Light twisted mass quarks

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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.

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

- the numerical simulation is faster,
- the lattice artifacts are reduced (“automatic” $\mathcal{O}(a)$ improvement),
- 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.

Twisted mass Wilson fermions

Aoki,... Frezzotti, Grassi, Sint, Weisz,... Frezzotti, Rossi,...

Fermion matrix for an unequal-mass doublet:
with masses $m_u = \mu_{(+)} - \mu_{(-)}, \;\; m_d = \mu_{(+)} + \mu_{(-)}$

$$\mu_{(+)} - \tau_3\mu_{(-)} - \frac{1}{2}\sum_{\mu=\pm1}^{\pm4} \delta_{y,x+\hat{\mu}} U_{x\mu}\gamma_\mu - i\gamma_5\tau_1 \left(-\frac{1}{2}\sum_{\mu=\pm1}^{\pm4} \delta_{y,x+\hat{\mu}} U_{x\mu} + \mu_{\kappa cr} \right)$$

where the notation $\mu_\kappa \equiv (2\kappa)^{-1} \equiv am_0 + 4$ is used.

More generally: $\mu_{\kappa cr} \to \mu_\kappa = \mu_{\kappa cr} + (\mu_\kappa - \mu_{\kappa cr})$.
Then the mass term becomes

$$\mu_{(+)} - \tau_3\mu_{(-)} - i\gamma_5\tau_1(\mu_\kappa - \mu_{\kappa cr})$$

This can be diagonalized by a chiral rotation.

Chiral transformation:

$$\psi_x \equiv e^{i\frac{\omega}{2}\gamma_5\tau_1}\chi_x = \left(\cos\frac{\omega}{2} + i\gamma_5\tau_1\sin\frac{\omega}{2}\right)\chi_x \,,$$

$$\overline{\psi}_x \equiv \overline{\chi}_x e^{i\frac{\omega}{2}\gamma_5\tau_1} = \overline{\chi}_x\left(\cos\frac{\omega}{2} + i\gamma_5\tau_1\sin\frac{\omega}{2}\right)$$

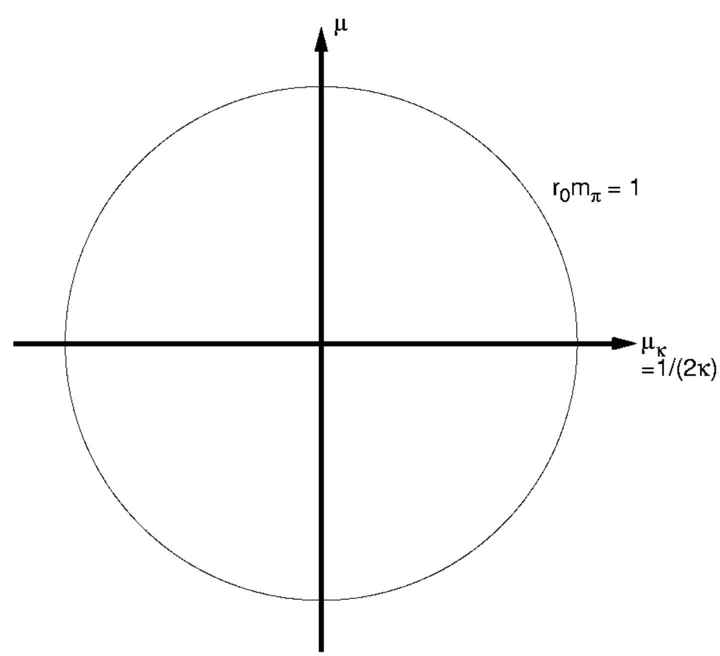
After an appropriate chiral transformation the mass term becomes $\mu'_{(+)} - \tau_3\mu_{(-)}$.

Conventional notation:
with a chiral transformation and an isospin rotation $\tau_1 \to \tau_3,\ \tau_3 \to -\tau_1$
one obtains

$$S_\chi = \sum_x \left\{ (\overline{\chi}_x[\mu_\kappa + i\gamma_5\tau_3\,\mu_{(+)} + \tau_1\mu_{(-)}]\chi_x) - \frac{1}{2}\sum_{\mu=\pm 1}^{\pm 4} (\overline{\chi}_{x+\hat{\mu}}U_{x\mu}[r+\gamma_\mu]\chi_x) \right\}$$

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

In the continuum limit the chiral symmetry is restored and ω becomes irrelevant.



At non-zero lattice spacing the circle is distorted.

Renormalization and Z-factors

In a mass-independent renormalization scheme the Z-factors can be defined at $\omega = \mu = 0$. The chiral multiplets of renormalized (composite) operators are obtained by a chiral rotation to $\omega \neq 0$.
For simplicity, from now on we deal with a degenerate doublet:
$\mu_{(+)} \equiv \mu,\ \mu_{(-)} = 0$.

Vector and axialvector currents:
one can introduce the twist angle ω as the chiral rotation angle between the renormalized (physical) vector and axialvector currents $\hat{V}^a_{x\mu}$, $\hat{A}^a_{x\mu}$ and the bare bilinears of the χ-fields

$$V^a_{x\mu} \equiv \overline{\chi}_x \frac{1}{2}\tau_a \gamma_\mu \chi_x \ , \qquad A^a_{x\mu} \equiv \overline{\chi}_x \frac{1}{2}\tau_a \gamma_\mu \gamma_5 \chi_x$$

With the renormalization constants Z_V and Z_A we have

$$\hat{V}^a_{x\mu} = Z_V V^a_{x\mu} \cos\omega + \epsilon_{ab} Z_A A^b_{x\mu} \sin\omega \ ,$$

$$\hat{A}^a_{x\mu} = Z_A A^a_{x\mu} \cos\omega + \epsilon_{ab} Z_V V^b_{x\mu} \sin\omega$$

where only charged currents are considered (a=1,2).
We define the two auxiliary angles

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

In terms of ω_V, ω_A one can write

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

where the overall multiplicative renormalization is ($X = V, A$)

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

The twist angle ω can be obtained as

$$\omega = \arctan\left(\sqrt{\tan\omega_V \tan\omega_A}\right)$$

A possibility to determine ω_V and ω_A is to impose the vector and axialvector Ward identities, respectively, with a suitable insertion operator $\hat{O}_x$.
For instance, in the vector case one can use the Ward identity

$$\sum_{\vec{x},\vec{y}} \langle \partial^*_\mu \hat{V}^+_{x\mu} \, \hat{O}^-_y \rangle = 0 \qquad \Longrightarrow \qquad \tan\omega_V = \frac{-i\sum_{\vec{x},\vec{y}} \langle \partial^*_0 V^+_{x0} \, \hat{O}^-_y \rangle}{\sum_{\vec{x},\vec{y}} \langle \partial^*_0 A^+_{x0} \, \hat{O}^-_y \rangle}$$

The indices $+$ and $-$ refer to the charged components $\tau_\pm \equiv \tau_1 \pm i\tau_2$ and ∂^*_μ denotes the backward lattice derivative.

Another possibility for determining the twist angles ω_V, ω_A and ω is to impose parity conservation for suitable matrix elements, for instance with the pseudoscalar density $P^\pm_x = \bar{\chi}_x \frac{\tau^\pm}{2} \gamma_5 \chi_x$:

$$\sum_{\vec{x},\vec{y}} \langle \hat{A}^+_{x0} \, \hat{V}^-_{y0} \rangle \;=\; \sum_{\vec{x},\vec{y}} \langle \hat{V}^+_{x0} \, P^-_y \rangle \;=\; 0 \; .$$

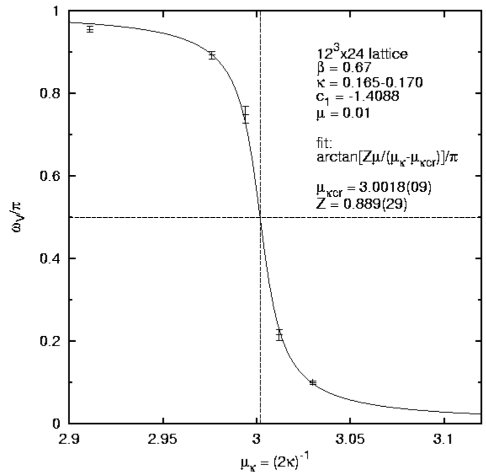
The solution is:

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

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

This method for determining the twist angle can also be used in case of simulations with partially quenched twisted mass quarks.
The estimate of ω is, of course, affected by $\mathcal{O}(a)$ ambiguities.

Example of a numerical simulation result:



The dependence of the twist angle ω_V on the bare untwisted quark mass $\mu_\kappa = (2\kappa)^{-1}$ at $\beta = 0.67$, $\mu = 0.01$ on a $12^3 \times 24$ lattice. The fit determines the critical hopping parameter to be $\kappa_{cr} = (2\mu_{\kappa cr})^{-1} = 0.16657(6)$ and $Z_A Z_S/(Z_V Z_P) = 0.889(29)$.

From a similar fit of ω_A one can obtain $Z_V Z_S/(Z_A Z_P)$.
Z_A can be obtained from the conserved axialvector current at $\omega = \pi/2$.

QCD phase structure with Wilson-type quarks

As a consequence of spontaneous chiral symmetry breaking, in QCD there is a singularity at zero quark mass.
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.

Phase structure with $N_f = 2$ Wilson-type quarks: Sharpe and Singleton WChPT.
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:

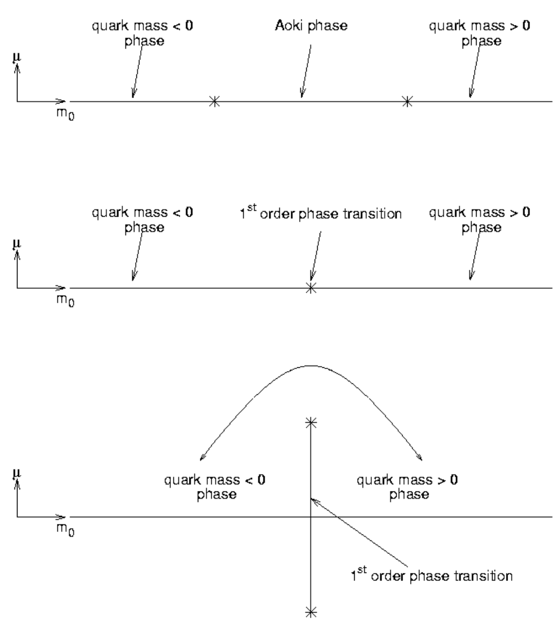
$$\Sigma = A + i \sum_{r=1}^{3} B_r \tau_r \ .$$

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.

The value of c_2 is characteristic for the lattice action:
clover, Symanzik-improved, Iwasaki, DBW2,...

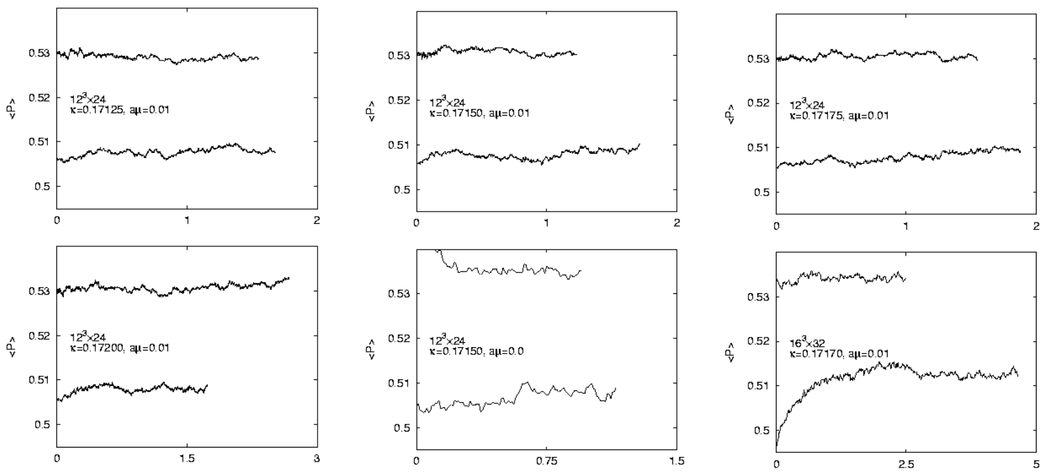
Possible phase structures: depending on the sign of c_2 between the positive and negative quark mass phases there is either an Aoki-phase or a first order phase transition.



QCD phase structure: numerical simulations

Hamburg-Münster-Zeuthen Collaboration:
Wilson quarks, Wilson plaquette action: hep-lat/0406039, hep-lat/0409098
Wilson quarks, DBW2 action: hep-lat/0410031

First order phase transition signals have been observed:



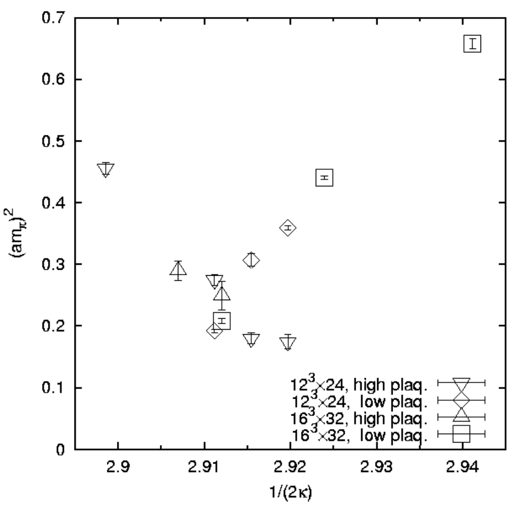
Recent numerical simulations show that the width of Aoki phase in the bare mass parameter shrinks to zero (or to a small value) at $\beta \leq 4.6$.
E.-M. Ilgenfritz et al., hep-lat/0309057.

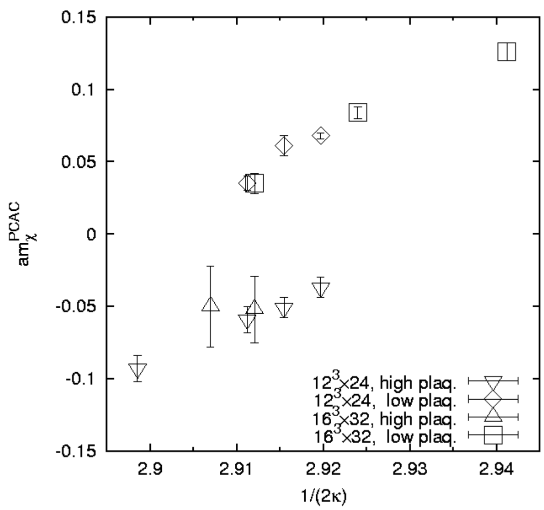
Earlier observations of strong first order phase transitions:
T. Blum et al., hep-lat/9404006;
JLQCD Collaboration, S. Aoki et al., hep-lat/0110088, hep-lat/0409016.

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.

In case of Wilson quarks and either plaquette or DBW2 gauge action the numerical data strongly suggest that the second $(c_2 < 0)$ Sharpe-Singleton scenario is realized.

Pion mass-squared and quark mass in the two (stable or metastable) phases: plaquette gauge action, $12^3 \cdot 24$ and $16^3 \cdot 32$ lattice, $\beta = 5.2,\ \mu = 0.01$





Renormalization group improved (RGI) gauge actions:
the Iwasaki-action or the DBW2 action:

$$S_g = \beta \sum_x \left(c_0 \sum_{\mu<\nu;\,\mu,\nu=1}^{4} \left\{ 1 - \frac{1}{3} \mathrm{Re}\, U_{x\mu\nu}^{1\times1} \right\} + c_1 \sum_{\mu,\nu=1}^{4} \left\{ 1 - \frac{1}{3} \mathrm{Re}\, U_{x\mu\nu}^{1\times2} \right\} \right)$$

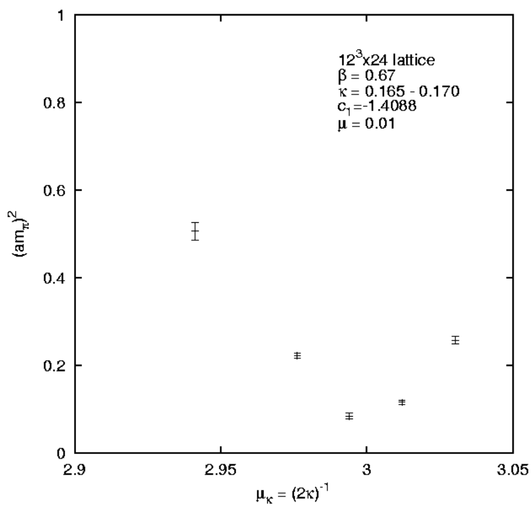
Normalization condition $c_0 = 1 - 8c_1$.
The coefficient c_1 takes different values for various choices of RGI actions:

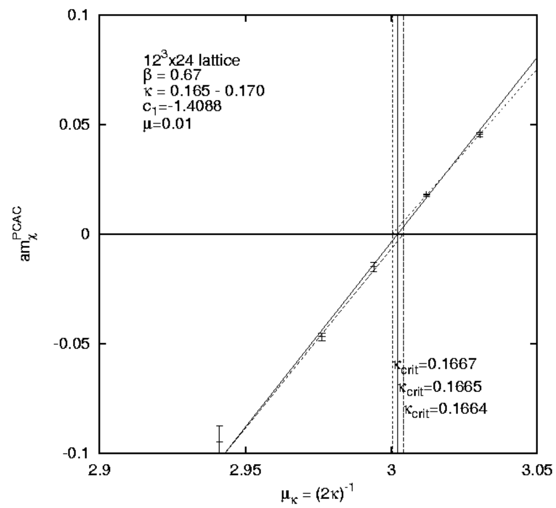
$$c_1 = \begin{cases} -1/12 & \text{tree-level Symanzik action,} \\ -0.331 & \text{Iwasaki action,} \\ -1.4088 & \text{DBW2 action.} \end{cases}$$

The Iwasaki-action and tree-level Symanzik action are often used in dynamical fermion simulations in combination with the clover fermion action.
Most recent dynamical domain-wall fermion simulations use the DBW2 action.

Pion mass-squared and quark mass:

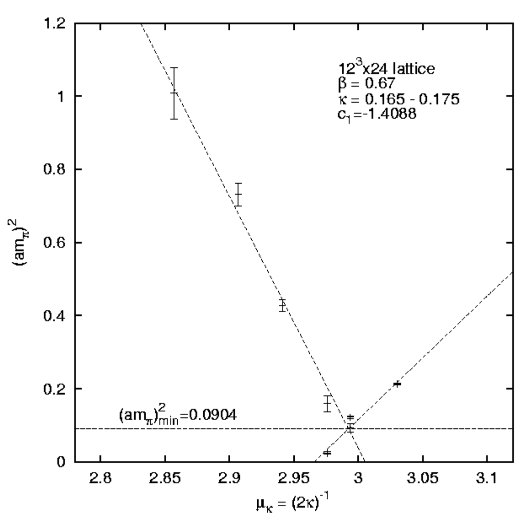
DBW2 gauge action, $12^3 \cdot 24$ lattice, $\beta = 0.67,\ \mu = 0.01$

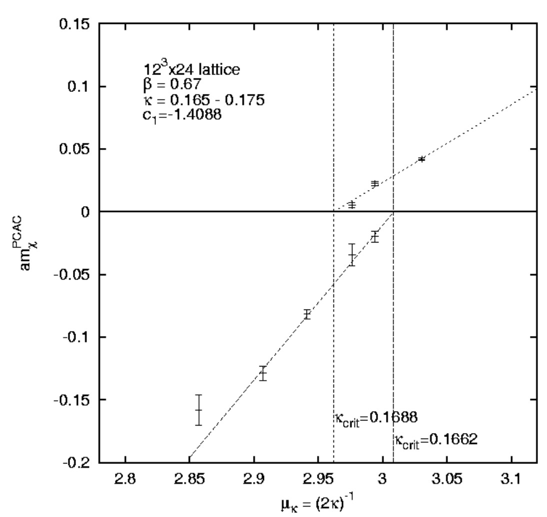




Pion mass-squared and quark mass:

DBW2 gauge action, $12^3 \cdot 24$ lattice, $\beta = 0.67,\ \mu = 0$





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.

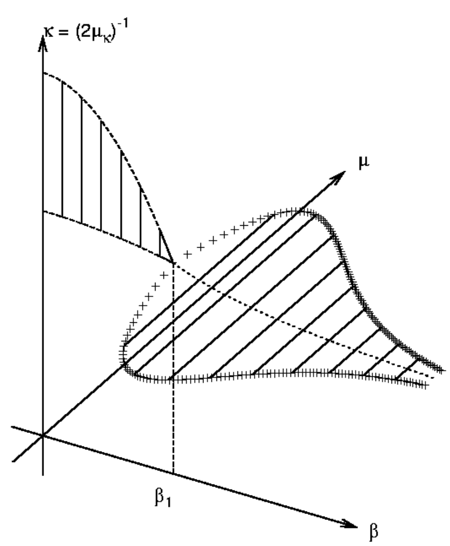
The origin of the jump of the average plaquette between the phases with positive and negative quark mass can be understood as a consequence of broken chiral symmetry allowing a mixing between the plaquette field and the condensates $\langle\bar{\chi}\chi\rangle$ and $\langle\bar{\chi}i\gamma_5\tau_3\chi\rangle$.

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.

The schematic view of the phase transitions in the (β, κ, μ) space for Wilson quarks with both DBW2 and Wilson plaquette gauge action (β=bare gauge coupling, κ=hopping parameter, μ=bare twisted quark mass, $\mu_\kappa \equiv (2\kappa)^{-1}$=bare untwisted quark mass.) The figure does not extend down to $\beta = 0$ and only one “finger” of the Aoki phase is shown.



PRELIMINARY!

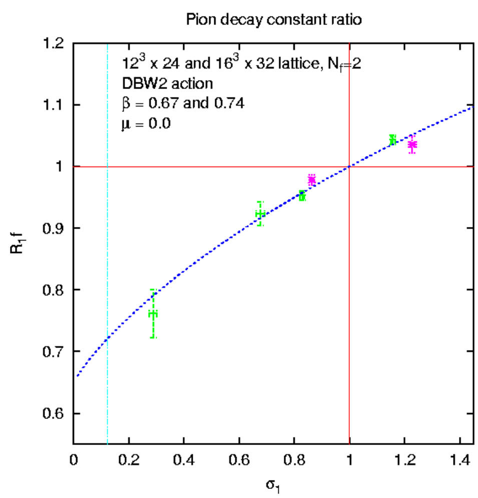
Plaquette action: $\beta = 5.1, \mu = 0.013 : \quad m_{\pi min} \simeq 530\,\mathrm{MeV}$

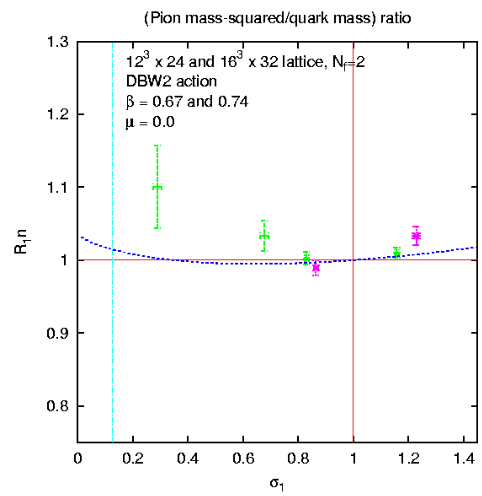
$\beta = 5.2, \mu = 0.010 : \quad m_{\pi min} \simeq 490\,\mathrm{MeV}$

$\beta = 5.3, \mu = 0.008 : \quad m_{\pi min} \simeq 420\,\mathrm{MeV}$

DBW2 action: $\beta = 0.67, \mu = 0.01 : \quad m_{\pi min} < 320\,\mathrm{MeV}$

$\beta = 0.67, \mu = 0.00 : \quad m_{\pi min} \simeq 250\,\mathrm{MeV}$





Discussion

Light dynamical quark simulations with twisted mass Wilson fermions are feasible with reasonable cost: $C_{\tau_{int}} = \mathcal{O}(10^7)(am_q)^{-1}\,\Omega$.

The phase structure near zero quark mass can be influenced by changing the gauge action alone.

Optimizing the effective potential: the singular structure near zero quark mass should be as close as possible to a pointlike singularity, as in the continuum limit. A point-singularity is exactly chiral symmetric!

(Example: Sharpe-Singleton model for $c_2 = 0$.)