Lattice QCD with a chiral twist (I)

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Topics:

- ∗ Classical continuum considerations
- ∗ Lattice QCD with standard Wilson quarks
- ∗ Adding a chirally twisted mass term
- ∗ Equivalence between the two
- ∗ Recipes and applications

Nara, 11/7/2005

A few references

- S. Aoki, *Phys. Rev.* **D30** (1984) 2653;

  first appearance of the tmQCD action (study of parity-flavour breaking phase with Wilson fermions)

- R. Frezzotti, A. Grassi, S.S. and P. Weisz (ALPHA collab.)

  Nucl. Phys. B (Proc. Suppl.) 83 (2000) 941; *JHEP* **08** (2001) 058 `hep-lat/0101001`

  relation between tmQCD and standard QCD, simplification of renormalization problems for F_π, chiral condensate and B_K

- R. Frezzotti, S.S. and P. Weisz (ALPHA collab.)

  JHEP **07** (2001) 048 `hep-lat/0104014`

  Symanzik O(a) improvement, definition of the transfer matrix

- R. Frezzotti and G.C. Rossi *JHEP* **08** (2004) 007 `hep-lat/0306014`;

  observation of "automatic" O(a) improvement

- C. Pena, S.S. and A. Vladikas *JHEP* **09** (2004) 069 `hep-lat/0405028`

  $\Delta I = 1/2$ rule from $K \to \pi$ transitions (valence = sea quarks)

- R. Frezzotti and G.C. Rossi *JHEP* **10** (2004) 070 `hep-lat/0407002`

  mixing problems for 4-quark operators (valence $\neq$ sea quarks)

- R. Frezzotti and G. C. Rossi, `hep-lat/0311008`

  non-degenerate quark flavours

- A. Shindler, plenary talk at Lattice 2005, PoS(LAT2005) 014;

  review of current activity:

  – numerical simulations,
  – O(a) improvement,
  – flavour and parity breaking,
  – analysis of phase structure,
  – chiral perturbation theory (cf. lectures by S. Sharpe)

Continuum considerations

Consider the continuum action of a doublet of massless quarks

$$S_{\mathrm{f}} = \int \mathrm{d}^4x\ \bar{\psi}(x)\partial_\mu\gamma_\mu\psi(x)$$

The massless action is symmetric under chiral transformations

$$\begin{aligned} \psi \to \psi' &= \exp(i\omega_{\mathrm{A}}^a\gamma_5\tau^a/2)\psi \\ \bar{\psi} \to \bar{\psi}' &= \bar{\psi}\exp(i\omega_{\mathrm{A}}^a\gamma_5\tau^a/2) \end{aligned}$$

When introducing a quark mass term the choices $\bar{\psi}\psi$ or

$$\bar{\psi}'\psi' = \bar{\psi}\exp(i\omega_{\mathrm{A}}^a\gamma_5\tau^a)\psi = \cos(\omega_{\mathrm{A}})\ \bar{\psi}\psi + i\sin(\omega_{\mathrm{A}})u_{\mathrm{A}}^a\ \bar{\psi}\gamma_5\tau^a\psi$$

are equivalent!

(ω_{A} denotes the module of $(\omega_{\mathrm{A}}^1, \omega_{\mathrm{A}}^2, \omega_{\mathrm{A}}^3)$ and $u^a = \omega_{\mathrm{A}}^a/\omega_{\mathrm{A}}$ is a unit vector)

- The choice of a mass term $\bar{\psi}\psi$ is a mere convention; in general one may pick any other direction in chiral flavour space

- The form of symmetry transformations depends on this choice:

  – by definition,the flavour (isospin) symmetry leaves the mass term invariant:

$$\begin{aligned} \psi &\rightarrow \exp(-i\omega_{\rm A}^a\gamma_5\tau^a/2)\exp(i\omega_{\rm V}^b\tau^b/2)\exp(i\omega_{\rm A}^c\gamma_5\tau^c/2)\,\psi \\ \bar{\psi} &\rightarrow \bar{\psi}\,\exp(i\omega_{\rm A}^a\gamma_5\tau^a/2)\exp(-i\omega_{\rm V}^b\tau^b/2)\exp(-i\omega_{\rm A}^c\gamma_5\tau^c/2) \end{aligned}$$

  – similarly for parity:

$$\psi(x)\rightarrow\gamma_0\exp(i\omega_{\rm A}^a\gamma_5\tau^a)\,\psi(x_0,-\mathbf{x}),\qquad \bar{\psi}(x)\rightarrow\bar{\psi}(x_0,-\mathbf{x})\,\exp(i\omega_{\rm A}^a\gamma_5\tau^a)\gamma_0$$

Question: why should one deviate from the standard convention for the quark mass term?

Standard Wilson quarks

Lattice action for Wilson quarks:

$$S_f = a^4 \sum_x \bar{\psi}(x)(D_{\rm W} + m_0)\psi(x)$$

$$D_{\rm W} = \sum_{\mu=0}^{3} \{\tfrac{1}{2}(\nabla_\mu + \nabla^*_\mu)\gamma_\mu - a\nabla^*_\mu \nabla_\mu\}$$

- exact SU($N_{\rm f}$) vector symmetry
- invariant under axis permutations, reflections such as parity and charge conjugation
- unitarity rigorously established; explicit construction of a self-adjoint positive transfer matrix (Lüscher '77)

HOWEVER: all axial symmetries are explicitly broken:

- additive quark mass renormalization,

$$m_{\mathrm{R}} = Z_m(m_0 - m_{\mathrm{c}}),$$

- non-trivial renormalization of the corresponding axial symmetry current ($Z_{\mathrm{A}} \neq 1$),

- mixing of operators with different chirality; additive renormalization of chiral order parameter (mixing with constant field)

$$(\bar{\psi}\psi)_{\mathrm{R}} = Z_{\mathrm{S}^0}\left\{\bar{\psi}\psi + c_{\mathrm{S}}(g_0, am_0)a^{-3}\right\}$$

- cutoff effects are <u>linear</u> in a

- The Wilson-Dirac operator $D_{\mathrm{W}} + m_0$ for a given gauge field U may have eigenvalues $\simeq 0$ even at finite physical quark mass (exceptional gauge field configurations)!

The problem with exceptional configurations

- for a given gauge background field the Wilson-Dirac operator may have zero modes, unless $m_0 > 0$

- In practice, due to the additive quark renormalization, $m_0 \geq 0$ corresponds to rather heavy quarks (charm quark region)

  $\Rightarrow$ the bare masses corresponding to light quarks are negative and do not protect against zero modes!

- the quenched approximation breaks down as the chiral limit is approached. With the O(a) improved action around $m_{\rm strange}/2$, long before finite volume effects from light pions become a problem!

- expect problems for partially quenched approximation, too!

- zero modes are no problem in principle, Grassmann integrals are always finite!

Consider a fermionic correlation function, e.g. the pion propagator:

$$G_{xy}^{ab} = -\int D[U,\psi,\bar{\psi}]\mathrm{e}^{-S}\,\bar{\psi}(x)\gamma_5\frac{\tau^a}{2}\psi(x)\bar{\psi}(y)\gamma_5\frac{\tau^b}{2}\psi(y),$$

integration over the quark and antiquark fields:

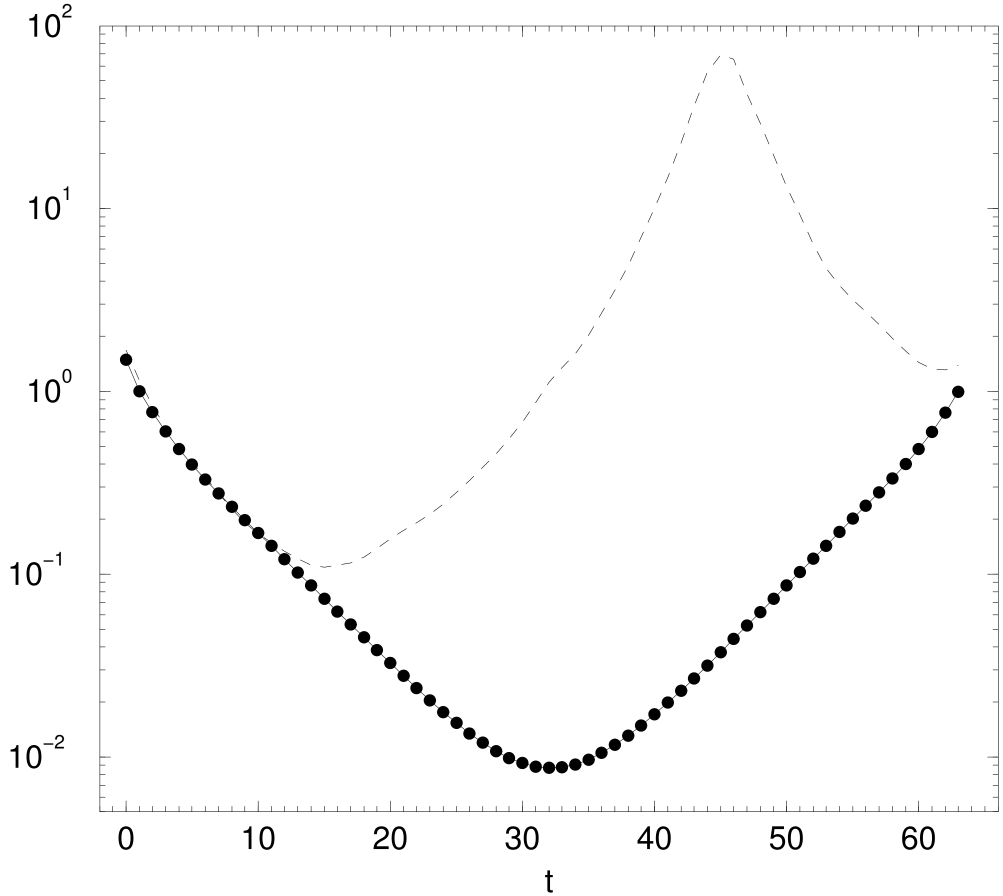
$$G_{xy}^{ab} = \tfrac{1}{2}\delta^{ab}\int D[U]\mathrm{e}^{-S_g}\,\det(D_{\mathrm{W}}+m_0)\,\mathrm{tr}\,\left(G_f(x,y)^\dagger G_f(x,y)\right), \quad G_f = (D_{\mathrm{W}}+m_0)^{-1}$$

NB: The result of the Grassmann integration is always a polynomial in the eigenvalues of the Wilson-Dirac operator: in a basis of eigenmodes ψ_i with eigenvalues λ_i the non-vanishing contributions to the Grassmann integral take the form

$$\int \mathrm{d}\psi_1\mathrm{d}\bar{\psi}_1\cdots\mathrm{d}\psi_n\mathrm{d}\bar{\psi}_n\mathrm{e}^{\sum_i\lambda_i\bar{\psi}_i\psi_i}\,\psi_k\bar{\psi}_k\psi_l\bar{\psi}_l = \prod_{i\neq k,l}\lambda_i$$

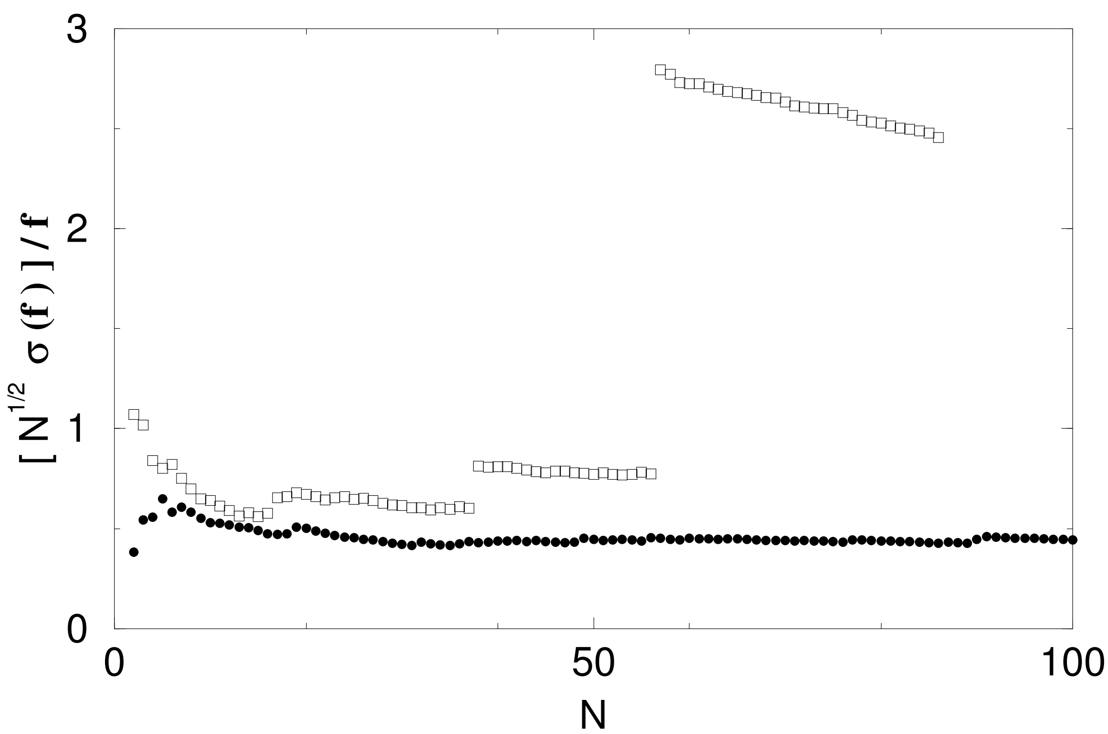
Divergences appear when the quark determinant is neglected (quenched approximation) or when the quark masses in the determinant do not coincide with the masses of the propagator computation (partially quenched approximation):

Example: (Göckeler et al, `hep-lat/9809165v1`) $32^3 \times 64$ lattice, quenched simulation at $\beta = 6.2$, $m_\pi/m_\rho \approx 0.5$, non-perturbatively O(a) improved action, measure pion propagator at zero spatial momentum as a function of $t = (x_0 - y_0)/a$



- Strictly speaking, the (partially) quenched approximation does not exist for Wilson quarks with $m_0 \leq 0$!

- in practice the frequency of (near-) zero modes depends strongly on the parameters and on the chosen gauge action. If near zero modes become frequent the statistical error σ does not decrease as $1/\sqrt{N}$:



(example from M. Della Morte et al, `hep-lat/0110166`: lattice size $24^3 \times 48$, $\beta = 6.0$, $m_{\rm PS}/m_{\rm V} \approx 0.47$)

Twisted Mass Lattice QCD

Lattice action for a doublet ψ of mass degenerate light Wilson quarks quarks (Aoki '84):

$$S_f = a^4 \sum_x \bar{\psi}(x) \left(D_{\rm W} + m_0 + i\mu_q \gamma_5 \tau^3\right) \psi(x)$$

$D_{\rm W}$: Wilson-Dirac operator with/without Sheikholeslami-Wohlert (clover) term

$\mu_{\rm q}$: bare twisted mass parameter

Properties:

- regularisation of QCD with $N_{\rm f} = 2$ mass degenerate quark flavours (see below)

- $\mu_\mathrm{q} \neq 0 \Rightarrow$ no unphysical zero modes:

$$
\begin{aligned}
&\det\Big(D_\mathrm{W} + m_0 + i\mu_q\gamma_5\tau^3\Big) \\
&= \det\begin{pmatrix} \gamma_5(D_\mathrm{W}+m_0)+i\mu_q & 0 \\ 0 & \gamma_5(D_\mathrm{W}+m_0)-i\mu_q \end{pmatrix} \\
&= \det\left([D_\mathrm{W}+m_0)]^\dagger[D_\mathrm{W}+m_0]+\mu_\mathrm{q}^2\right) > 0
\end{aligned}
$$

- positive and selfadjoint transfer matrix provided μ_q is real and $|\kappa| < 1/6$ $(\kappa = (2am_0+8)^{-1}) \Rightarrow$ unitarity

- flavour symmetry reduced to U(1) with generator $\tau^3/2$

- symmetries: C, axis permutations, reflections with flavour exchange, e.g.

$$\psi(x) \to \gamma_0\tau^1\psi(x_0,-\mathbf{x}), \qquad \bar\psi(x) \to \bar\psi(x_0,-\mathbf{x})\gamma_0\tau^1$$

Equivalence between tmQCD and QCD

Classical continuum limit of twisted mass lattice QCD:

$$S_f = \int \mathrm{d}x \; \bar{\psi}(x)\big(\not{D} + m + i\mu_{\mathrm{q}}\gamma_5\tau^3\big)\psi(x).$$

Perform a global chiral (non-singlet) rotation of the fields:

$$\psi' = R(\alpha)\psi, \quad \bar{\psi}' = \bar{\psi}R(\alpha), \quad R(\alpha) = \exp\left(i\alpha\gamma_5\frac{\tau^3}{2}\right).$$

For $\tan\alpha = \mu_{\mathrm{q}}/m$ the action reads:

$$\begin{aligned} S'_f &= \int \mathrm{d}x \; \bar{\psi}'(x)(\not{D} + M)\psi'(x), \qquad M = \sqrt{m^2 + \mu_q^2} \\ \bar{\psi}'\psi' &= \bar{\psi}\exp(i\alpha\gamma_5\tau^3)\psi = \cos(\alpha)\bar{\psi}\psi + i\sin(\alpha)\bar{\psi}\gamma_5\tau^3\psi \end{aligned}$$

corresponds to $\omega_{\mathrm{A}}^a = \alpha\delta^{3a}$ in the previous discussion.

Introduce polar mass coordinates

$$m = M\cos(\alpha), \qquad \mu_{\rm q} = M\sin(\alpha),$$

and consider the formal functional integral

$$\langle O[\psi,\bar\psi]\rangle_{(M,\alpha)} = \mathcal{Z}^{-1}\int D[U,\psi,\bar\psi]\,O[\psi,\bar\psi]\,{\rm e}^{-S[m,\mu_{\rm q}]}$$

The change of variables leads to the identity:

$$\left\langle O[\psi,\bar\psi]\right\rangle_{(M,0)} = \left\langle O[R(\alpha)\psi,\bar\psi R(\alpha)]\right\rangle_{(M,\alpha)}$$

For a member $\phi_A^{(r)}$ of a chiral multiplet in the representation r,

$$\phi_A^{(r)}[R(\alpha)\psi,\bar\psi R(\alpha)] = R_{AB}^{(r)}(\alpha)\phi_B^{(r)}[\psi,\bar\psi]$$

The identity for n-point functions of such fields becomes

$$\left\langle \phi_{A_1}^{(r_1)}(x_1)\cdots\phi_{A_n}^{(r_n)}(x_n)\right\rangle_{(M,0)} = \left\{\prod_{i=1}^{n} R_{A_iB_i}^{(r_i)}(\alpha)\right\}\left\langle \phi_{B_1}^{(r_1)}(x_1)\cdots\phi_{B_n}^{(r_n)}(x_n)\right\rangle_{(M,\alpha)}$$

Examples: chiral multiplets (A_μ^a, V_μ^a) and $(\frac{1}{2}S^0, P^a)$

$$A_\mu^a = \bar\psi\gamma_\mu\gamma_5\tfrac{\tau^a}{2}\psi, \qquad V_\mu^a = \bar\psi\gamma_\mu\tfrac{\tau^a}{2}\psi,$$
$$P^a = \bar\psi\gamma_5\tfrac{\tau^a}{2}\psi, \qquad S^0 = \bar\psi\psi.$$

With $\psi' = R(\alpha)\psi$, $\bar\psi' = \bar\psi R(\alpha)$, $O' \equiv O[\psi', \bar\psi']$, $c \equiv \cos(\alpha)$, $s \equiv \sin(\alpha)$ one finds:

$$A'^1_\mu = cA^1_\mu + sV^2_\mu, \qquad V'^1_\mu = cV^1_\mu + sA^2_\mu,$$
$$A'^2_\mu = cA^2_\mu - sV^1_\mu, \qquad V'^2_\mu = cV^2_\mu - sA^1_\mu,$$
$$A'^3_\mu = A^3_\mu, \qquad V'^3_\mu = V^3_\mu,$$
$$P'^a = P^a, \quad (a = 1, 2), \qquad P'^3 = cP^3 + is\,\tfrac{1}{2}\bar\psi\psi.$$

For instance:

$$\left\langle A_\mu^1(x)P^1(y)\right\rangle_{(M,0)} = \cos(\alpha)\left\langle A_\mu^1(x)P^1(y)\right\rangle_{(M,\alpha)} + \sin(\alpha)\left\langle V_\mu^2(x)P^1\right\rangle_{(M,\alpha)}$$

The PCAC and PCVC relations,

$$\partial_\mu A_\mu^a = 2mP^a + \delta^{3a} i\mu_q S^0, \qquad \partial_\mu V_\mu^a = -2\mu_q \varepsilon^{3ab} P^b,$$

take their standard form in the primed basis

$$\partial_\mu {A'}_\mu^a = 2M{P'}^a, \qquad \partial_\mu {V'}_\mu^a = 0.$$

Remarks:

- We refer to the basis of primed fields as "physical" because the mass term takes its standard form in this basis
- We still need to explain how the relationship between QCD with a standard mass term and twisted mass QCD works out beyond the formal continuum theory.

Beyond the formal continuum theory

* If tmQCD is regularized with Ginsparg-Wilson quarks the same identities can be derived in the bare theory

* If the renormalization procedure respects the chiral multiplet structure and the multiplicative renormalization constants do not depend on α (e.g. mass independent renormalization schemes)

  $\Rightarrow$ the formal continuum relations hold between renormalized theories.

  N.B.: no reference to perturbation theory! Assuming universality the correspondence is established non-perturbatively. In PT it works out order by order in the loop expansion.

* The angle α is given by the ratio between renormalized PCVC and PCAC masses: $\tan\alpha = \mu_{\mathrm{R}}/m_{\mathrm{R}}$

Lattice tmQCD with Wilson quarks

1. restore the chiral multiplets in the massless bare theory by imposing the chiral flavour Ward identities, e.g. $(Z_{\rm A}A_\mu^a, \tilde{V}_\mu^a)$ where $\tilde{V}_\mu^a$ is the conserved vector current (at $\mu_{\rm q} = 0$).

2. If necessary renormalize a given chiral multiplet by imposing a renormalization condition on one of its members. Choose a mass independent renormalization scheme!

3. Renormalization of the parameters:

$$g_{\rm R}^2 = Z_g g_0^2, \qquad m_{\rm R} = Z_m(m_0 - m_{\rm c}), \qquad \mu_{\rm R} = Z_\mu \mu_{\rm q},$$

From the exact PCVC relation

$$\partial_\mu^* \tilde{V}_\mu^2 = 2\mu_{\rm q} P^1 = 2\mu_{\rm R}(P_{\rm R})^1 \quad \Rightarrow Z_\mu Z_{\rm P} = 1.$$

$\Rightarrow$ to define α measure a bare PCAC mass m

$$m = \frac{\langle \partial_\mu A^1_\mu(x) O \rangle}{\langle P^1(x) O \rangle} \qquad \Rightarrow \qquad \tan\alpha = \frac{\mu_\mathrm{R}}{m_\mathrm{R}} = \frac{Z_\mathrm{P}^{-1}\mu_\mathrm{q}}{Z_\mathrm{P}^{-1} Z_\mathrm{A} m} = \frac{\mu_\mathrm{q}}{Z_\mathrm{A} m}.$$

the definition of α requires Z_A, except for $\alpha = \pi/2$, where $m = 0$.

4. Although α is an unphysical paramater and can be set to any value, the continuum limit should be taken at fixed α, keeping the physical conditions in its definition fixed (PCAC relation)

The freedom of introducing more general mass terms can be used to avoid lattice renormalization problems:

1. F_π can be obtained from the 2-point function

$$\begin{aligned}\big\langle (A_\mathrm{R})^1_0(x)(P_\mathrm{R})^1(y)\big\rangle_{(M_\mathrm{R},0)} &= \cos(\alpha)\,\big\langle (A_\mathrm{R})^1_0(x)(P_\mathrm{R})^1(y)\big\rangle_{(M_\mathrm{R},\alpha)} \\ &\quad + \sin(\alpha)\big\langle \widetilde{V}^2_0(x)(P_\mathrm{R})^1(y)\big\rangle_{(M_\mathrm{R},\alpha)}.\end{aligned}$$

   At $\alpha = \pi/2$ one has $\cos(\alpha) = 0$ and F_π is obtained from the vector current. The determination of Z_A is avoided!

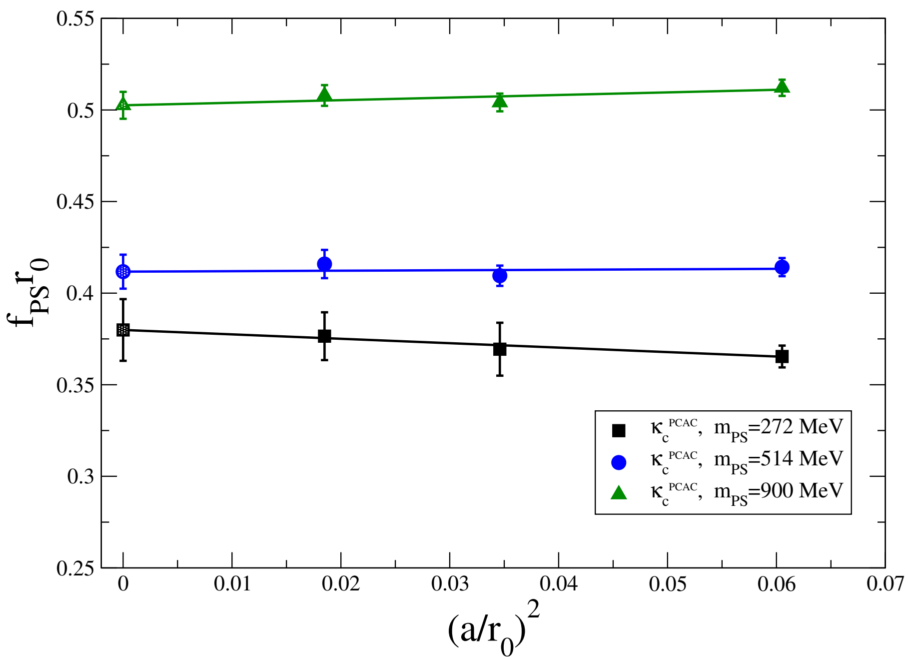
2. The chiral condensate:

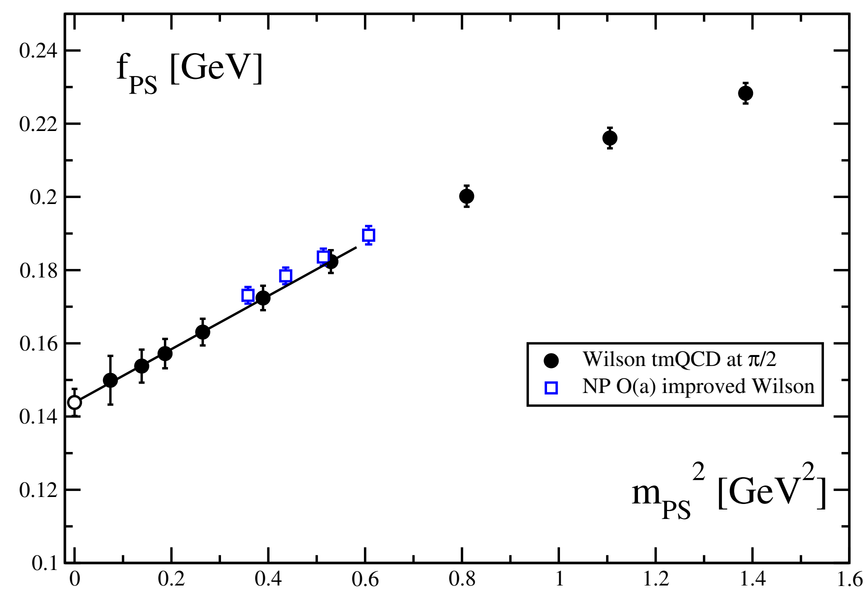
$$\big\langle (S_\mathrm{R})^0(x)\big\rangle_{(M_\mathrm{R},0)} = \cos(\alpha)\,\big\langle (S_\mathrm{R})^0(x)\big\rangle_{(M_\mathrm{R},\alpha)} + 2i\sin(\alpha)\big\langle (P_\mathrm{R})^3(x)\big\rangle_{(M_\mathrm{R},\alpha)}.$$

   At $\alpha = \pi/2$ the chiral condensate is represented by P^3 which only renormalizes multiplicatively in the chiral limit!

Example: computation of F_π

Quenched simulations at least down to pion masses of $\approx 270\,\mathrm{MeV}$ are possible





reference: K. Jansen et al. (χLF collaboration) (2005), as presented by A. Shindler at Lattice 2005

An application to the computation of B_K

The B_K parameter is defined in QCD with dynamical u, d, s quarks:

$$\langle \bar{K}^0 | O^{\Delta S=2}_{(\mathrm{V-A})(\mathrm{V-A})} | K^0 \rangle = \tfrac{8}{3} F_K^2 m_K^2 B_K$$

The local operator

$$O^{\Delta S=2}_{(\mathrm{V-A})(\mathrm{V-A})} = \sum_{\mu} \left[\bar{s} \gamma_\mu (1 - \gamma_5) d \right]^2$$

is the effective local interaction induced by integrating out the massive gauge bosons and t, b, c quarks in the Standard Model.

- only the parity-even part contributes to B_K

$$O_{(\mathrm{V-A})(\mathrm{V-A})} = \underbrace{O_{\mathrm{VV+AA}}}_{\mathrm{parity-even}} - \underbrace{O_{\mathrm{VA+AV}}}_{\mathrm{parity-odd}}$$

- Operator mixing problem with Wilson type quarks:

$$
\begin{aligned}
[O_{\mathrm{VV+AA}}]_{\mathrm{R}} &= Z_{\mathrm{VV+AA}}\Big\{O_{\mathrm{VV+AA}} + \sum_{i=1}^{4} z_i\ O_i^{d=6}\Big\} \\
[O_{\mathrm{VA+AV}}]_{\mathrm{R}} &= Z_{\mathrm{VA+AV}} O_{\mathrm{VA+AV}}
\end{aligned}
$$

$\Rightarrow$ parity-odd component renormalizes multiplicatively!

Question: Can we avoid the mixing problem by using the multiplicatively renormalized operator $O_{\mathrm{VA+AV}}$ to compute B_K?

- consider continuum theory for a light quark doublet ψ and the s-quark:

$$
\begin{aligned}
\mathcal{L}_f &= \bar{\psi}\left(\not{D} + m + i\mu_q\gamma_5\tau^3\right)\psi + \bar{s}\left(\not{D} + m_{\mathrm{s}}\right)s \\
\Rightarrow \quad O'_{\mathrm{VV+AA}} &= \cos(\alpha)O_{\mathrm{VV+AA}} - i\sin(\alpha)O_{\mathrm{VA+AV}} \\
&= -iO_{\mathrm{VA+AV}} \quad (\alpha = \pi/2)
\end{aligned}
$$

Non-perturbative renormalization of $O_{\mathrm{VA+AV}}$

We use a finite volume scheme based on the Schrödinger functional which

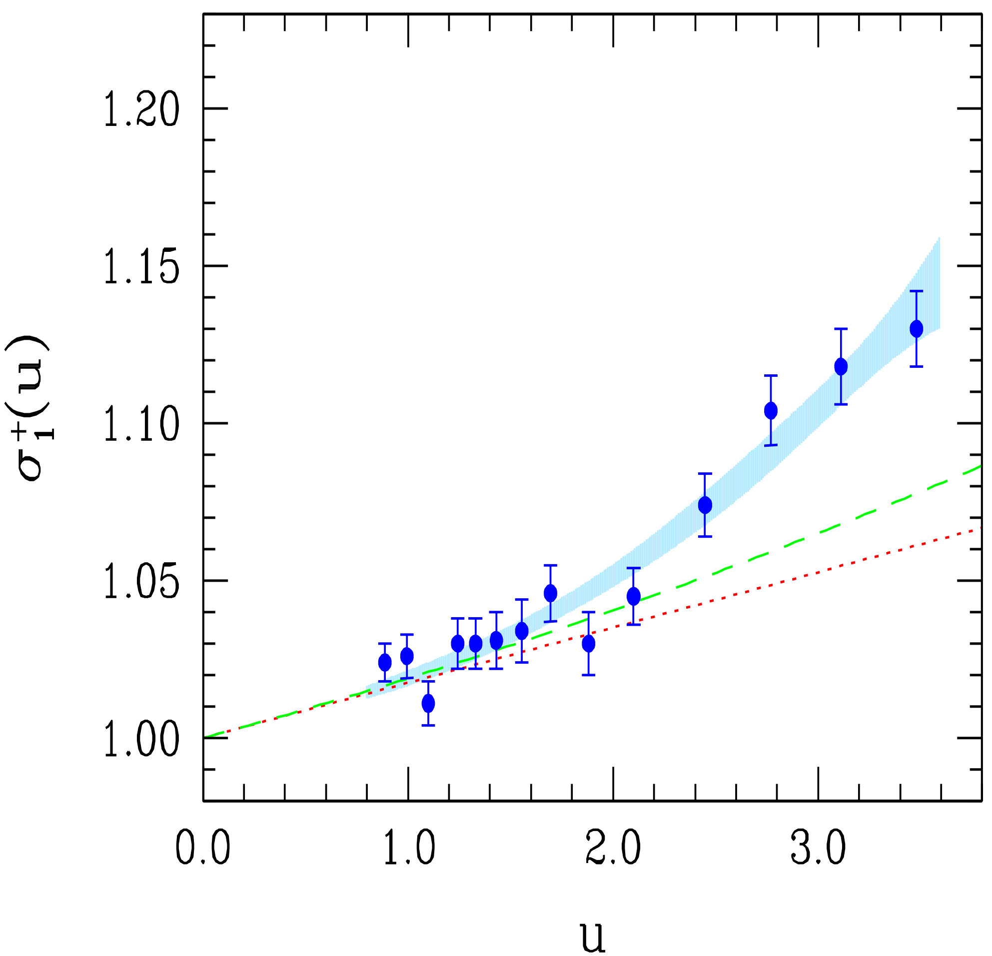
- is gauge invariant
- is quark mass independent: renormalization conditions are imposed in the chiral limit (S. Weinberg '73)
- allows for simulations at zero quark mass, due to SF boundary conditions (Dirichlet conditions in time direction)
- has the renormalization scale set by the space-time volume, $\mu = 1/L$

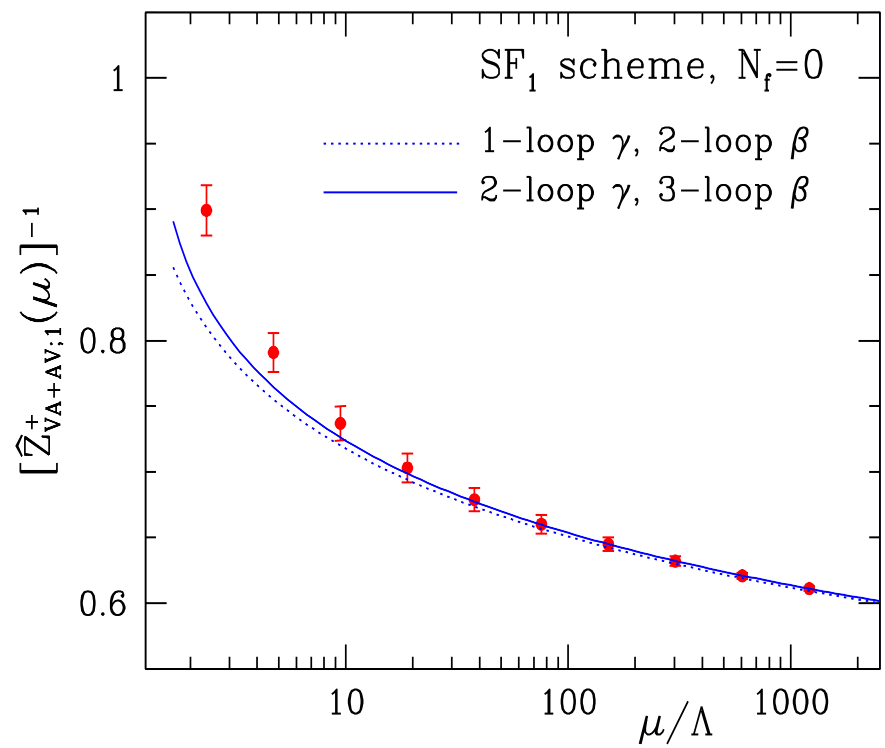
⇒ recursive procedure allows to connect scales which differ by orders of magnitude

⇒ renormalization fully controlled at the non-perturbative level

refs.: Guagnelli, Heitger, Palombi, Pena, S., Vladikas (Alpha collaboration), `hep-lat/0505002 & hep-lat/0505003`

Renormalization group evolution of B_K (SF scheme)





Conclusions

Twisted mass QCD with Wilson type quarks is a regularisation which

- is equivalent to standard QCD (based on universality, established to all orders in perturbation theory),
- is unitary (with plain Wilson gauge and quark actions; Symanzik improvement terms are expected to cause unitarity violations close to the cutoff scale),
- is free of unphysical zero modes (no exceptional configurations),
- has an additional unphysical parameter, the twist angle α. This angle determines the physical interpretation (flavour vs. chiral symmetries, parity) and can be used to circumvent certain lattice specific renormalization problems: F_π without Z_{A}, the chiral order parameter without cubic divergence, B_K without mixing ....

One expects

- the breaking of flavour and parity symmetries to cause some technical complications (see later),
- that parity and flavour symmetries are restored in the continuum limit (just as axial symmetry with standard Wilson quarks).