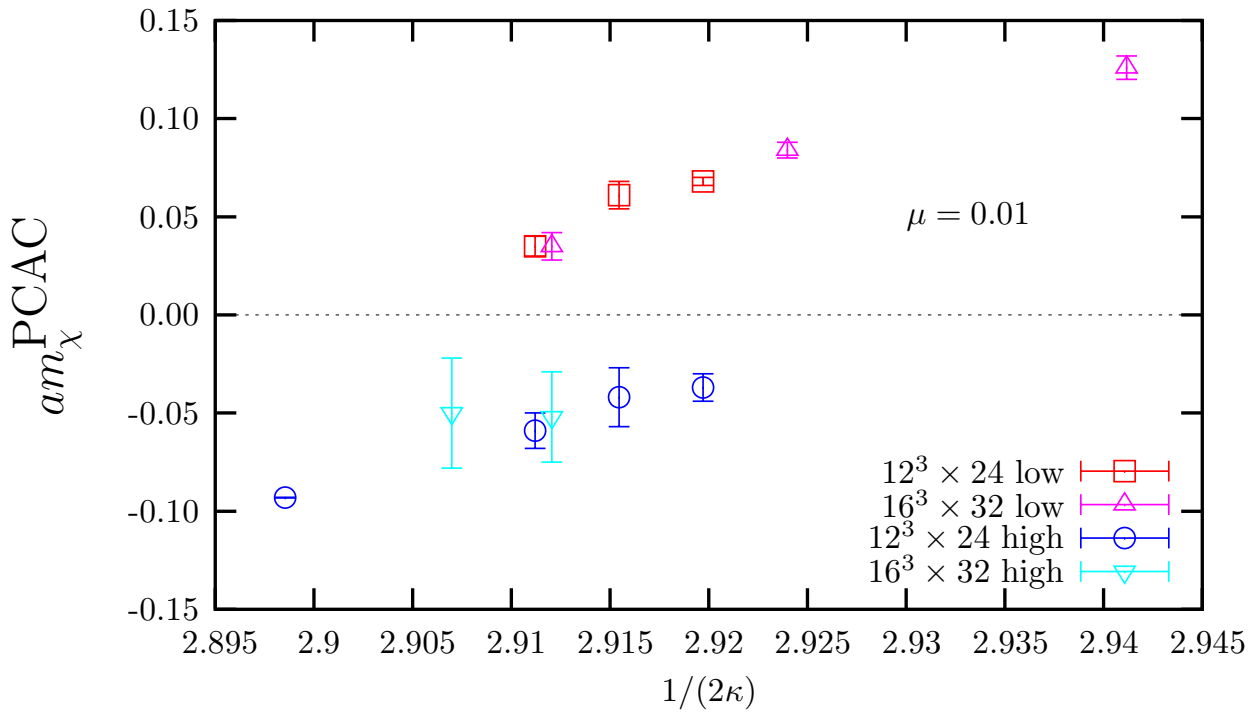
Metastabilities



Metastabilities



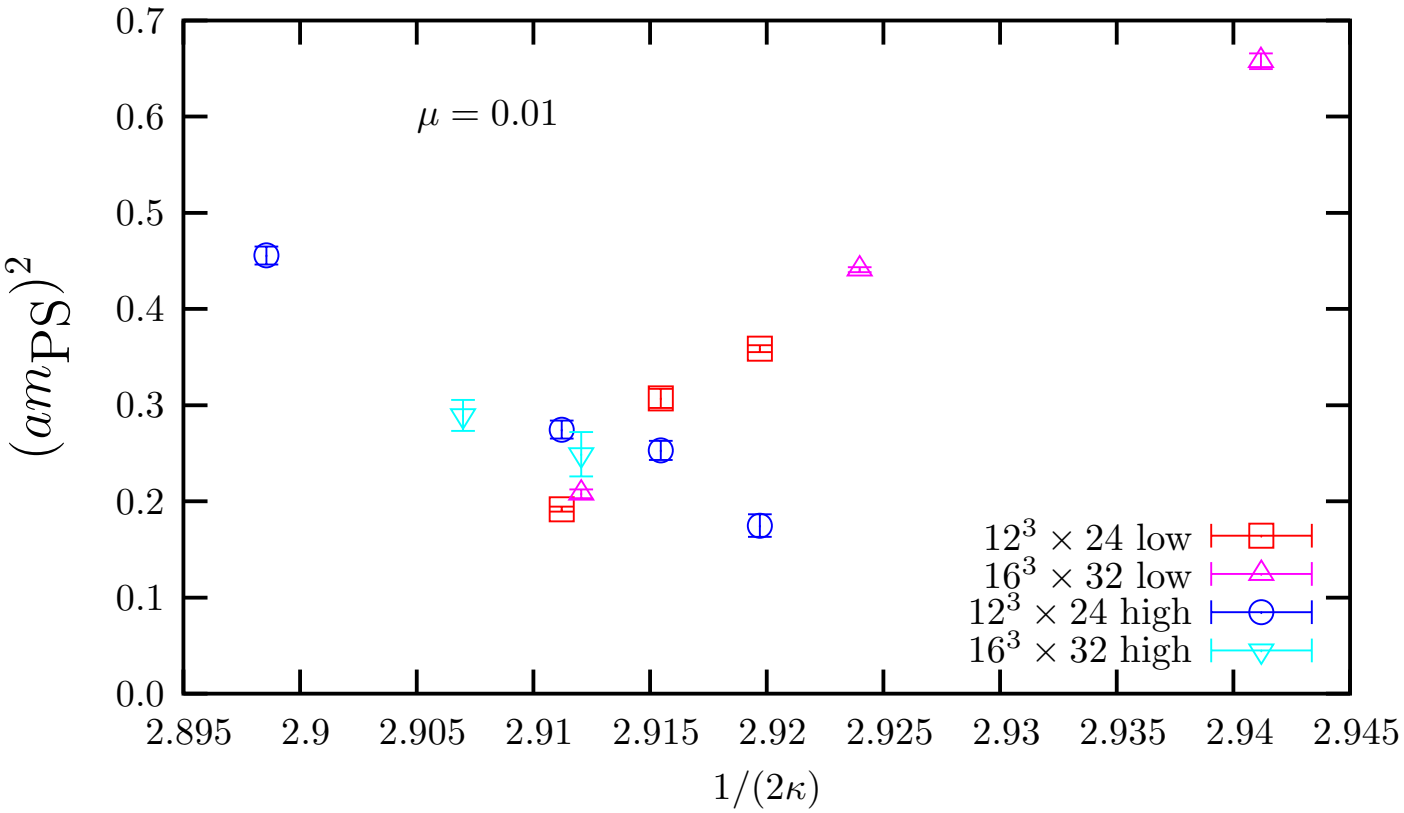
PCAC quark mass in the twisted base



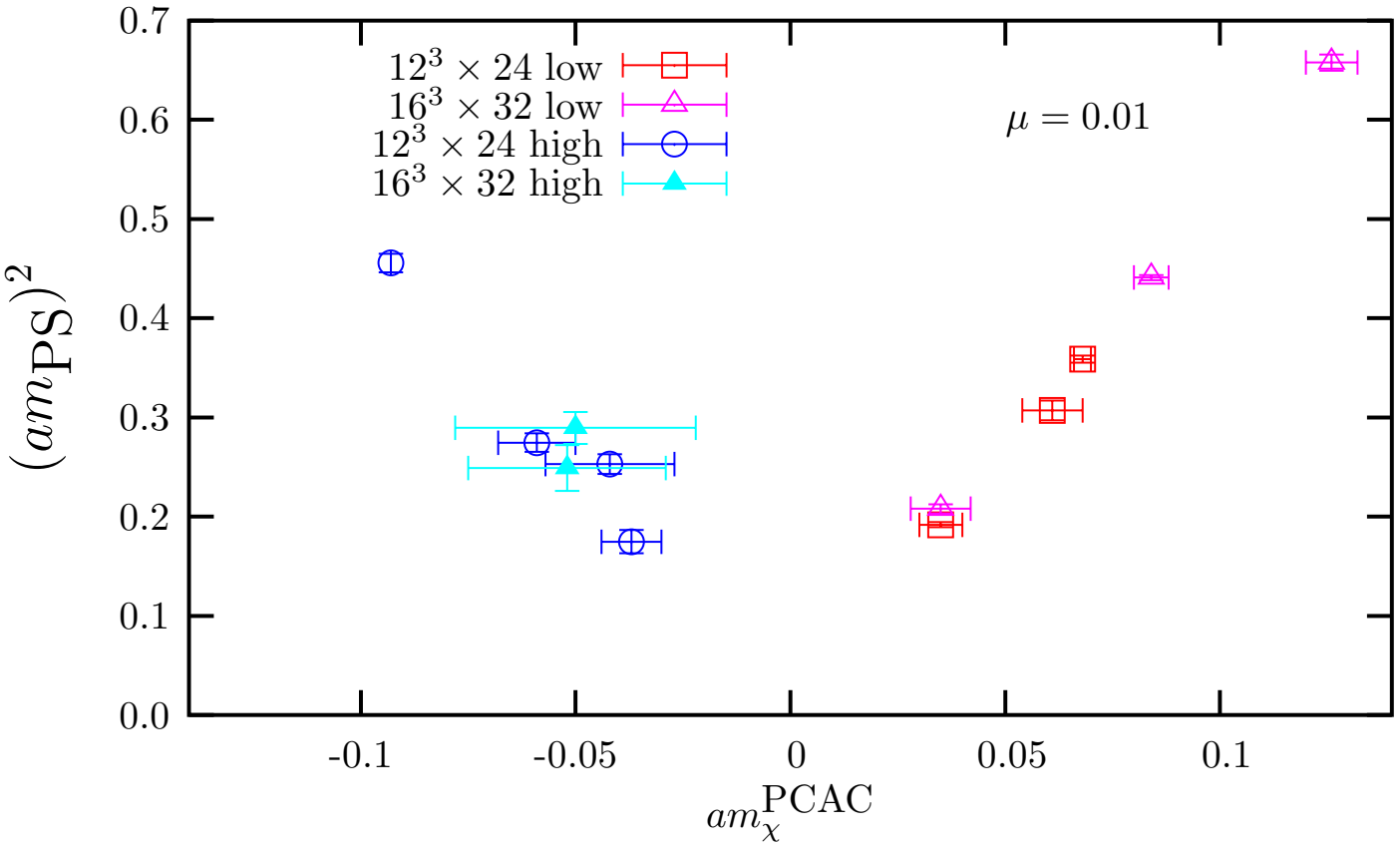
$$m_\chi^{\rm PCAC} = \frac{\langle P(y)\partial_0 A(x)\rangle}{2\langle P(y)P(x)\rangle}$$

with:
A: axialvector current
P: pseudoscalar density
in the twisted base.

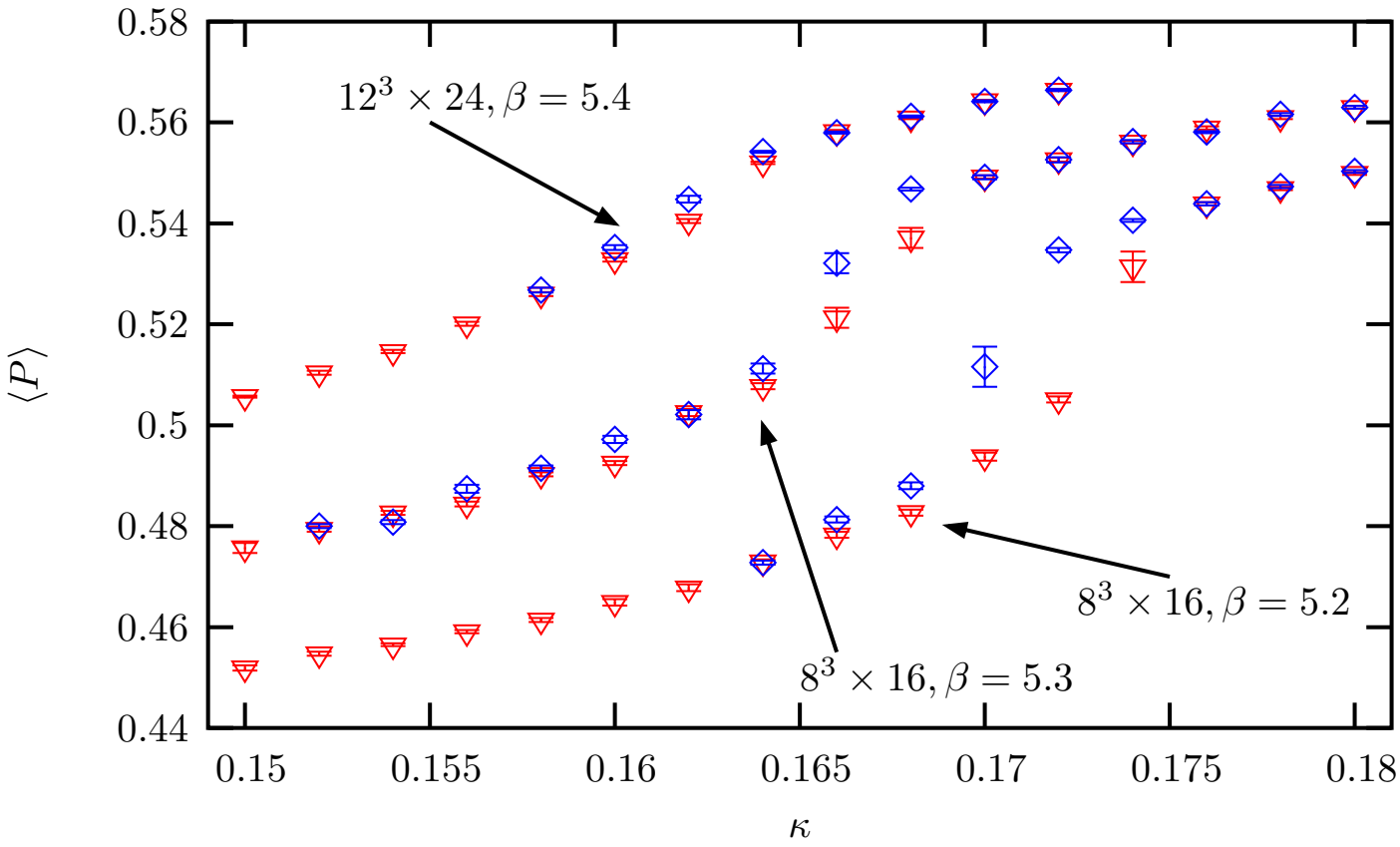
Pseudo scalar mass (charged)



Pseudo scalar mass versus m_χ^{PCAC}



. . . again thermal cycles



Intermediate summary

- We find strong metastabilities:
  - m_χ^{PCAC} and m_{PS} have two different values at the same κ-value.
  - m_{PS} develops a minimum with non zero value.
- How does this phenomenon depend on β and μ?
  There are signs that it is weakening with
  - increasing values of μ.
  - increasing values of β.
- We have an interpretation $\longrightarrow$ talk of F. Farchioni.

Untwisting tmQCD

Important quantities depend upon the twist (e.g. m_q^{PCAC}, f_{PS}): these must be rotated back to the untwisted theory.

Currents in the twisted (χ) basis:

$$V_\mu^a(x) = \bar{\chi}(x)\gamma_\mu t^a \chi(x)$$
$$A_\mu^a(x) = \bar{\chi}(x)\gamma_\mu\gamma_5 t^a \chi(x)$$

Physical currents normalized as in the continuum with no twist:
charged, a=1,2,

$$\hat{V}_\mu^a = \cos\hat{\omega}\,(Z_V V_\mu^a) + \epsilon_{ab}\,\sin\hat{\omega}\,(Z_A A_\mu^b)$$
$$\hat{A}_\mu^a = \cos\hat{\omega}\,(Z_A A_\mu^a) + \epsilon_{ab}\,\sin\hat{\omega}\,(Z_V V_\mu^b)$$

Alternative representation of the currents ($\hat{\omega} \to \omega_{A,V}$)

$$\hat{V}^a_\mu = \mathcal{N}_V \left(\cos\omega_V V^a_\mu + \epsilon_{ab} \sin\omega_V A^b_\mu\right)$$
$$\hat{A}^a_\mu = \mathcal{N}_A \left(\cos\omega_A A^a_\mu + \epsilon_{ab} \sin\omega_A V^b_\mu\right)$$

Normalization:

$$\mathcal{N}_X = \frac{Z_X}{\cos\omega_X \sqrt{1 + \tan\omega_V \tan\omega_A}}$$

Relations:

$$\omega_V = \arctan(Z_A Z_V^{-1} \tan\hat{\omega})$$
$$\omega_A = \arctan(Z_V Z_A^{-1} \tan\hat{\omega})$$
$$\hat{\omega} = \arctan\sqrt{\tan\omega_V \tan\omega_A}$$

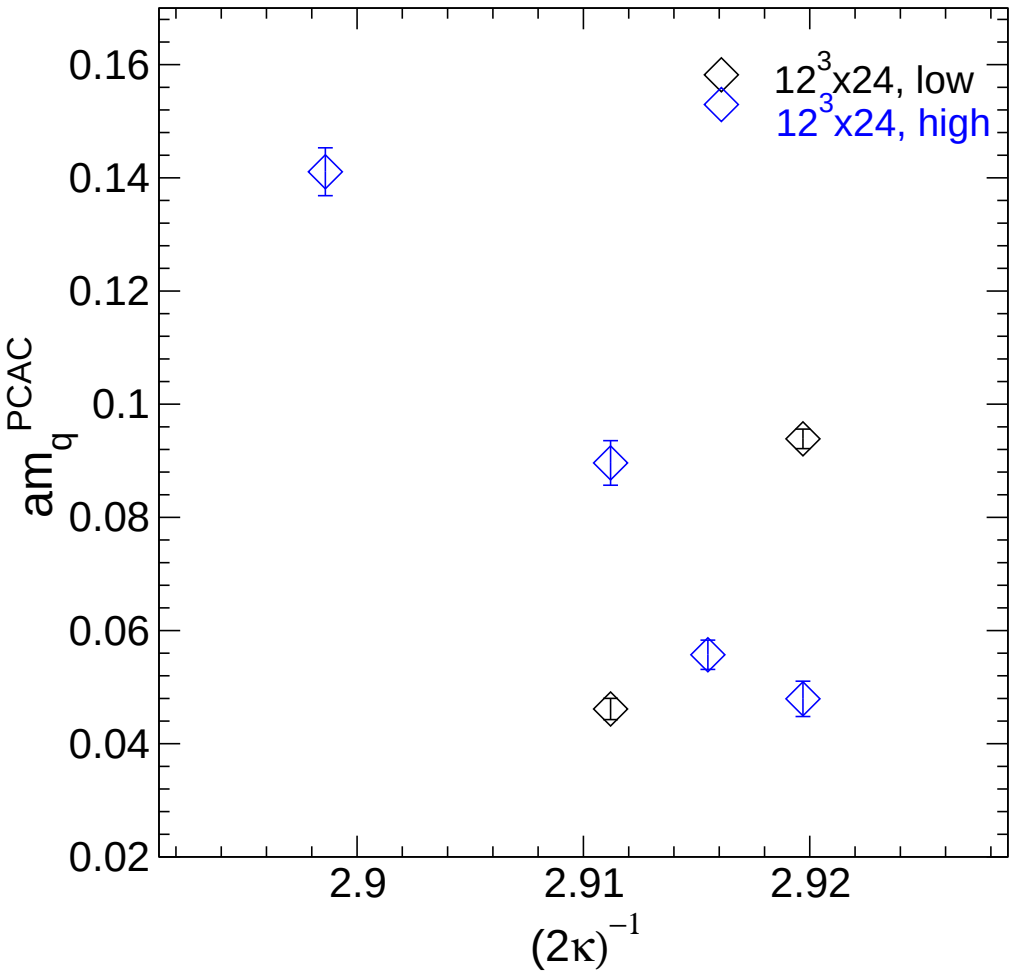
Determination of $\omega_{A,V}$

Parity conservation: $\sum_{\vec{x},\vec{y}} \langle P(y)\, \hat{V}_0(x)\, \rangle = \sum_{\vec{x},\vec{y}} \langle \hat{V}_0(y)\, \hat{A}_0(x) \rangle = 0$

$$\rightarrow \begin{cases} \tan\omega_V = \dfrac{-i \sum_{\vec{x},\vec{y}} \langle P(y) V_0(x) \rangle}{\sum_{\vec{x},\vec{y}} \langle P(y) A_0(x) \rangle} \\ \\ \tan\omega_A = \dfrac{i \sum_{\vec{x},\vec{y}} \langle V_0(y) A_0(x) \rangle + \tan\omega_V \sum_{\vec{x},\vec{y}} \langle A_0(y) A_0(x) \rangle}{\sum_{\vec{x},\vec{y}} \langle V_0(y) V_0(x) \rangle - i \tan\omega_V \sum_{\vec{x},\vec{y}} \langle A_0(y) V_0(x) \rangle} \end{cases}$$

Vector symmetry: $\langle O(y)\, \partial \hat{V}(x) \rangle = 0 \quad \rightarrow \quad \tan\omega'_V = \dfrac{-i \langle O(y)\, \partial V(x) \rangle}{\langle O(y)\, \partial A(x) \rangle}$

$O(a)$ ambiguity

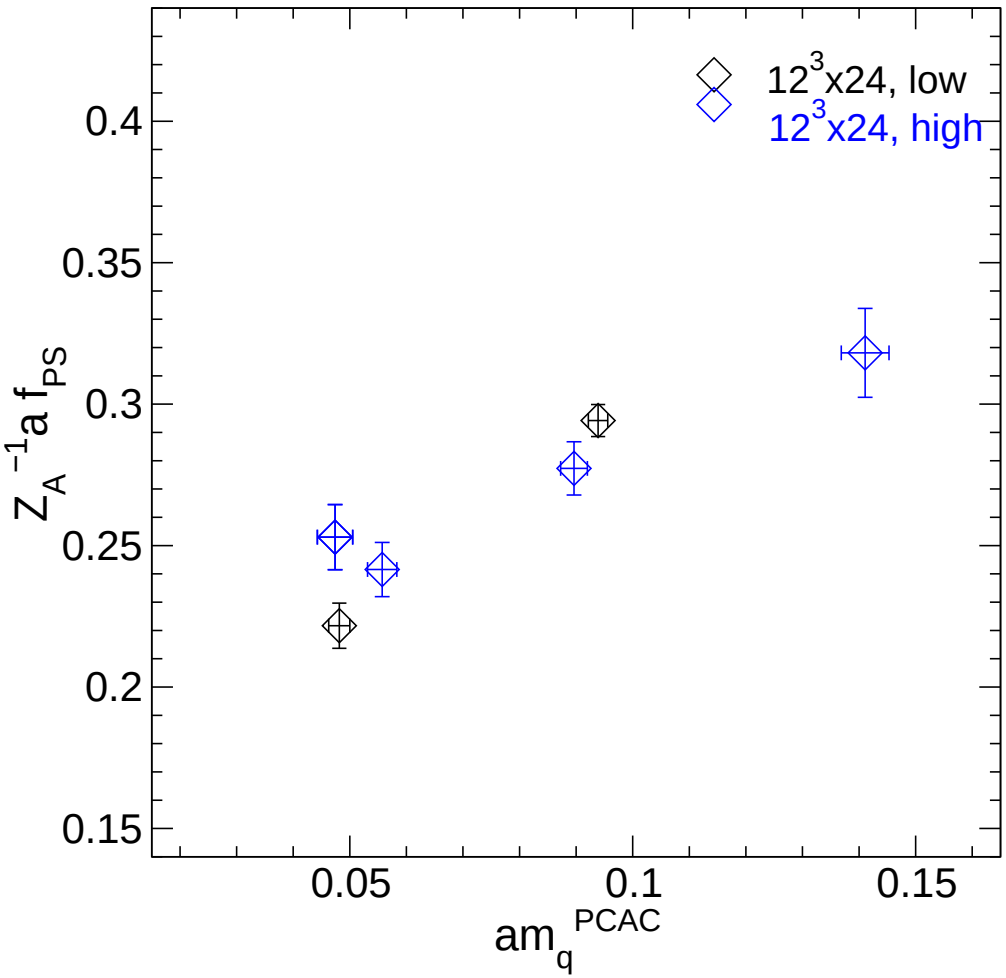


PCAC quark mass

$$m_q^{PCAC} = \frac{Z_A{}^{-1}\langle P(y)\,\partial_0\hat{A}(x)\rangle}{2\langle P(y)\,P(x)\rangle}$$

low: $\hat{\omega}/\pi = 0.05 - 0.1$

high: $\hat{\omega}/\pi = 0.87 - 0.96$



PS decay constant

vs

m_q^{PCAC}

$$f_{PS} = m_\pi^{-1} \langle \pi | \hat{A}_0(0) | 0 \rangle$$

Phase structure of Wilson fermions

Framework: chPT including up to $O(m^2, a^2, am)$ corrections, $N_f = 2$ (no twist!). Sharpe and Singleton, 1998

Two possible scenarios depending on the sign of a coefficient (c_2) in the effective potential:

S1. $c_2 > 0$: lattice artifacts induce region of quark masses with spontaneously broken vector symmetry and parity (Aoki Phase).

S2. $c_2 < 0$: region of quark masses with two competing (meta)stable minima with opposite sign of the condensate and PCAC quark mass (1st order PT).

Our observations indicate that S2 is the scenario valid in our case ($\beta = 5.2$).

(Cf. Ilgenfritz, Kerler, Müller-Preussker, Sternbeck and Stüben, `hep-lat/0309057`: no Aoki phase observed for $\beta \geq 4.6$.)

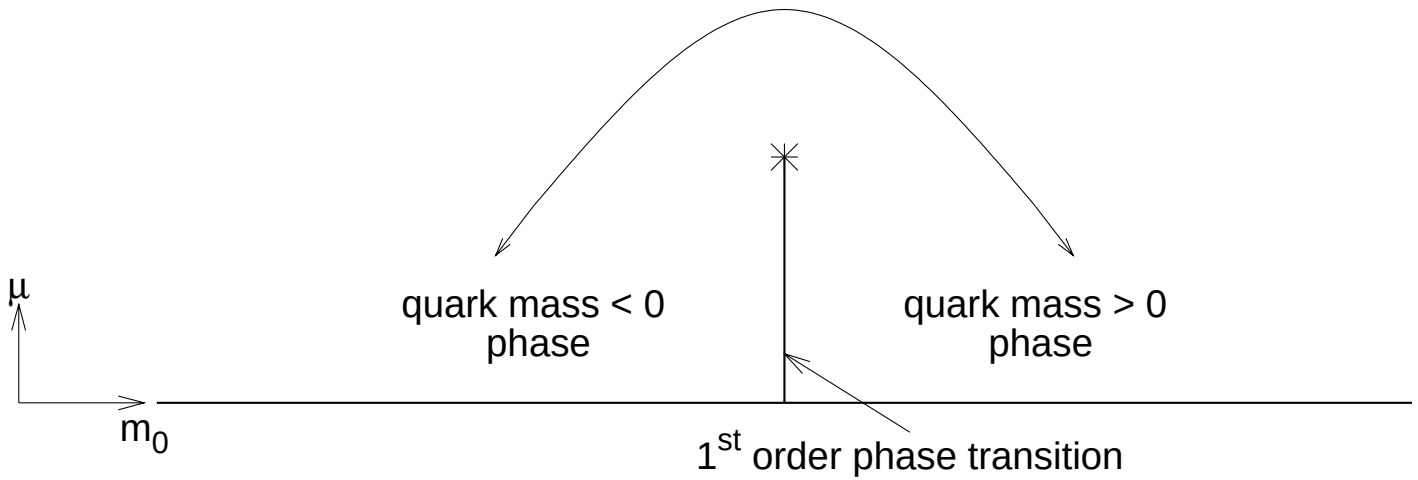
S2 in the case of twisted mass Wilson fermions ($\mu \neq 0$):

Microscopic interpretation of metastability: cloud of eigenvalues of the Dirac operator with small modulus crossing the imaginary axis.

vanishing of the determinant $\rightarrow$ potential barrier

$\det D_{TM}(\mu) = \det\left[(\gamma_5 D_W)^2 + \mu^2\right] \rightarrow$ barrier dumped by $\mu \neq 0$

The phase diagram for $\mu \neq 0$ from chPT analysis, cf. Gernot Münster's talk at this conference



Conclusions

- Twisted mass quarks: nice framework for the exploration of the phase structure of lattice QCD

- We see metastabilities and signs of a first order phase transition:
  $\Longrightarrow \mu = 0$: explaination within the model of Sharpe and Singleton.
  $\Longrightarrow \mu \neq 0$: talk by Gernot Münster at this conference.

Outlook/open questions

- Extend the investigation with different values of β.
- What is the lowest quark mass that can be simulated at a given value of β?
- Is the observed metastability related to that found in Wilson simulations with a clover term? [JLQCD, `hep-lat/0110088`]
- Is there a gauge action with $c_2 = 0$?