Realistic simulations w/ exact chiral symmetry

T. Kaneko for the JLQCD/TWQCD collaborations

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1. introduction: JLQCD/TWQCD collaborations

JLQCD collaboration

- study lattice QCD on super computer system at KEK

KEK:	S.Hashimoto, H.Ikeda, TK, M.Matsufuru, J.Noaki, N.Yamada
YITP:	H.Ohki, T.Onogi, E.Shintani, T.Umeda
Tsukuba:	S.Aoki, K.Takeda, T.Yamazaki
Nagoya:	H.Fukaya
Hiroshima:	K-I.Ishikawa, M.Okawa

- –FY2000: w/ Fujitsu VPP500 (128GFLOPS)

  $N_f = 0$: KS or Wilson/clover: B_K, $f_{B,D}$, B_B, m_s, ...

- –FY2005: w/ Hitachi SR8000 (1.2TFLOPS)

  $N_f = 2$: clover : M_{msn}, M_{brn}, $f_{\pi,K}$, B_B

  $N_f = 2 + 1$: clover : only M_{msn}, M_{brn}, $f_{\pi,K}$ (w/ CP-PACS Collab.)

chiral symmetry breaking due to lattice action

$\Rightarrow$ severely limits applications of gauge ensembles!

1. introduction: chiral symmetry on the lattice

chiral symmetry

characterize low-energy dynamics of QCD through SSB

$M_{\rm msn}^2 \propto m_q$, ...

price of chiral symmetry breaking

- operator mixing in renormalization : ~~B_K~~
- modified ChPT : ex. Wilson ChPT *(Sharpe-Singleton, 1998, ...)*

  additional LECs, $a^2 \ln[m_q]$ singularities

  OK for $M_{\rm msn}, f_{PS}$ at NLO; maybe not for others / NNLO

Nielsen-Ninomiya no-go theorem, 1981

The following properties can NOT hold simultaneously:

- locality
- translational invariance
- no doublers unphys.species, ~~anomaly~~
- chiral sym. : $\{\gamma_5, D\} = 0$

$\Leftrightarrow$

Ginsparg-Wilson fermions, 1982

- GW relation :

  $\{\gamma_5, D\} = aD\gamma_5 D/m_0$
- modified chiral symmetry

  $\delta\bar{q} = \bar{q}\gamma_5, \quad \delta q = \gamma_5(1 - aD/2)q$
- correct anomaly, no mixing
- examples of D ....?

1. introduction: dynamical overlap simulations

overlap fermions *(Neuberger, 1998)*

$$S_q = \sum \bar{q}\, D(m)\, q,$$

$$D(m) = \left(m_0 + \frac{m}{2}\right) + \left(m_0 - \frac{m}{2}\right) \gamma_5\, \mathrm{sgn}[H_{\mathrm{w}}(-m_0)]$$

(m = quark mass, m_0 = a tunable parameter)

- satisfies GW relation exactly!
- computationally demanding...

JLQCD/TWQCD's project

- precise determination of MEs $\Rightarrow$ test of Standard Model, ...
- current supercomputer system @ KEK (FY2006 – FY2010)

  IBM Blue Gene/L + Hitachi SR11K : 59 TFLOPS in total

$\Rightarrow$ embark large-scale unquenched simulations with overlap fermion

in collaboration w/ T.-W.Chiu and T.H.Sheh in Taiwan (TWQCD)

Outline

outline

- Introduction
- simulation method

  implementation; parameters
- fixed topology
- physics results

  for $N_f = 2$:

  on-going $N_f = 3$ runs

  $\langle J_\mu(x)\, J_\nu(0) \rangle \Rightarrow$ talk by E. Shintani (Kyoto)
- summary

2. simulation method

2.1 implementation: overlap action

- overlap-Dirac operator $\ni \mathrm{sgn}[H_{\mathrm{W}}]$

$$D(m) \quad = \quad \left(m_0 + \frac{m}{2}\right) + \left(m_0 - \frac{m}{2}\right)\gamma_5\,\mathrm{sgn}[H_{\mathrm{w}}(-m_0)], \qquad m_0 = 1.6$$

- $\mathrm{sgn}[H_{\mathrm{W}}] \sim$ polynomial / rational approx.

  Zolotarev (min-max) approx: $\mathrm{sgn}[H_{\mathrm{W}}] = H_{\mathrm{W}}\{p_0 + \sum_{l=1} p_l/(H_{\mathrm{W}}^2 + q_l)\}$

  - nested inversion of Dirac operators : very time consuming

    $$D(m)^{-1} \;\ni\; Dx \;\ni\; H_{\mathrm{W}}^{-1}$$

  - discontinuity in S_q

    $\Rightarrow$ modified HMC *(Fodor-Katz-Szabo, 2004)* : very time consuming

  - locality

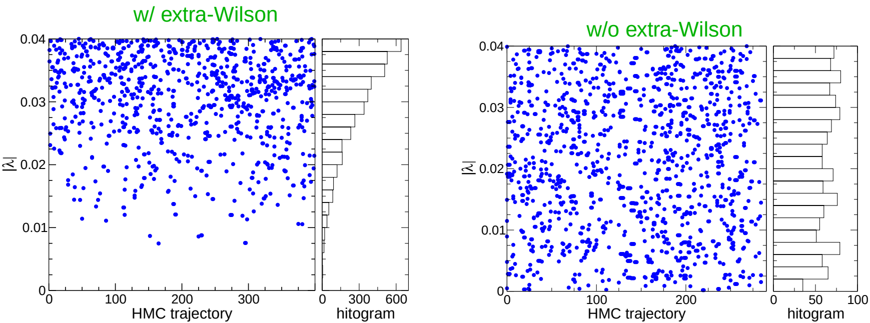
    $\Leftarrow$ OK, if $\sigma[H_{\mathrm{W}}]$ has a positive lower bound

$\Rightarrow$ suppress (near-)zero modes of H_{W} by auxiliary Boltzman weight *(JLQCD, 2006)*

$$\Delta_{\mathrm{W}} \quad = \quad \frac{\det[H_W(-m_0)^2]}{\det[H_W(-m_0)^2 + \mu^2]}, \quad \mu = 0.2$$

2.1 implementation: auxiliary determinant

- Δ_W : modification of gauge action $\Rightarrow$ modification of a dependence
- Δ_W : suppress (near)zero modes of H_W $\Rightarrow$ locality, reduced cost



- Δ_W : fix *global* topology during HMC $\Rightarrow$ effects should be studied

2.1 implementation: other techniques

other techniques

- multiplications of D : accuracy of $\mathrm{sgn}[H_W]$ = accuracy of chiral sym.
  - $\sigma[H_W] \Rightarrow [\lambda_{min}, \lambda_{thrs}] \cup [\lambda_{thrs}, \lambda_{max}]$
  - low modes : Lanczos $\Rightarrow$ low mode projection
  - high modes : Zolotarev approx. (min-max)

    $\Rightarrow \quad \langle \nabla_4 A_4 P^\dagger \rangle / \langle P P^\dagger \rangle |_{m=0} \lesssim 0.1(0.1)$ MeV
- D solver = 5D solver *(Edwards et al.,2005)* :
  - Schur decomposition ($D \Rightarrow M_5$) + even/odd precond. $\Rightarrow$ CPU cost $\times 1/2$
- HMC algorithm
  - mass preconditioning +multiple time scale MD $\Rightarrow$ CPU cost $\times 1/5$

    Hasenbusch, 2001; Sexton-Weingargen, 1992
  - no reflection/refraction steps : $\Rightarrow$ CPU cost $\times 1/4$
- assembler code for H_W multiplications : $\Rightarrow$ CPU cost $\times 1/3$

2.2 parameters

$N_f = 2$ runs : completed

- Iwasaki-gauge + overlap + Δ_W
- $\beta = 2.30 \Rightarrow a \approx 0.118(2)$ fm ($r_0 = 0.49$ fm)
- $16^3 \times 32$ lattice $\Rightarrow L \simeq 2$ fm
- 6 values of $m_{ud} \in [m_{s,\text{phys}}/6, m_{s,\text{phys}}]$ for $Q = 0$
- 10000 HMC trajectories at each m_{ud}
- $Q = -2, -4$ at $m_{\text{ud}} \sim m_{\text{s,phys}}/2$

$N_f = 2+1$ runs : on-going

- $\beta = 2.30 \Rightarrow a \approx 0.107(1)$ fm ($r_0 = 0.49$ fm)
- $16^3 \times 48$ lattice $\Rightarrow L \simeq 1.7$ fm
  - 2 m_s's $= m_{s,\text{phys}}, 1.3 \times m_{s,\text{phys}}$; 5 m_{ud}'s $\in [m_{s,\text{phys}}/6, m_s]$; 2500 traj.
- $24^3 \times 48$ lattice $\Rightarrow L \simeq 2.6$ fm, $M_\pi L \gtrsim 3.7$
  - $m_s \sim m_{s,\text{phys}}$; $m_{ud} \sim m_{s,\text{phys}}/6, m_{s,\text{phys}}/4$; 2500 traj.
- simulations with $Q \neq 0$ are on-going

2.3 measurements: low-mode averaging

low-mode averaging (LMA)

- 100 low-modes $\Leftarrow$ Lanczos

$$D\,u^{(k)} = \lambda^{(k)} u^{(k)}$$

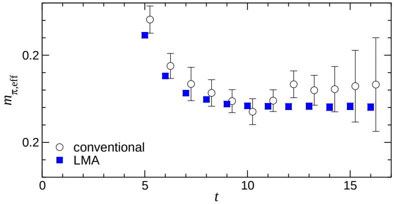
$$(D^{-1})_{\text{low}} = \sum_k \frac{1}{\lambda_k} u_k\, u_k^\dagger$$

$$C_\Gamma = \left\langle \left\{ (D^{-1})_{\text{low}} + (D^{-1})_{\text{high}} \right\} \Gamma \times \left\{ (D^{-1})_{\text{low}} + (D^{-1})_{\text{high}} \right\} \Gamma \right\rangle$$

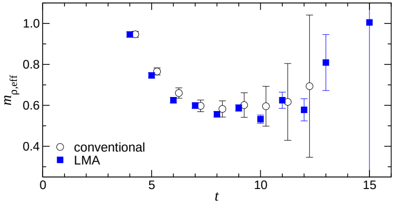
$$= C_{\Gamma,LL} + C_{\Gamma,HL} + C_{\Gamma,LH} + C_{\Gamma,HH}$$

- exact low-mode contrib.
  $\Rightarrow$ reduce stat. error remarkably
- preconditioning for D^{-1} solver
  100 modes $\Rightarrow$ $\times$ 8 speed up
- $\rho(\lambda)$, χ_t, spectrum, B_K, ...

PS correlator



vector correlator



2.3 measurements: all-to-all propagator

all-to-all quark propagator *(TrinLat, 2005)*

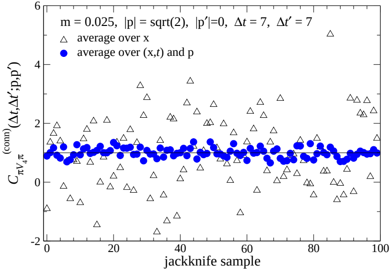
- high mode $\Leftarrow$ noise method

$$D\, x^{(r)} = (1 - P_{\text{low}})\eta^{(r)}$$
$$(D^{-1})_{\text{high}} = \frac{1}{N_r} \sum_r x^{(r)} \eta^{(r)\dagger}$$

- can construct any correlators w/o small additional CPU costs
  - smearing function
  - meson momenta

    $\Rightarrow$ form factors, hadron decays

$\langle \pi | V_4 | \pi \rangle$



- needs large N_r for M_{HL}, M_N, ... $\Leftrightarrow$ $O(100)$ TB disk
- pion form factors

3. fixed topology

3.1 fixed topology

fixed topology simulations

auxiliary determinant Δ_W $\Rightarrow$ fix global topology during HMC : problematic ?

- do NOT suppress local topological fluctuations

  $\Rightarrow$ χ_t is calculable from fixed Q simulations (next slide)

- suppressed by $1/V$: small effects ($\lesssim 1\,\%$) in MEs

- effects can be corrected systematically *(Aoki et al., 2007)*

$$G_{\theta=0} - G_Q = \frac{G^{(2)}_{\theta=0}}{2\chi_t V}\left(1 - \frac{Q^2}{\chi_t V} - \frac{c_4}{2\chi_t^2 V}\right) + O(V^{-3})$$

- topological tunneling will be suppressed at $a \to 0$

  $\Rightarrow$ fixing Q is inevitable for any lattice regularization

  (w/o modifications of HMC)

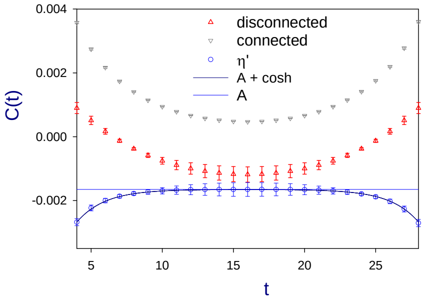
3.2 topological susceptibility: determination

determination from η' correlator ($N_f = 2$)

η' correlator $\Rightarrow$ a constant term $\Rightarrow$ χ_t

$$m_q^2 \langle \eta'(t+\Delta t)\eta'(t)\rangle_Q = -\frac{\chi_t}{V}\left(1 - \frac{Q^2}{\chi_t V} + \frac{c_4}{2\chi_t^2 V}\right) + O(e^{-M_\eta \Delta t}) + O(V^{-3})$$

η' correlator for $Q = 0$



- $Q = 0$: 2nd term vanishes
- 4pt function $\Rightarrow$ $c_4/(2\chi^2 V)$: small
- η' contamination rapidly damps
  $(M'_\eta > M_\pi)$ $\Rightarrow$ clear plateau
- 3 sectors $Q = 0, -2, -4$ at $m_{ud} = 0.050$
  $\Rightarrow$ consistent results for χ_t

3.2 topological susceptibility: chiral behavior

chiral behavior ($N_f = 2$)

LO ChPT *(Leutwyler-Smilga, 1992)*

$$\chi_t = \frac{\Sigma}{m_u^{-1} + m_d^{-1} + m_s^{-1}} \rightarrow \frac{m_{ud}\Sigma}{2}$$

- expected linear m_{ud} dependence at $m_{ud} \lesssim m_{s,\mathrm{phys}}/2$

  $\chi_t = c + m_{ud}\Sigma/2 \;\Rightarrow\; c = 0.0(1) \times 10^{-5}$

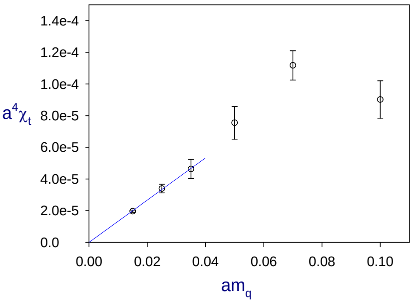
  not clear in previous studies

  - ill-determined w/o chiral symmetry (~~index theorem~~; $F\tilde{F}$ needs cooling)
  - insufficient sampling of topological sectors at small m_{ud}

- provides a determination of Σ

  $\Sigma = \{242(5)(10)\ \mathrm{GeV}\}^3$

χ_t vs m_{ud}



fixed topology strategy :

- introduced to reduce CPU cost...
- an effective way to study topological properties of QCD

4. selected results
(mainly from $N_f = 2$)

4.1 chiral condensate

chiral condensate $\langle \bar{q}q \rangle$ $\Rightarrow$ SSB of chiral symmetry

JLQCD/TWQCD's determinations

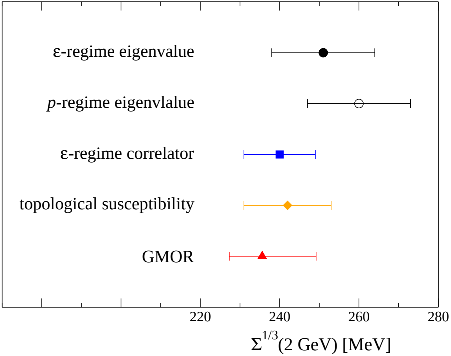
- topological susceptibility
  $\chi_t = \Sigma m_q / N_f$ (degenerate flavors)
  $\Leftarrow$ needs a reliable estimate of χ_t
- GMOR relation
  $M_{\rm NG}^2 = 2B(m_{q,1} + m_{q,2}) + ...$ $\Rightarrow$ $\Sigma = BF^2$
  $\Leftarrow$ WChPT modifies the LEC: $B \to B(1 - H''/F^2)$
- eigenvalue distribution in ϵ-regime
  comparison w/ ChRMT *(Damgaard-Nishigaki, 2001)*
  $\langle \zeta_k \rangle_{\rm ChRMT} = \langle \lambda_k \rangle_{\epsilon\text{-regime}} \Sigma V$
- meson correlators in ϵ-regime
  PS correlator $\ni$ Σ F at NNLO
  $\Leftarrow$ chiral symmetry + fixed topology in ϵ-regime

ChPT in ϵ-regime

- $M_\pi L \lesssim 1$
- $M_\pi \sim 1/L^2 \sim \epsilon^2$
- modified m_q-dep.
- Q dependence

4.1 chiral condensate

results for $\langle \bar{q}q \rangle$



- all results are determined w/ $\lesssim 5\,\%$ accuracy
- $\langle \bar{q}q \rangle$ from various sources are consistent with each other

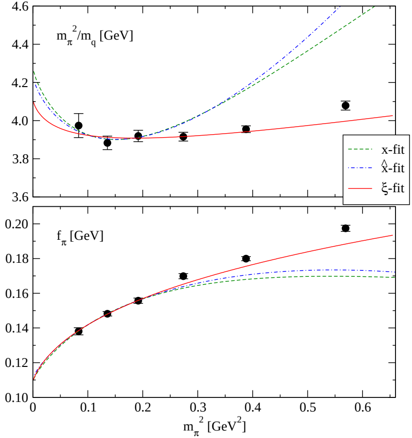
$\Rightarrow$ quantitative confirmation of spontaneous chiral symmetry breaking !!

4.2 pion mass and decay constant

pion mass and decay constant

- basic quantities to examine convergency of chiral expansion
  - reliability of LQCD
  - applicability of ChPT
- corrections : few % - few % = small
  - FVC $\Leftarrow$ NLO ChPT + resummation, *(Colangelo et al., 2005)*
  - fixed Q $\Leftarrow$ NLO ChPT w/ fixed Q *(Aoki et al., 2007)*
- choice of expansion parameters
  $x \equiv m_q/F^2$, $\hat{x} \equiv M_\pi^2/F^2$, $\xi \equiv M_\pi^2/F_\pi^2$
  - our data at $m_{ud} < m_{s,\text{phys}}/2$: NLO
  - at $m_{ud} \lesssim m_{s,\text{phys}}$: NNLO w/ ξ
    $\Leftarrow$ resummation (?)

"NLO" fits to M_π^2 and f_π



4.2 pion mass and decay constant

low-energy constant

- large deviation in l_4 between NLO and NNLO
  - $\Rightarrow$ NNLO is needed for a reliable estimate of LECs
- results from NNLO fit w/ ξ

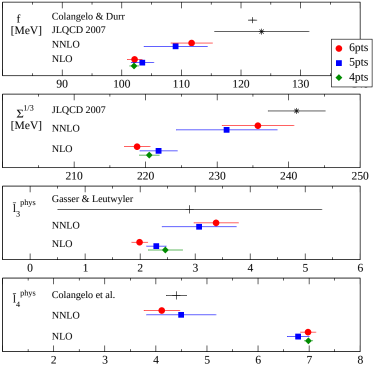
$$\Sigma = BF^2 = \{235.7(5.0)(^{+13}_{-2})\mathrm{GeV}\}^3$$

$$F = 79.0(2.5)(^{+4.3}_{-0.7})\mathrm{MeV}$$

$$l_3^r = 3.38(40)(^{+39}_{-24})$$

$$l_4^r = 4.12(35)(^{+43}_{-30})$$

results for LECs



consistent w/ phenomenology *(Gasser-Leutwyler, 1984; Colangelo et al., 2001,2004)*

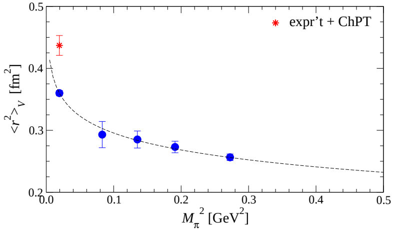
4.3 pion form factors

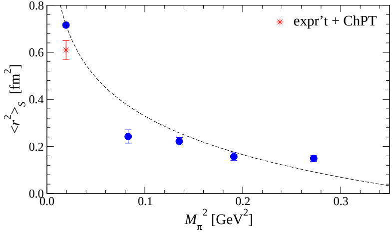
pion form factors

$$\langle \pi(p')|V_\mu|\pi(p)\rangle = (p+p')_\mu F_V(q^2)$$
$$\langle \pi(p')|S|\pi(p)\rangle = F_S(q^2)$$
$$\langle r^2\rangle_{V,S} = 6(\partial F_{V,S}(q^2)/\partial q^2)_{q^2=0}$$

- next simplest to test convergency
- $\langle r^2\rangle_S$
  - 6 times larger chiral log
  - determination of $l_4 \Leftrightarrow F_\pi$
  - no experimental process
- measurements w/ all-to-all
  - precise estimate of $F_{V,S}(q^2)$
  - first calc. of F_S w/ disc.
- NLO ChPT fit is not successful
  - $\langle r^2\rangle_V$ is inconsistent w/ expr't
  - fails to reproduce M_π^2 dep. of $\langle r^2\rangle_S$

NLO fits to $\langle r^2\rangle_{V,S}$





4.3 pion form factors

NNLO fit

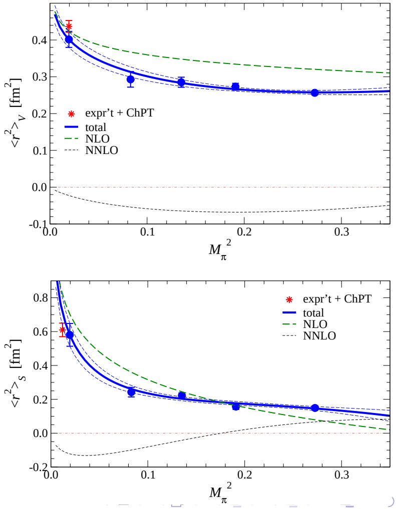
- 4 $O(p^4)$ LECs, 3 $O(p^6)$ LECs
  - include $c_V = \partial^2 F_X(q^2)/\partial(q^2)^2$
  - $\bar{l}_3$: fixed to that from M_π^2
  - $\hat{x}$ is used to reduce LECs
- consistent results w/ experiment

$$\langle r^2 \rangle_V = 0.402(22)(36)\text{fm}^2$$
$$\langle r^2 \rangle_S = 0.581(67)(96)\text{fm}^2$$
$$\bar{l}_4 = 4.05(55)$$

$\Leftrightarrow$ $\langle r^2 \rangle_V = 0.437(16)\text{fm}^2$ (expr't)
$\langle r^2 \rangle_S = 0.61(4)\text{fm}^2$ (expr't)
$\bar{l}_4 = 4.12(56)$ (F_π)

- NNLO contrib. is important in analysis of form factors

NNLO fits to $F_{V,S}(q^2)$



4.4 B_K

- $B_K \;\Rightarrow\;$ tests of Standard Model

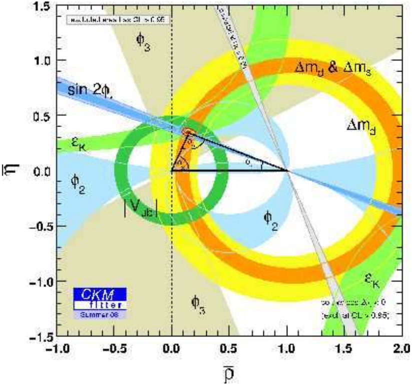
  $B_K \Rightarrow \epsilon_K \Rightarrow$ unitarity triangle
- use of overlap quarks

  $\Rightarrow$ avoid large error due to op. mixing

  VV – AA $\Leftrightarrow$ VV + AA, PP + SS, TT + TT
- chiral extrap.
  - $M_\pi, F_\pi, \langle r^2 \rangle_{V,S} \;\Rightarrow\;$ NNLO ChPT?
  - NNLO formula is not available

  $\Rightarrow$ use NLO formula w/ NNLO analytic terms

constraints on unitarity triangle



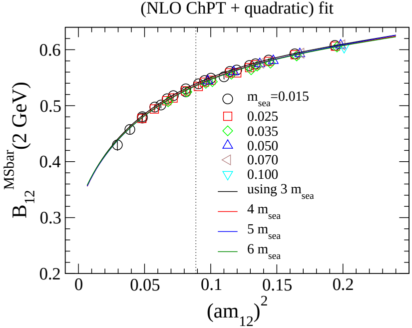
4.4 B_K

- systematic uncertainties
  - FVC : 5 %
    NLO ChPT + resummation
  - fixed Q : 1.4 %
    measurement at $Q \neq 0$
  - scaling violation : 5 %
    naive order counting
  - $N_f < 3$: missing
    small ? : *cf. RBC :* $N_f = 2 \Leftrightarrow 3$

$$B_K^{\overline{\mathrm{MS}}}(2\ \mathrm{GeV}) = 0.537(4)(40)$$

$\Leftrightarrow \quad B_K^{\overline{\mathrm{MS}}} = 0.524(10)(28)$
($N_f = 3$; RBC/UKQCD, 2008)

chiral fit of B_K



expect a better control of sys. error w/ $N_f = 3$ confs at $M_\pi L \gtrsim 3.7$

4.5 baryon quark contents

πN σ term

$$\sigma_{\pi N} = m_{ud}\langle N|\bar{u}u + \bar{d}d|N\rangle$$

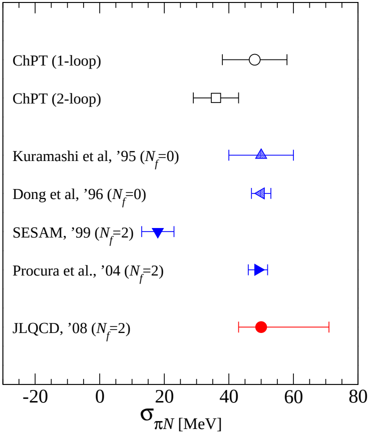
cf. $$M_N = M_0 + \sigma_{\pi N} + \ldots$$

- use Feynman-Hellman theorem

$$\frac{\partial M_N}{\partial m_q} = N_{f,q} m_q \langle N|\bar{q}q|N\rangle$$

- chiral fit of M_N
  - $O(p^3)$ BChPT
  - $g_A = 1.267$
  - ignore some small $O(M_\pi^{4,5})$ terms
  - FVC from BChPT (known up to $O(p^4)$)

ChPT and lattice estimates of $\sigma_{\pi N}$



$\sigma_{\pi N} = 52(2)(^{+21}_{-7})$ MeV $\Leftrightarrow$ consistent w/ previous estimates

4.5 baryon quark contents

y parameter

$$y = \frac{2\langle N|\bar{s}s|N\rangle}{\langle N|\bar{u}u + \bar{d}d|N\rangle}$$

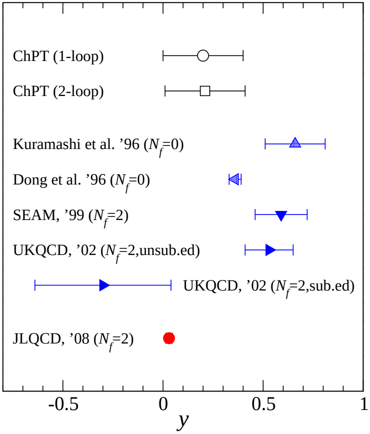
$\Rightarrow$ direct search of dark matter (XMASS, ...)

- chiral fit + Feynman-Hellman
  - $O(p^3)$ PQBChPT
  - g_A, $g_{1,\eta NN}$ fixed
- chiral symmetry removes a large contamination in "$\partial M_N / \partial m_{\text{sea}}^{\text{bare}}|_{m_{\text{val}}^{\text{bare}}}$"

  (UKQCD, 2002)

$$\left.\frac{\partial M_N}{\partial m_{\text{sea}}^{\text{phys}}}\right|_{m_{\text{val}}^{\text{phys}}} + \left.\frac{\partial M_N}{\partial m_{\text{val}}^{\text{phys}}}\right|_{m_{\text{sea}}^{\text{phys}}} \left.\frac{\partial m_{\text{val}}^{\text{phys}}}{\partial m_{\text{sea}}^{\text{bare}}}\right|_{m_{\text{sea}}^{\text{phys}}}$$

ChPT and lattice estimates of y

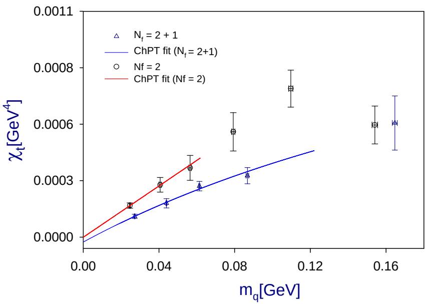


$y = 0.030(16)(^{+6}_{-2})$ $\Leftrightarrow$ smaller but natural ?; need to extend to $N_f = 3$

4.6 in $N_f = 3$ QCD

topological susceptibility

χ_t vs m_{ud}



- consistent w/ LO ChPT

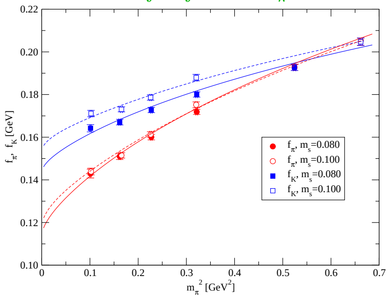
$$\chi_t = \Sigma/(2m_{ud}^{-1} + m_s^{-1})$$

- $\Sigma = \{249(4)(2)\ \text{MeV}\}^3$

$\Leftrightarrow \quad \Sigma = \{242(5)(10)\ \text{MeV}\}^3\ (N_f = 2)$

spectroscopy

f_π, f_K vs M_π^2



- NNLO ChPT fits w/ NPR

$$m_{ud}^{\overline{MS}}(2\,\text{GeV}) = 3.80(7)\ \text{MeV}$$
$$m_s^{\overline{MS}}(2\,\text{GeV}) = 115(2)\ \text{MeV}$$
$$f_\pi = 121.5(4.1)\ \text{MeV}$$
$$f_K = 148.3(4.7)\ \text{MeV}$$
$$f_K/f_\pi = 1.220(10)$$

summary

- JLQCD/TWQCD's dynamical overlap project:
  - advantage : chiral symmetry
    - essential to calculate general matrix elements (4 quark op., multi. bilinear, ...)
    - study chiral behavior based on continuum ChPT
  - drawback : not on physical point $\Leftrightarrow$ PACS-CS *(talk by Ukita)*

    $\Leftrightarrow$ quantities w/ poor convergency of chiral expansion
- future possibilities w/ ensembles at ($m_{ud} \gtrsim m_{s,\text{phys}}/6$, $M_\pi L \gtrsim 3.7$)
  - current KEK supercomputer system : till FY2010

    $\Rightarrow$ $Q \neq 0$, ϵ-regime, degenerate $N_f = 3$, high T, ...
  - what can be done for hyperon physics ?
    - single body problem : may be OK

      matrix elements ($\Leftarrow$ overlap), disconnected diagram ($\Leftarrow$ all-to-all), ...
    - baryon interaction ?

      $M_\pi L \gtrsim 4$ is safe for multi-baryon system?
      chiral symmetry plays important roles ?