Dynamical Wilson twisted mass fermions

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Contents

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Introduction

In order to be conclusive, the numerical simulations of QCD have to be performed at small quark masses.

"Small" means: close to the physical values ($m_{u,d}/\Lambda_{QCD} \simeq 0.02$, $m_s/\Lambda_{QCD} \simeq 0.5$) or, at least, in the range of applicability of low-order ChPT.

This is a great challenge for algorithms and computers.

Once this is achieved, since the quark masses are free variables, one can obtain more information about QCD than it is available in experiments.

Using twisted-mass Wilson fermions is a promising way to proceed.

Twisted mass quarks

Frezzotti, Grassi, Sint, Weisz, hep-lat/9909003, hep-lat/0101001;
Frezzotti, Rossi, hep-lat/0306014, hep-lat/0311008, hep-lat/0407002,...

Lattice action: for a mass-degenerate doublet, with the twisted mass μ

$$S_\chi = \sum_x \left\{ (\overline{\chi}_x[\mu_1 + i\gamma_5\tau_3\,\mu]\chi_x) - \frac{1}{2}\sum_{\mu=\pm 1}^{\pm 4} (\overline{\chi}_{x+\hat{\mu}} U_{x\mu}[r+\gamma_\mu]\chi_x) \right\}$$

$$\equiv \sum_{x,y} \overline{\chi}_y Q_{(\chi)yx}\chi_x$$

where $\mu_1 \equiv (2\kappa)^{-1} \equiv \mu_0 + 4r$, with the hopping parameter κ.
In numerical simulations the Wilson parameter is usually set to $r = 1$.

Non-degenerate doublet: by the substitution $\mu \to \mu_{(+)} + \gamma_5\tau_2\,\mu_{(-)}$.

Introducing the single-flavour fermion matrix

$$Q_{(\mu_1)yx} \equiv \mu_1 \delta_{yx} - \frac{1}{2} \sum_{\mu=\pm 1}^{\pm 4} \delta_{y,x+\hat{\mu}} U_{x\mu} [r + \gamma_\mu]$$

one has

$$Q_{(\chi)} = i\gamma_5 \tau_3 \, \mu + Q_{(\mu_1)}$$

In order to display μ as the mass, one can define

$$Q_{(tm)} \equiv -i\gamma_5 \tau_3 \, Q_{(\chi)} = \mu - i\gamma_5 \tau_3 Q_{(\mu_1)} = \mu - i\tau_3 \tilde{Q}_{(\mu_1)}$$

where $\tilde{Q}_{(\mu_1)} \equiv \gamma_5 Q_{(\mu_1)}$ denotes the hermitean single-flavour fermion matrix.

$Q_{(tm)}$ has an eigenvalue spectrum as, for instance, staggered fermions.
The eigenvalues are on a line perpendicular to the real axis, at a distance μ from the origin. The parameter μ_1 can be tuned to its critical value $\mu_1 = \mu_{1cr}$.

For the determinant one has:

$$\det(Q_{(tm)}) = \det(\mu^2 + \tilde{Q}^2_{(\mu_1)}) = \det(Q_{(\chi)})$$

The continuum limit and renormalization can be best investigated in the physical basis of fermion fields. This is related to $\chi_x, \overline{\chi}_x$ by the chiral transformation

$$\psi_x \equiv e^{i\frac{\omega}{2}\gamma_5\tau_3}\chi_x = \left(\cos\frac{\omega}{2} + i\gamma_5\tau_3\sin\frac{\omega}{2}\right)\chi_x \ ,$$

$$\overline{\psi}_x \equiv \overline{\chi}_x e^{i\frac{\omega}{2}\gamma_5\tau_3} = \overline{\chi}_x\left(\cos\frac{\omega}{2} + i\gamma_5\tau_3\sin\frac{\omega}{2}\right)$$

where the twist angle ω depends on the critical untwisted bare quark mass μ_{1cr} and is defined together with μ_q (the magnitude of the bare fermion mass) by

$$\mu_1 - \mu_{1cr} = \mu_0 - \mu_{0cr} = \mu_q\cos\omega \ , \qquad \mu = \mu_q\sin\omega$$

In case of $\mu_1 = \mu_{1cr} = (2\kappa_{cr})^{-1}$ we have “full twist”: $\omega = \pi/2,\ \mu_q = \mu$.

The lattice action in the physical basis can be written as

$$\begin{aligned} S_\psi \quad &= \quad \sum_x \Bigg\{ \mu_q\overline{\psi}_x\psi_x - \frac{1}{2}\sum_{\mu=\pm1}^{\pm4} \overline{\psi}_{x+\hat{\mu}}U_{x\mu}\gamma_\mu\psi_x \\ &+ \quad \left[\mu_{0cr}\overline{\psi}_x - \frac{r}{2}\sum_{\mu=\pm1}^{\pm4}\left(\overline{\psi}_{x+\hat{\mu}}U_{x\mu} - \overline{\psi}_x\right)\right] e^{-i\omega\gamma_5\tau_3}\psi_x \Bigg\} \end{aligned}$$

Advantages of twisted mass LQCD compared to untwisted Wilson-type LQCD:

- the numerical simulation is faster,
- the lattice artifacts are reduced,
- the operator mixing in the renormalization procedure can be made simpler,
- there exists an exactly conserved axialvector current;

Disadvantage:

- there is an explicit flavour symmetry breaking.

QCD phase structure: continuum and lattice

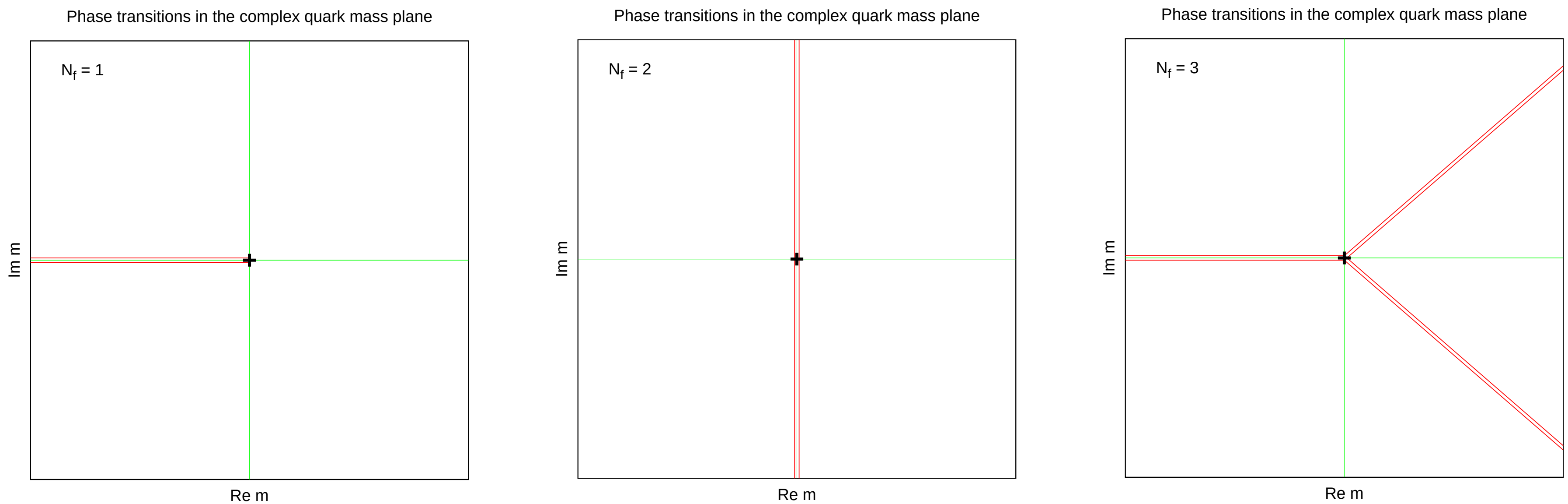
As a consequence of spontaneous chiral symmetry breaking, in QCD there is a singularity at zero quark mass, which is a first order phase transition point. The simplest manifestation of this singularity is that the scalar quark condensate changes sign if one approaches zero from positive and negative quark mass.

The phase structure in the complex quark mass plane near zero quark mass is described by the low energy chiral Lagrangian.

A partial list of the literature:

E. Witten, Annals of Phys. 128 (1980) 363; M. Creutz, hep-th/9505112, hep-ph/9608216; A. V. Smilga, hep-ph/9805214; I. M., hep-lat/9909020.

First order phase transitions in QCD in the complex quark mass plane with N_f equal mass quarks, as obtained from the low energy chiral Lagrangian.



For an odd number of flavours there is spontaneous CP-violation for negative quark mass.
The phase structure of supersymmetric Yang-Mills theory with gauge group $SU(N_f)$ is similar.

Chiral effective Lagrangian: for three equal (complex) mass quarks.

$$\mathcal{L} = \frac{f_\pi^2}{2}\left[\mathrm{Tr}\,\left(\partial_\mu U\,\partial_\mu U^{-1}\right) + 2\,\mathrm{Re}\,\mathrm{Tr}\,\left(m_q e^{-i\theta} U\right)\right]$$

With an $SU(3) \otimes SU(3)$-transformation U can be transformed to

$$U = e^{i\Phi_r \lambda_r / f_\pi} \Longrightarrow \begin{pmatrix} e^{i\alpha} & 0 & 0 \\ 0 & e^{i\beta} & 0 \\ 0 & 0 & e^{-i(\alpha+\beta)} \end{pmatrix}$$

This gives for the effective potential

$$E(\alpha,\beta) \propto cos(\alpha-\theta) + cos(\beta-\theta) + cos(\alpha+\beta+\theta)$$

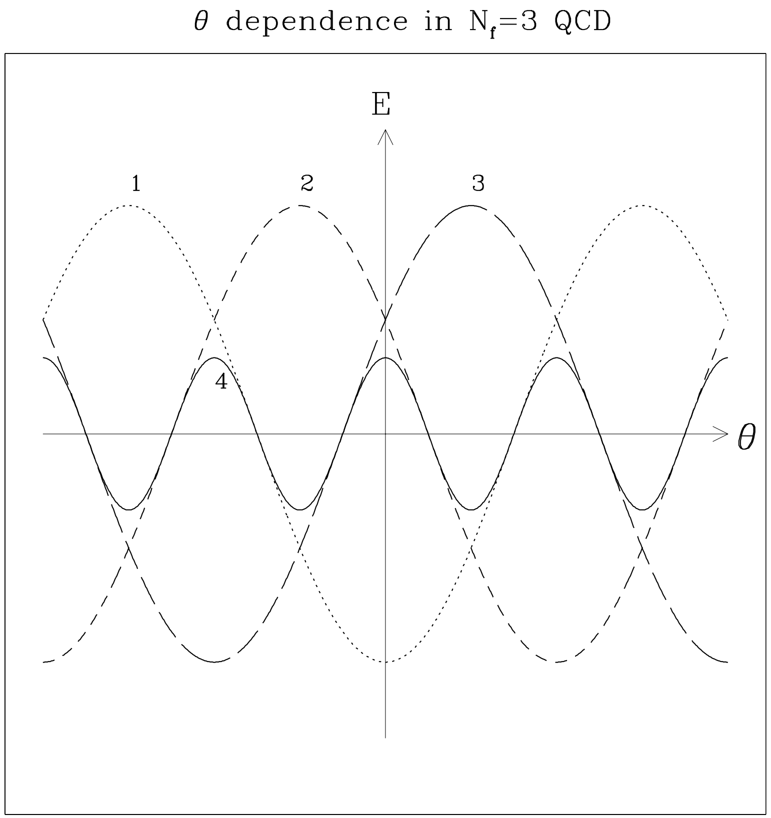
The stationary points of the effective potential, for given θ, are at:

$$\begin{aligned} 1: \quad \alpha &= \beta = 0 \\ 2: \quad \alpha &= \beta = 2\pi/3 \\ 3: \quad \alpha &= \beta = -2\pi/3 \\ 4: \quad \alpha &= \beta = \pi - 2\theta \ldots \end{aligned}$$

First order phase transition between $1 \leftrightarrow 2$ at $\theta = \pi/3$:

$$U = \begin{pmatrix} 1 & 0 & \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Longleftrightarrow \begin{pmatrix} e^{2i\pi/3} & 0 & 0 \\ 0 & e^{2i\pi/3} & 0 \\ 0 & 0 & e^{2i\pi/3} \end{pmatrix}$$

Similarly at $\theta = \pi$ $2 \leftrightarrow 3$ and $\theta = 5\pi/3$ $3 \leftrightarrow 1$.



In the complex mass plane the phase transition at $\theta = \pi$ is at real negative values which are available to numerical simulations.

The situation is analogous to SYM with $SU(3)$ gauge group.

Phase structure with $N_f = 2$ Wilson-type quarks:

Sharpe and Singleton, hep-lat/9804028.

Up to order $\mathcal{O}(a^2)$ in lattice artifacts the effective potential can be brought to the form:

$$\mathcal{V}_\chi = -c_1 A + c_2 A^2 \; .$$

A is the flavour singlet component of the SU(2) matrix valued field Σ in the low energy effective chiral Lagrangian:

$$\Sigma = A + i \sum_{r=1}^{3} B_r \tau_r \; .$$

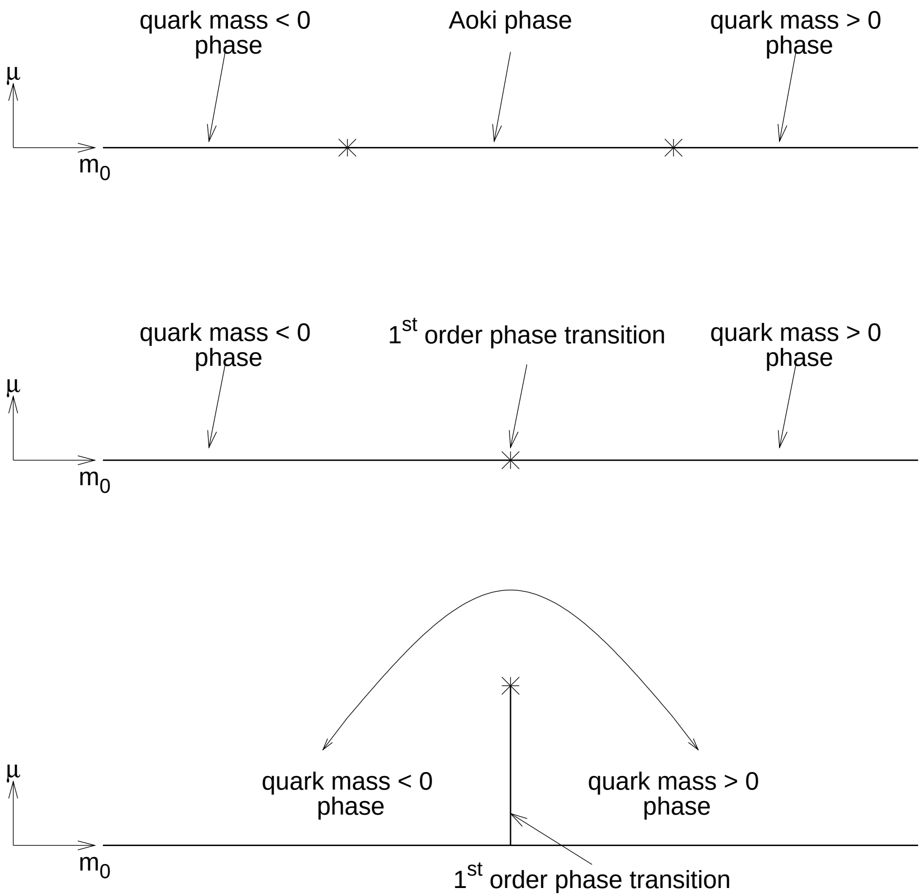
Because of $1 = A^2 + \sum_{r=1}^{3} B_r B_r$ the variable A lies in the interval $[-1, +1]$.

In the vicinity of the critical quark mass the constant $c_2 = \mathcal{O}(a^2)$ and the other parameter c_1 is proportional to the bare quark mass.

Possible phase structures: between the positive and negative quark mass phases there is either an Aoki-phase or a first order phase transition.

Possible phase structures in the Sharpe-Singleton model:

depending on (the sign of) the parameter c_2



QCD phase structure: numerical simulations

Recent numerical simulations show that the width of Aoki phase in the bare mass parameter shrinks to zero (or to a small value) at $\beta \leq 4.6$.
E.-M. Ilgenfritz et al., hep-lat/0309057.

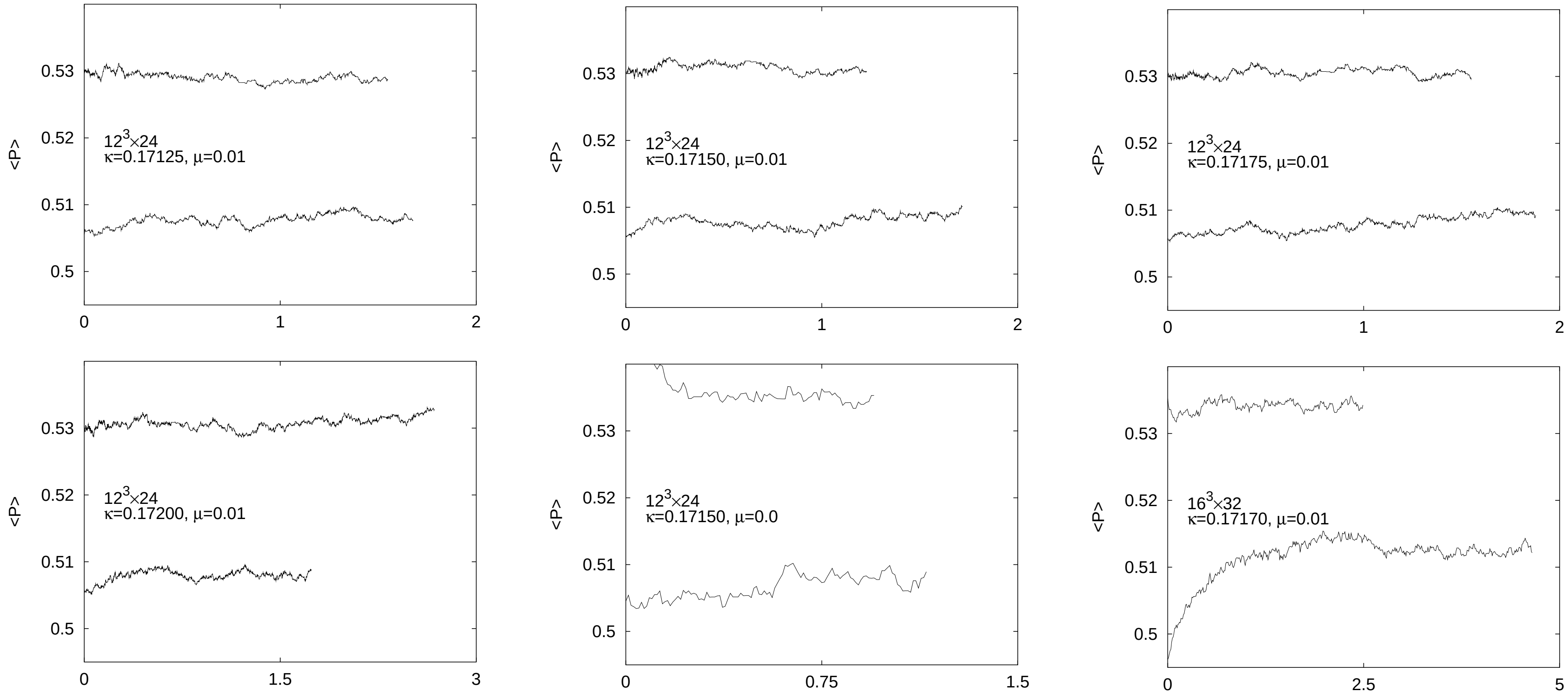
Earlier observations of strong first order phase transitions:
T. Blum et al., hep-lat/9404006;
JLQCD Collaboration, S. Aoki et al., hep-lat/0110088, hep-lat/0409016.

At present, the interpretation of these results is unclear.
The use of different fermion-gauge-action combinations and different number of quark flavours requires a case-by-case study.

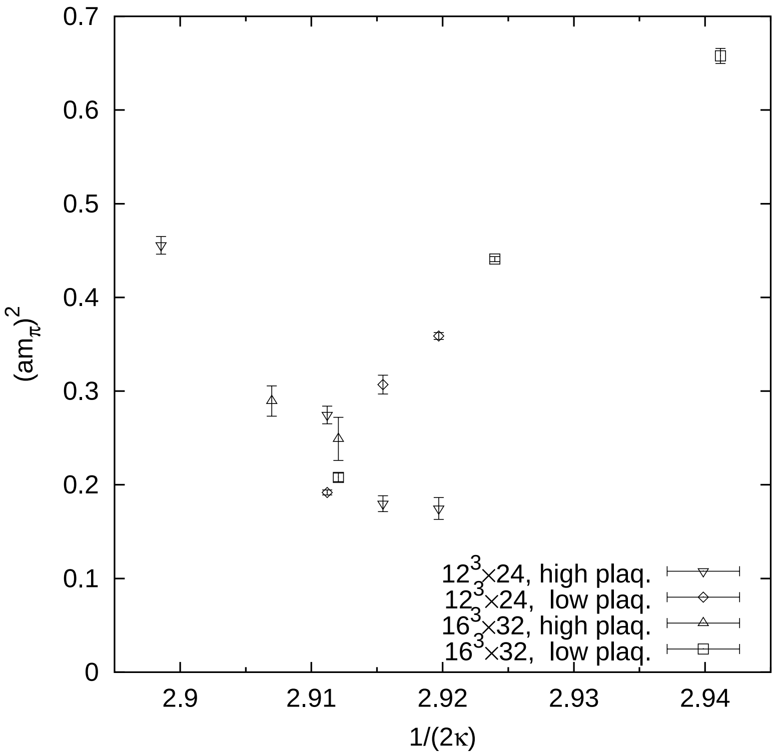
It is not excluded that all these observations are due to the realization of the second ($c_2 < 0$) Sharpe-Singleton scenario.

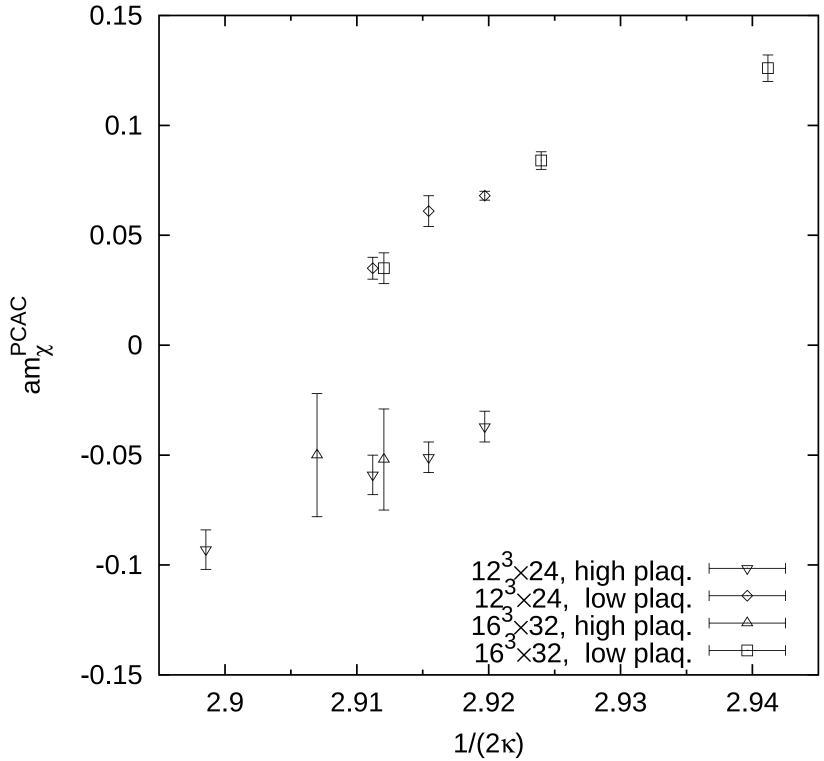
Recent results on the phase structure of Wilson-quarks: $N_f = 2$

Farchioni et al., hep-lat/0406039, hep-lat/0409098. Metastable states at $\beta = 5.2$.
The number of sweeps is given in thousands. The lattice size is $12^3 \times 24$, except for the right panel in the bottom line where it is $16^3 \times 32$. The twisted mass is $\mu = 0.01$, exept for the middle panel in the bottom line where it is $\mu = 0$.

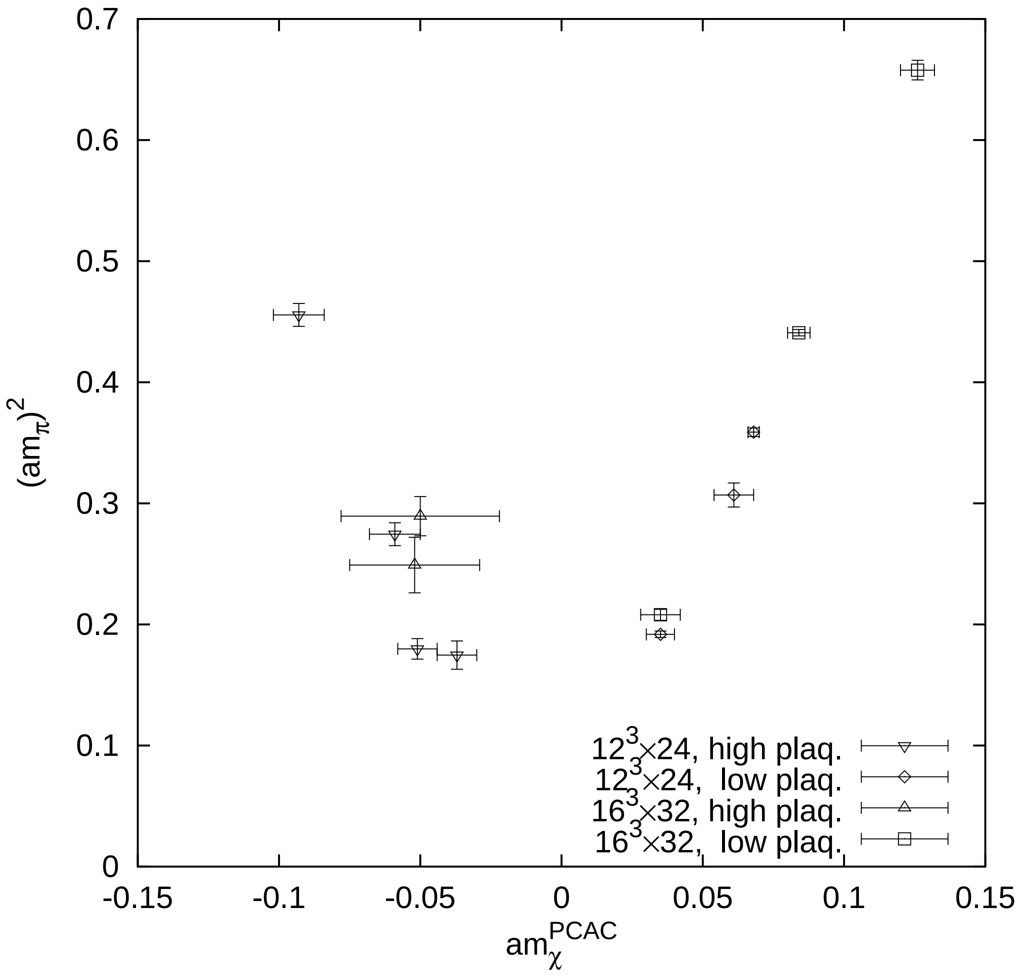


Pion mass-squared and quark mass in the two (stable or metastable) phases:





Pion mass-squared versus quark mass:
the gap in the middle should be filled at larger β



The presence of a non-zero twisted mass has been very helpful because the simulations become easier. In spite of this, the small quark masses and the metastability represent a serious challenge for the update algorithms.

Two optimized updating algorithms have been used:
Multiple Pseudofermion Hybrid Monte Carlo (MPHMC)
M. Hasenbusch, hep-lat/0107019; M. Hasenbusch, K. Jansen, hep-lat/0211042.
Two-Step Multi-Boson (TSMB)
I. M., hep-lat/9510042; qq+q Collaboration, F. Farchioni et al., hep-lat/0206008.

The origin of the jump of the average plaquette between the phases with positive and negative quark mass can be understood as a consequence of broken chiral symmetry allowing a mixing between the plaquette field and the condensates $\langle\bar{\chi}\chi\rangle$ and $\langle\bar{\chi}i\gamma_5\tau_3\chi\rangle$.

Extension of the Sharpe-Singleton model to non-zero twisted mass:
G. Münster, hep-lat/0407006; L. Scorzato, hep-lat/0407023;
S. Sharpe, J. Wu, hep-lat/0407025, hep-lat/0407035; S. Aoki, O. Baer, hep-lat/0409006.

Numerical simulations with Wilson-fermion+DBW2 lattice action:

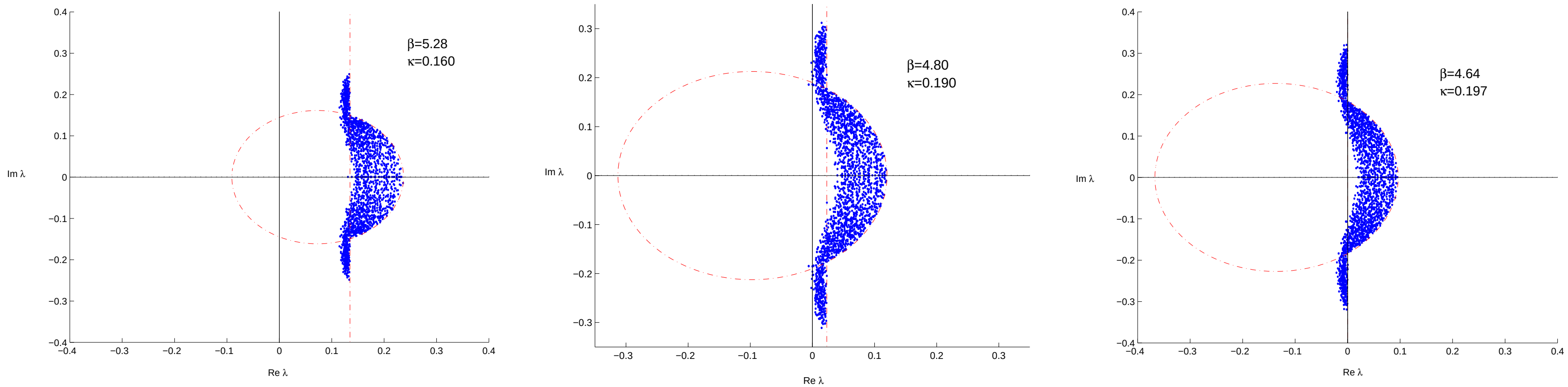
Farchioni et al., DESY 04-162.

The first order phase transition can be related to the existence of a large number of non-physical ("exceptional") small eigenvalues of the Wilson-Dirac operator on the gauge fields generated by the interplay of the Wilson fermion and Wilson gauge action.

qq+q Collaboration, hep-lat/0206008.

Numerical simulations with Wilson action on $8^3 \cdot 16$ lattice,

$a \simeq 0.27\,\mathrm{fm}$ for decreasing quark mass: $m_q \simeq 5/3\,m_s \rightarrow m_q \simeq 1/5\,m_s$



The small unphysical eigenvalues can be suppressed by taking renormalization group improved (RGI) gauge actions as the Iwasaki-action or the DBW2 action:

$$S_g = \beta \sum_x \left(c_0 \sum_{\mu<\nu;\, \mu,\nu=1}^{4} \left\{ 1 - \frac{1}{3} \mathrm{Re}\, U_{x\mu\nu}^{1\times 1} \right\} + c_1 \sum_{\mu,\nu=1}^{4} \left\{ 1 - \frac{1}{3} \mathrm{Re}\, U_{x\mu\nu}^{1\times 2} \right\} \right)$$

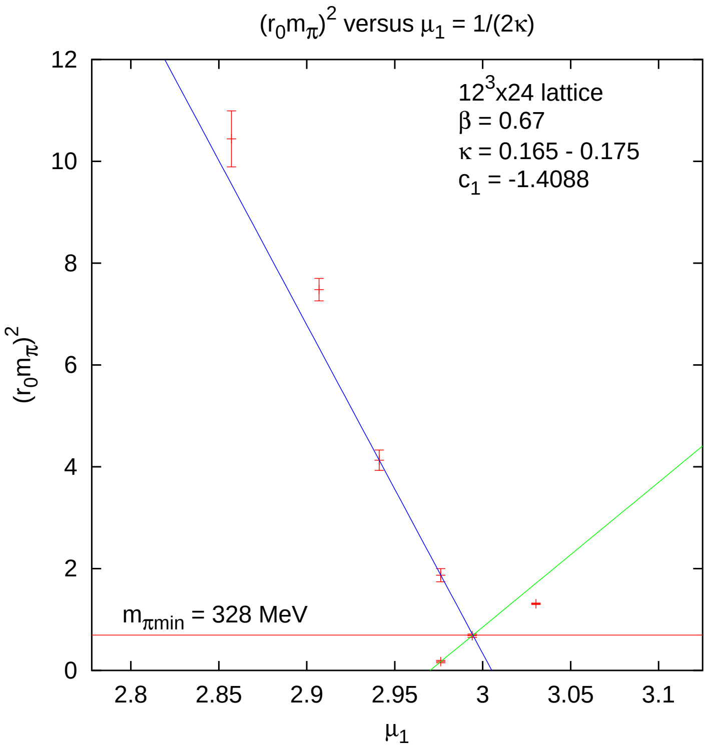
Normalization condition $c_0 = 1 - 8c_1$.
The coefficient c_1 takes different values for various choices of RGI actions:

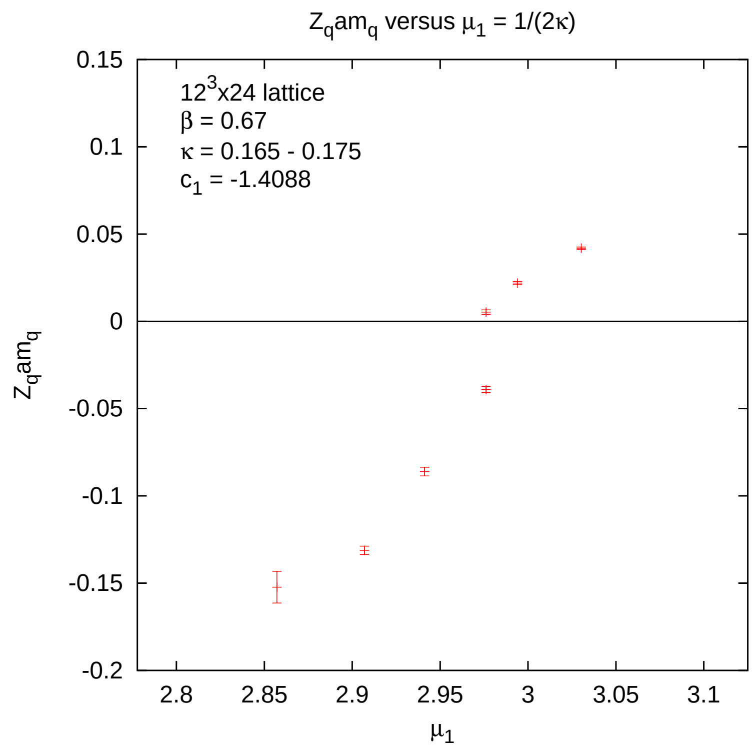
$$c_1 = \begin{cases} -0.331 & \text{Iwasaki action,} \\ -1.4088 & \text{DBW2 action.} \end{cases}$$

The Iwasaki-action is often used in dynamical fermion simulations in combination with the clover fermion action.
Most dynamical domain-wall fermion simulations use the DBW2 action.
We have chosen the original Wilson fermion action.

The lattice spacing (defined by r_0/a) has been tuned to the same value $a \simeq 0.2\,\mathrm{fm}$ as at $\beta = 5.2$ for the Wilson-plaquette action.

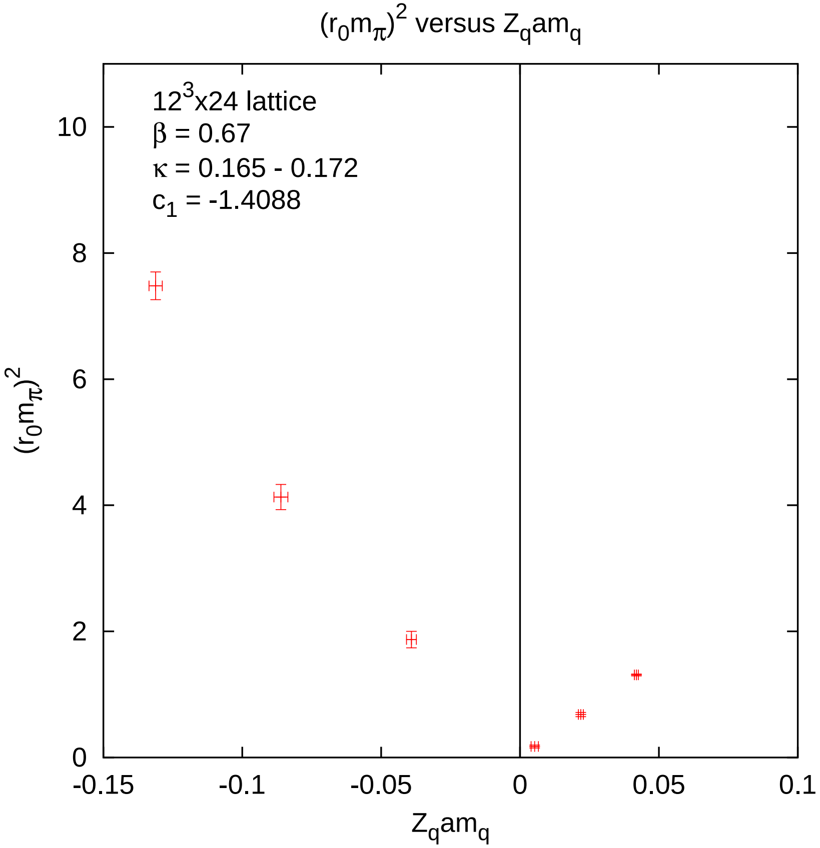
Results on $12^3 \cdot 24$ lattice at vanishing twisted mass $\mu = 0$:





At $\beta = 0.55$ $(a \simeq 0.3\,\mathrm{fm})$ there is an Aoki-phase between $\kappa = 0.190 - 0.191$.

The dependence of $M_r \equiv (r_0 m_\pi)^2$ on the (bare) PCAC quark mass $Z_q a m_q$:



The point close to the origin has a pion mass $m_\pi \simeq 160\,\mathrm{MeV}$, but at this point the positive quark mass phase is metastable. The computational cost is less than with the Wilson-plaquette action, it behaves as $C \simeq F(am_q)^{-1}\Omega$.

The metastability at $\beta = 0.67, \ \mu = 0.01$ is barely visible on a $12^2 \cdot 24$ lattice: The jump of the plaquette is at least by a factor of 10 smaller than with the Wilson-plaquette gauge action at $\beta = 5.2, \ \mu = 0.01$.

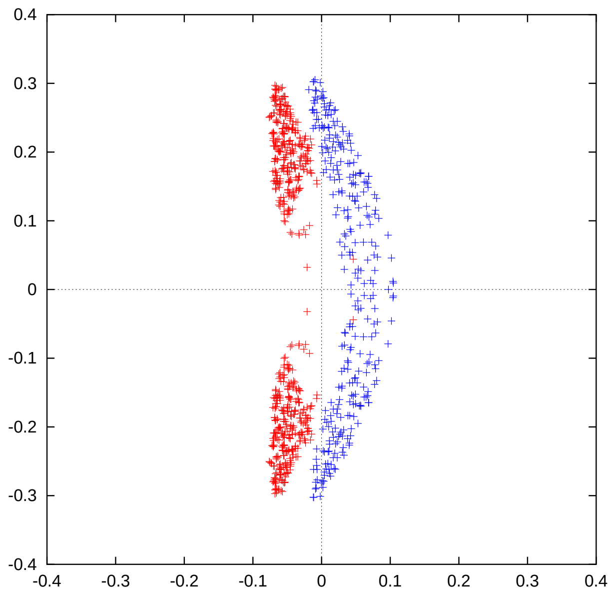
The "half-moons" of the eigenvalue distributions are straightened:

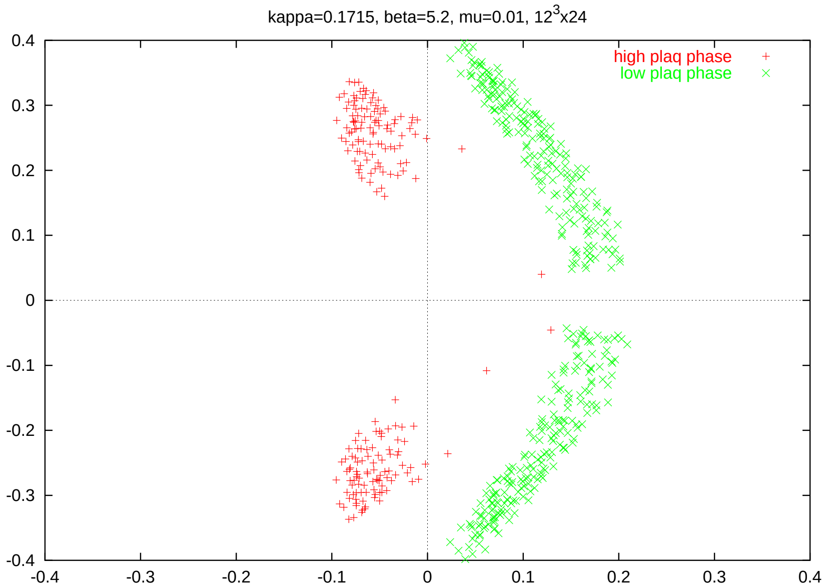
blue $= \beta = 0.67, \ \mu = 0, \ \kappa = 0.168$;

red $= \beta = 0.67, \ \mu = 0.01, \ \kappa = 0.168$.

Right panel: Wilson-plaquette action

$\beta = 5.20, \ \mu = 0.01, \ \kappa = 0.1715$.





Discussion

The introduction of a twisted mass in simulations with Wilson-type quarks is an alternative to staggered quarks.

Before starting phenomenologically relevant simulations with u, d, s (or u, d, s, c) quarks, further exploratory work is needed.

In particular, the β-dependence of the phase structure has to be investigated. It is expected that the minimal pion mass and the jump in the plaquette decrease for increasing β. In the continuum limit the first order phase transition line is expected to shrink to a first order phase transition point.

The effective potential (i.e. the phase structure) can be improved by changing the gauge action only. With RGI gauge actions the updating is faster.

Question: the phase structure of QCD in staggered quark simulations?

Discussion session: twist angles

Frezzotti, Grassi, Sint, Weisz, hep-lat/0101001 (FGSW);

Frezzotti, Rossi, hep-lat/0306014 (FR1).

Vector and axialvector currents: in the "physical"

$$V^{\psi}_{Sx\mu} \equiv \overline{\psi}_x \frac{1}{2} \tau_S \gamma_\mu \psi_x \ , \qquad A^{\psi}_{Sx\mu} \equiv \overline{\psi}_x \frac{1}{2} \tau_S \gamma_\mu \gamma_5 \psi_x$$

and "twisted" basis:

$$V^{\chi}_{Sx\mu} \equiv \overline{\chi}_x \frac{1}{2} \tau_S \gamma_\mu \chi_x \ , \qquad A^{\chi}_{Sx\mu} \equiv \overline{\chi}_x \frac{1}{2} \tau_S \gamma_\mu \gamma_5 \chi_x$$

The relations between them are

$$V^{\psi}_{Sx\mu} = \cos\omega_0 V^{\chi}_{Sx\mu} + \sin\omega_0 A^{\chi}_{\tilde{S}x\mu} \ , \qquad A^{\psi}_{Sx\mu} = \cos\omega_0 A^{\chi}_{Sx\mu} + \sin\omega_0 V^{\chi}_{\tilde{S}x\mu}$$

where we used

$$\psi_x = \left(\cos\frac{1}{2}\omega_0 + i\gamma_5\tau_3 \sin\frac{1}{2}\omega_0\right)\chi_x \ , \quad \overline{\psi}_x = \overline{\chi}_x \left(\cos\frac{1}{2}\omega_0 + i\gamma_5\tau_3 \sin\frac{1}{2}\omega_0\right)$$

First let us neglect the Z-factors of multiplicative renormalization: $Z = 1$.
The physical currents satisfy the WT-identities

$$\left\langle O_y \cdot \Delta^b_{x\mu} V^{\psi}_{Sx\mu} \right\rangle = \mathcal{O}(a) \; , \qquad \left\langle O_y \cdot \Delta^b_{x\mu} A^{\psi}_{Sx\mu} \right\rangle = 2m_{q0} \left\langle O_y P_{Sx} \right\rangle + \mathcal{O}(a)$$

Here we shall consider the charged components $S \to \pm$ with $\tau_\pm \equiv \frac{1}{2}(\tau_1 \pm i\tau_2)$. m_{q0} is some bare quark mass, Δ^b_μ denotes the backward lattice derivative and the pseudoscalar density is

$$P_{Sx} \equiv \overline{\psi}_x \frac{1}{2} \tau_S \gamma_5 \psi_x = \overline{\chi}_x \frac{1}{2} \tau_S \gamma_5 \chi_x$$

If in the vector WT-identity we choose for the quantity $O^{(-)}_y = P^{(-)}_y$ then we obtain a possible definition of ω_0:

$$\tan \omega_0 = \frac{\left\langle P^{(-)}_y \cdot \Delta^b_{x\mu} V^{\chi(+)}_{x\mu} \right\rangle}{i \left\langle P^{(-)}_y \cdot \Delta^b_{x\mu} A^{\chi(+)}_{x\mu} \right\rangle} + \mathcal{O}(a)$$

The twist angle ω_0 is defined for any fixed (μ_1, μ). One can also define the bare PCAC (or Axial-Ward-Identity-) quark mass by the axialvector current:

$$\mu_{q0} \equiv \mu_{q0}^{PCAC} \equiv Z_A^{-1} a m_q^{AWI} \equiv \frac{\left\langle P_y^{(-)} \cdot \Delta_{x\mu}^b A_{x\mu}^{\psi(+)} \right\rangle}{2 \left\langle P_y^{(-)} P_x^{(+)} \right\rangle} + \mathcal{O}(a)$$

$$= \frac{\cos\omega_0 \left\langle P_y^{(-)} \cdot \Delta_{x\mu}^b A_{x\mu}^{\chi(+)} \right\rangle - i \sin\omega_0 \left\langle P_y^{(-)} \cdot \Delta_{x\mu}^b V_{x\mu}^{\chi(+)} \right\rangle}{2 \left\langle P_y^{(-)} P_x^{(+)} \right\rangle} + \mathcal{O}(a)$$

Combining this with the definition of ω_0 one can also write

$$\mu_{q0} = \frac{\sqrt{\left\langle P_y^{(-)} \cdot \Delta_{x\mu}^b A_{x\mu}^{\chi(+)} \right\rangle^2 - \left\langle P_y^{(-)} \cdot \Delta_{x\mu}^b V_{x\mu}^{\chi(+)} \right\rangle^2}}{2 \left\langle P_y^{(-)} P_x^{(+)} \right\rangle} + \mathcal{O}(a)$$

Introducing the Z-factors:
Since up to now the vector WT-identity is used for the definition of ω_0, let us rename it now as $\omega_0 \equiv \omega_{0V}$.

One can define for the axialvector current another $\omega_0 \equiv \omega_{0A}$ by the axialvector WT-identity. A possibility is to require

$$\frac{\left\langle \left(\cos\omega_{0A}\Delta^b_{y\nu}A^\chi_{-y\nu} + i\sin\omega_{0A}\Delta^b_{y\nu}V^\chi_{-y\nu}\right)\left(\cos\omega_{0A}\Delta^b_{x\mu}A^\chi_{+x\mu} - i\sin\omega_{0A}\Delta^b_{x\mu}V^\chi_{+x\mu}\right)\right\rangle}{\left\langle \left(\cos\omega_{0A}\Delta^b_{y\nu}A^\chi_{-y\nu} + i\sin\omega_{0A}\Delta^b_{y\nu}V^\chi_{-y\nu}\right) P_{+x}\right\rangle}$$

$$= \frac{\left\langle P_{-y}\left(\cos\omega_{0A}\Delta^b_{x\mu}A^\chi_{+x\mu} - i\sin\omega_{0A}\Delta^b_{x\mu}V^\chi_{+x\mu}\right)\right\rangle}{\langle P_{-y}P_{+x}\rangle} = 2m_{q0}^{PCAC} \ .$$

The last equality shows that, in general, if $\omega_{0V} \neq \omega_{0A}$ then the definition of the bare PCAC quark mass involves ω_{0A} and not ω_{0V}.

The definition of the renormalized currents is, according to FR1:

$$\hat{V}_{S\mu} = \frac{1}{Z_M(\omega)} \left[Z_V z_m \cos\omega V^{\chi}_{S\mu} + Z_A \sin\omega A^{\chi}_{\bar{S}\mu} \right] \;,$$

$$\hat{A}_{S\mu} = \frac{1}{Z_M(\omega)} \left[Z_A z_m \cos\omega A^{\chi}_{S\mu} + Z_V \sin\omega V^{\chi}_{\bar{S}\mu} \right]$$

where $Z_M(\omega) = [(z_m \cos\omega)^2 + (\sin\omega)^2]^{\frac{1}{2}}$. Then with

$$\tan\omega_{0V} = \frac{Z_A}{Z_V z_m} \tan\omega \;, \qquad \tan\omega_{0A} = \frac{Z_V}{Z_A z_m} \tan\omega$$

we have

$$\hat{V}_{S\mu} = \frac{\sqrt{(Z_V z_m \cos\omega)^2 + (Z_A \sin\omega)^2}}{\sqrt{(z_m \cos\omega)^2 + (\sin\omega)^2}} \left[\cos\omega_{0V} V^{\chi}_{S\mu} + \sin\omega_{0V} A^{\chi}_{\bar{S}\mu} \right] \;,$$

$$\hat{A}_{S\mu} = \frac{\sqrt{(Z_A z_m \cos\omega)^2 + (Z_V \sin\omega)^2}}{\sqrt{(z_m \cos\omega)^2 + (\sin\omega)^2}} \left[\cos\omega_{0A} A^{\chi}_{S\mu} + \sin\omega_{0A} V^{\chi}_{\bar{S}\mu} \right]$$

Comparison with $V^{\psi}_{S\mu}$, $A^{\psi}_{S\mu}$ implies

$$\hat{V}_{S\mu} = \frac{\sqrt{(Z_V z_m \cos\omega)^2 + (Z_A \sin\omega)^2}}{\sqrt{(z_m \cos\omega)^2 + (\sin\omega)^2}} V^{\psi}_{S\mu} \ ,$$

$$\hat{A}_{S\mu} = \frac{\sqrt{(Z_A z_m \cos\omega)^2 + (Z_V \sin\omega)^2}}{\sqrt{(z_m \cos\omega)^2 + (\sin\omega)^2}} A^{\psi}_{S\mu}$$

These relations show, respectively, the multiplicative renormalization of $V^{\psi}_{S\mu}$ defined with $\omega_0 = \omega_{0V}$ and $A^{\psi}_{S\mu}$ defined with $\omega_0 = \omega_{0A}$.

Since the renormalized PCAC quark mass m_q^{PCAC} is defined by the renormalized axialvector current $\hat{A}$, the renormalization of the PCAC quark mass is given by

$$m_q^{PCAC} = \frac{\sqrt{(Z_A z_m \cos\omega)^2 + (Z_V \sin\omega)^2}}{Z_P \sqrt{(z_m \cos\omega)^2 + (\sin\omega)^2}} m_{q0}^{PCAC} \ .$$

In the above formulas ω denotes the twist angle used in the definition of the physical basis for the fermion field. Its relation to ω_{0V} and ω_{0A} is given, for instance, by

$$\tan\omega_{0V}\tan\omega_{0A} = \left(\frac{\tan\omega}{z_m}\right)^2$$

The relations between ω_{0V} and ω_{0A} to ω simplify for $\omega = \omega_{0V} = \omega_{0A} = 0,\ \pi/2$. For a general ω let us define $Z_i \equiv 1 + \delta Z_i$, then assuming that δZ_i is small, an expansion gives:

$$\sin\omega_{0V} = \sin\omega\left\{1 + cos^2\omega\left[\delta Z_A - \delta Z_V - \delta Z_m\right] + \mathcal{O}((\delta Z)^2)\right\},$$

$$\sin\omega_{0A} = \sin\omega\left\{1 + cos^2\omega\left[\delta Z_V - \delta Z_A - \delta Z_m\right] + \mathcal{O}((\delta Z)^2)\right\}.$$

ω is defined by the bare untwisted mass $\mu_1 \equiv 1/(2\kappa)$ and bare twisted mass μ as

$$\omega = \arctan\frac{\mu}{(\mu_1 - \mu_{1cr})}$$

where $\mu_{1cr} \equiv 1/(2\kappa_{cr})$ is the “critical” bare untwisted quark mass.

Connection to FGSW: another twist angle can also be introduced:

$$\alpha \equiv \arctan \frac{\mu_r}{\mu_{1r}}$$

where μ_{1r} and μ_r are the renormalized untwisted and twisted mass, respectively. It is related to ω by $\tan\alpha = \tan\omega/z_m$. With this "renormalized" twist angle the expressions of the renormalized currents are simplified to

$$\hat{V}_{S\mu} = Z_V \cos\alpha V^{\chi}_{S\mu} + Z_A \sin\alpha A^{\chi}_{\bar{S}\mu} ,$$

$$\hat{A}_{S\mu} = Z_A \cos\alpha A^{\chi}_{S\mu} + Z_V \sin\alpha V^{\chi}_{\bar{S}\mu}$$

The twist angles in the vector and axialvector currents are defined now by

$$\tan\omega_V = \frac{Z_A}{Z_V}\tan\alpha , \qquad \tan\omega_A = \frac{Z_V}{Z_A}\tan\alpha ; \qquad \tan^2\alpha = \tan\omega_V \tan\omega_A$$

In the previous relations we have to replace:

$$\omega \to \alpha , \quad \omega_{0V} \to \omega_V , \quad \omega_{0A} \to \omega_A , \quad z_m \to 1 , \quad \delta z_m \to 0$$

Using parity restauration: (F. Farchioni)
The numerical determination of ω_V and ω_A from the Ward-Takahashi identities is possible but not very easy.
A simpler possibility is to impose for the renormalized currents the restauration of parity conservation. Suitable matrix elements are, for instance,

$$\sum_{\vec{x},\vec{y}} \langle \hat{A}_{+x0}\, \hat{V}_{-y0} \rangle = \mathcal{O}(a) \ , \qquad \sum_{\vec{x},\vec{y}} \langle \hat{V}_{+x0}\, P_{-y} \rangle = \mathcal{O}(a)$$

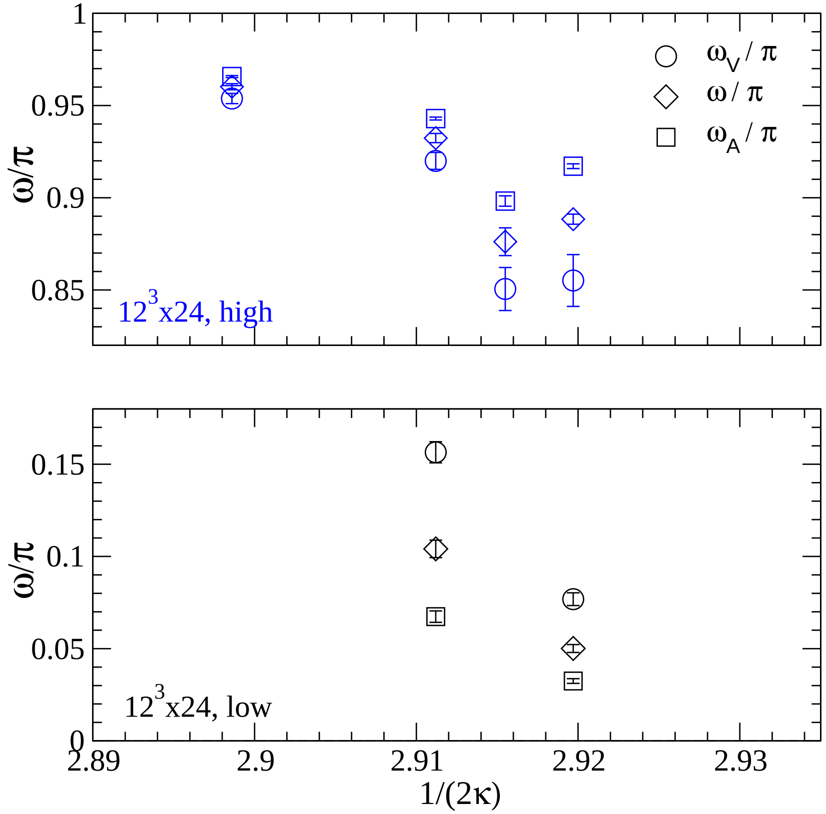
This has for the vector and axialvector twist angle the solution

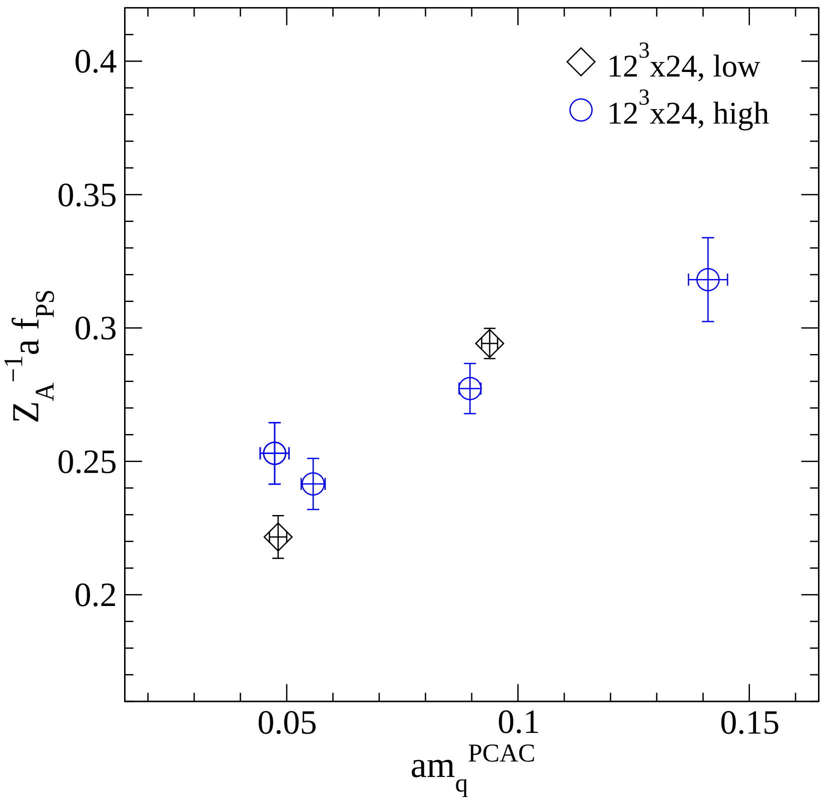
$$\tan \omega_V = \frac{-i \sum_{\vec{x},\vec{y}} \langle V^{\chi}_{+x0}\, P_{-y} \rangle}{\sum_{\vec{x},\vec{y}} \langle A^{\chi}_{+x0}\, P_{-y} \rangle} \ ,$$

$$\tan \omega_A = \frac{i \sum_{\vec{x},\vec{y}} \langle A^{\chi}_{+x0}\, V^{\chi}_{-y0} \rangle + \tan \omega_V \sum_{\vec{x},\vec{y}} \langle A^{\chi}_{+x0}\, A^{\chi}_{-y0} \rangle}{\sum_{\vec{x},\vec{y}} \langle V^{\chi}_{+x0}\, V^{\chi}_{-y0} \rangle - i \tan \omega_V \sum_{\vec{x},\vec{y}} \langle V^{\chi}_{+x0}\, A^{\chi}_{-y0} \rangle}$$

Numerical results at $\beta = 5.2$ on $12^3 \cdot 24$ lattice:

left: $\omega \equiv \alpha$, right: pseudoscalar decay constant





Discussion session: split doublets

Let us introduce another fermion matrix by

$$Q_{(ft)} \equiv \frac{1}{2}(1 - i\gamma_5\tau_3)Q_{(\chi)}(1 - i\gamma_5\tau_3) = \mu + N - i\tau_3\tilde{W}_{(\mu_1)}$$

where

$$N_{yx} = -\frac{1}{2}\sum_{\mu=\pm1}^{\pm4} \delta_{y,x+\hat{\mu}}U_{x\mu}\gamma_\mu \, , \quad R_{yx} = -\frac{1}{2}\sum_{\mu=\pm1}^{\pm4} \delta_{y,x+\hat{\mu}}U_{x\mu} \, , \quad \tilde{W}_{(\mu_1)} = \gamma_5(\mu_1{+}R)$$

and we tune μ_1 to its critical value $\mu_1 = \mu_{1cr}$.
This means that we are at full twist.

The mass splitting in the doublet is introduced by the replacement
$\mu \longrightarrow \mu_{(+)} + \tau_1\mu_{(-)}$ in $Q_{(ft)}$.
Becasue of

$$Q_{(\chi)} = i\gamma_5\tau_3[\mu_{(+)} + \gamma_5\tau_2\mu_{(-)}] + Q_{(\mu_1)} \, ,$$

on the twisted mass basis we have to substitute $\mu \longrightarrow \mu_{(+)} + \gamma_5 \tau_2 \mu_{(-)}$.

The hermitean fermion matrix is now

$$\tilde{Q}_{(\chi)} \equiv \gamma_5 \tau_1 Q_{(\chi)} = \tau_2 \mu_{(+)} + \gamma_5 \mu_{(-)} + \tau_1 \tilde{Q}_{(\mu_1)} \ ,$$

with the single-flavour hermitean matrix $\tilde{Q}_{(\mu_1)} \equiv \gamma_5 Q_{(\mu_1)}$.

The masses can be diagonalized by an isospin rotation: $\tau_3 \longrightarrow \tau_1,\ \tau_1 \longrightarrow -\tau_3$.
The (bare) mass eigenvalues are: $\mu_s \equiv \mu_{(+)} - \mu_{(-)}$ and $\mu_c \equiv \mu_{(+)} + \mu_{(-)}$.

One can show (Frezzotti, Rossi, hep-lat/0311008) that the fermion determinant $\det Q_{(ft)} = \det Q_{(\chi)} = \det \tilde{Q}_{(\chi)}$ is positive for $|\mu_{(+)}| > |\mu_{(-)}|$.

The sign problem of negative determinants starts to occur at the singularity corresponding to the zero of the smaller (renormalized) mass in the doublet.