

# Remarks on $N_f = 2 + 1 + 1$ LQCD at maximal twist

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# Action for 2+1+1 MtmLQCD

$$S^{\text{latt}} = S_{\text{YM}} + \alpha^4 \sum_x [L_{\text{Mtm}}^\ell + L_{\text{Mtm}}^h]$$

with  $S_{\text{YM}}$  a suitable (chosen: Iwasaki) gluonic action and

a)  $N_f = 2$  light degenerate flavours ( $\psi_\ell = (u, d)^t$ ) with  $\gamma_5\tau^3$ -twist

$$L_{\text{Mtm}}^\ell = \bar{\psi}_\ell [\gamma \cdot \tilde{\nabla} - i\gamma_5\tau^3(W + m_0) + \mu_\ell] \psi_\ell, \quad W \equiv -r(a/2)\nabla^* \cdot \nabla$$

b)  $N_f = 1 + 1$  flavours ( $\psi_h = (c, s)^t$ ) with  $\gamma_5\tau^1$ -twist

$$L_{\text{Mtm}}^h = \bar{\psi}_h [\gamma \cdot \tilde{\nabla} - i\gamma_5\tau^1(W + m_0) + \mu_h + \epsilon_h\tau^3] \psi_h$$

Mass parameter renormalization:

$m_0 = M_{\text{cr}}$  for max. twist -  $\mathcal{O}(a)$  part of  $m_0$  tunable to reduce  $\mathcal{O}(a^2)$  artifacts

$$\hat{m}_{ud} = Z_P^{-1} \mu_\ell$$

$$\hat{m}_s = Z_P^{-1} (\mu_h - Z_P Z_S^{-1} \epsilon_h), \quad \hat{m}_c = Z_P^{-1} (\mu_h + Z_P Z_S^{-1} \epsilon_h)$$

Gauge links in  $L_{\text{Mtm}}^{\ell,h}$  can be replaced with stout ones without affecting symmetries and renormalization pattern...

# Symanzik LEL and optimal $M_{\text{cr}} - I$

Symanzik expansion of lattice operator vev's in terms of continuum ones

$$\langle O \rangle^{\text{MtmL}} = \langle O \rangle^{\text{cont}} - a \int d^4 y \langle O \mathcal{L}_5^{\text{Mtm}}(y) \rangle^{\text{cont}} + a \langle \Delta_1 O \rangle^{\text{cont}} + a^2 \langle \Delta_1 O \rangle^{\text{cont}} + \\ + \frac{a^2}{2} \int d^4 y d^4 z \langle O \mathcal{L}_5^{\text{Mtm}}(y) \mathcal{L}_5^{\text{Mtm}}(z) \rangle^{\text{cont}} - a^2 \int d^4 y \langle O \mathcal{L}_6^{\text{Mtm}}(y) \rangle^{\text{cont}} + \dots$$

with matched renorm. cond. on the two sides above and

$$\mathcal{L}_5^{\text{Mtm}} = \mathcal{L}_5^\ell + \mathcal{L}_5^h,$$

$$\mathcal{L}_5^\ell = \eta_{1\text{SW}} \bar{\psi}_\ell \sigma \cdot F \gamma_5 \tau^3 \psi_\ell + (\eta_{1a}^\ell \mu_\ell^2 + \eta_{1b}^\ell \mu_h^2 + \eta_{1c}^\ell \epsilon_h^2) \bar{\psi}_\ell i \gamma_5 \tau^3 \psi_\ell + \Lambda_{\text{QCD}}^2 \delta_1 \bar{\psi}_\ell i \gamma_5 \tau^3 \psi_\ell,$$

$$\mathcal{L}_5^h = \eta_{1\text{SW}} \bar{\psi}_h \sigma \cdot F \gamma_5 \tau^1 \psi_h + (\eta_{1a}^h \mu_\ell^2 + \eta_{1b}^h \mu_h^2 + \eta_{1c}^h \epsilon_h^2) \bar{\psi}_h i \gamma_5 \tau^1 \psi_h + \Lambda_{\text{QCD}}^2 \delta_1 \bar{\psi}_h i \gamma_5 \tau^1 \psi_h$$

The structure of  $\mathcal{L}_5^{\text{Mtm}}$  follows from (spurionic) symmetries (see JHEP 0410 (2004) 070)

$H(4)$ , charge conjugation,  $P \times \mathcal{D}_d \times (\mu_\ell \rightarrow -\mu_\ell) \times (\mu_h \rightarrow -\mu_h) \times (\epsilon_h \rightarrow -\epsilon_h)$

Vector $_{\pi/2}^{3\ell}$ , Axial $_{\pi/2}^{2\ell} \times (\mu_\ell \rightarrow -\mu_\ell)$ , Axial $_{\pi/2}^{1\ell} \times (\mu_\ell \rightarrow -\mu_\ell)$

Vector $_{\pi/2}^{1h} \times (\epsilon_h \rightarrow -\epsilon_h)$ , Axial $_{\pi/2}^{2h} \times (\mu_h \rightarrow -\mu_h)$ , Axial $_{\pi/2}^{3h} \times (\mu_h \rightarrow -\mu_h) \times (\epsilon_h \rightarrow -\epsilon_h)$

Terms containing  $\Lambda_{\text{QCD}}^2$  are needed to describe N.P.  $\mathcal{O}(a)$  artifacts in the determination of  $M_{\text{cr}}$   
(its value is part of the specification of  $\langle \rangle^{\text{MtmL}}$ )

# Symanzik LEL and optimal $M_{\text{cr}}$ – II

Generic estimate of  $M_{\text{cr}}$ : the Symanzik expansion of  $\langle O \rangle^{\text{MtmL}}$  contains powers of  $[\xi_\pi m_\pi^{-2} \Lambda_{\text{QCD}}^{-1}]_{\mu_\ell, (\mu_h, \epsilon_h)}$  with

$$\xi_\pi|_{\mu_\ell, (\mu_h, \epsilon_h)} \equiv \langle \Omega | a \mathcal{L}_5^{\text{Mtm}} | \pi \rangle_{\mu_\ell, (\mu_h, \epsilon_h)}^{\text{cont}} = \langle \Omega | a \mathcal{L}_5^\ell | \pi \rangle_{\mu_\ell, (\mu_h, \epsilon_h)}^{\text{cont}}$$

- last equality above follows from vector $^{2\ell, 1\ell}$ -invariance of continuum theory;
- $\mathcal{L}_5^\ell = \eta_{1\text{SW}} \bar{\psi}_\ell \sigma \cdot F \gamma_5 \tau^3 \psi_\ell + (\eta_{1a}^\ell \mu_\ell^2 + \eta_{1b}^\ell \mu_h^2 + \eta_{1c}^\ell \epsilon_h^2) \bar{\psi}_\ell i \gamma_5 \tau^3 \psi_\ell + \Lambda_{\text{QCD}}^2 \delta_1 \bar{\psi}_\ell i \gamma_5 \tau^3 \psi_\ell$

As in the  $N_f = 2$  theory (see Frezzotti-Martinelli-Papinutto-Rossi'05), also here

$$C_{VP}^{\ell\ell}(x_0) \equiv a^3 \sum_{\vec{x}} \langle V_0^{2\ell}(x) P^{1\ell}(0) \rangle^{\text{MtmL}} = 0 \quad \Rightarrow \quad \xi_\pi|_{\mu_\ell, (\mu_h, \epsilon_h)} = \mathcal{O}(a\mu_\ell) \Lambda_{\text{QCD}}^3 + \dots$$

Define the optimal critical mass  $m_0 = M_{\text{cr}}^{\text{opt}}[\mu_\ell, (\mu_h, \epsilon_h)]$  by

$$|m_{\text{PCAC}}| = |\partial_{x_0} C_{VP}^{\ell\ell}(x_0) / C_{PP}^{\ell\ell}(x_0)|_{m_0, \mu_\ell, (\mu_h, \epsilon_h)} = 0 \quad (\text{in practice } \ll \mu_\ell)$$

$M_{\text{cr}}^{\text{opt}}$  (in the sense of FMPR'05 – and also of  $\chi\text{PT}$ : Aoki-Bär'04 and Sharpe-Wu'04) depends significantly on  $(\mu_h, \epsilon_h)$  – however the mild  $\mu_\ell$ -dependence is treated

# $m_0$ -value for evaluation of $Z$ 's

For practical reasons: mass-independent renormalization schemes (RIMOM, SF)

$\Rightarrow$  must work at small  $\rightarrow$  zero mass parameters, e.g. with

$[\mu_\ell, (\mu_h, \epsilon_h)] = [\mu, (\mu, 0)] \rightarrow [0, (0, 0)]$  and  $m_0 \rightarrow M_{\text{cr}}$  (generic).

How to choose  $m_0$  if the  $Z$ 's "feel"  $\chi$ SSB-enhanced (e.g.  $\sim a/m_\pi^2$ ) cutoff effects?

A) work at  $[\mu, (\mu, 0)]$ ,  $\mu$  small and  $m_0 = M_{\text{cr}}^{\text{opt}}[\mu_\ell, (\mu_h, \epsilon_h)] \Rightarrow$

$$\xi_\pi|_{\mu, (\mu, 0)}^{m_0} = O(a\mu_h^2, a\epsilon_h^2)\Lambda_{\text{QCD}}^2 + O(a\mu_\ell)\Lambda_{\text{QCD}}^3 \gg O(a\mu)\Lambda_{\text{QCD}}^3$$

$m_0$  already known,  $m_{\text{PCAC}}|_{\mu, (\mu, 0)}^{m_0} \neq 0$ : any  $\chi$ SSB-enhanced cutoff effects in  $Z$ 's?

B) work at  $[\mu, (\mu, 0)]$ ,  $\mu$  small and  $m'_0 = M_{\text{cr}}^{\text{opt}}[\mu, (\mu, 0)] \Rightarrow$

$$\xi_\pi|_{\mu, (\mu, 0)}^{m_0} = O(a\mu)\Lambda_{\text{QCD}}^3 \quad \text{by construction,}$$

extra tuning to find  $m'_0$ :  $m_{\text{PCAC}}|_{\mu, (\mu, 0)}^{m'_0} \simeq 0$  ! Can show:  $m'_0 - m_0 \sim a$

Exploit suppression of  $\chi$ SSB-enhanced artifacts at small  $L$  (SF) or large  $q$  (RIMOM)

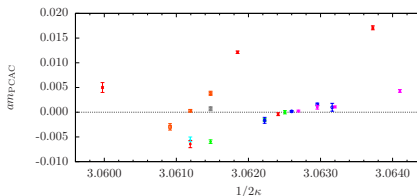
# Choice A): $m_{\text{PCAC}}$ at $[\mu_\ell, (\mu_h, \epsilon_h)]$ and $[\mu, (\mu, 0)]$

Theory & data at  $\beta = 1.9 \rightarrow \Delta(am_{\text{cr}}^{\text{opt}}) \sim 0.40\Delta(a^2\epsilon_h^2) - 0.71\Delta(a^2\mu_h^2)$

With choice  $m_0 = M_{\text{cr}}^{\text{opt}}[\mu_\ell, (\mu_h, \epsilon_h)]$  : expect  $\Delta(am_{\text{cr}}^{\text{opt}}) \simeq -0.0015$

i.e.  $am_{\text{PCAC}}|_{\sim 0, (\sim 0, 0)}^m \simeq 0.0075$  or (bare)  $m_{\text{PCAC}}|_{\sim 0, (\sim 0, 0)}^{m_0} \simeq 16 \text{ MeV}$

To get an idea of  $\chi$ SSB vs FS effects at  $L = 1 \text{ fm}$ :  $(L^2 2Bm_{\text{PCAC}})^{1/2} \simeq \sqrt{2}$



$\beta = 1.90$	$\mu = 0.0040$	$\mu_\sigma = 0.110$	$\mu_\delta = 0.090$	
$\beta = 1.90$	$\mu = 0.0040$	$\mu_\sigma = 0.110$	$\mu_\delta = 0.120$	
$\beta = 1.90$	$\mu = 0.0060$	$\mu_\sigma = 0.110$	$\mu_\delta = 0.120$	
$\beta = 1.90$	$\mu = 0.0040$	$\mu_\sigma = 0.150$	$\mu_\delta = 0.190$	
$\beta = 1.90$	$\mu = 0.0060$	$\mu_\sigma = 0.150$	$\mu_\delta = 0.190$	
$\beta = 1.90$	$\mu = 0.0080$	$\mu_\sigma = 0.150$	$\mu_\delta = 0.190$	
$\beta = 1.90$	$\mu = 0.0100$	$\mu_\sigma = 0.150$	$\mu_\delta = 0.190$	
$\beta = 1.90$	$\mu = 0.0040$	$\mu_\sigma = 0.185$	$\mu_\delta = 0.236$	

# $\det(D_{\text{Mtm}}^h)$ and the case of $\mu_h^2 < \epsilon_h^2$

$\mu_h^2 > \epsilon_h^2 \Rightarrow \det(D_{\text{Mtm}}^h) > 0$  on each gauge configuration, for any  $V$ .

$\mu_h^2 < \epsilon_h^2$ :  $\det(D_{\text{Mtm}}^h)$  has fixed sign on the relevant  $U$ -ensembles, as we find

- median of the spectral gap of  $Q_h \equiv \gamma_5 \tau^3 D_{\text{Mtm}}^h = Q_h^\dagger$  (though EO-precond.) well  $> 0$  and nearly proportional to  $\mu_h - Z_P Z_S^{-1} \epsilon_h = Z_P \hat{m}_s$  (Gregorio's plot)
- width of the spectral gap of  $Q_h$  seems to decrease with  $1/\sqrt{V}$  (G.'s plots)

This makes plausible the hypothesis that in infinite volume  $Q_h^2$  has zero (positive) eigenvalue density for  $\alpha < \bar{\alpha}$  ( $\alpha = \bar{\alpha}$ ) – at least for sufficiently small  $\alpha$

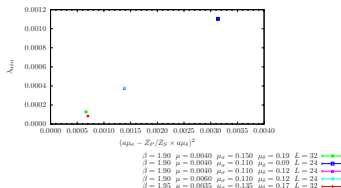
Under this hypothesis and in infinite volume:  $\bar{\alpha} = (\mu_h - Z_P Z_S^{-1} \epsilon_h)^2 + O(\alpha^2)$

renormalization of eigenvalue density (and gap) understood and related to that of quark mass(es), up to  $O(\alpha^2) \Leftrightarrow$  consistent with G.'s plot

Proof parallels that in hep-lat/0512021 (Del Debbio *et al.*) ( $\gamma_5$ -hermiticity of  $D_m$  and individual valence quarks there  $\rightarrow \gamma_5 \tau^3$ -hermiticity of  $D_{\text{Mtm}}^h$  and pairs of valence quarks here)

# The case of $\mu_h^2 < \epsilon_h^2$ on finite lattices

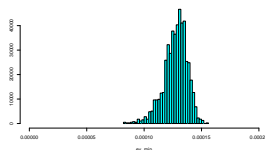
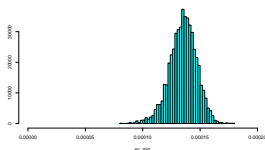
Spectral gap of  $Q_h^2$  vs  $(\mu_h - Z_P Z_S^{-1} \epsilon_h)^2$  (but EO-preconditioned)



Hypothesis on the spectral density: true in the continuum; can and should be checked (for the unpreconditioned  $Q_h$ ) on our lattices (large  $V$ , small  $a$ )

# The case of $\mu_h^2 < \epsilon_h^2$ on finite lattices – cont'd

$\beta = 1.9$ ,  $(a\mu_h, a\epsilon_h) = (0.15, 0.19)$ : distribution of  $\mathcal{Q}_h^2$  (but EO-preconditioned)



$L/a = 24, a\mu_\ell = 0.006$       and       $L/a = 32, a\mu_\ell = 0.004$

Width of the  $\mathcal{Q}_h^2$  spectral gap distribution: check whether it scales with  $a/\sqrt{V}$

Philosophy: if in our small  $a$ , large  $V$  simulations, by numerical checks of this type, we find good evidence that  $\det(D_{\text{Mtm}}^h)$  has constant sign on the relevant (for PHMC importance sampling)  $U$ -ensembles, then we also understand why: because we work close enough to the continuum and  $V = \infty$  limits.  $\Rightarrow$  self-consistent picture supporting the safety of our MC simulations at  $\epsilon_h^2 > \mu_h^2$ .

# Unitary vs. mixed action setup

Possibility of using OS fermions for the valence strange and charm quarks: avoid  $s$ - $c$  mixings, retain unitarity in the continuum limit.

Easy matching of  $s$  and  $c$  bare masses (requires knowledge of  $Z_P/Z_S$ ):

$$m_s = (\mu_h - Z_P/Z_S \epsilon_h) \quad \text{and} \quad m_c = (m u_h + Z_P/Z_S \epsilon_h)$$

No anomalously large cutoff effects seen in  $N_f = 2$  observables (other than  $m_\pi^{\text{OS}}$ ): see e.g.  $B_K$ . Indeed no such problems expected for masses and matrix elements involving only one-particle states.