Lattice QCD with chirally twisted Wilson fermions

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tmLQCD: lattice QCD with chirally twisted quarks

Key point: disentangle quark mass, m_q, and Wilson term,

$W = -(a/2)\nabla^* \cdot \nabla$, by chiral twist of $W + M_{\rm cr}$ $(N_f = 2, 4, ...)$

E.g. for $N_f = 2 \Leftrightarrow \psi = (u, d)^{\rm t}$ maximal twist is given by

$$L^{N_f=2} = L_{\rm YM} + \bar{\psi}\,[\,\gamma \cdot \widetilde{\nabla} - i\gamma_5\tau^3(W + M_{\rm cr}) + m_q\,]\,\psi$$

- m_q gives IR cutoff, no quark zero modes if $m_q \neq 0$
- lattice artifacts only $O(a^2)$ in physical quantities
- action with $m_0 = M_{\rm cr}$: need to know it up to $O(a)$

  (included, in practice: fine tuning of m_0)

Some questions on tmLQCD $\Rightarrow$ Outline

1. Why is it needed?

   (Problems with Wilson quarks; other lattice fermions and systematic errors)

2. Why is it possible?

   (Chiral twist of the term $W + M_{\rm cr}$: a change of irrelevant operators)

3. How well does it work? Pro's and con's...

   (Multiplicatively renormalized quark mass. Automatic O(a) improvement. Determining $M_{\rm cr}$ precisely enough. Flavour–chiral and parity breaking.)

4. How general is it?

   ($N_f > 2$ sea flavours. Operator renormalization and mixed actions.)

5. A few selected physical results

Brief history of twisted mass fermions

- Aoki ’84 (twisted mass pre-history)
- RF–Grassi–Sint–Weisz ’99–’01 (equivalence to QCD)
- Alpha ’00–’02 (numerical test, IR safety, scaling: clover)
- Alpha ’03–’06 (application of tmLQCD to B_K: clover)
- RF–Rossi ’03–’04 (automatic O(a) improvement)
- ETMC proto-group ’04–’05 (scaling and phase structure)
- Regina group (baryons, form factors; scaling)

"Twisters" in Europe: the ETM Collaboration

- Germany — B. Blossier, F. Farchioni, K. Jansen, I. Montvay, K. Nagai, S. Schäfer, A. Shindler, C. Tarantino, G. Münster, O. Bär
- Italy — T. Chiarappa, P. Dimopoulos, R. Frezzotti, G. Herdoiza, V. Lubicz, G. Martinelli, M. Papinutto, G.C. Rossi, L. Scorzato, S. Simula, A. Vladikas
- UK — C. McNeile, C. Michael, J. Pickavance, C. Urbach
- France — R. Baron, M. Brinet, Ph. Boucaud, J. Carbonell,Z. Liu, B. Haas, O. Pène
- Spain — V. Gimenez, D. Palao
- Switzerland — U. Wenger
- Cyprus — D. Alexandrou, G. Koutsou

Control of errors in Lattice QCD

Lattice regularization may break symmetries: O(4), flavour-chiral, parity

As $a \to 0$ all the non–anomalous symmetries of QCD are recovered

Non-perturbative path-integrals on finite lattices ; (with $(L/a)^3 T/a$ sites)

can be evaluated via numerical algorithms (linear solvers and MC's)

Errors are controllable and systematically reducible

- systematics: operator renormalization, $O(a)$ effects, finite-L effects; (partial) quenching of quark flavours, values of quark masses
- statistics: finite n.r of decorrelated estimators for each observable

In addition one must keep negligibly small any possible systematic errors due to
i) imperfect equilibration of (unquenched) gauge ensembles
ii) misidentification of transfer–matrix eigenstate contributions to correlators

Systematic errors in LQCD – I

Choice of lattice fermions is crucial for control of systematics

- operator renormalization:

  $\hat{O}|_{\mu}^{\rm RS} = Z_O^{\rm RS}(g_0^2, a\mu)\{O|_{\rm bare} + \zeta_i(g_0^2, am_q)a^{n_i}\Delta_i^O|_{\rm bare}\}$

  scale–independent mixing with Δ_i^O of dim. $d_i = d_O + n_i$, *relevant* if $n_i \leq 0$;

  non-perturbative lattice ren. schemes (RI-MOM, SF) $\Rightarrow$ $\hat{O}_{RGI}$.

- O(a^n) cutoff effects:

  irrelevant terms in the action and external operators $\Rightarrow$ artifacts of order $(a\Lambda_{\rm QCD})^n$, $(am_q)^n$, $(ap_{\rm ext})^n$ in correlators and derived quantities

  Note: Wilson fermions & model with chiral SSB $\Rightarrow n = 1$;

  O(a) improved Wilson or "more chiral" fermions: $\Rightarrow n = 2$.

  Typically: $1/a \sim 2 \div 4$ GeV $\Leftrightarrow$ $a \sim 0.1 \div 0.05$ fm.

Systematic errors in LQCD – II

- finite size effects (negligible only if $m_{PS}L \gg 1$):
  increase with hadron radius and as $m_q \to 0$; decrease as $L \to \infty$
  (behaviour in L first power-like, then exponential). Typically: $L \sim 2 \div 3$ fm
- neglected sea quark effects:
  (sea) u and d quarks important; s expected to be important for specific observables; c almost irrelevant ? ($m_c \gg \Lambda_{\rm QCD}$)
- unphysical values of (u, d; b) quark masses:
  ChPT–inspired extrapolations to realistic values of m_u, m_d; interpolation between static limit (HQET–QCD) and charm mass region

Systematic errors of different type mutually entangled in practice.

Typically: more symmetric (ideally chiral–invariant) lattice action $\Rightarrow$ fewer operator mixings and $O(a)$ artifacts reduced or absent, but more CPU time requested (especially for unquenching)

$\Rightarrow$ smaller L/a–values, thus larger cutoff and/or finite size effects.

Lattice fermions: generalities

Lattice Dirac operators $D = D[U]$ cannot enjoy simultaneously locality, chirality and correct continuum limit with no doublers (Nielsen–Ninomiya, '81).

In particular $D_{\rm free} \equiv D[1]$ cannot satisfy simultaneously

1. $D_{\rm free}$ is analytic in momentum space (local in position space)
2. $D_{\rm free}$ in momentum space is given for $ap \ll 1$ by $p_\mu \gamma_\mu + O(ap^2)$
3. $D_{\rm free}$ in momentum space (1st BZ) has only one pole at $p = 0$
4. $D_{\rm free}\gamma_5 + \gamma_5 D_{\rm free} = 0$ (formal chirality)

Consistent with QCD physics: axial-$U(1)$ anomaly, η' massive as $m_q \to 0$.

Wilson's approach: keep 1.-2.-3. (D ultralocal) and break 4. while preserving all vector symmetries of the chiral group (and parity).

Ginsparg–Wilson (GW) approach: keep 1.-2.-3. and chiral–vector symmetries; replace 4. with $D\gamma_5 + \gamma_5 D = aDR\gamma_5 D$ where $R = R[U]$ is local.

Wilson quarks for LQCD

Wilson's approach: keep 1.-2.-3. and break 4. while preserving all vector symmetries of the chiral group (and parity). This leads to

$$L^{N_f}_{\rm Latt} = L_{\rm YM} + \bar{\psi}_f \, [\, \gamma \cdot \widetilde{\nabla} + W + m_{0f} \,] \, \psi_f \, , \quad W = -\frac{a}{2} \nabla^* \cdot \nabla \, , \quad m_{0f} = M_{\rm cr} + m_{qf}$$

Pro: all symmetries useful to label QCD–Hamiltonian eigenstates exact.

Con: axial symmetries hardly broken, possibly spurious quark zero modes

$\Rightarrow$ simulations with $m_q \leq a\Lambda^2_{\rm QCD}$ may be statistically unstable; chiral–violating operator mixings in renormalization; large O(a) artifacts.

On-shell O(a) improved action: $W \rightarrow W + c_{\rm SW} \frac{i}{4} \sigma \cdot F$ with suitable c_{SW}, $M_{\rm cr}$.

Note: on-shell O(a) improvement does not eliminate the first two problems; unquenching u and d softens the first ($m_q \sim 20$ MeV stable at $a^{-1} = 3$ GeV).

Chiral invariant (overlap) quarks for LQCD

GW approach: keep 1.-2.-3. and vector symmetries; replace 4. with

$D\gamma_5 + \gamma_5 D = aDR\gamma_5 D$ (GW–relation), where $R = R[U]$ is local.

Solutions: perfect fermions (Hasenfratz '97); overlap fermions (Neuberger '97); domain wall fermions with $N_5 = L_5/a \to \infty$ (Kaplan, Shamir, Kikukawa, ...-'99).

Overlap solution $\Rightarrow$ $L^{N_f}_{\mathrm{Latt}} = L_{\mathrm{YM}} + \bar\psi\,[(1 - \frac{am_{qf}}{2\rho})D_{\mathrm{ov}} + m_{qf}\,]\,\psi$, where

$D_{\mathrm{ov}} = a^{-1}\rho(1 + X(X^\dagger X)^{-1/2}) \qquad X = \gamma\cdot\tilde\nabla + W - a^{-1}\rho,$

satisfies the GW–relation with $R = \rho^{-1}$ (ρ is a free O(1) parameter).

Axial symmetries exact with correct singlet anomaly if (Lüscher '98):

$\delta\psi = \hat\gamma_5\psi\,, \quad \delta\bar\psi = \bar\psi\gamma_5\,,$ with $\hat\gamma_5 \equiv (1 - a\rho^{-1}D_{\mathrm{ov}})\gamma_5$ and $\hat\gamma_5 = \hat\gamma_5{}^\dagger = \hat\gamma_5{}^{-1}$.

Note: D_{ov} contains X (W-like) and $(X^\dagger X)^{-1/2}$ (zeros of X are critical).
$\Rightarrow$ CPU cost $\sim$ 50 larger than for W-like actions & $D_{\mathrm{ov}}[U]$ discontinuous at the boundaries of U-regions with different $Q_{\mathrm{top}}[U] = \mathrm{Tr}[\gamma_5 D_{\mathrm{ov}}[U]]$.

Osterwalder–Seiler fermions – I

Basic building block of max. twisted Wilson quarks: one flavour field q with

$$L_{OS}^{N_f=1} = L_{\rm YM} + \bar{q}\,[\,\gamma\cdot\widetilde{\nabla} - i\gamma_5(W+m_0) + \mu\,]\,q\,, \qquad W = -r(a/2)\nabla^*\cdot\nabla$$

One–flavour lattice theory reflection positive and with a continuum limit:

QCD with (UV–finite) θ–term ($\theta = \arctan(\hat{\mu}/\hat{m})$), provided

g_0^2, μ, m are suitably multiplicatively renormalized, where

$m \equiv m_0 - M_{\rm cr}$ with appropriate $M_{\rm cr} = a^{-1} f_{\rm cr}(g_0^2, r) = -a^{-1} f_{\rm cr}(g_0^2, -r)$

Lattice quark determinant complex: unquenching by means of ordinary MC simulations very problematic

Sea quark effects induce $\tilde{F}F$–term: parity-violations in correlators (as $a \to 0$)!

Osterwalder–Seiler fermions – II

Proof of renormalizability for case $m = 0$ (by power counting and symmetry)

This is the only case treated by OS; extension to $m \neq 0$ straightforward

1. $d = 4$: $\bar{q}\gamma_5\gamma\cdot\nabla q$ forbidden by charge conjugation
2. $d = 4$: $\bar{q}q[1, \mu]$ inv. $P \times R_5 \times (\mu \to -\mu)$ allows only term with μ
3. $d = 3, 4$: $-\bar{q}i\gamma_5 q[r, m_0]$ see inv. $P \times (r \to -r) \times (m_0 \to -m_0)$
4. $d = 5$: $i\tilde{F}F[1, \mu]$ as in 3 with an IR cutoff in place; μ/m: UV–finite
5. extra factors of i forbidden by $\Theta_{l,s}$ reflection-inv.

$$R_5 \ : \ q(x) \to \gamma_5 q(x) \ , \qquad \bar{q}(x) \to -\bar{q}(x)\gamma_5$$

$$P \ : \ q(x) \to \gamma_0 q(x_P) \ , \qquad \bar{q}(x) \to \bar{q}(x_P)\gamma_0 \ , \qquad (U_0, U_k)(x) \to (U_0, U_k^\dagger)(x_P)$$

μ multiplicatively renormalized, $O(a)$ artifacts from P–violations only $\Rightarrow$
OS-like quarks useful as valence quarks in mixed action lattice formulations

Osterwalder–Seiler fermions – III

Origin of UV–finite θ–term: proof by universality & use of GW–formulation

$$S_{OS}^{N_f=1} = S_{\rm YM} + \{\bar{q}\,[\gamma\cdot\widetilde{\nabla} - i\gamma_5(W + M_{\rm cr} + m) + \mu\,]\,q\}\,,$$

$$\chi = \exp(-i\pi\gamma_5/4)q\,, \qquad \bar{\chi} = \bar{q}\exp(-i\pi\gamma_5/4) \qquad \text{(non–anomalous)}$$

$$S_{OS}^{N_f=1} = S_{\rm YM} + \{\bar{\chi}\,[\gamma\cdot\widetilde{\nabla} + (W + M_{\rm cr} + m) + i\gamma_5\mu\,]\,\chi\}\,,$$

universality

$$S_{GW}^{N_f=1} = S_{\rm YM} + \{\bar{\chi}_L D_{\rm ov}\chi_L + \bar{\chi}_R D_{\rm ov}\chi_R + (m + i\mu)(\bar{\chi}_L\chi_R) + (m - i\mu)(\bar{\chi}_R\chi_L)\}$$

$$q = \exp(i\theta\gamma_5/2)\chi\,, \qquad \bar{q} = \bar{\chi}\exp(i\theta\hat{\gamma}_5[U]/2) \qquad (U(1)_A \text{ anomaly})$$

$$S_{GW}^{N_f=1} = S_{\rm YM} + i\theta Q_{\rm topo}[U] + \{\bar{q}_L D_{\rm ov} q_L + \bar{q}_R D_{\rm ov} q_R + \sqrt{m^2+\mu^2}(\bar{q}_L q_R + \bar{q}_R q_L)\}$$

with $\tan\theta = \mu/m$ (parameters of GW lattice action) & $\{\ldots\} = a^4\sum_x \ldots$

From two OS flavours to one Mtm doublet

Lattice QCD with $N_f = 2$ quarks at maximal twist: in quark basis $\psi = (u, d)^t$

$$L_{Mtm}^{N_f=2} = L_{\rm YM} + \bar{\psi}\,[\,\gamma \cdot \tilde{\nabla} - i\gamma_5\tau^3(W + M_{\rm cr}) + \mu\,]\,\psi\,, \qquad W = -r(a/2)\nabla^* \cdot \nabla$$

$\Leftrightarrow$ pairing two OS quark flavours ($m = 0$) with opposite r–values

- action contains $M_{\rm cr}$: need to determine it, i.e. tune m_0 to $M_{\rm cr} = M_{\rm cr}(r)$
- three conserved lattice currents: V_λ^3 (exactly), $A_\lambda^{1,2}$ (up to $O(\mu)$)
- power counting renormalizability obvious (symmetry not less than for OS)
- additional inv. $P \times (u \leftrightarrow d)$ $\Rightarrow$ no θ-term: $N_f = 2$ QCD as $a \to 0$
- real $\det[\,\gamma \cdot \tilde{\nabla} - i\gamma_5\tau^3(W + M_{\rm cr}) + \mu\,] > 0$ provided $\mu \neq 0$

$D_{\rm tm} = [\,\gamma \cdot \tilde{\nabla} - i\gamma_5\tau^3(W + M_{\rm cr}) + \mu\,]_{\rm 2fl.}$ and $Q_{\rm cr} \equiv \gamma_5[\,\gamma \cdot \tilde{\nabla} + W + M_{\rm cr}]_{\rm 1fl.} = Q_{\rm cr}^\dagger$

$\Rightarrow$ $\det[D_{\rm tm}[U]] = \det[Q_{\rm cr}[U]^2 + \mu^2]$; spectrum of D_{tm} away from imaginary axis by μ.

$N_f = 2$ Mtm-LQCD: symmetries – I

Besides lattice gauge invariance, translations and rotations (H(4)) one has

- charge conjugation, I_3 (U(1) isospin subgroup with generator τ^3)
- $P \times (u \leftrightarrow d)$, with P the physical parity

  $$P \;:\quad \psi(x) \to \gamma_0 \psi(x_P)\,,\quad \bar\psi(x) \to \bar\psi(x_P)\gamma_0\,,\quad (U_0, U_k)(x) \to (U_0, U_k^\dagger)(x_P)$$

- $R_5 \times \mathcal{D}_d$ with (note $-i = e^{3i\pi/2}$)

  $$R_5 \;:\quad \psi(x) \to \gamma_5 \psi(x)\,,\quad \bar\psi(x) \to -\bar\psi(x)\gamma_5$$

  $$\mathcal{D}_d \;:\quad \psi(x) \to -i\psi(-x)\,,\quad \bar\psi(x) \to -i\bar\psi(-x)\,,\quad U_\mu(x) \to U_\mu^\dagger(-x - a\hat\mu)$$

- $P \times \mathcal{D}_d \times (\mu \to -\mu)$ or equivalently $(u \leftrightarrow d) \times \mathcal{D}_d \times (\mu \to -\mu)$

  $\Rightarrow$ terms of odd dimensionality in $\mathcal{L}^{\rm Mtm}_{\rm Sym}$ are odd under P and $(u \leftrightarrow d)$

$N_f = 2$ Mtm-LQCD: symmetries – II

- invariance under $\mu \to -i[(\theta_1\tau^1 + \theta_2\tau^2)\gamma_5]\mu$ & oblique global $SU(2)$:
  $\psi \to i[(\theta_1\tau^1 + \theta_2\tau^2)\gamma_5 + \theta_3\tau^3]/2\,\psi\,, \quad \bar\psi \to i\bar\psi\,[-\theta_3\tau^3 + (\theta_1\tau^1 + \theta_2\tau^2)\gamma_5]/2$
  $\Leftrightarrow$ in the limit $\mu \to 0$ three conserved currents A^1_μ, A^2_μ, V^3_μ
  (analogous to W, where the three conserved currents are of vector type)
- $R_5 \times (\mu \to -\mu) \times [(r \to -r) \times (M_{\rm cr} \to -M_{\rm cr})] \quad \Rightarrow \quad$ odd r-parity of $M_{\rm cr}$
- $(\mu \to -\mu)$ & pseudo λ–axis inversion (or pseudo parity):
  $\psi(x) \to i\tau^3\gamma_\lambda\psi(x')\,, \quad \bar\psi(x) \to \bar\psi(x')i\tau^3\gamma_\lambda\,, \quad x'_\mu = x_\mu(1 - 2\delta_{\mu,\lambda})\,,$
  $U_\lambda(x) \to U^\dagger_\lambda(x' - a\hat\lambda)\,, \quad U_\mu(x) \to U_\mu(x')\,, \quad \mu \neq \lambda$

⋆ Tuning m_0 to $M_{\rm cr}$: restore P or $I_{1,2}$ in a given correlator or matrix element (analogous to W, different symmetry restored). P or $I_{1,2}$ still broken elsewhere.

⋆ In the QM analysis of correlators intermediate states with different P– and I–properties; beware of states with smaller energy than those surviving as $a \to 0$

Mtm-LQCD: automatic O(a) improvement – I

Mtm-LQCD action is not O(a) improved. However (RF–Rossi '03; ...) :

no O(a) artefacts in $\langle O\rangle|^{L}_{M_{\rm cr},\mu}$ from which physical quantities are extracted.

In general these are (F.T.'ed) vev's of multilocal operators of the form $O = [{\rm F.T.} \prod_{j=1}^{n} \Phi_j(x_j)](\{p\})K(\{p\})$, with kinematical factor K : $\langle O\rangle|^{\rm cont}_{\mu} \neq 0$

Symanzik local effective Lagrangian (LEL) for Mtm-LQCD with $m_0 = M^{e}_{\rm cr}$:

$$\mathcal{L}^{\rm Mtm}_{\rm Sym} = -\frac{1}{2}F\cdot F + \bar\psi[D+\mu]\psi + a\mathcal{L}^{\rm Mtm}_5 + a^2\mathcal{L}^{\rm Mtm}_6 + \ldots$$

$$\mathcal{L}^{\rm Mtm}_5 = b_{5;SW}\bar\psi\gamma_5\tau^3\sigma\cdot F\psi + b_{5;P}\mu^2\bar\psi i\gamma_5\tau^3\psi + \delta^{e}_{5;NP}\Lambda^2_{\rm QCD}\bar\psi i\gamma_5\tau^3\psi$$

Symanzik description of vev's of multilocal operators:

$$\langle\prod_{j=1}^{n}\Phi_j(x_j)\rangle|^{L}_{M^{e}_{\rm cr},\mu} = \langle\prod_{j=1}^{n}\Phi_j(x_j)\rangle|^{\rm cont}_{\mu} - a\int d^4y\langle\prod_{j=1}^{n}\Phi_j(x_j)\mathcal{L}^{\rm Mtm}_5(y)\rangle|^{\rm cont}_{\mu} +$$

$$+a\sum_{j=1}^{n}\langle\Delta_1\Phi_j(x_j)\prod_{k\neq j}\Phi_k(x_k)\rangle|^{\rm cont}_{\mu} + {\rm O}(a^2)\ ,$$

where $\mathcal{L}^{\rm Mtm}_5$ is P-odd and $\Delta_1\Phi_j$ has parity opposite to Φ_j.

Mtm-LQCD: automatic O(a) improvement – II

If F.T. and kinematical factors are s.t. $O = [\mathrm{F.T.} \prod_{j=1}^{n} \Phi_j(x_j)](\{p\})K(\{p\})$ is

P–even $\Rightarrow$ coefficients of terms of order a, a^3, ... vanish by P

$(u \Leftrightarrow d)$–even $\Rightarrow$ coeff. of terms of order a, a^3, ... vanish by flavour symmetry

More generally, provided $\prod_{j=1}^{n} \Phi_j(x_j)$ is O(3)–covariant, one can choose F.T. and kinematical factor s.t. O is O(3)–scalar $\Rightarrow$ P-even $\Rightarrow$ no O(a) artefacts, since

- terms non–invariant under O(3) (O(4)) in Symanzik's LEL can contribute only at O(a^2) – this is why they are usually not even mentioned;
- all terms of order a in the Symanzik expansion of $\langle O \rangle|^L_{M_{\rm cr},\mu}$ vanish because $\int d^4y O \mathcal{L}_5^{\rm Mtm}(y)$ and $\Delta_1 O$ are O(3)–scalars and P–odd.

Key point: symmetry $P \times \mathcal{D}_d \times (\mu \rightarrow -\mu)$ resp. $(u \leftrightarrow d) \times \mathcal{D}_d \times (\mu \rightarrow -\mu)$

(This proof: RF-Martinelli–Papinutto–Rossi '05; Aoki–Bär '06; RF @ETMC–meeting, Florence '07)

tm flavour doublet at generic twist angle

Lattice QCD with $N_f = 2$ quarks at twist angle ω: in quark basis $\psi = (u, d)^t$

$$L_{tm}^{N_f=2} = L_{\rm YM} + \bar\psi\,[\,\gamma\cdot\widetilde\nabla + \exp(-i\omega\gamma_5\tau^3)(W + M_{\rm cr}) + m_q\,]\,\psi\,,$$

- m_q : bare quark mass, renormalizes multiplicatively ($m_\pi^2 \sim m_q + O(a)$)
- ω : UV regularization label, controls $O(a)$, unphysical ($\omega = 0, \pi \;\leftrightarrow\;$ Wilson)
- quark det. is $\det[(Q_{\rm cr} + \gamma_5 m_q \cos\omega)^2 + m_q^2 \sin^2\omega] > 0$ if $m_q \sin\omega \neq 0$

Whatever the chosen ω-value, the (unphysical) basis where the action reads

$$L_{tm}^{N_f=2} = L_{\rm YM} + \bar\chi\,[\,\gamma\cdot\widetilde\nabla + W + m_0 + i\mu\gamma_5\tau^3\,]\,\chi\,, \qquad m_0 = M_{\rm cr} + m\,,$$

$$m = m_q \cos\omega\,, \qquad \mu = m_q \sin\omega;\,, \qquad \chi = e^{-i\omega\gamma_5\tau^3/2}\psi\,, \qquad \bar\chi = \bar\psi e^{-i\omega\gamma_5\tau^3/2}$$

is convenient for determination of $M_{\rm cr}$ and operator renormalization. Note:

$\omega = 0, \pi \;\Leftrightarrow\;$ standard W. & $\omega = \pm\pi/2 \;\Leftrightarrow\;$ maximally twisted W.

Determination of $M_{\rm cr}$ and maximal twist

Except for the cases $\omega = 0, \pi$, the tmLQCD action in the physical basis is defined only once $M_{\rm cr}$ is known. Start with the action in the $(\chi, \bar{\chi})$–basis:

$$L_{tm}^{N_f=2} = L_{\rm YM} + \bar{\chi}\,[\,\gamma\cdot\widetilde{\nabla} + W + m_0 + i\mu\gamma_5\tau^3\,]\,\chi\,, \qquad m_0 = M_{\rm cr} + m\,.$$

In this basis, two chiral–WTI are sensitive to $m_0 - M_{\rm cr}$ (and not to μ):

$$\partial_\lambda[\bar{\chi}\gamma_\lambda\gamma_5\tau^{1,2}\chi](x) \;\propto \{2(m_0 - M_{\rm cr})[\bar{\chi}\gamma_5\tau^{1,2}\chi](x) + \mathrm{O}(a)\}.$$

A numerically robust n.p. estimate of $M_{\rm cr}$ is obtained by imposing

$$a^3\sum_{\vec{x}}\partial_\lambda\langle[\bar{\chi}\gamma_\lambda\gamma_5\tau^{1,2}\chi](x)[\bar{\chi}\gamma_5\tau^{1,2}\chi](0)\rangle|^L_{M_{\rm cr},\mu} = 0$$

for $\mu \neq 0$ and suitable kinematics (e.g. zero three-momentum, large x_0);

in phys. quark basis of Mtm-LQCD: $\quad a^3\sum_{\vec{x}}\partial_\lambda\langle V_\lambda^{2,1}(x)P^{1,2}(0)\rangle|^L_{M_{\rm cr},\mu} = 0.$

A specific determination of $M_{\rm cr}$ $\Leftrightarrow$ a specific definition of maximal twist

(with a generic estimate of $M_{\rm cr}$ max. twist is defined only up to $\mathrm{O}(a)$).

$N_f = 2$ Mtm-LQCD: operator renormalization

Most conveniently discussed (and Z's named) in the $(\chi\ ,\bar{\chi})$–basis, as

- log. divergent (& UV–finite) renormalization unaffected by soft terms $\propto \mu\,, m = m_0 - M_{\rm cr}\,;$ they possibly enter only in the relation bare–to–m.r. operators: $Q_{\chi;{\rm m.r.}} \;=\; Q_\chi \,+\, \sum_i\, b_i^Q(a\mu, am)\, a^{-n_i} Q_\chi^i$
- mass independent schemes obtained for $\mu = 0$, $m_0 = M_{\rm cr}$

Examples: renormalization of isotriplet quark bilinears (subscripts $\Leftrightarrow$ quark basis)

$$(\hat{A}^1_\mu)_\psi = Z_V (V^2_\mu)_\chi\,, \quad (\hat{A}^2_\mu)_\psi = -Z_V (V^1_\mu)_\chi\,, \quad (\hat{A}^3_\mu)_\psi = Z_A (A^3_\mu)_\chi\,,$$

$$(\hat{V}^1_\mu)_\psi = Z_A (A^2_\mu)_\chi\,, \quad (\hat{V}^2_\mu)_\psi = -Z_A (A^1_\mu)_\chi\,, \quad (\hat{V}^3_\mu)_\psi = Z_V (V^3_\mu)_\chi\,,$$

$$(\hat{S}^0)_\psi = Z_P [i(P^3)_\chi + b_3((a\mu)^2) a^{-2} \mu]\,, \qquad (\hat{P}^1)_\psi = Z_P (P^1)_\chi$$

$$i(\hat{P}^3)_\psi = Z_{S^0} [(S^0)_\chi + b_0((a\mu)^2) a^{-3}]\,, \qquad (\hat{P}^2)_\psi = Z_P (P^2)_\chi$$

Generalization: if O^i_ψ reads $\sum_j\, f^{ij}_{A3}\, Q^j_\chi$ in the $(\chi\ ,\bar{\chi})$–basis, f_{A3} trivial,

then $\hat{O}^i_\psi \;=\; \sum_j\, f^{ij}_{A3}\, Z_{Q^j_\chi}\, Q^j_{\chi;{\rm m.r.}}\,,$ i.e. no new Z wrt ordinary Wilson's

$N_f = 2$ Mtm-LQCD: automatic O(a) improvement of the RI-MOM renormalization constants

Lattice N.P. gauge-fixing ($\partial_\mu G_\mu = 0$) procedure $\Leftrightarrow$ correlators evaluated with

$$S^L_{\rm Landau\ G.} = S^L_{\rm G.I.} + a^4 \sum_x [\lim_{\xi\to 0} \frac{1}{2\xi} (\tilde\partial\cdot G[U])^2(x) + (\bar c\,, (\tilde\partial\cdot\tilde D)[U]c)(x)]$$

(barring Gribov ambiguities) i.e. preserves the key relevant symmetry:

$$P \times \mathcal{D}_d \times (\mu \to -\mu) \quad \text{or equivalently} \quad (u \leftrightarrow d) \times \mathcal{D}_d \times (\mu \to -\mu)$$

O(a) improved renorm. constants Z_q, Z_O as usual, e.g. for quark bilinear O_Γ:

$$Z_q^{-1} \frac{i}{12} {\rm Tr}\{(\gamma\cdot p)/p^2 S_q^{-1}(p)\}|^{\mu\to 0}_{p^2=q^2} = 1 \qquad \leftrightarrow \qquad \hat\chi = Z_q^{1/2}\chi$$

$$G_\Gamma^{u,d}(p,p) \equiv a^8 \sum_{x,y} \langle u(x) O_\Gamma^{u,d}(0) \bar d(y)\rangle e^{-ip(x-y)}$$

$$Z_{O_\Gamma} Z_q^{-1} {\rm Tr}\{P_\Gamma S_u^{-1}(p) G_\Gamma^{u,d}(p,p) S_d^{-1}(p)\}|^{\mu\to 0}_{p^2=q^2} = 1 \qquad \leftrightarrow \qquad \hat O = Z_{O_\Gamma} O_\Gamma$$

$\star$ because $Z^{u,d}_{q,O}$'s $\Leftrightarrow$ O(4)–scalar form factors of amputated correlators

$\star$ average $\frac{1}{2}(Z^{u,d}_{q,O} + Z^{d,u}_{q,O})$: statistics increased, O(a) improvement obvious

Chiral SSB and Wilson–term induced artifacts

In tm-LQCD Wilson term breaks $SU(2) \times SU(2)$ symmetry (action in $(\chi, \bar\chi)$–basis)

$$L_{tm}^{N_f=2} = L_{\rm YM} + \bar\chi [\gamma \cdot \widetilde\nabla + W + + m_0 + i\mu\gamma_5\tau^3] \chi$$

$O(a\Lambda^2_{\rm QCD})$ breaking: analogous to mass terms $\propto m, \mu$, but with non-trivial gauge-field dependence. In the presence of SχSB in order to get reliable results for $m_{\rm PS} \lesssim 400$ MeV (typically @ $a \lesssim 0.01$ fm) need

- to tune m_0 (to $M_{\rm cr}^{\rm opt}$) so that the impact of the term $\bar\chi(W + M_{\rm cr}^{\rm opt})\chi$ on the chiral polarization of the vacuum is minimized (see "optimal critical mass");
- to work where χ–breaking $O(a^2)$ terms in Symanzik's LEL are small enough that the term $\mu\bar\chi i\gamma_5\tau^3\chi \rightarrow \mu\bar\psi\psi$ effectively determines the chiral phase of the vacuum (away from peculiar lattice phase structure: Aoki; Singleton–Sharpe) ;
- to check that this happens without large statistical fluctuations driven by the (subtracted) Wilson term (fluctuations suppressed by increasing L and $1/a$)

Once this is done, $O(a^2)$ errors on physical observables are in general small, with the π^0–mass being a remarkable (understood) exception.

Optimal critical mass

Many legitimate non-perturbative estimates of $M_{\rm cr}$ can be obtained for a given LQCD formulation with Wilson–like fermions: differences are $O(a\Lambda^2_{\rm QCD})$

Analysis à la Symanzik of Mtm-LQCD correlators with m_0 set to a generic estimate of $M_{\rm cr}$ shows chirally enhanched cutoff effects of the form:

$(\xi_\pi/m_\pi^2)^2,\ a\xi_\pi/m_\pi^2, \ldots \qquad \xi_pi \equiv \langle\Omega|(\,a\,\mathcal{L}_5^{\rm Mtm} + a^3\,\mathcal{L}_5^{\rm Mtm} + \ldots)|\pi^0(\vec{0})\rangle|^{\rm cont}_\mu = O(a)$

The determination of the critical mass discussed above, i.e. in the phys. quark basis of Mtm-LQCD

$$a^3 \sum_{\vec{x}} \partial_\lambda \langle V_\lambda^{2,1}(x) P^{1,2}(0)\rangle|^L_{M_{\rm cr},\mu} = 0 \qquad \text{(at } x_0 \text{ s.t. charged pion dominates)}\ ,$$

reduces the (leading) chirally enhanced $O(a^2)$ terms to “regular” $O(a^2)$ since $\xi_\pi = O(a\mu\Lambda^3_{\rm QCD}) \qquad \Rightarrow \xi_\pi/m_\pi^2 = O(a\Lambda^2_{\rm QCD})$.

Among the residual cutoff effects in correlators the leading ones (close to the chiral limit) are of (relative) order $a^2\Lambda^4_{\rm QCD}/m_\pi^2$. Strong lattice artifacts avoided if $\mu > \rho a^2 \Lambda^3_{\rm QCD}$ (ρ from simulations) (R.F.–Martinelli–Papinutto–Rossi '05; Sharpe '05)

Mtm flavour pair with non-degenerate masses

$N_f = 1 + 1$ flavours ($\psi = (s, c)^t$) with $\omega = \pi/2$ & $\gamma_5\tau_1$–twist (R.F.–Rossi, '03)

$$L_{\rm Mtm}^{N_f=1+1} = \bar{\psi}[\gamma\cdot\widetilde{\nabla} - i\gamma_5\tau_1(W + M_{\rm cr}) + \mu - \epsilon\tau_3]\psi$$

- fermionic determinant: real and positive for $|\epsilon| \neq |\mu|$

zero modes of Dirac matrix only if $|\epsilon| = |\mu|$ as only then ${\rm Re}(\lambda) = 0$ possible

sketch of the proof for the case $|\epsilon| < |\mu|$:

$${\rm det}[Q_{\rm cr}^2 + \mu^2 - \epsilon^2]\ {\rm det}[1 + 2\epsilon B] \ \geq\ {\rm det}[Q_{\rm cr}^2 + \mu^2 - \epsilon^2]$$

$$Q_{\rm cr} \equiv \gamma_5[\gamma\cdot\widetilde{\nabla} + W + M_{\rm cr}] = Q_{\rm cr}^\dagger \qquad B = (Q_{\rm cr}^2 + \mu^2 - \epsilon^2)^{-1/2}\ \gamma\cdot\widetilde{\nabla}\ (Q_{\rm cr}^2 + \mu^2 - \epsilon^2)^{-1/2} = -B^\dagger$$

analogous proof also for the case $|\epsilon| > |\mu|$ (new!)

- renormalized quark masses: $\hat{m}^{\pm} = Z_P^{-1}\mu \pm Z_S^{-1}\epsilon$

only restriction on $\hat{m}^{\pm}$: avoid values (close to) $(Z_P^{-1} \pm Z_S^{-1})\ \mu$; immaterial for s, c.

- automatic O(a) improvement $\Leftarrow$ $P \times \mathcal{D}_d \times (\mu \to -\mu) \times (\epsilon \to -\epsilon)$

Mtm flavour non–degenerate pair: some remarks

- due to $\gamma_5\tau^1$–twist the oblique SU(2) group is here generated by the charges associated to the currents $V_\mu^1, A_\mu^2, A_\mu^3$
  with V_μ^1 softly broken by $-\epsilon\bar{\psi}\tau^3\psi$ and A_μ^2, A_μ^3 softly broken by $\mu\bar{\psi}\psi$
- due to $\gamma_5\tau^1$–twist the propagator of the flavour pair is not flavour diagonal: O(a) parity–odd "mixing" of flavours in the propagator $\Rightarrow$ O(a^2) artifacts in physical quantities & need of disentangling strange and charmed states in data analysis (feasible...)
- if the flavour pair is $(s\,,\,c)$ with $\hat{m}_c = \hat{m}^+ \sim 0.5 \div 0.25a^{-1}$ the "mixing" of flavours in the pair propagator gives potentially significant O(a^2) pollution even in non-charmed observables with strangeness $\Rightarrow$ whether use of the flavour pair for valence is convenient needs be checked...
- flavour pair $(s\,,\,c)$ was proposed as sea quark pair; valence s and c can be introduced as flavour–diagonal OS quarks
- no (known) way of introducing three maximally twisted sea flavours with real quark determinant and automatic O(a) improvement

Mixed action approach: general setup

Local renormalizable model with 4 sea and N_v valence quarks (R.F. – Rossi '04)

$$L^{4sNv}_{\rm Mtm} = L_{\rm YM} + L^{2s}_{\rm Mtm}[\psi_\ell] + L^{2s}_{\rm Mtm}[\psi_h] + + \sum_{f=1}^{N_v} L^f_{OS}[q_f;\phi_f]$$

$$L^f_{OS} = \bar{q}_f[\gamma\cdot\widetilde{\nabla} - i\gamma_5[W + M_{\rm cr}](r_f) + m_f]q_f + \phi^\dagger \frac{m_f}{|m_f|}[\gamma\cdot\widetilde{\nabla} - i\gamma_5[W + M_{\rm cr}](r_f) + m_f]\phi_f$$

- observables involve only gluons and valence quarks $\{q_f\ ,\ {\rm all}\ f's\}$ with suitably chosen r_f's (the unitary setup is included as a particular case)
- ϕ_f is a spin–1/2 bosonic ghost: it cancels the contribution of q_f to the matter determinant in a local way $\Rightarrow$ no θ–term generated via radiative corrections (Morel '87; Sharpe & Shoresh '01)
- (valence) flavour is exactly conserved, parity is broken at O(a)
- automatic O(a) improvement from invariance of the lattice model under (generalized) $P \times \mathcal{D}_d \times (M \to -M)$ (M including m_ℓ, $m_h^\pm$, m_f's)

Mixed action approach: applications

Mixed action (Mtm sea pairs & several OS valence flavours) approach:

- allows to obtain lattice QCD correlators in the continuum limit without cutoff effects linear in a
- is very flexible, i.e. allows to adapt the regularization of the valence quark operators of interest so as to avoid lattice–peculiar mixings under renormalization: play with replica of the same valence flavour $(f, f', f'' \ldots)$ with suitable values of $(r_f, r'_f, r''_f \ldots)$
- examples: method to evaluate B_K, amplitudes $K \to \pi\pi$ and $K \to \pi$ with no lattice–peculiar operator mixings (R.F. – Rossi '04)
- observable–dependent (case by case) method, but computationally cheap

Example 1: K^0–$\overline{K}^0$ mixing and B_K

QCD with $N_f = 4$ (qcd4): B_K is extracted from (FT's of)

$$C^{(\mathrm{qcd4})}_{K\mathcal{O}K} = \langle (\bar{d}\gamma_5 s)(x)[(\bar{s}\gamma_\mu d)^2 + (\bar{s}\gamma_\mu\gamma_5 d)^2](0)\bar{d}\gamma_5 s)(y)\rangle^{(\mathrm{qcd4})}$$

4s6v model: different regularizations for sea and valence quarks

- sea quarks $(u_{\mathrm{sea}}, d_{\mathrm{sea}})$, $(s_{\mathrm{sea}}, c_{\mathrm{sea}})$ in pairs (FR action)
- valence species u, d, d', s, s', c with OS action
- B_K can be extracted from the 4s6v–model correlator

$$C^{(\mathrm{4s6v})}_{K'\mathcal{Q}K} = \langle (\bar{d}'\gamma_5 s')(x) 2\mathcal{Q}^{\Delta S=2}_{VV+AA}(0)(\bar{d}\gamma_5 s)(y)\rangle^{(\mathrm{4s6v})}$$

$$\mathcal{Q} = (\bar{s}\gamma_\mu d)(\bar{s}'\gamma_\mu d') + (\bar{s}\gamma_\mu\gamma_5 d)(\bar{s}'\gamma_\mu\gamma_5 d') + (\bar{s}\gamma_\mu d')(\bar{s}'\gamma_\mu d) + (\bar{s}\gamma_\mu\gamma_5 d')(\bar{s}'\gamma_\mu\gamma_5 d)$$

- $\underline{r_d = \pm r_{d'} = r_s = \mp r_{s'}} \;\Rightarrow\; \mathcal{Q}^{\Delta S=2}_{VV+AA}$ has no mixings
- $a \to 0$ @ $\hat{m}_d = \hat{m}_{d'} = \hat{m}_{d_{\mathrm{sea}}}$, $\hat{m}_s = \hat{m}_{s'} = \hat{m}_{s_{\mathrm{sea}}}$
- $\lim_{a\to 0}[C^{(\mathrm{4s6v})}_{K'\mathcal{Q}K}]_R \overset{\mathrm{Wick\_thm}}{=} \lim_{a\to 0}[C^{(\mathrm{qcd4})}_{K\mathcal{O}K}]_R$, if $\hat{m}^{(\mathrm{4s6v})}_f = \hat{m}^{(\mathrm{qcd4})}_f$, $f = u, d, s, c$

Extended to B^{stat}_B: use valence d, d' (relativistic) and h^+ (static) (Della Morte '04)

Example 2: $K \to \pi\pi$ decay

Strategy analogous to that for B_K, but based on an auxiliary 4s10v model with

- valence OS flavours $u, u', u'', u''', d, s, c, c', c'', c'''$
- two sea pairs $(u_{\rm sea}, d_{\rm sea}), (s_{\rm sea}, c_{\rm sea})$ (FR action)
- same renormalized mass for all quarks of a given physical flavour

1. $K \to \pi\pi$ amplitudes can be extracted from

$$C^{(4s10v)}_{\pm,\pi\pi} = \langle \Phi_\pi(x)\Phi_\pi(y)\mathcal{Q}^{\pm}_{VA+AV}(0)\Phi_{K^0}(y)\rangle^{(4s10v)}$$

$\Phi_{\pi^\pm}$, Φ_{π^0}, Φ_{K^0} with only valence u, d, s quarks

$$\mathcal{Q}^{\pm}_{VA+AV} = \mathcal{Q}^{\pm\,(u,c)}_{VA+AV} + \mathcal{Q}^{\pm\,(u',c')}_{VA+AV} - \frac{1}{2}\mathcal{Q}^{\pm\,(u'',c'')}_{VA+AV} - \frac{1}{2}\mathcal{Q}^{\pm\,(u''',c''')}_{VA+AV}$$

i) $\underline{r_d = r_s}$, $r_d = r_u$ ii) $\underline{r_u = r_c = r_{u''} = r_{c''} = -r_{u'} = -r_{c'} = -r_{u'''} = -r_{c'''}}$

$\Rightarrow$ $\mathcal{Q}^{\pm}_{VA+AV}$ mixes only with $(m_c^2 - m_u^2)(m_s - m_d)\,(\bar{s}\gamma_5 d)$

2. $K \to \pi$ amplitudes from matrix elements of

$$\mathcal{Q}^{\pm}_{VV+AA} = \mathcal{Q}^{\pm\,(u,c)}_{VV+AA} + \mathcal{Q}^{\pm\,(u',c')}_{VV+AA} - \frac{1}{2}\mathcal{Q}^{\pm\,(u'',c'')}_{VV+AA} - \frac{1}{2}\mathcal{Q}^{\pm\,(u''',c''')}_{VV+AA}$$

with i) $\underline{r_d = -r_s}$, $r_d = r_u$ and ii).

Our implementation of maximal twist

Thanks to G. Herdoiza for this collection of recent results by ETMC:

this presentation ⇔ his talk @ Benasque workshop '07 + updates

- Fix the value of $m_0 = M_{\rm cr}$ at the smallest $\mu \equiv \mu_{\rm min}$ by imposing

$$a m_{\rm PCAC}(t \gg (\text{PS meson energy gap})^{-1}; L \gg \frac{1}{m_{\rm PS}}; \mu_{\rm min}) = 0$$

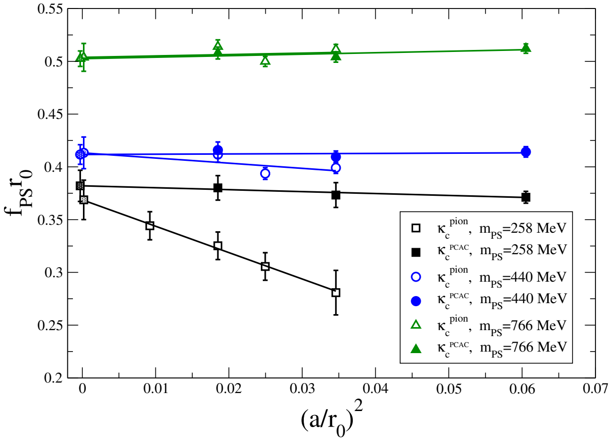
within statistical errors or up to numerical errors $\ll a^2 \Lambda_{\rm QCD} \mu_{\rm min}$

- $\mu_{\rm min}$ is the smallest μ–value of interest where:
  - simulations are stable for all lattice spacings
  - chirally enhanced terms are suppressed

$$\Rightarrow \quad \mu_{\rm min} > a^2 \Lambda^3_{\rm QCD}$$

- $\mathrm{O}(a)$ improvement is not harmed: determining $M_{\rm cr}$ at $\mu = \mu_{\rm min}$ (rather than in the limit $\mu \to 0$) merely induces $\mathrm{O}(a \mu_{\rm min} \Lambda_{\rm QCD})$ corrections in $M_{\rm cr}$, hence $\mathrm{O}(a^2 \mu_{\rm min} \Lambda_{\rm QCD})$ relative corrections in physical quantities

tmLQCD: scaling in quenched approximation



(K. Jansen, M. Papinutto, A. Shindler, C. Urbach, I. Wetzorke, 2005)

Choice of the gauge action

- Wilson-type fermions (plain and twisted) have a non-trivial phase structure at finite lattice spacing (Aoki; Sharpe, Singleton)
- The strength of the phase transition depends on details of the action
  - gluonic: b_1
  - fermionic: c_{sw}
- tree-level Symanzik improved (tlSym) gauge action

$$S_g = \frac{\beta}{3} \sum_x \Big[(1 - 8b_1) \sum_{\mu<\nu}^{4} \Big(1 - \mathrm{ReTr}\left(U^{1\times 1}_{x,\mu,\nu}\right)\Big) + b_1 \sum_{\mu\neq\nu}^{4} \Big(1 - \mathrm{ReTr}\left(U^{1\times 2}_{x,\mu,\nu}\right)\Big) \Big]$$

with $b_1 = -1/12$

- tlSym:
  - weakens the first order phase transitions compared to Wilson gauge action ($b_1 = 0$)
  - better scaling than DBW2 ($b_1 = -1.4088$)

(Farchioni *et.* al., 2004-2005)

- Consequence of first order phase transitions:
  - For a given a, simulation is safe if $\mu > \mu_{\mathrm{end-point}} \sim a^2 \Lambda^3_{\mathrm{QCD}}$
  - For a given value of m_{PS} one can find a lattice spacing $a_{\max}$ such that simulations at $a < a_{\max}$ can be safely performed

Algorithm: speeding-up the HMC Wilson fermions

- Variant of the HMC algorithm
  (C. Urbach, K. Jansen, A. Shindler, U. Wenger, 2005)
  - even/odd preconditioning
  - mass preconditioning (Hasenbusch, 2001)
  - multiple time scale integration
- Other variants: all of them are efficient to reach small quark masses
  - domain decomposition (Lüscher, 2003-2004)
  - RHMC (Clark, Kennedy, 2003)
  - QCDSF collab. (2003)
- Wilson fermions are back in the game

Simulations: plan

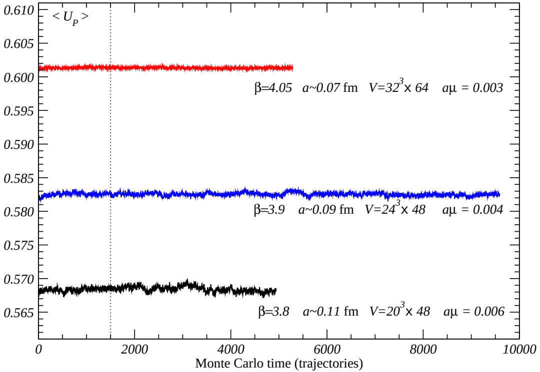
- fermion: $N_{\mathrm{f}} = 2$ maximally twisted mass QCD
- gauge: tlSym
- three lattice spacings: $0.075 - 0.115$ fm
- $270 \lesssim m_{\mathrm{PS}} \lesssim 550$ MeV
- $L > 2$ fm

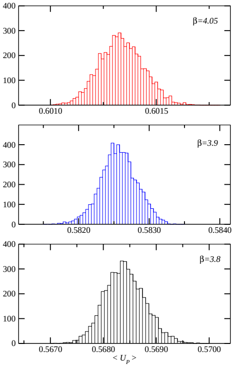
Simulations at three lattice spacings

β	target a (fm)	$L^3 \cdot T$	κ_{crit}	$a\mu$	$N_{traj}\|_{\tau=0.5}$ i	target m_{PS} (MeV)
4.05	$\sim$ 0.07	$32^3 \cdot 64$	0.15701	0.0030	5000	$\sim$ 270
				0.0060	5000	$\sim$ 380
				0.0080	5000	$\sim$ 430
				0.0120	5000	$\sim$ 530
		$24^3 \cdot 48$		0.0060	5000	$\sim$ 380
		$20^3 \cdot 48$		0.0060	5000	$\sim$ 380
3.9	$\sim$ 0.09	$24^3 \cdot 48$	0.160856	0.0040	9400	$\sim$ 300
				0.0064	5000	$\sim$ 380
				0.0085	5000	$\sim$ 440
				0.0100	5000	$\sim$ 480
				0.0150	5000	$\sim$ 580
		$32^3 \cdot 64$		0.0040	5000	$\sim$ 300
3.8	$\sim$ 0.11	$20^3 \cdot 48$	0.164111	0.0060	6000	$\sim$ 320
				0.0080	5000	$\sim$ 380
				0.0110	5000	$\sim$ 430
				0.0165	5000	$\sim$ 530

Evaluation of correlators (phys. observables): advanced @ $\beta = 3.9$; only basic ones done @ $\beta = 4.05$; just started @ $\beta = 3.8$

Monte Carlo histories of plaquette

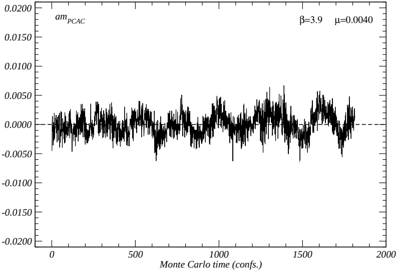


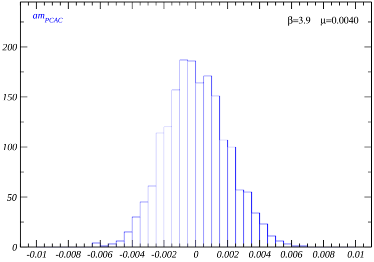


Autocorrelations $\beta = 3.9$

- plaquette : $\tau_{\rm int}(P) \in [10 - 55]$ (in units of $\tau = 0.5$)
- $f_{\rm PS}$: $\tau_{\rm int}(af_{\rm PS}) \in [4 - 7]$
- configurations saved every 2 trajectories
- ILDG

Monte Carlo history of $m_{\rm PCAC}$ $\beta = 3.9$

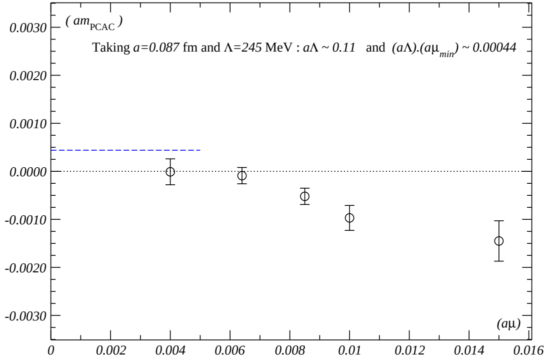




- $V = 24^3 \cdot 48, \;\; \beta = 3.9, \;\; a\mu = a\mu_{\rm min} = 0.004$

$$am_{\rm PCAC}(a\mu = a\mu_{\rm min}) = 0 \pm \mathcal{O}((a\mu_{\rm min})(a\Lambda_{\rm QCD}))$$

$am_{\rm PCAC}$ vs. $a\mu$ $\beta = 3.9$

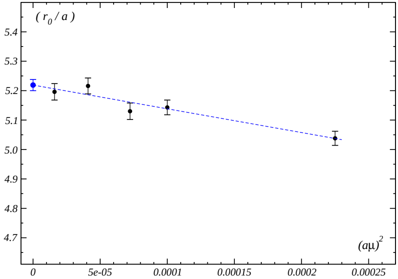


- $am_{\rm PCAC}(a\mu_{\rm min}) = -0.00001(27)$
- for all μ values: $am_{\rm PCAC} \lesssim (a\mu)(a\Lambda_{\rm QCD})$
- The weak μ-dependence of $m_{\rm PCAC}$ is an $\mathcal{O}(a)$ effect

$\rightsquigarrow$ $\mathcal{O}(a^2)$ artifacts in physical quantities

Determination of r_0/a: data vs. $a^2\mu^2$ $\beta = 3.9$

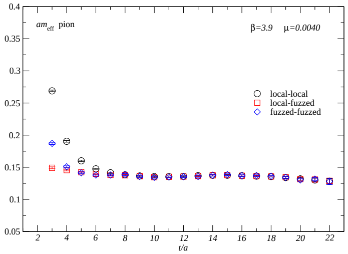
- Sommer parameter r_0: static inter-quark force

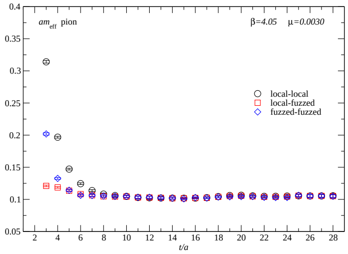


- dependence on μ^2
- good accuracy: $r_0/a = 5.22(2)$
- very useful to check scaling; in the end not used to set the scale

Pion sector: correlators and effective masses

- quark propagator: stochastic sources to include all spatial sources
- Change the location of the time-slice source: reduce autocorrelations
- Fuzzing





- stable masses $\rightsquigarrow$ isolate ground state from excited states
- small statistical errors

Pion: decay constant and χPT fits

Pseudo-scalar decay constant:

$$f_{\rm PS} = \frac{2\mu}{m_{\rm PS}^2} |\langle 0|P^1(0)|\pi\rangle|$$

- obtained from exact lattice Ward identity for maximally twisted mass fermions
- no need of renormalization factors : $Z_{\rm P} = 1/Z_\mu$

Can chiral perturbation theory (χPT) reproduce the data? $\beta = 3.9$

- we use continuum χPT to describe the dependence on:
  - finite spatial size L
  - the mass μ
- Simultaneous fit to $N_{\rm f} = 2$ χPT at NLO

(Gasser, Leutwyler, 1987; Colangelo *et* al., 2005)

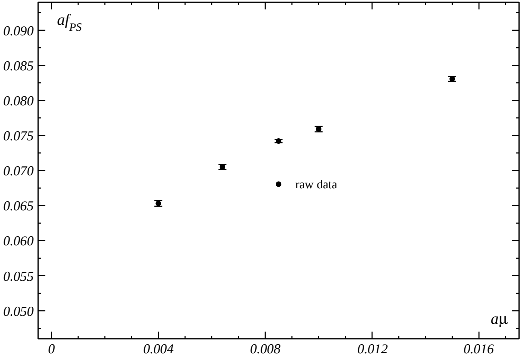
$$m_{\rm PS}^2(L) = 2B_0\mu \left[1 + \frac{1}{2}\xi\tilde{g}_1(\lambda)\right]^2 \left[1 + \xi\log(2B_0\mu/\Lambda_3^2)\right] ,$$

$$f_{\rm PS}(L) = F\,[1 - \xi\tilde{g}_1(\lambda)] \left[1 - 2\xi\log(2B_0\mu/\Lambda_4^2)\right]$$

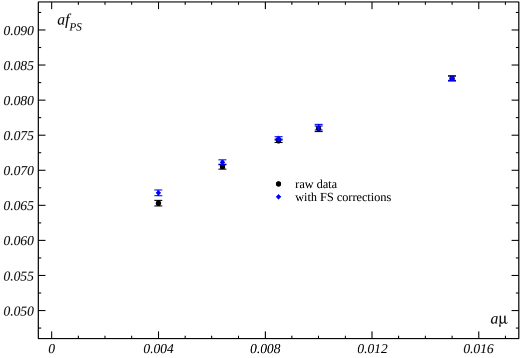
where $\xi = 2B_0\mu/(4\pi F)^2$, $\lambda = \sqrt{2B_0\mu L^2}$, $\tilde{g}_1(\lambda)$ is a known function

- fit parameters: B_0, F, Λ_3 and Λ_4
- extract low-energy constants: $\bar{l}_{3,4} \equiv \log(\Lambda_{3,4}^2/m_\pi^2)$

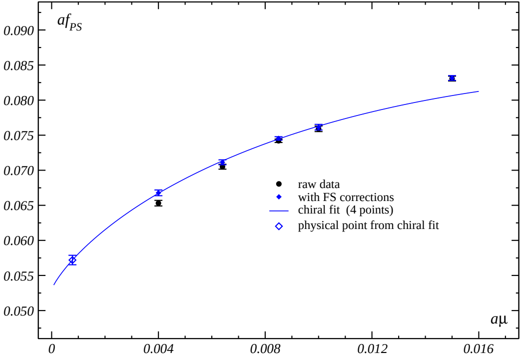
Pion sector: af_{PS} vs. $a\mu$ $\beta = 3.9$



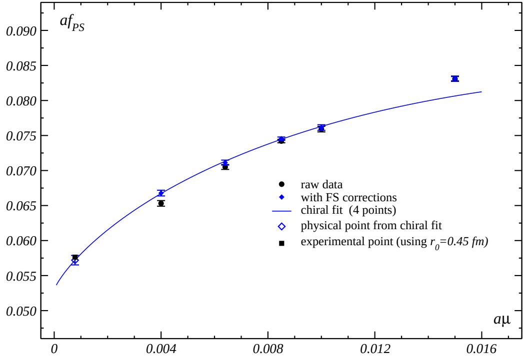
Pion sector: af_{PS} vs. $a\mu$ $\beta = 3.9$



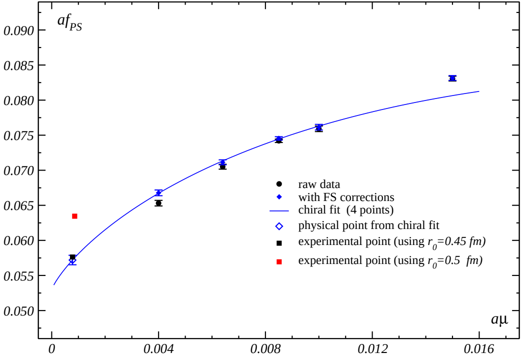
Pion sector: af_{PS} vs. $a\mu$ $\beta = 3.9$



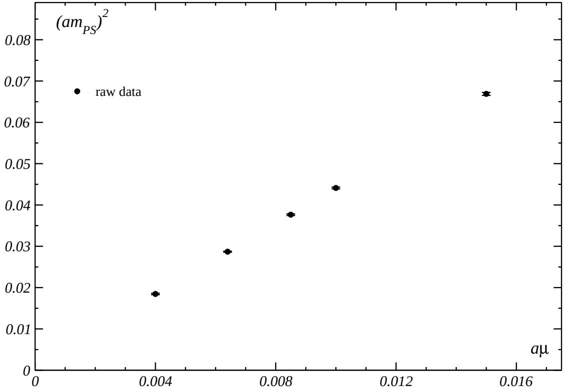
Pion sector: af_{PS} vs. $a\mu$ $\beta = 3.9$



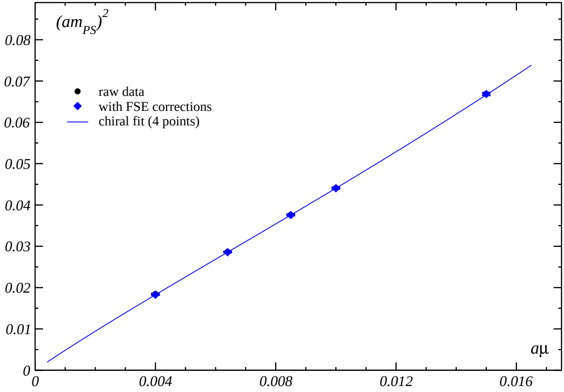
Pion sector: af_{PS} vs. $a\mu$ $\beta = 3.9$



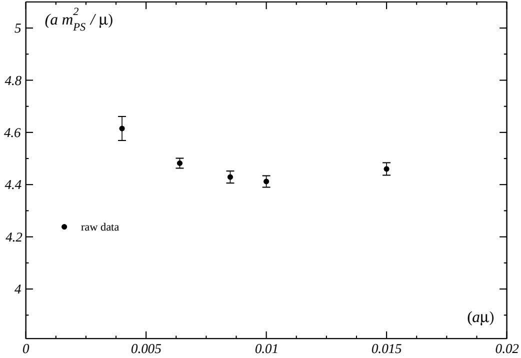
Pion sector: $(am_{PS})^2$ vs. $a\mu$ $\beta = 3.9$



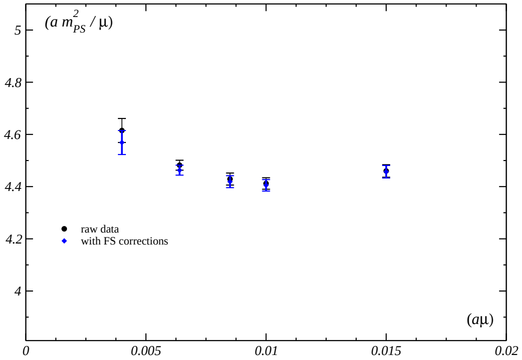
Pion sector: (am_{PS}^2) vs. $a\mu$ $\beta = 3.9$



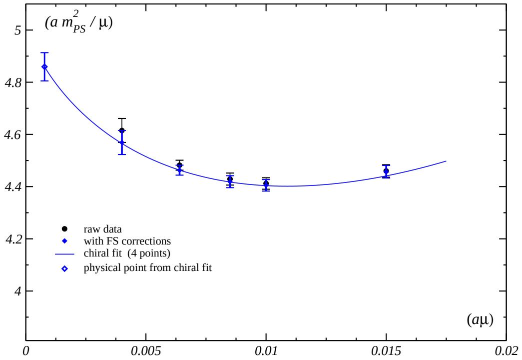
Pion sector: m_{PS}^2/μ vs. μ $\beta = 3.9$



Pion sector: m_{PS}^2/μ vs. μ $\beta = 3.9$



Pion sector: m_{PS}^2/μ vs. μ $\beta = 3.9$



Pion: results from χPT fits

$$m^2_{\rm PS}(L) = 2B_0\mu \left[1 + \frac{1}{2}\xi\tilde{g}_1(\lambda)\right]^2 \left[1 + \xi \log(2B_0\mu/\Lambda_3^2)\right]$$

$$f_{\rm PS}(L) = F\,[1 - \xi\tilde{g}_1(\lambda)]\,\left[1 - 2\xi \log(2B_0\mu/\Lambda_4^2)\right]$$

where $\xi = 2B_0\mu/(4\pi F)^2\,, \qquad \lambda = \sqrt{2B_0\mu L^2}$

$$2aB_0 = 4.99(6)$$
$$aF = 0.0534(6)$$
$$\log(a^2\Lambda_3^2) = -1.93(10)$$
$$\log(a^2\Lambda_4^2) = -1.06(4)$$
$$\chi^2/dof = 3.5/4 \sim 0.9$$

- The "physical point" $a\mu_\pi$ is determined by requiring $m_{\rm PS}/f_{\rm PS} = 139.6/130.7 = 1.068$ $\leadsto$ we get: $a\mu_\pi = 0.00078(2)$
- Taking $f_\pi = 130.7$ MeV, we obtain $a = 0.087(1)$ fm
- Using $r_0/a = 5.22(2)$ we get: $r_0 = 0.454(7)$ fm
- We determine : $\bar{l}_{3,4} \equiv \log(\Lambda^2_{3,4}/m^2_\pi)$

Pion: low-energy constants $\beta = 3.9$

Accurate determinations of $\bar{l}_{3,4} \equiv \log(\Lambda^2_{3,4}/m^2_\pi)$

$$\bar{l}_3 = 3.65 \pm 0.12$$

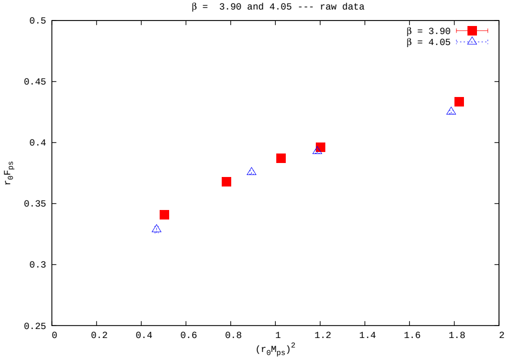
$$\bar{l}_4 = 4.52 \pm 0.06$$

Other estimates (Leutwyler, hep-ph/0612112)

- $\bar{l}_3$:
  - $\bar{l}_3 = 2.9 \pm 2.4$ from the mass spectrum of the pseudoscalar octet
  - $\bar{l}_3 = 0.8 \pm 2.3$ from MILC
  - $\bar{l}_3 = 3.0 \pm 0.6$ from lattice CERN group
- $\bar{l}_4$:
  - $\bar{l}_4 = 4.3 \pm 0.9$ from f_K/f_π
  - $\bar{l}_4 = 4.4 \pm 0.2$ from the radius of the scalar pion form factor
  - $\bar{l}_4 = 4.0 \pm 0.6$ from MILC

$f_{PS} r_0$ vs $m_{PS}^2 r_0^2$: raw data at $a \simeq (0.087 \ \& \ 0.067)$ fm

check scaling of f_{PS} vs m_{PS}^2 in units of r_0 (PRELIMINARY)

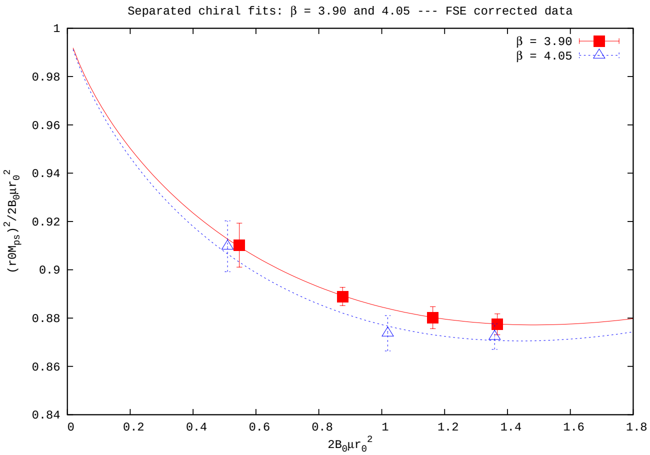


use $r_0/a|_{\beta=3.9} = 5.22$ and $r_0/a|_{\beta=4.05} = 6.60$ (PRELIMINARY)

statistical errors on r_0 not shown here and in the following...

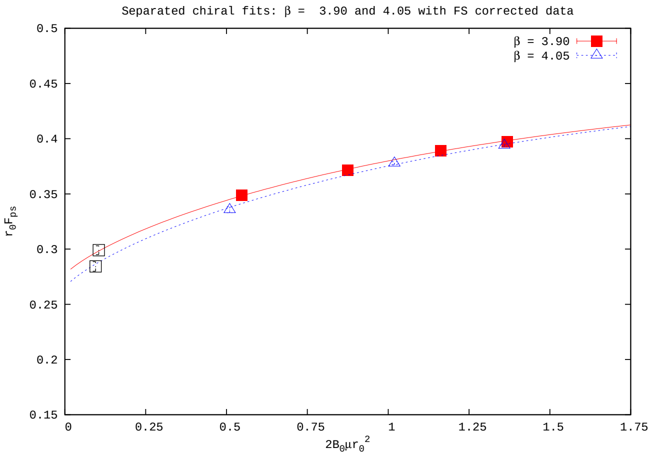
they are $\sim 0.4\%$ at $\beta = 3.9$, still $\sim 1\%$ at $\beta = 4.05$

$m_{\rm PS}^2/2B_0\mu$ vs $2B_0\mu r_0^2$: one chiral fit for each β



Recall: simultaneous fit of data for both $m_{\rm PS}$ and $f_{\rm PS}$ (at each β)

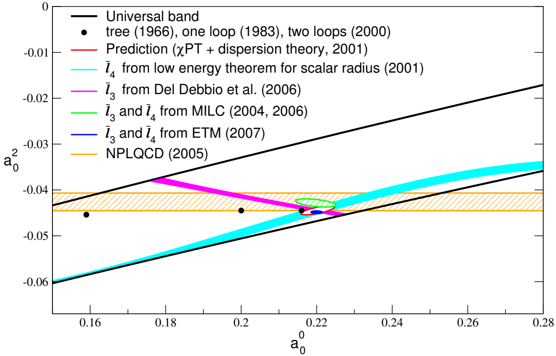
$f_{\rm PS} r_0$ vs $2B_0\mu r_0^2$: one chiral fit for each β



Recall: simultaneous fit of data for both $m_{\rm PS}$ and $f_{\rm PS}$ (at each β)

$\pi\pi$ scattering $\beta = 3.9$

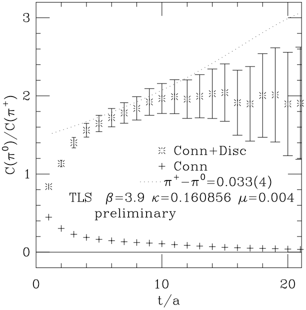
S-wave scattering lengths a_0^0 and a_0^2 (Leutwyler, 2007)

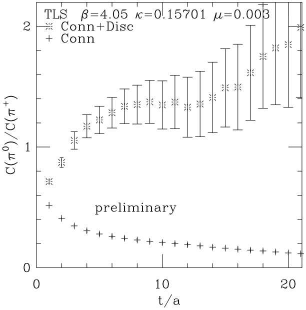


- radius of the scalar pion form factor :
  - This work: $\langle r^2 \rangle = 0.637 \pm 0.026\ \mathrm{fm}^2$ (statistical)
  - Colangelo *et. al*, 2001 : $\langle r^2 \rangle = 0.61 \pm 0.04\ \mathrm{fm}^2$

Large O(a^2) in the π^0–mass $\beta = 3.9$ and 4.05

in part PRELIMINARY: thanks to C. Michael and C. Urbach



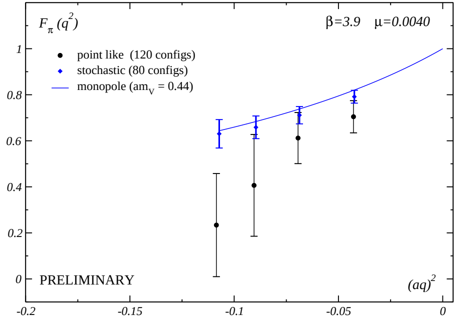


- @ $\beta = 3.9, L/a = 24$: $am_{\rm PS}^{\pm} = 0.136(1)$ and $am_{\rm PS}^{0} = 0.111(11)$ (hep-lat/0701012)
- $r_0^2((m_{\rm PS}^0)^2 - (m_{\rm PS}^{\pm})^2) = c(a/r_0)^2$ with $c = -4.5(1.8)$; estimate $a\mu_{\rm end} \sim 0.0013$

  coeff. c two times smaller than in quenched and with opposite sign
- @ $\beta = 4.05$: π^0–mass closer to $\pi^{\pm}$–mass (as expected)
- for the vector meson the mass splitting compatible with zero

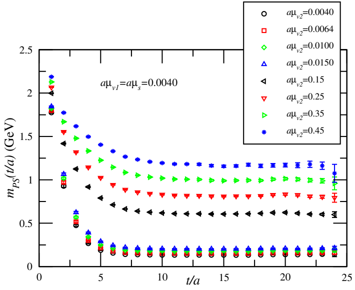
Pion form factor $\beta = 3.9$

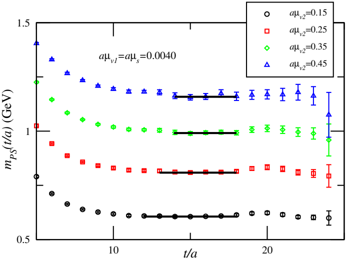
PRELIMINARY: thanks to S. Simula

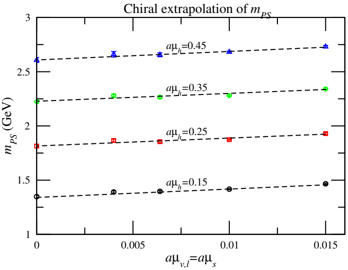


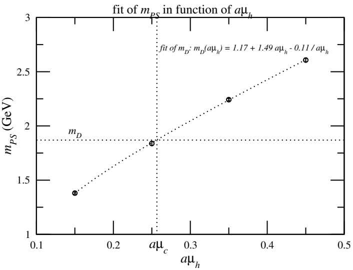
- As an example: $\beta = 3.9$ $a\mu = 0.004$ $m_{\rm PS} \sim 300$ MeV
- Improvement: stochastic propagators with θ boundary conditions
- More values of $m_{\rm PS}$ and q^2 with larger statistics in progress; more a's later...

Charm sector (PRELIMINARY)









Renormalization & quark masses ($\beta = 3.9$ only)

VERY PRELIMINARY; O(a^2) errors and finite size effects not yet under full control

- renormalization constants of bilinear quark operators: RI-MOM
- preliminary estimates of quark masses:

$$m_{u,d}[\overline{\rm MS}, 2\ {\rm GeV}] = 4.24\ (07)\ [37]\ [??]\ {\rm MeV}$$

$$m_s[\overline{\rm MS}, 2\ {\rm GeV}] = 111\ (2)\ [8]\ [??]\ {\rm MeV}$$

$$m_c[\overline{\rm MS}, 2\ {\rm GeV}] = 1.30\ (02)\ [05]\ [??]\ {\rm GeV}$$

- Strange sector: $m_s/m_{ud} \sim 25.3\ (0.2)\ [0.7]\ [??]$,

  $f_K \sim 159.6\ (0.5)\ [2.1]\ [??]\ {\rm MeV}$ $\qquad$ $f_K/f_\pi \sim 1.221\ (004)\ [016]\ [??]$

- Charm sector (stat. uncertainty still about few percents plus (??)):

  $f_D \sim 214\ {\rm MeV}$ $(\sim 220$ exp.) $\qquad$ $m_{D_s}/m_D \sim 1.07$ $(\sim 1.054$ exp.)

from PQ analyses: thanks to B. Blossier, V. Lubicz and C. Tarantino

Numerical results: conclusions

Summary:

- maximally twisted mass QCD has been successfully employed for large scale simulations with two light sea quarks
- for $a \lesssim 0.1$ fm simulations are stable down to $m_{\rm PS} \sim 300$ MeV (at least)
- small statistical errors $\Rightarrow$ precise results for hadron spectrum, LEC's, weak matrix elements... provided
- systematic errors are fully checked: $O(a^2)$ and finite volume effects ?
- good scaling for π mass and decay constant at $\beta = 3.9$ & 4.05 (prelim.)

Perspectives:

- contact with phenomenology
- mixed action (sea: tmQCD; valence: overlap or OS quarks) : $B_K, K \to (\pi)\pi$: $\mathcal{O}(a)$ improved without mixing
- $N_{\rm f} = 2 + 1 + 1$ simulations feasible and planned (setup definition started)