Lattice QCD simulation with exact chiral symmetry

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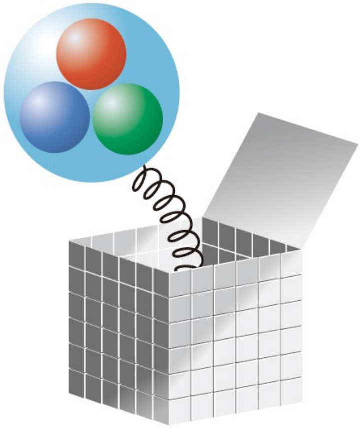
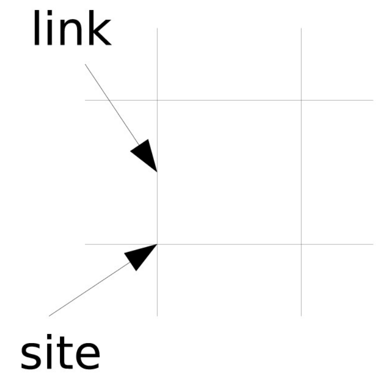
Introduction



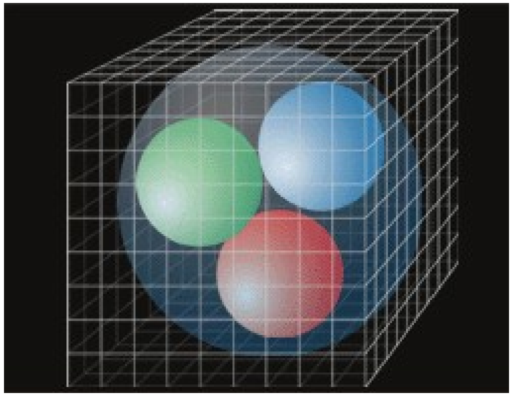
Lattice QCD

Lattice QCD: gauge theory on 4D Euclidean lattice

- Regularized by lattice
  - gluon: SU(3) link variables
  - quark: Grassmann field on sites
- Continuum limit ($a \to 0$) → QCD
- Numerical simulation by Monte Carlo
- Nonperturbative calculation



- Quantitative calculation has become possible
  - Matrix elements for flavor physics
  - Phase structure/plasma properties
  - Nuclear force in near future



Introduction

Our goals:

- Quantitative QCD calculation
  - To the level required by flavor physics
- Explore chiral dynamics
  - Mechanism of chiral symmetry breaking

Three extrapolations must be under control:

- Continuum limit ($a \to 0$)
- Thermodynamic limit (infinite $V \to \infty$)
- Chiral limit ($m \to 0$)

In particular, taming chiral symmetry is most significant

Introduction

Recent progress:

- Breakthrough: domain-wall fermion
- Realization of exact chiral symmetry on the lattice
  - Ginsparg-Wilson relation
- Fermion actions satisfying G-W relation

Our choice: overlap fermion --- Why overlap ?

- Exact chiral symmetry (theoretically clean)
  - No unwanted operator mixing
  - Continuum ChPT is applicable
  - Direct access to symmetry breaking properties
    - Epsilon regime, etc
- Large simulation costs (numerically challenging!)
  - Let's get rid of by algorithmic progress and large machine
- First large-scale dynamical simulation

Members

KEK: T. Aoyama, S. Hashimoto, T. Kaneko, H. Matsufuru, J. Noaki, N. Yamada, H. Ikeda

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Nagoya: H. Fukaya

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Hiroshima: K.-I. Ishikawa, M. Okawa

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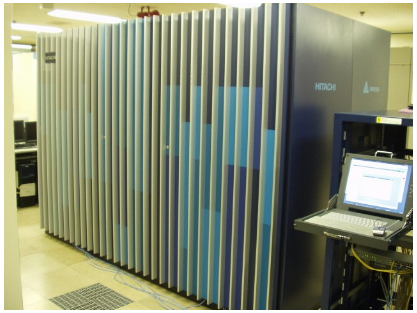
Machines

Main machine: IBM Blue Gene/L at KEK(2006~)

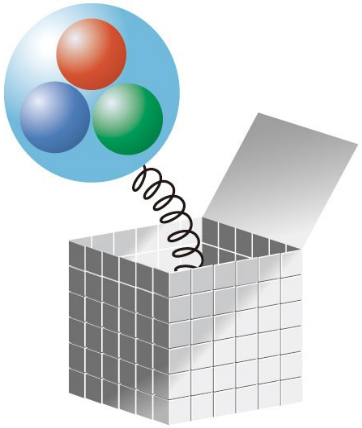
- 57.6 Tflops peak (10 racks)
- 0.5TB memory/rack
- 8x8x8(16) torus network
- About 30% performance for Wilson kernel (thanks to IBM staffs)
- 10-15% for overlap HMC

- Hitachi SR11000 (KEK)
  - 2.15TFlops/0.5TB memory



- NEC SX8 (YITP, Kyoto)
  - 0.77TFlops/0.77TB memory

Lattice fermion actions



Fermion doubling

Fermion doubling

- naïve discretization causes 16-fold doubling

$$S_F = \sum_x \bar{\psi}(x) \left[\frac{1}{2} \sum_\mu [U_\mu(x)\psi(x) - U_\mu(x-\hat{\mu})\psi(x-\hat{\mu})] + m\psi(x) \right]$$

$$a = 1,\ U_\mu \simeq 1 + igA_\mu,\ \hat{\mu} : \text{unit vector in } \mu\text{-th direction}$$

$$S_q(p)_{free} = \frac{1}{\sum_\mu \gamma_\mu \sin(p_\mu a) + ma}$$

- Nielsen-Ninomiya's No-go theorem
  - Doublers appear unless chiral symmetry is broken

$$D\gamma_5 + \gamma_5 D = 0$$

Staggered fermion

- Wilson fermion
  - adds Wilson term to kill 15 doublers
  - breaks chiral symmetry explicitly → additive mass renorm.
  - Improved versions, twisted mass versions are widely used

$$S_F = \frac{1}{2}\sum_{x,s}\bar{\psi}(x)\left[\gamma_\mu U_\mu(x)\psi(x+\hat{\mu}) - \gamma_\mu U_\mu(x-\hat{\mu})\psi(x-\hat{\mu}) - \frac{r}{2}\Delta^{(2)}\psi(x)\right]$$

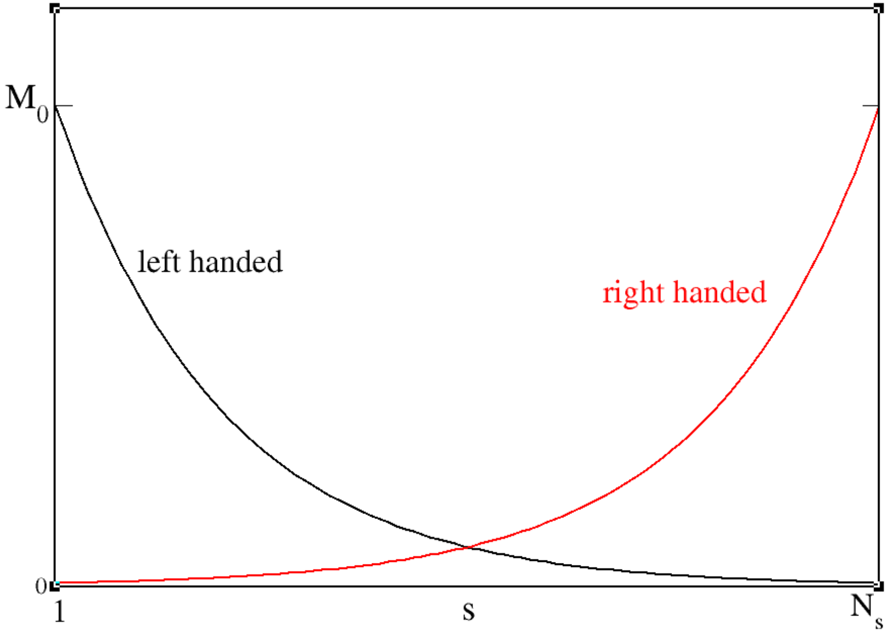
- Staggered fermion
  - 16=4 spinors x 4 flavors ('tastes')
  - Remnant U(1) symmetry
  - Fourth root trick: still debated
  - Numerical cost is low

Domain-wall fermion

- Domain-wall fermion (Kaplan 1992, Shamir 1993)
  - 5D formulation, light modes appear at the edges
  - Symmetry breaking effect $m_{res} \to 0$ as $N_5 \to \infty$

$$S_F = \frac{1}{2}\sum_{x,s} \bar{\psi}(x,s)\left[D_W(x,s;-M_0)\psi(x,s) + (1+\gamma_5)\psi(x,s+1) + (1-\gamma_5)\psi(x,s-1) - 2\psi(x,s)\right]$$

  - Costs O(20) times than Wilson fermions



Chiral symmetry on lattice

Ginsparg-Wilson relation (1982)

$$\gamma_5 D + D\gamma_5 = aRD\gamma_5 D$$

– Exact chiral symmetry on the lattice (Luscher 1998)

$$\delta\psi = \gamma_5 \left(1 - \frac{aR}{2} D\right) \psi \qquad \delta\bar{\psi} = \bar{\psi} \left(1 - D\frac{aR}{2}\right) \gamma_5$$

- Satisfied by
  - Overlap fermion (Neuberger, 1998)
  - Fixed point action (Bietenholz and Wiese, 1996)

Overlap fermion

$$D = \frac{1}{Ra}\left[1 + \gamma_5 \,\mathrm{sign}(H_W(-m_0))\right]$$

H_W : hermitian Wilson-Dirac operator

(Neuberger, 1998)

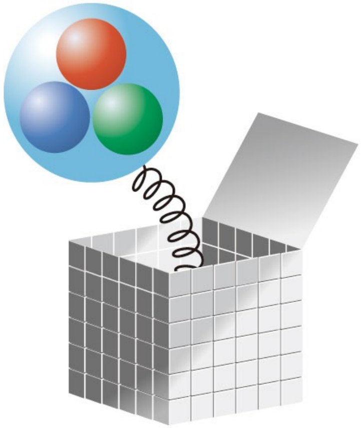
- Theoretically elegant
  - Satisfies Ginsparg-Wilson relation
  - *Infinite* N_s limit of Domain-wall fermion (No m_{res})
- Numerical cost is high
  - Calculation of sign function
  - Discontinuity at zero eigenvalue of H_W
- Has become feasible with
  - Improvement of algorithms
  - Large computational resources

Costs

Large-scale dynamical simulation projects

Fermion	Chiral symmetry	flavor structure	cost	Collab.
Wilson-type	explicitly broken	simple	modest	PACS-CS, etc
Twisted mass	explicitly broken	simple	modest	ETM
Staggered	remnant U(1)	complex	low	MILC, etc
Domain-wall	good	simple	high	RBC, UKQCD
Overlap	best	simple	very high	JLQCD

Overlap fermion



Overlap fermion

$$D(m) = \left(M_0 + \frac{m}{2}\right) + \left(M_0 - \frac{m}{2}\right) \gamma_5 \mathrm{sign}(H_W)$$

H_W : hermitian Wilson-Dirac operator

- Sign function means:

$$\mathrm{sign} H_W \cdot v = \sum_\lambda \mathrm{sign}(\lambda)(\psi_\lambda, v)\psi_\lambda$$

(λ, ψ_λ): eigenvalue/vector of H_W

In practice, all eigenmodes cannot be determined

- Reasonable solution:
  - Eigenmodes determined at low frequency part
  - Approximation formula for high mode part
    - Chebychev polynomial, partially fractional, etc.

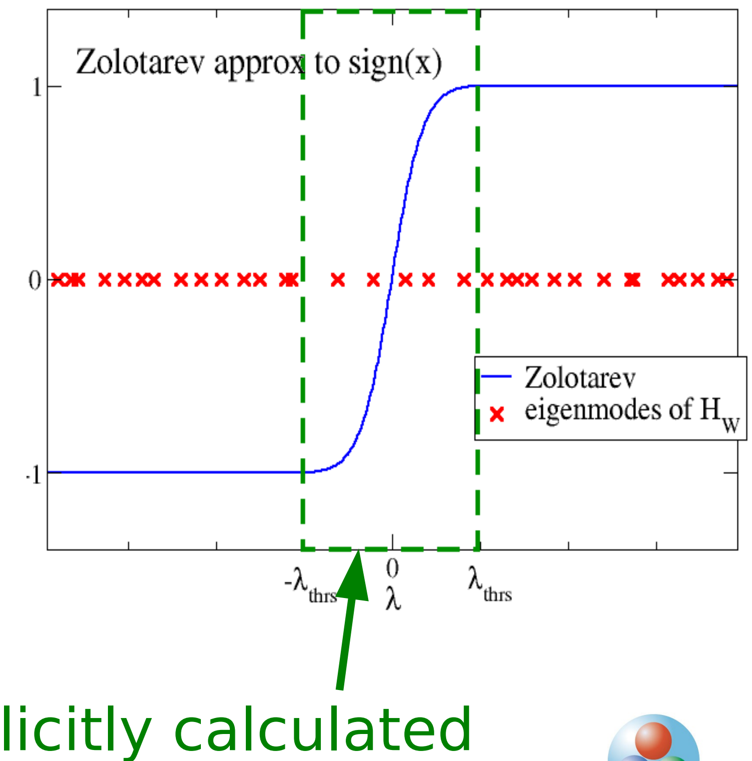
Sign function

Zolotarev's Rational approximation

$$\mathrm{sign}(H_W) = \frac{H_W}{\sqrt{H_W^2}} = H_W \left(p_0 + \sum_{l=1}^{N} \frac{p_l}{H_W^2 + q_l} \right)$$

- $(H_W^2 + q_l)^{-1}$: calculable simultaneously
- Valid for |λ| (eigenmode of H_W) ∈ [λ_{thrs} , λ_{max}]
- Projecting out low-modes of H_W below λ_{thrs} $\rightarrow$ $\mathrm{sign}(\lambda)$ $(\lambda < \lambda_{thrs})$
- Cost depends on the low-mode density

(λ_{thrs}=0.045, N=10 in this work)



Sign function discontinuity

Overlap operator is discontinuous at λ=0

--- Needs care in HMC when λ changes sign, thus changing topological charge Q

- Reflection/refraction

  (Fodor, Katz and Szabo , 2004)

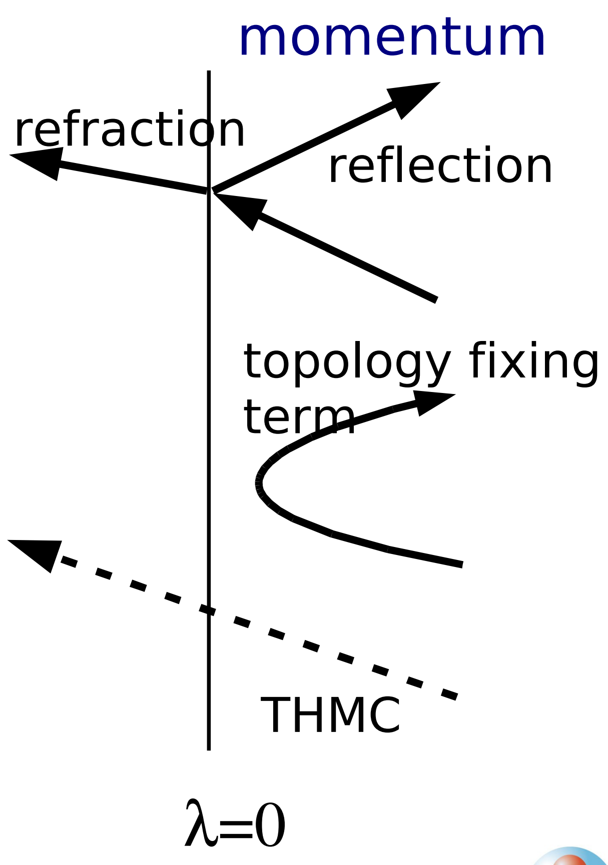
  - Change momentum at λ=0
  - Additional inversions at λ=0
- Topology fixing term

  (Vranas, 2000, Fukaya, 2006)

  - $\lambda\sim0$ modes never appear
- Tunneling HMC

  (Golterman and Shamir, 2007)

  - Project out low modes in MD steps
  - Needs practical feasibility test



Suppressing near-zero modes of H_W

<u>Topology fixing term</u>: extra Wilson fermion/ghost

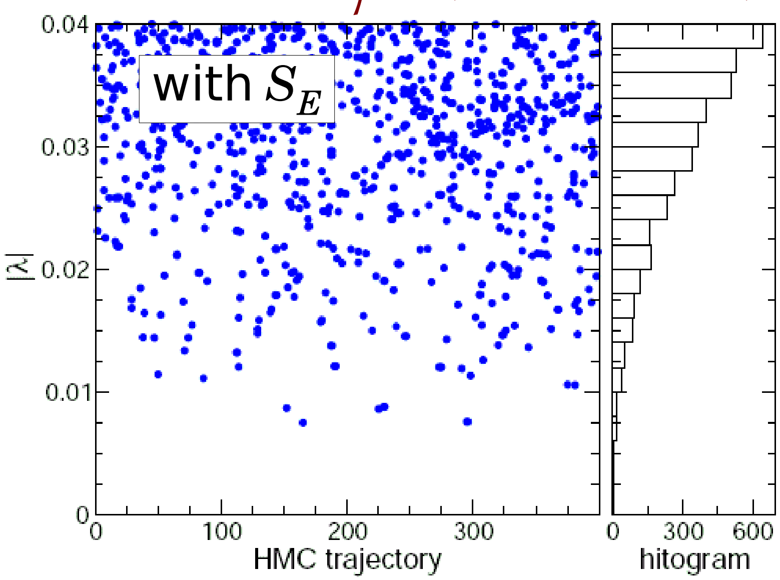
(Vranas, 2000, Fukaya, 2006, JLQCD, 2006)

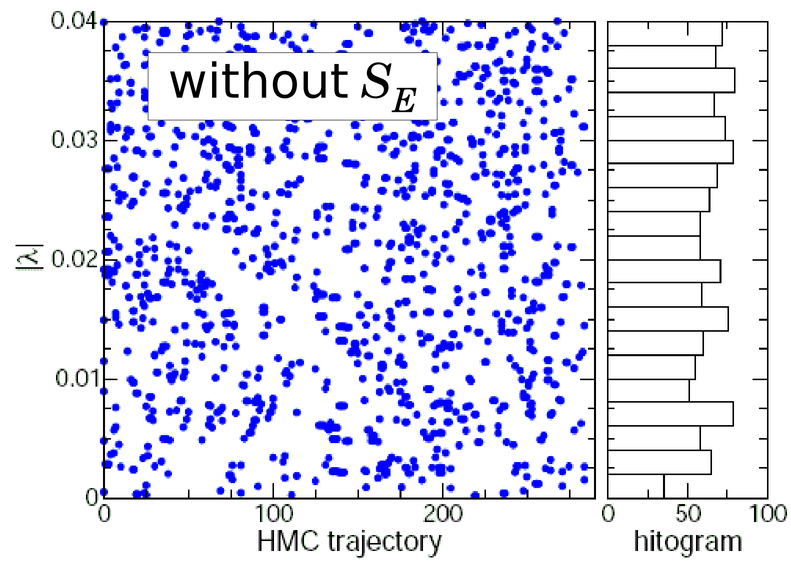
$$\det\left(\frac{H_W^2}{H_W^2+\mu^2}\right) = \int \mathcal{D}\chi^\dagger \mathcal{D}\chi \exp[-S_E]$$

--- avoids λ~0 during MD evolution

- No need of reflection/refraction
- cheeper sign function

$N_f = 2$, a~0.125fm, $m_{sea} \sim m_s$, μ =0.2

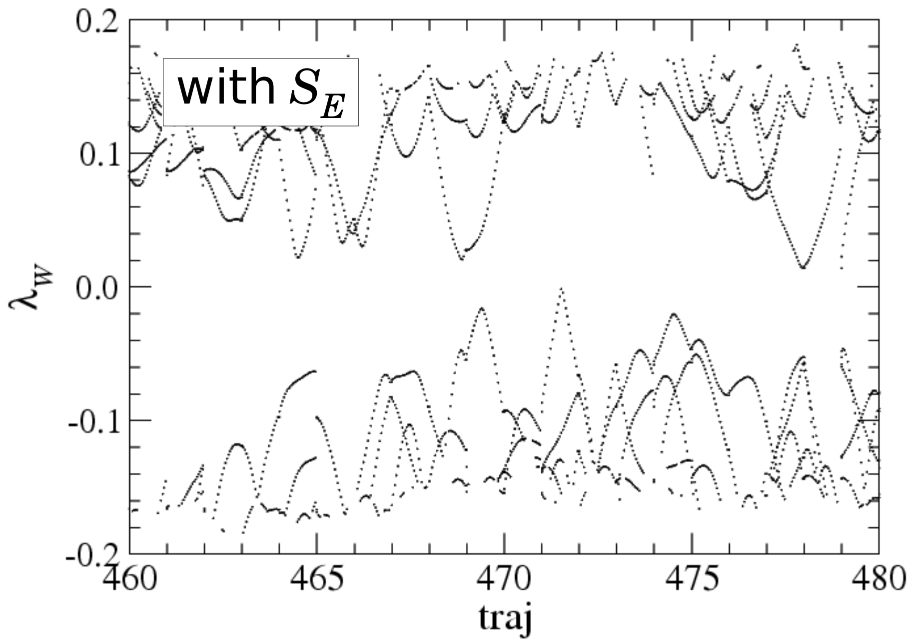


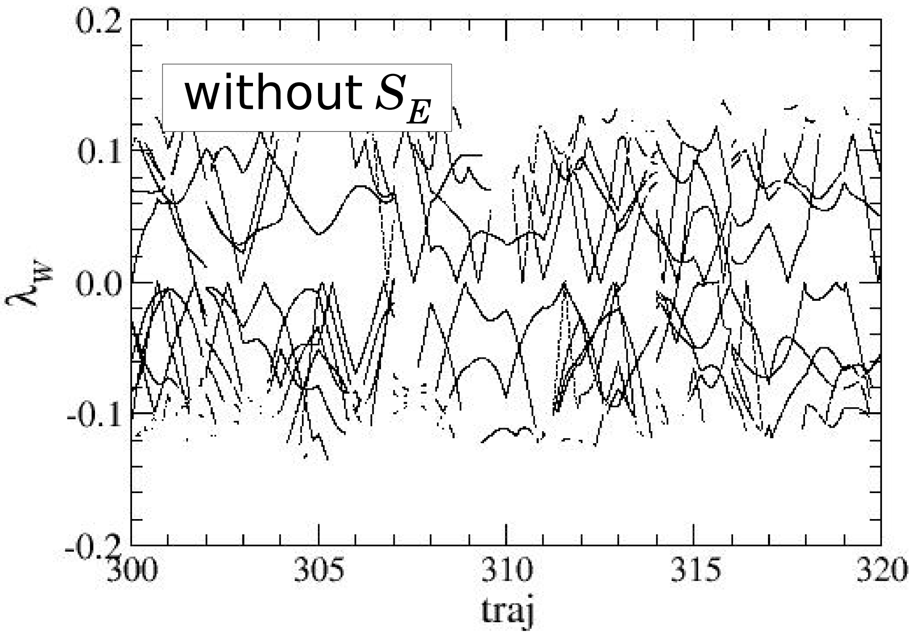


Suppressing near-zero modes of H_W

HMC/MD history of lowest eigenvalue

$N_f = 2$, $a\sim 0.125$fm, $m_{sea} \sim m_s$, $\mu = 0.2$





With extra Wilson fermion/ghost, λ=0 does not occur

Locality

Fermion operator should be local

- Overlap operator is exponentially local, if
  - No low mode of H_W below some threshold

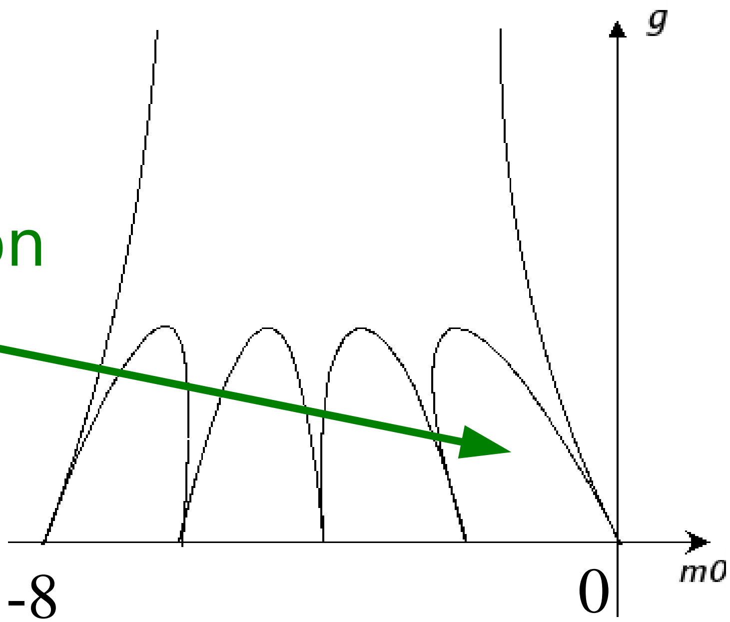
    Hernandez, Jansen, Luscher, 1999

  Near-zero mode is itself exponentially local

    Golterman, Shamir, 2003; Golterman, Shamir, Svetitsky, 2003

  ⟺ Out of Aoki phase
  (parity broken phase

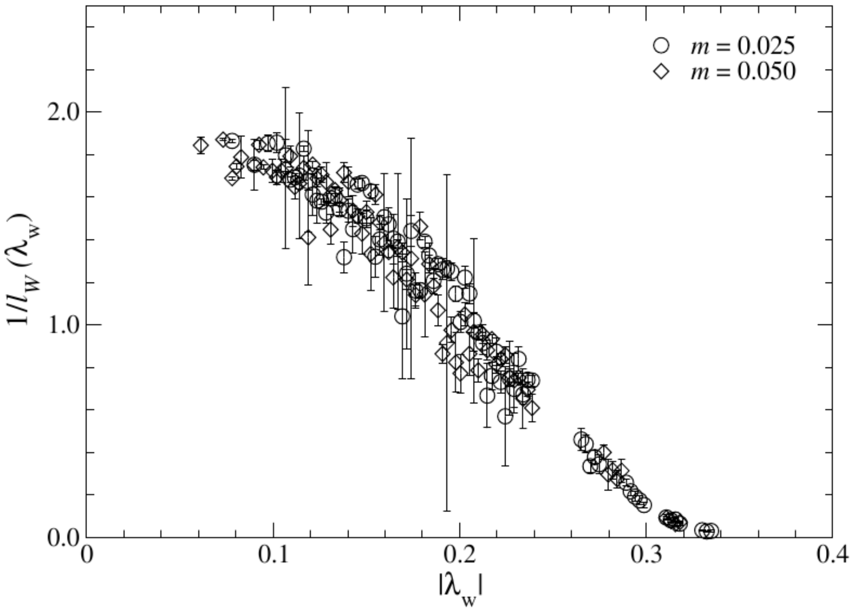
Should be in this region



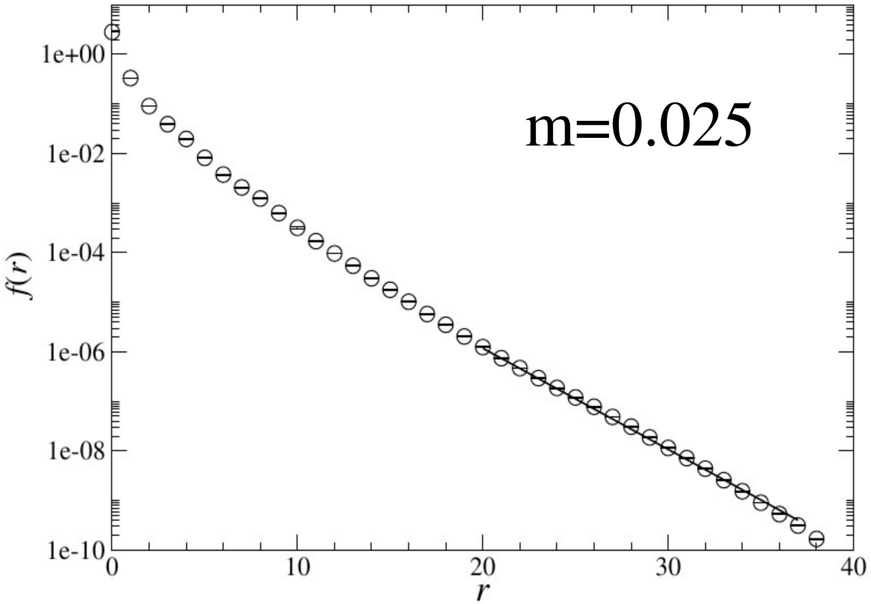
Locality

JLQCD, 2008; JLQCD (Yamada et al.), Proc. of Lattice 2006

- At beta=2.3 (Nf=2)



Localization length of low eigenmodes of H_W



Localization of overlap operator $l = 0.25\text{fm}\ (\sim 2a)$

Simulation at fixed topology

Forbidding near-zero mode of $H_W \Leftrightarrow$ fixing topology

Is fixing topology a problem ?

- In the infinite V limit,
  - Fixing topology is irrelevant
  - Local fluctuation of topology is active
- In practice, V is finite
  - Topology fixing $\Rightarrow$ finite V effect
  - $\theta=0$ physics can be reconstructed
    - Finite size correction to fixed Q result (with help of ChPT)
  - Must check local topological fluctuation

    $\Rightarrow$ topological susceptibility, η' mass
  - Remaining question: Ergodicity ?

Physics at fixed topology

One can reconstruct fixed θ physics from fixed Q physics

(Bowler et al., 2003, Aoki, Fukaya, Hashimoto, & Onogi, 2007)

- Partition function at fixed topology

$$Z_Q = \frac{1}{2\pi}\int_{-\pi}^{\pi} Z(\theta)\exp(i\theta Q) \quad \Rightarrow \quad Z(\theta) = \sum\nolimits_Q Z_Q \exp(-i\theta Q)$$

  – For $Q \ll \chi_t V$, Q distribution is Gaussian

- Physical observables
  – Saddle point analysis

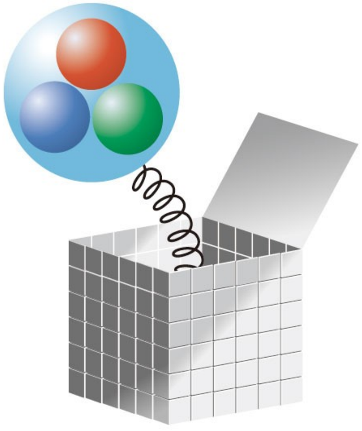
$$\Rightarrow \langle O\rangle_\theta = \langle O\rangle_Q + (\text{finite } V \text{ correction}) \quad \text{for} \quad Q \ll \chi_t V$$

  – Example: pion mass

$$m_\pi^Q = m_\pi(\theta=0) + \frac{1}{2V\chi_t}\left(1 - \frac{Q^2}{V\chi_t}\right)\frac{\partial^2 m_\pi(\theta)}{\partial\theta^2}\bigg|_{\theta=0} + O(V^{-2})$$

Implementation of overlap simulation

- Solver algorithm for overlap operator
- Hybrid Monte Carlo algorithm



Overlap solver

Solver algorithm for overlap operator

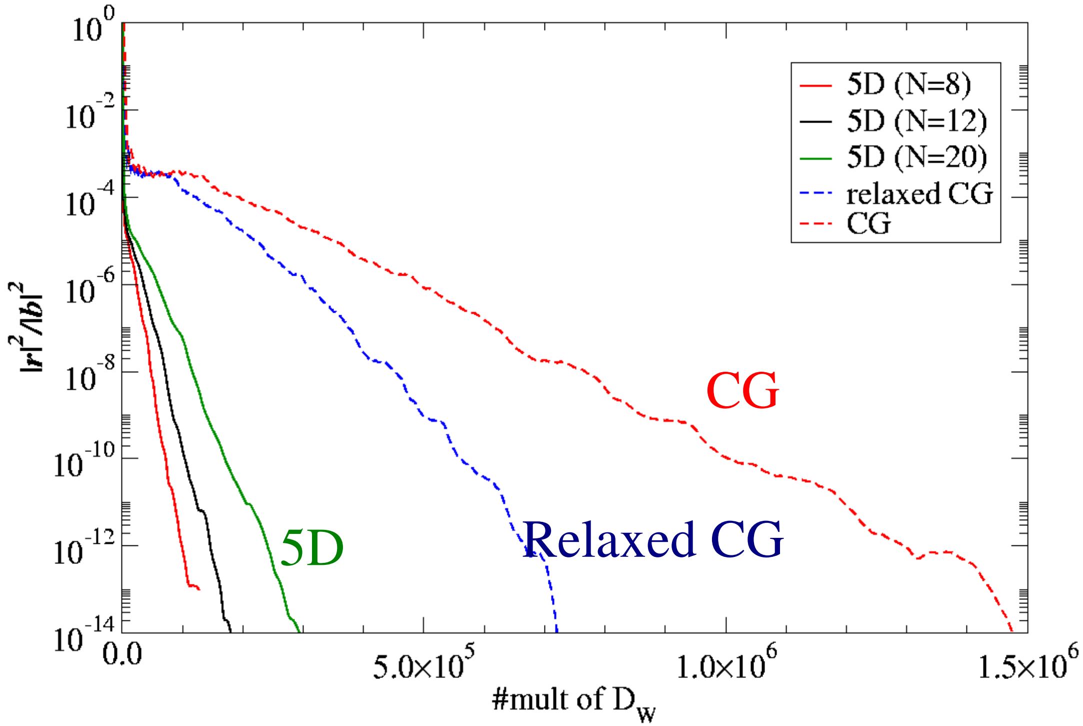
$$D_{ov}\, x = b \quad \text{must be solved}$$

- Most time-consuming part of HMC
- Needed to obtain quark propagator

- Two algorithms were used
  - Nested (4D) CG
  - 5D CG

4D solver

- Nested CG (Fromer et al., 1995, Cundy et al., 2004)
  - Outer CG for $D(m)$, inner CG for $(H_W^2 + q_l)^{-1}$ (multishift)
  - Relaxed CG: ε_{in} is relaxed as outer loop iteration proceeds
  - Cost mildly depends on N



Nf=2, a=0.12fm, on single config.
Without low-mode projection

5D solver

Borici, 2004, Edwards et al., 2006

- Schur decomposition
  - One can solve $S\psi_4 = \chi_4$ by solving (example: N=2 case)

$$M_5 \begin{pmatrix} \phi \\ \psi_4 \end{pmatrix} = \begin{pmatrix} 0 \\ \chi_4 \end{pmatrix}, \quad M_5 = \left(\begin{array}{cccc|c} H_W & -\sqrt{q_2} & & & 0 \\ -\sqrt{q_2} & -H_W & & & \sqrt{p_2} \\ & & H_W & -\sqrt{q_1} & 0 \\ & & -\sqrt{q_1} & -H_W & \sqrt{p_1} \\ \hline 0 & \sqrt{p_2} & 0 & \sqrt{p_1} & R\gamma_5 + p_0 H \end{array}\right) = \left(\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right)$$

$S = D - CA^{-1}B$: overlap operator (rational approx.)

  - Even-odd preconditioning
  - Low-mode projection of H_W in lower-right corner

5D solver

Schur decomposition:

$$M_5 = \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ CA^{-1} & 1 \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} 1 & A^{-1}B \\ 0 & 1 \end{pmatrix} \equiv \tilde{L}\tilde{D}\tilde{U},$$

where $S = D - CA^{-1}B$. S is called the Schur complement. Consider a linear equation

$$M_5 \begin{pmatrix} \phi \\ \psi_4 \end{pmatrix} = \begin{pmatrix} 0 \\ \chi_4 \end{pmatrix}.$$

Using $M_5 = \tilde{L}\tilde{D}\tilde{U}$ and multiplying $\tilde{L}^{-1}$ from the left to the above equation,

$$\begin{pmatrix} A & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} \phi + A^{-1}B\psi_4 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} 0 \\ \chi_4 \end{pmatrix}.$$

Namely, by solving 5-dimensional equation (4.3), one can solve $S\psi_4 = \chi_4$.

(This page is added after seminar for explanation.)

5D solver

In general, A B, and C has the following structure.

$$A = \begin{pmatrix} A_N & & \\ & A_{N-1} & \\ & & \ddots \end{pmatrix}, \quad B = \begin{pmatrix} B_N \\ B_{N-1} \\ \vdots \end{pmatrix}, \quad C = (C_N, C_{N-1}, \cdots)$$

$$A^{-1} = \begin{pmatrix} A_N^{-1} & & \\ & A_{N-1}^{-1} & \\ & & \ddots \end{pmatrix}$$

$$A_i^{-1} = \frac{1}{H_W^2 + q_i} \begin{pmatrix} H_W & -\sqrt{q_i} \\ -\sqrt{q_i} & -H_W \end{pmatrix} \qquad (i = 1, \ldots, n)$$

Then

$$\begin{aligned} S &= D - CA^{-1}B = D - \sum_i C_i A_i^{-1} B_i \\ &= R\gamma_5 + p_0 H_W + H_W \sum_{i=1}^{N} \frac{p_i}{H_W^2 + q_i}. \end{aligned}$$

Even-odd preconditioning

- Acceleration by solving $(1 - M_{ee}^{-1} M_{eo} M_{oo}^{-1} M_{oe}) x_e = b'$
  - Need fast inversion of the "ee" and "oo" block; easy if there is no projection operator
  - $M_{ee(oo)}^{-1}$ mixes in the 5th direction, while $M_{eo(oe)}$ is confined in the 4D blocks
- Low-mode projection
  - Lower-right corner must be replaced by

$$R(1 - P_H)\gamma_5(1 - P_H) + p_0 H_W + \left(m_0 + \frac{m}{2}\right) \sum_{j=1}^{N_{ev}} \mathrm{sign}(\lambda_j) v_j \otimes v_j^\dagger$$

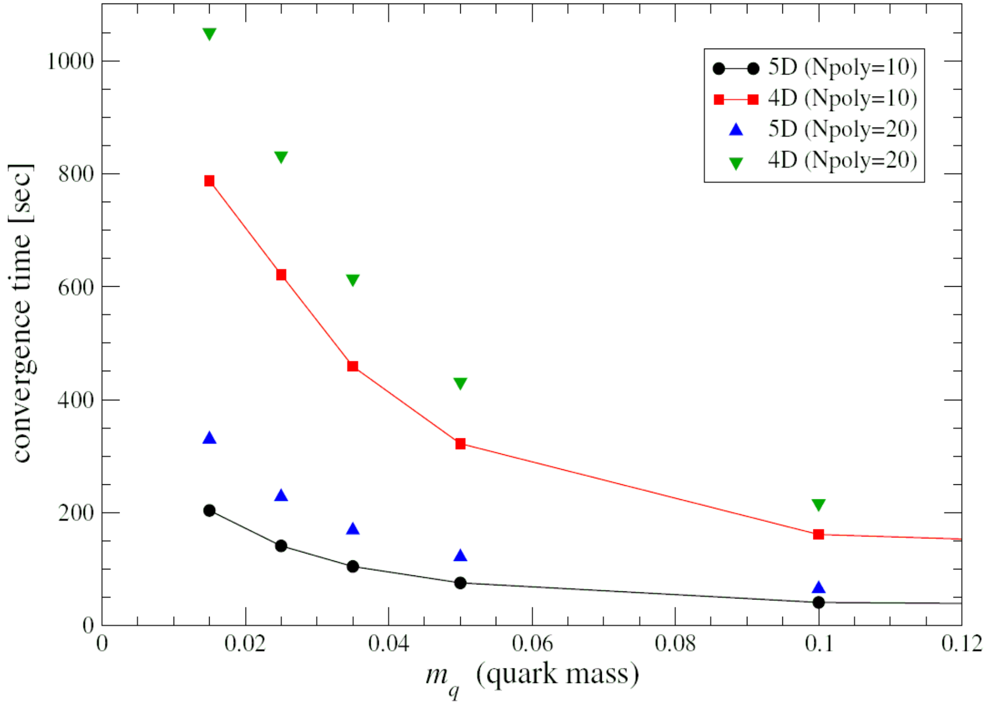
$$P_H = 1 - \sum_{j=1}^{N_{ev}} v_j \otimes v_j^\dagger$$

  - Inversion of $M_{ee(oo)}$ becomes non-trivial, but can be calculated

$$\{x_e, \gamma_5 x_e, v_{je}, \gamma_5 v_{je} (j = 1, \ldots, N_{ev})\}$$

5D solver

- Comparison on 16^3x48 lattice



On BG/L 1024-node

(N_{sbt}=8)

$|r|/|b| < 10^{-10}$

  - 5D solver is 3-4 times faster than 4D solver

Comparison with Domain-wall

- Overlap 5DCG (N=2 case)

$$M_5 = \left(\begin{array}{cccc|c} H_W & -\sqrt{q_2} & & & 0 \\ -\sqrt{q_2} & -H_W & & & \sqrt{p_2} \\ & & H_W & -\sqrt{q_1} & 0 \\ & & -\sqrt{q_1} & -H_W & \sqrt{p_1} \\ \hline 0 & \sqrt{p_2} & 0 & \sqrt{p_1} & R\gamma_5 + p_0 H \end{array}\right)$$

- Domain-wall (N_s=4 case)

$$D_{DW} = \begin{pmatrix} D_W & -P_L & & mP_R \\ -P_R & D_W & -P_L & \\ & -P_R & D_W & -P_L \\ mP_L & & -P_R & D_W \end{pmatrix}$$

Cf. Optimal domain-wall fermion (T.-W. Chiu, 2003)

CG iteration/#D_W-mult for D^{-1}

At $m=m_s/2$, a^{-1}=1.7GeV, 16^3x32/48, up to residual 10^{-10}:

- Overlap(N=10): O(1200) / O(50,000) (m_{res} = 0 MeV)
- DW(Ns=12): O(800) / O(20,000) (m_{res} =2.3 MeV)

(Y.Aoki et al., Phys.Rev.D72,2005)

- Factor ~2.5 difference

Hybrid Monte Carlo algorithm

- Standard algorithm for dynamical simulation
  - Introduce momenta conjugate to link var. U
  - Fermion determinant: pseudo-fermion → external field

$$\det(D^\dagger D) = \int \mathcal{D}\phi^\dagger \mathcal{D}\phi \exp[-\phi(D^\dagger D)^{-1}\phi]$$

  - Hamiltonian governing ficticious time variable

$$\mathcal{H} = \frac{1}{2}\sum_{x,\mu} \mathrm{tr} H_\mu^2(x) + S_G[U] + S_{PF}[U, \phi^\dagger, \phi]$$

  - Molecular dynamics evolution: Hamilton eq.

$$\frac{d}{d\tau}U_\mu(x;\tau) = H_\mu(x;\tau) \qquad \frac{d}{d\tau}H_\mu(x;\tau) = -\frac{\partial}{\partial U_\mu}(S_G + S_{PF})$$

    - Leapfrog integrator (symplectic)

Hybrid Monte Carlo algorithm

- Initial momenta: given by Gaussian distribution
- Fermion field: treated as external field

$$P[\phi] \propto \exp\left[-\phi^\dagger (D^\dagger D)^{-1}\phi\right]$$

$$\leftarrow \;\; P[\xi] \propto \exp\left[-\xi^\dagger \xi\right], \quad \phi = D^\dagger \xi$$

  - ϕ is kept const. During evolution of U and H
- Metropolis test at the end of evolution
  - Eliminate finite step size error $\Rightarrow$ detailed balance
  - Accept new configuration with probability

$$P_{acc} = \min\{1, \exp(-\mathcal{H}[U_{new}] + \mathcal{H}[U_{new}])\}$$

Hybrid Monte Carlo algorithm

- As update algorithm, straightfoward for overlap fermions
  - Except for singularity at $\lambda=0$ (absent in our case)
    - If topology is not fixed, reflection/refraction prescription must be employed --- additional overlap inversion
  - Monitoring low-lying eigenmodes of H_W
    - Implicitly restarted Lanczos algorithm
- Nf=2 simulation
  - 5D solver without projection of low-modes of H_W
  - Noisy Metropolis (Kennedy and Kuti, 1985)

    --> correct error from low modes of H_W
  - At early stage, 4D solver w/o noisy Metropolis (twice slower)
- Nf=2+1 simulation
  - 5D solver with low-mode projection (w/o noisy Metropolis)

Odd number of flavors

Bode et al., 1999, DeGrand and Schaefer, 2006

- $H^2 = D^\dagger(m)D(m)$ commutes with γ_5
  - Decomposition to chiral sectors is possible

$$H^2 = P_+ H^2 P_+ + P_- H^2 P_- \Rightarrow \det H^2 = \det(P_+ H^2 P_+) \cdot \det(P_- H^2 P_-)$$

  - $P_+H^2P_+$ and $P_-H^2P_-$ share eigenvalues except for zero-modes
  - 1-flavor: one chirality sector
  - Zero-mode contribution is constant throughout MC, thus neglected
- Pseudo-fermion: $S_{PF} = \sum_x \phi_\sigma^\dagger(x) Q_\sigma^{-1} \phi_\sigma(x), \quad Q_\sigma = P_\sigma H^2 P_\sigma$

  σ is either + or -
  - Refreshing ϕ from Gaussian distributed ξ as $\phi_\sigma(x) = Q_\sigma^{1/2}\xi(x)$
  - sqrt is performed using a rational approximation
  - Other parts are straightforward

Improving HMC

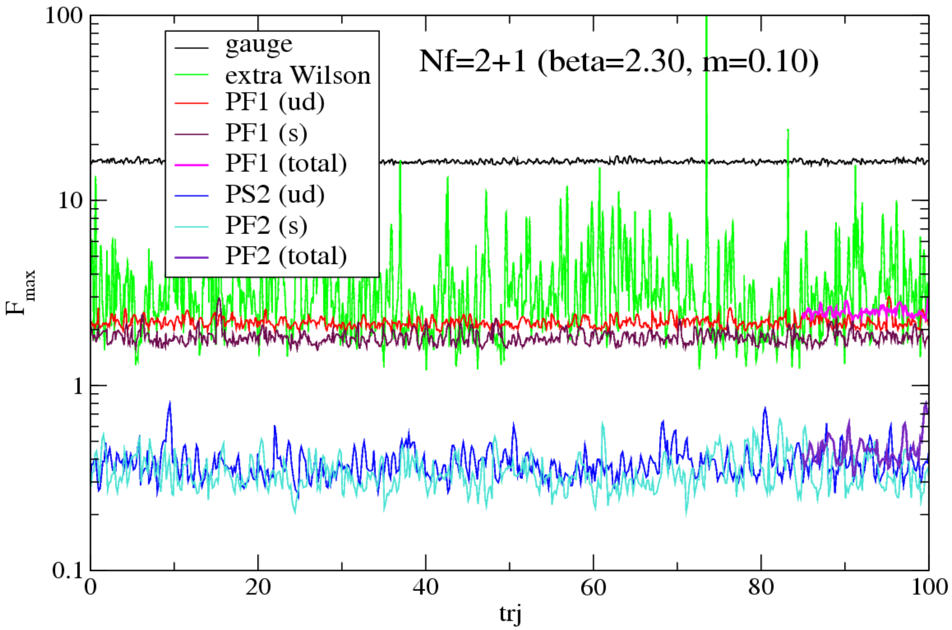
- Mass preconditioning (Hasenbusch, 2001)

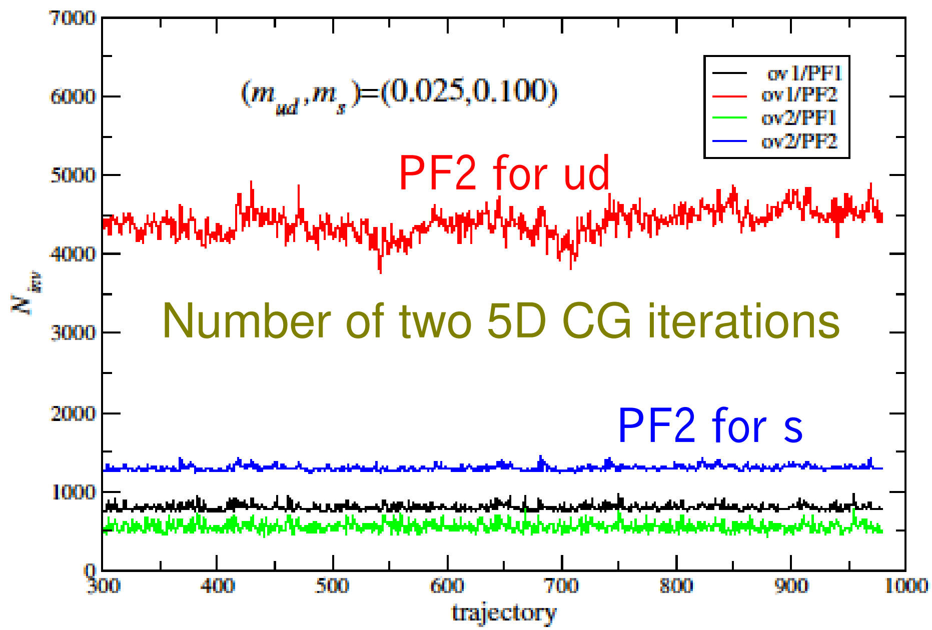
$$S_{ov}^{(1)} = \phi_1^\dagger [D(m')^\dagger D(m')]^{-1} \phi_1,$$
$$S_{ov}^{(2)} = \phi_2^\dagger \left\{ D(m')[D(m)^\dagger D(m)]^{-1} D(m')^\dagger \right\} \phi_2,$$

- Multi-time step (Sexton-Weingarten, 1992)

different time steps for overlap, preconditioner, gauge/exWg

$$F_G \sim F_E \gg F_{PF1} \gg F_{PF2}. \quad \Rightarrow \quad \Delta\tau_{(PF2)} \gg \Delta\tau_{(PF1)} \gg \Delta\tau_{(G)} = \Delta\tau_{(E)}.$$





Omelyan integrator

Omelyan et al., 2002; 2003, Takaishi and de Forcrand, 2006

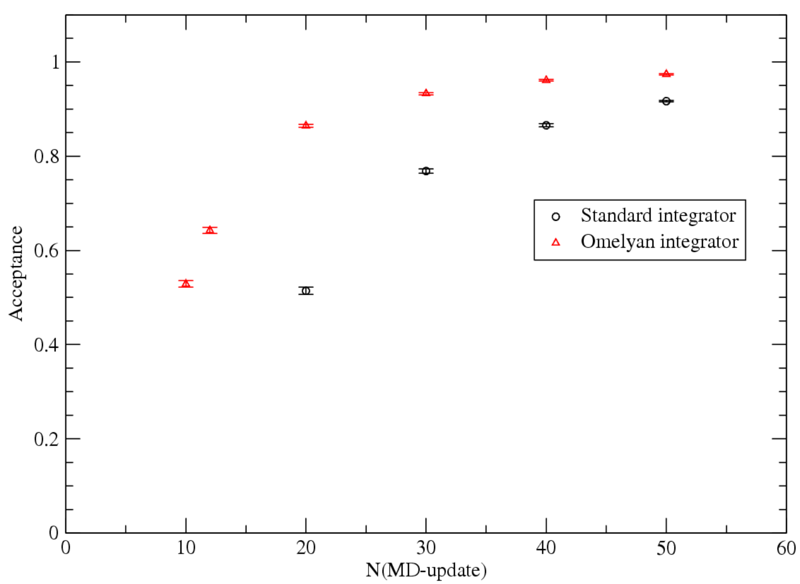
– Standard leapfrog:

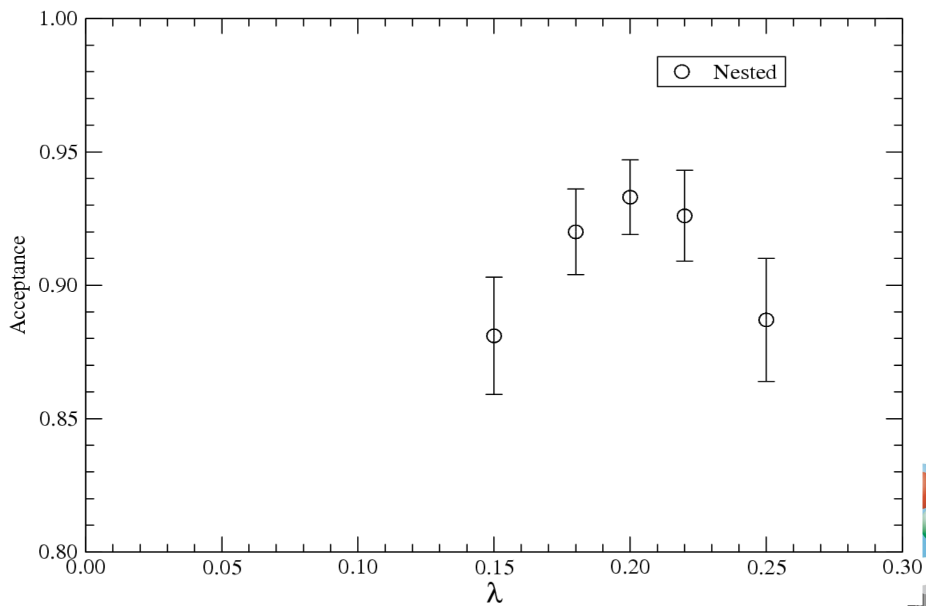
$$e^{\Delta\tau(T+V)} = e^{(1/2)\Delta\tau T} e^{\Delta\tau V} e^{(1/2)\Delta\tau T} + O(\Delta\tau^3)$$

– Integrator proposed by Omelyan et al., 2002; 2003

$$e^{\Delta\tau(T+V)} = e^{\lambda\Delta\tau T} e^{(1/2)\Delta\tau V} e^{(1-2\lambda)\Delta\tau T} e^{(1/2)\Delta\tau V} e^{\lambda\Delta\tau T} + O(\Delta\tau^3)$$

- Discretization error is minimized at $\lambda_c \simeq 0.1932$
- About 1.5 times accelration (test at Nc=2)





Other possible acceleration

- Improved solver algorithm
  - Better solver algorithm ?
  - Multi-grid or domain decomposition ?
  - Adoptive 5D CG solver (change N as solver proceeds)
- Acceleration of HMC
  - Chronological estimator
- Better algorithm to monitor low-lying eigenmodes of H_W

JLQCD's overlap project

Runs

S.Hashimoto, PoS(LAT2008)
H.Matsufuru for JLQCD-TWQCD, PoS(LAT2007)

- Iwasaki gauge (rectangular, RG improved)
- Topology fixing term (with twisted mass ghost: μ=0.2)
- Overlap fermion with m_0=1.6

Nf=2: 16^3x32, a=0.12fm (production run finished)

- 6 quark masses covering (1/6~1) m_s
- 10,000 trajectories with length 0.5
- 20-60 min/traj on BG/L 1024 nodes
- Q=0, Q=−2,−4 ($m_{sea} \sim m_s/2$)
- ε-regime ($m_{sea} \sim$ 3MeV)

Runs

Nf=2+1 : 16^{3}x48, a=0.11fm (production run finished)

- 2 strange quark masses around physical m_s (=0.080, 0.100)
- 5 ud quark masses covering (1/6~1)m_s
- 2500 trajectories with length 1
- About 2 hours/traj on BG/L 1024 nodes
- Q=1 (m_{ud}=0.015, m_s=0.080)

Nf=2+1 : 24^{3}x48 (in progress)

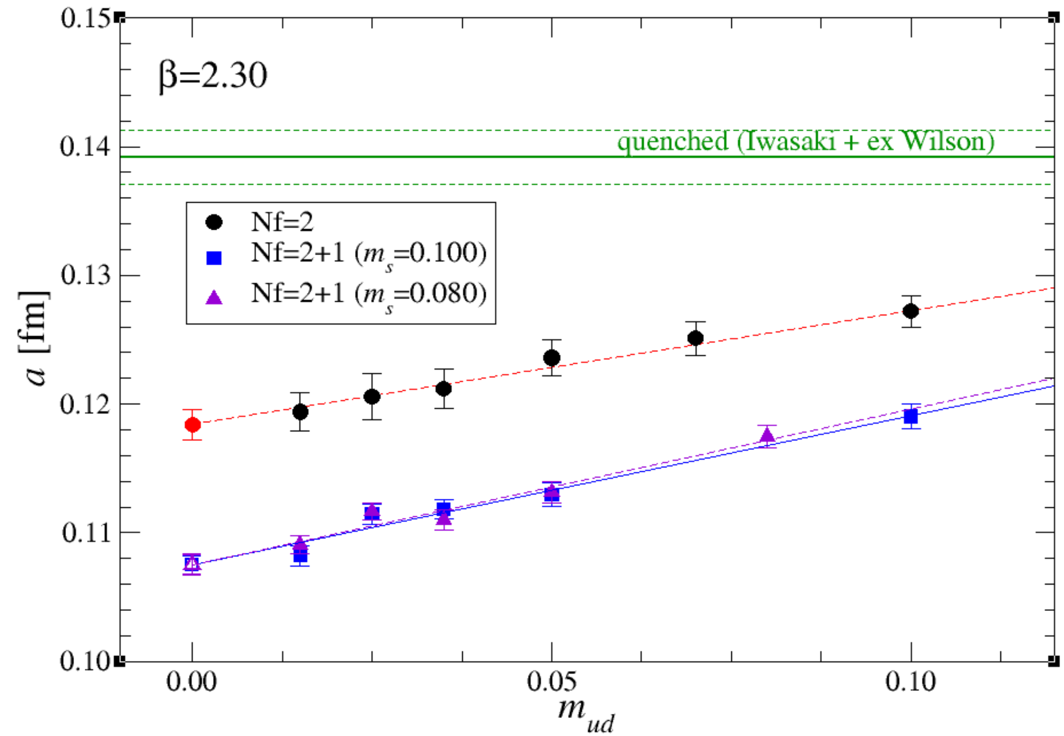
- Same parameters as 16^{3}x48
- m_{ud}=0.015, 0.025, m_s=0.080

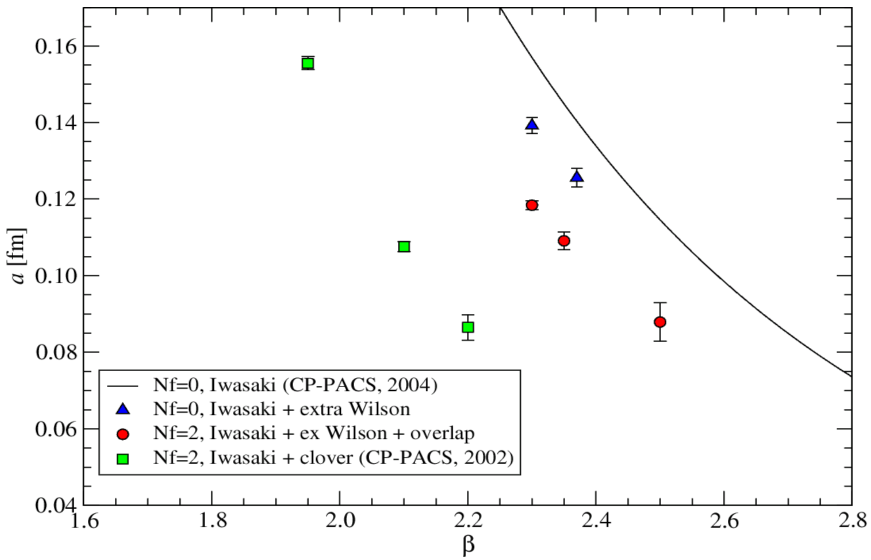
Lattice scale

- Scale: set by r_0 = 0.49fm
  - Static quark potential

$$r^2 \frac{\partial V(r)}{\partial r}\bigg|_{r=r_0} = 1.65$$

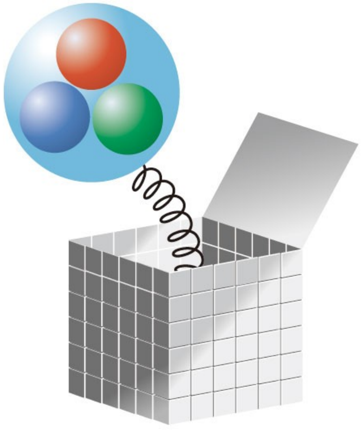
  - Milder β-shift than Wilson-type fermion





Physics results

- Epsilon regime
- Topological susceptibility
- Meson spectrum and ChPT test



Chiral condensate

- Banks-Casher relation (Banks & Casher, 1980)

$$\Sigma = \langle \bar{q}q \rangle = \lim_{m\to 0} \lim_{V\to\infty} \frac{\pi\rho(0)}{V}$$

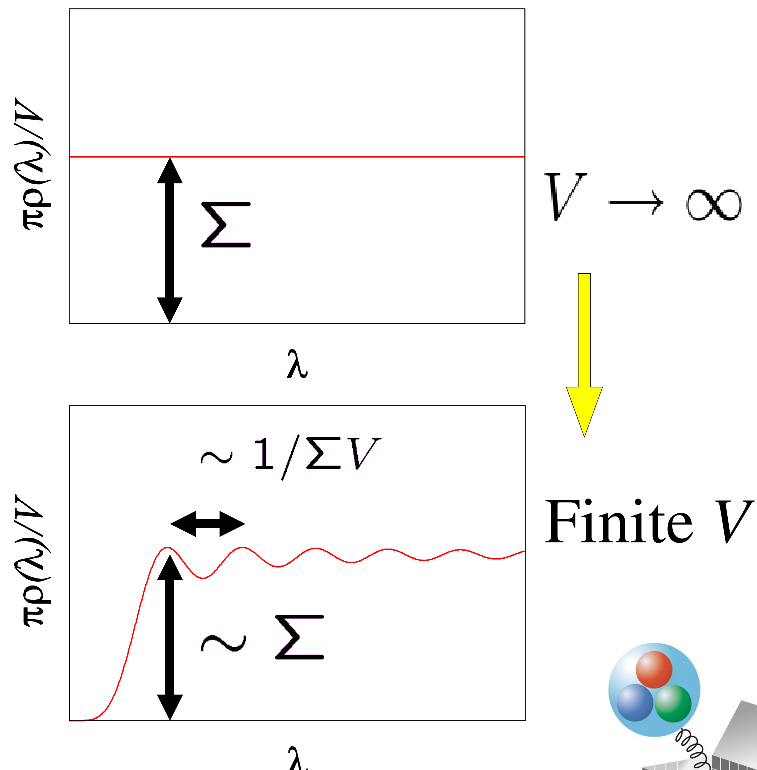
$\rho(\lambda) = \sum_k \langle \delta(\lambda - \lambda_k) \rangle$: spectral density of D

  - Accumulation of low modes $\Longleftrightarrow$ Chiral SSB
  - $V \to \infty$, then $m \to 0$

- ε-regime: $m << 1/\Sigma V$ at finite V

$$1/\Lambda_{QCD} \ll L \ll 1/m_\pi$$

  - Low-energy effective theory
  - Q-dependence is manifest
  - Random Matrix Theory (RMT)



ε-regime

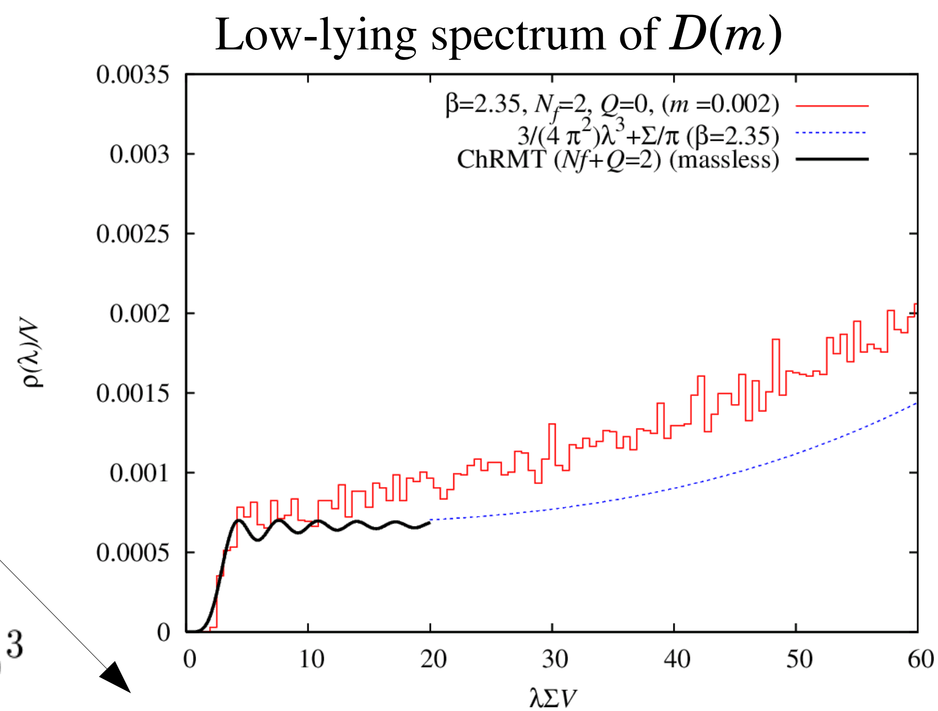
(JLQCD, 2007, JLQCD and TWQCD, 2007)

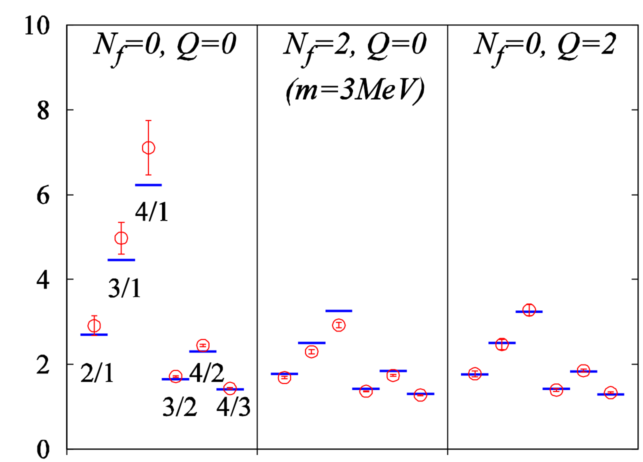
- Nf=2, 16^3x32, a=0.11fm
- m~3MeV

- Good agreement with RMT
  - lowest level distrib. $\longrightarrow \Sigma$
  - Flavor-topology duality
- Chiral condensate:
  - Nonperturbative renorm.

$$\Sigma^{\overline{MS}}(2\,\mathrm{GeV}) = (251 \pm 7(\mathrm{stat}) \pm 11(\mathrm{syst})\,\mathrm{MeV})^3$$

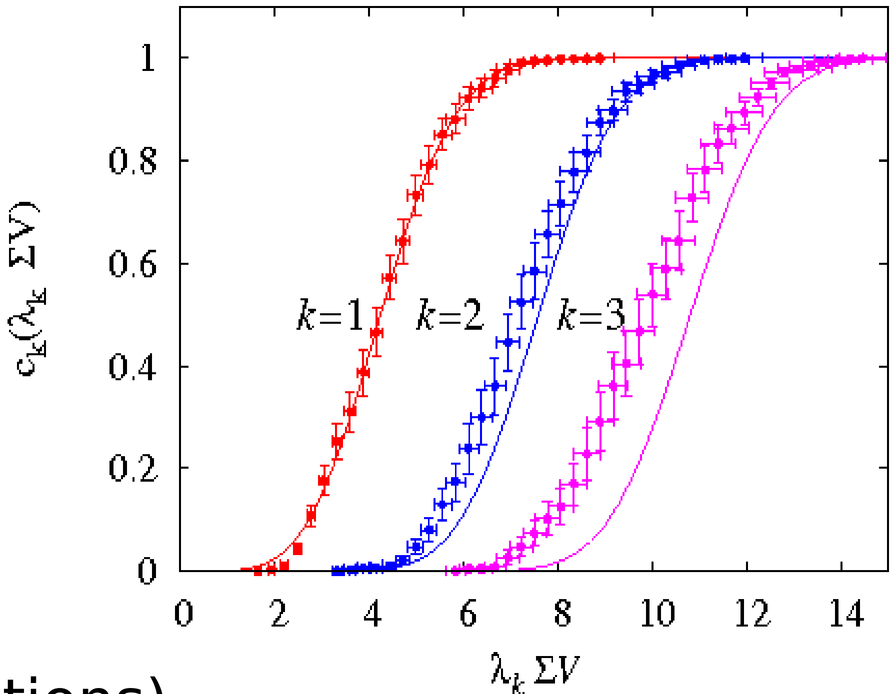
$O(\varepsilon^2)$ effect: correctable by meson correlator





Result in the ε-regime

- Low-lying mode distribution



- Matching with ChRMT
  - Σ=[251(7)(11) MeV]^3 (distributions)
  - Σ=[240(4)(7) MeV]^3 (correlators)
- Extension to *p*-regime is in progress

Damgaard and Fukaya (2009)

  - Nf=2+1
  - Reanalyzing Nf=2 data

Topological susceptibility

JLQCD-TWQCD, PLB665(2008)294; PoS(Lattice2008)072

Is local topological fluctuation sufficient ?

- In the infinite V limit,
  - Fixing topology is irrelevant
  - Local fluctuation of topology is responsible to physics
- In practice V is finite
  - Topology fixing $\Rightarrow$ finite V effect
  - θ=0 physics can be reconstructed
  - Must check local topological fluctuation

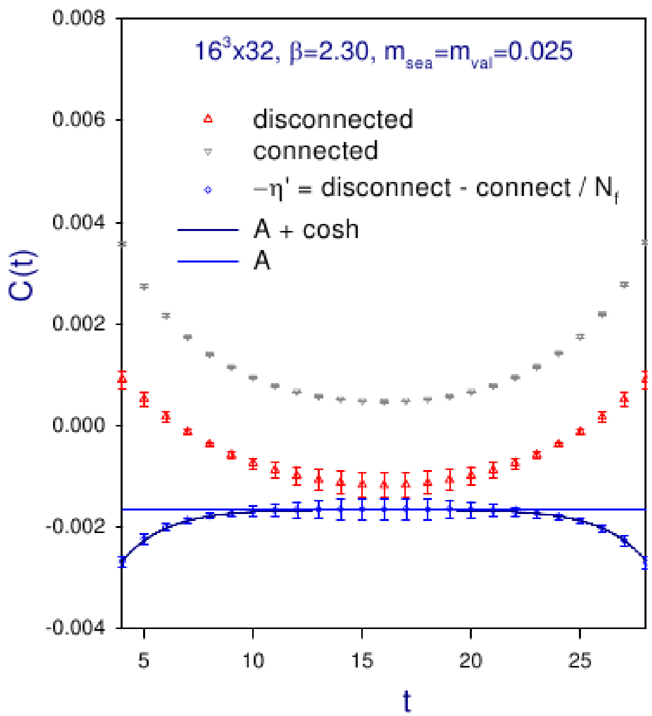
$\Rightarrow$ topological susceptibility, η' mass

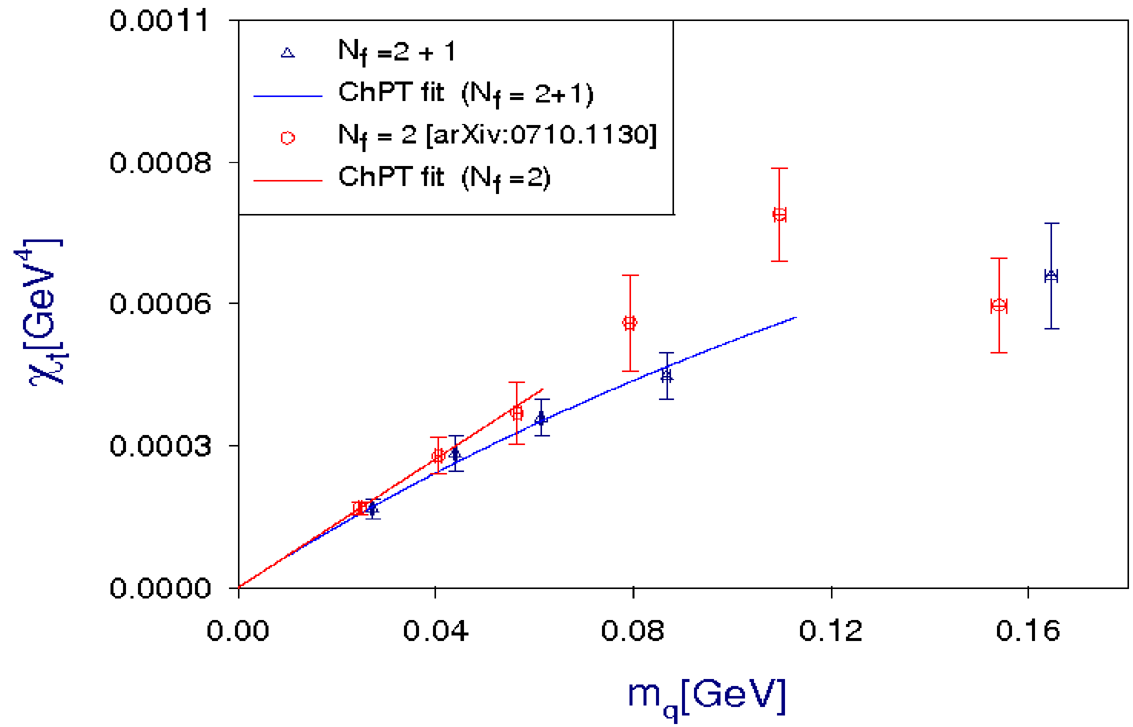
Topological susceptibility

- Topological susceptibility χ_t can be extracted from correlation functions (Aoki et al., 2007)

$$\frac{1}{L^3}\langle mP^0(\vec{x},t)mP^0(\vec{0},0)\rangle_Q \underset{t\gg 1}{\rightarrow} \frac{1}{V}\left[\frac{Q^2}{V} - \chi_t - \frac{c_4}{2\chi_t V}\right] + O(V^{-3}) + O(e^{-m_{\eta'}t})$$

where $$P^0 \equiv \frac{1}{N_f}\sum_{f=1}^{N_f} \bar{q}_f \gamma_5 \left(1 - \frac{D}{2m_0}\right) q_f$$





Topological susceptibility

- Fit with NLO ChPT prediction
  - Σ=[245(5)(10) MeV]^3 (Nf=2)
  - Σ=[240(5)(2) MeV]^3 (Nf=2+1, m_s=0.100)
- Good agreement with other approaches (epsilon regime, meson spectrum)
  - Local fluctuation is enough active
  - Volume is sufficiently large

(The quoted value of Σ for Nf=2+1 was replaced with correct value after seminar.)

Meson spectrum

"Touchstone" for quantitative measurements

- Controlled chiral extrapolation ?
- Is finite volume effects under cotrol ?
  - Fixed topology effect as well as ordinary one
- Is consistent with chiral perturbation theory ?
  - Virtue of overlap: continuum formulae are applicable
  - Extraction of low energy constants
  - Which expansion parameter is efficient ?
- How large is strange quark effect ?

Nf=2: JLQCD-TWQCD (Noaki et al.), PRL 101 (2008)202004
Nf=2+1: JLQCD-TWQCD (Noaki et al.), arXiv:0810.1360

Getting data

- Improvements with low-lying modes

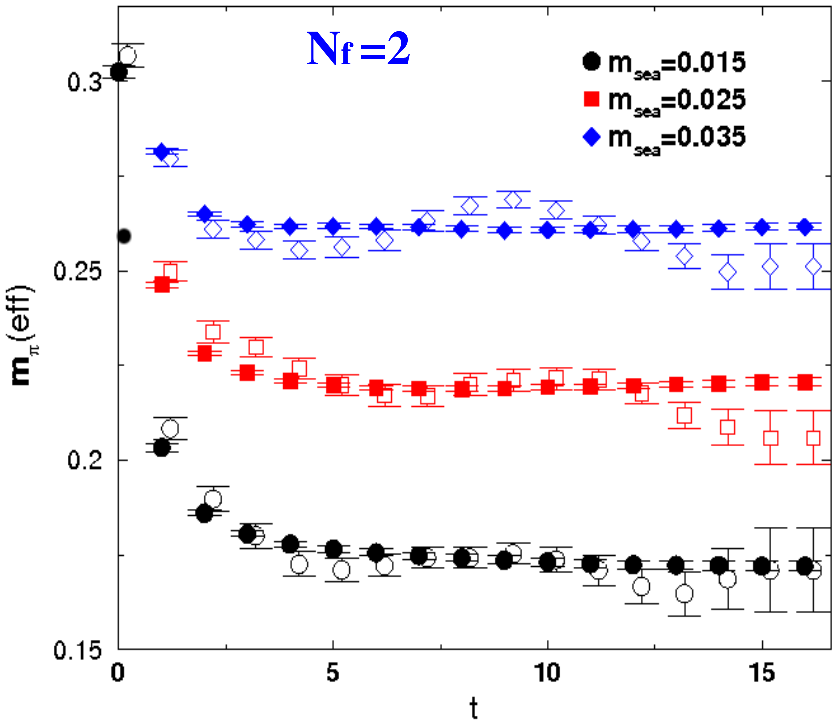
  Giusti et al., 2003; DeGrand & Schaefer, 2004

$$D_{ov} v_j = \lambda_j v_j$$

$$S_q(x,y) = \boxed{\sum_{j=1}^{N_{ev}} \frac{v_j(x) v_j^\dagger(y)}{\lambda_j + m}} + S_q^{high}(x,y)$$

$$C(t) = C^{HH}(t) + C^{HL}(t) + C^{LH}(t) + \boxed{C^{LL}(t)}$$

averaging



  - 50 lowest conjugate pairs of eigenmodes
  - Improvement of signal
  - Accelerating solver (8 times faster)

- Nonperturbative renormalization (RI-MOM scheme)

  Martinelli et al., 1995

Finite volume correction

$$\left(m_\pi^2\right)^{\text{corrected}} = \frac{m_\pi^2}{(1+R_m)^2(1+T_m)^2}, \qquad (f_\pi)^{\text{corrected}} = \frac{f_\pi}{(1+R_f)(1+T_f)}$$

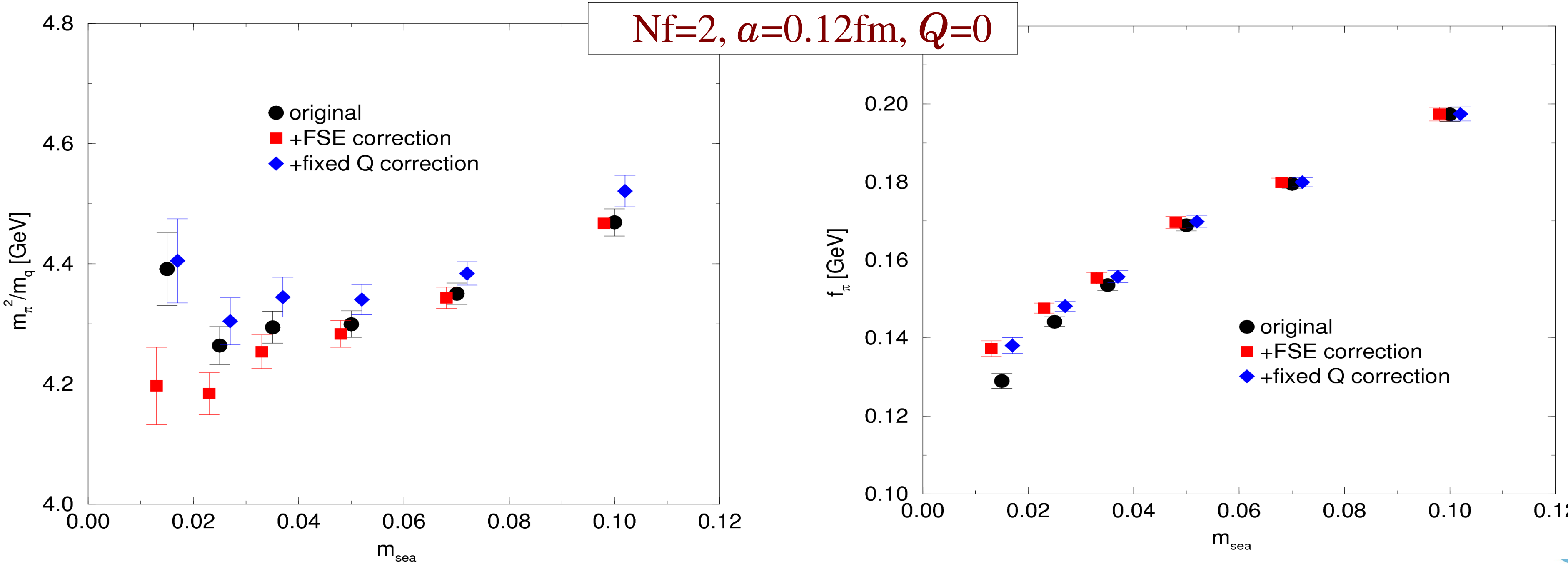
- R: ordinary finite size effect (Luscher's formula)

  Estimated using two-loop ChPT (Colangelo et al, 2005)

- T: Fixed topology effect (Aoki et al, 2007)

– At most 5% effect --- largely cancel between R and T

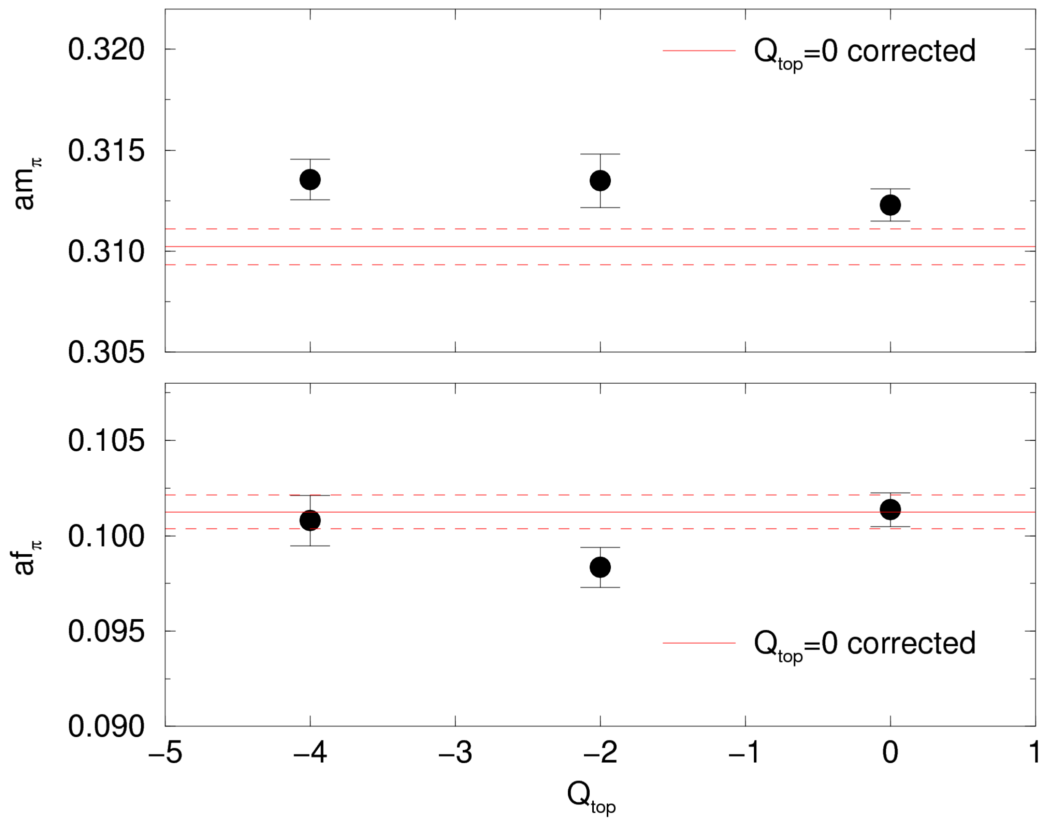
Nf=2, a=0.12fm, Q=0



Q-dependnece

Nf=2, m_{sea} = 0.050 Q = 0, -2, -4

- No large Q-dependence (consistent with expectation)



Nf=2 NLO ChPT

Region of convergence

- NLO formulae:

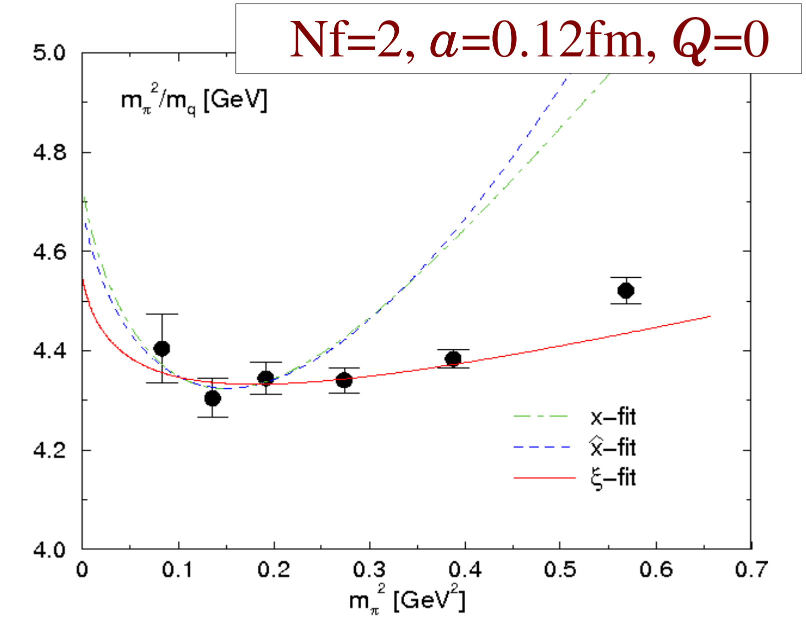
$$\frac{m_\pi^2}{m_q} = 2B[1 + x\ln(x) + c_3 x + O(x^2)]$$

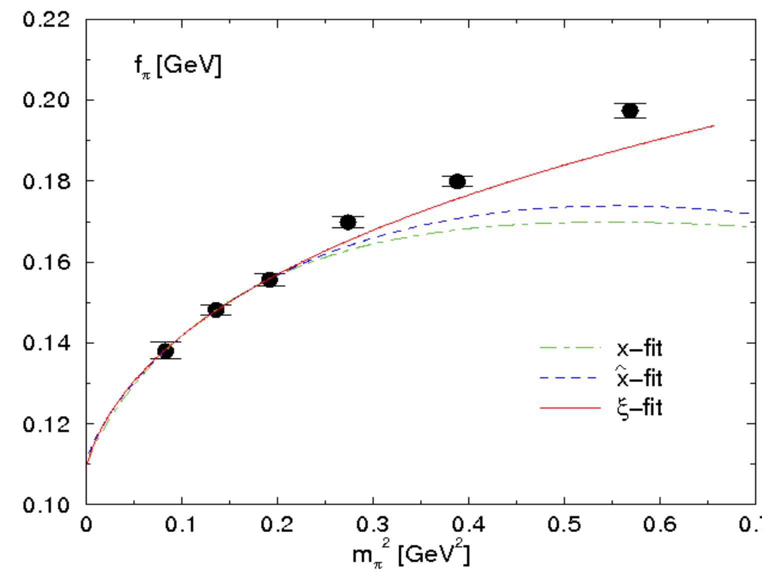
$$f_\pi = f[1 - 2x\ln(x) + c_4 x + O(x^2)]$$

- Expand either with

$$x \equiv \frac{m^2}{(4\pi f)^2},\ \hat{x} \equiv \frac{m_\pi^2}{(4\pi f)^2},\ \xi \equiv \frac{m_\pi^2}{(4\pi f_\pi)^2}$$

- At NLO, not converged beyond m_π~450 MeV
- ξ Expands the region significantly (resummation from f_π)



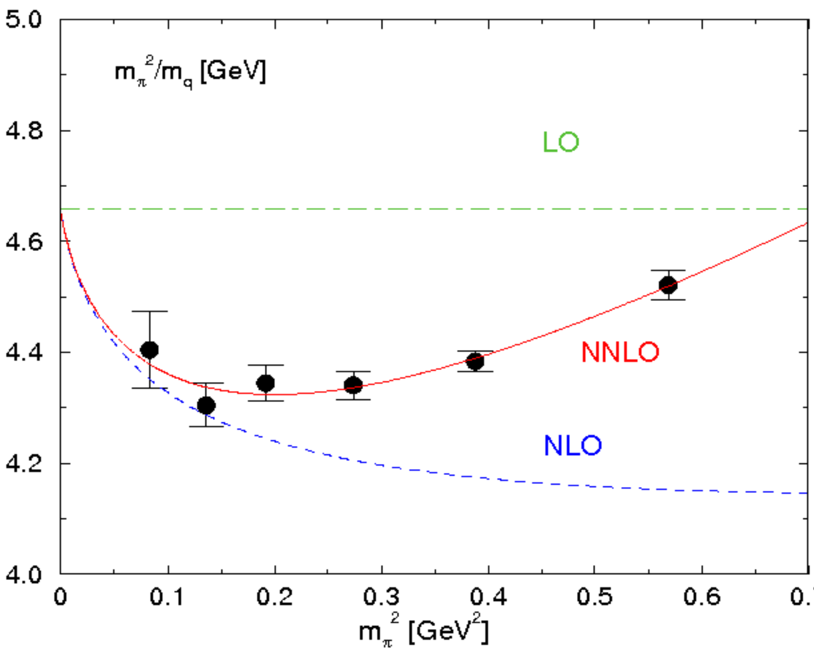


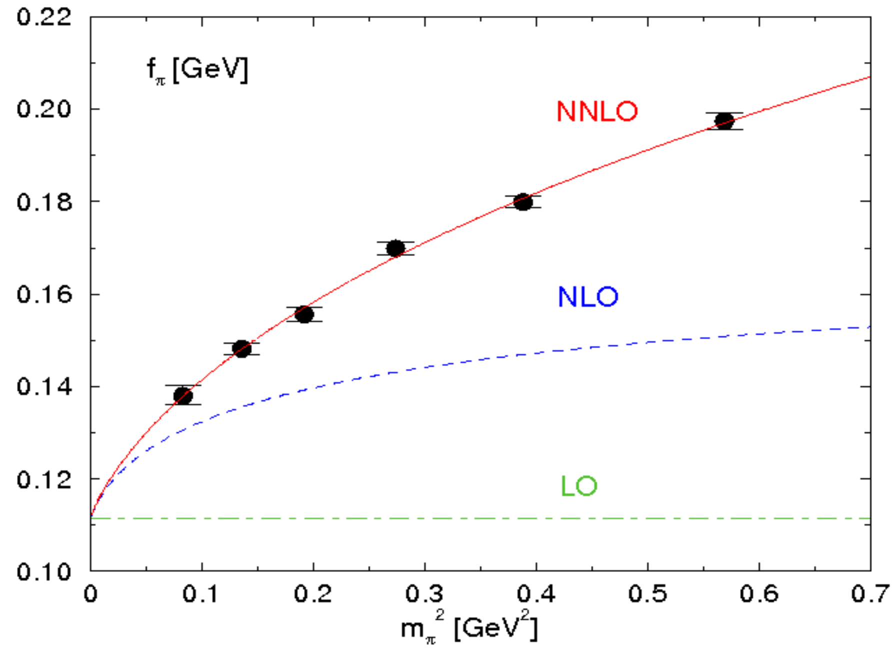
Nf = 2, NNLO ChPT

- NNLO: 2-loop effects and analytic terms (full NNLO)

Colangelo et al., 2001

  - Input: $7l^r_1+8l^r_2$, ambiguity took into account
  - Simultaneous correlated fit: 6x2=12 data points, 6 parameters





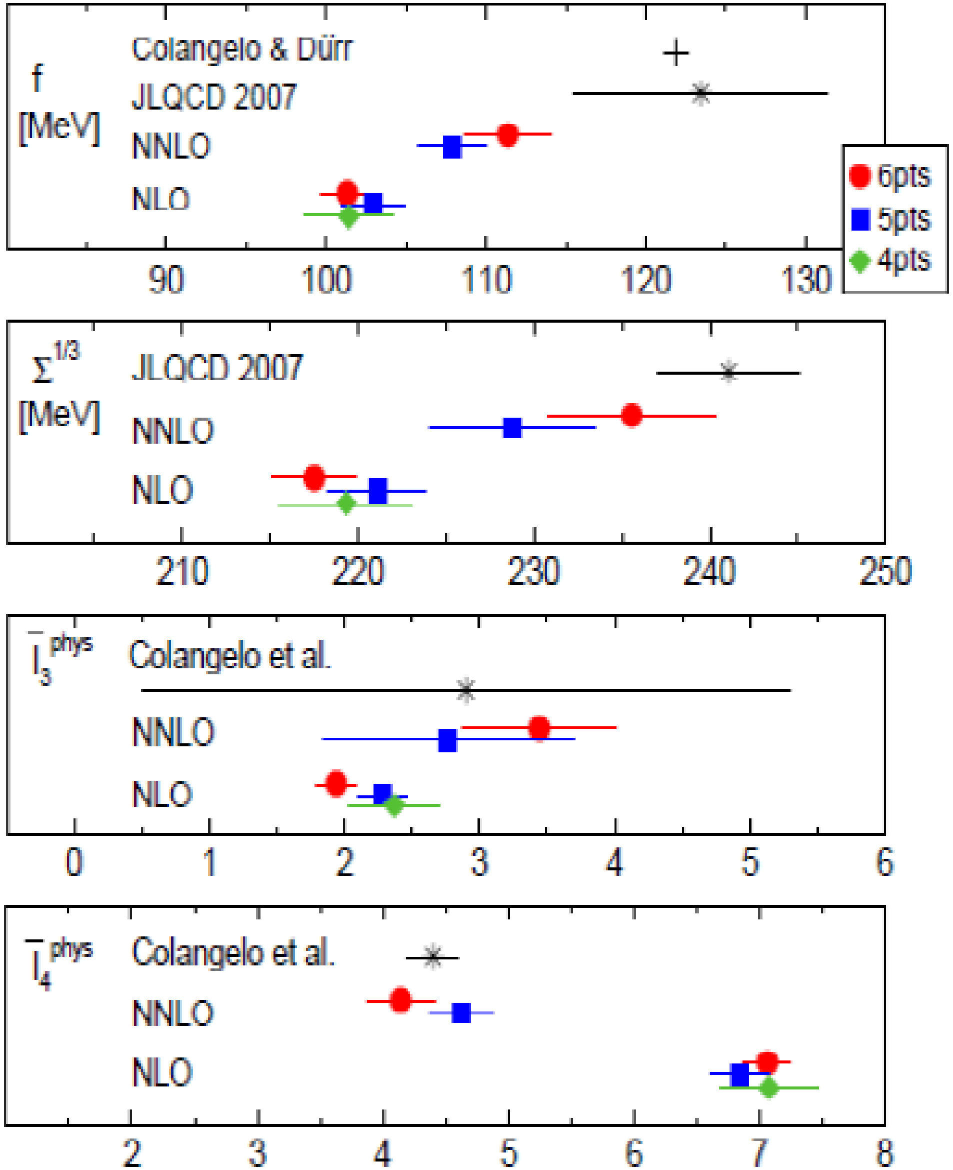
NNLO converges well and gives consistent values of f and Σ with other approaches.

Meson spectrum: low energy consts

Low energy constants

--- NNLO fit with ξ

For reliable extraction of low energy constant, NNLO terms are mandatory
(For NLO even fit is possible,
result is not reliable)



Extension to Nf=2+1

- How to treat K mesons (m_K^2, f_K) ?
  - Apply NNLO (SU(3) ChPT, natural extension)
  - Apply NLO within m_{ud} << m_s

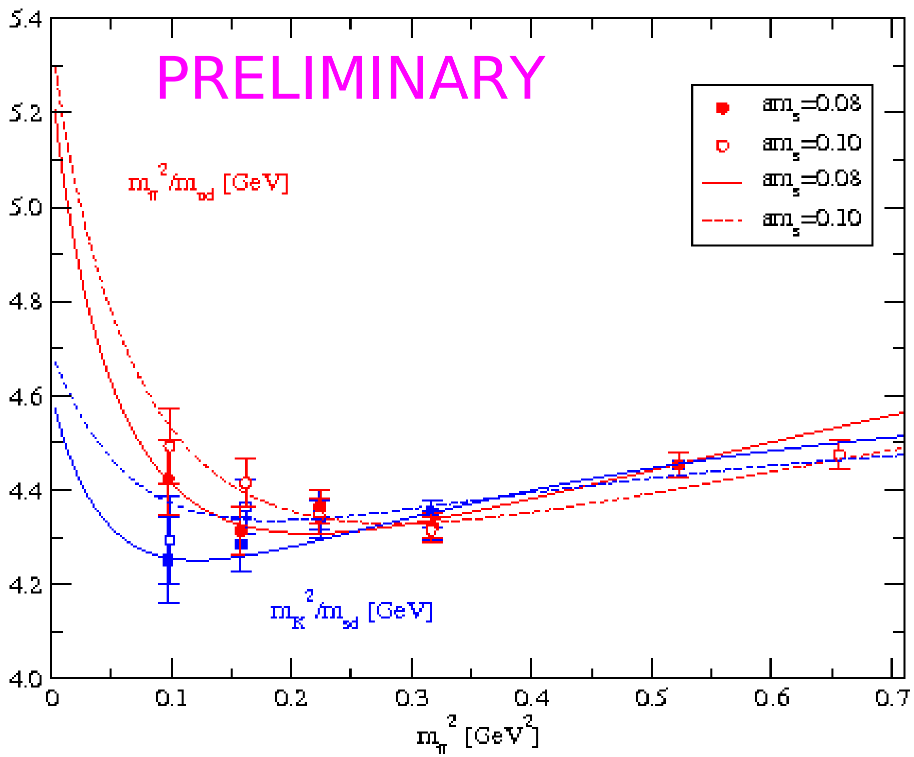
    Integrate out strange quark a → reduced SU(2) ChPT

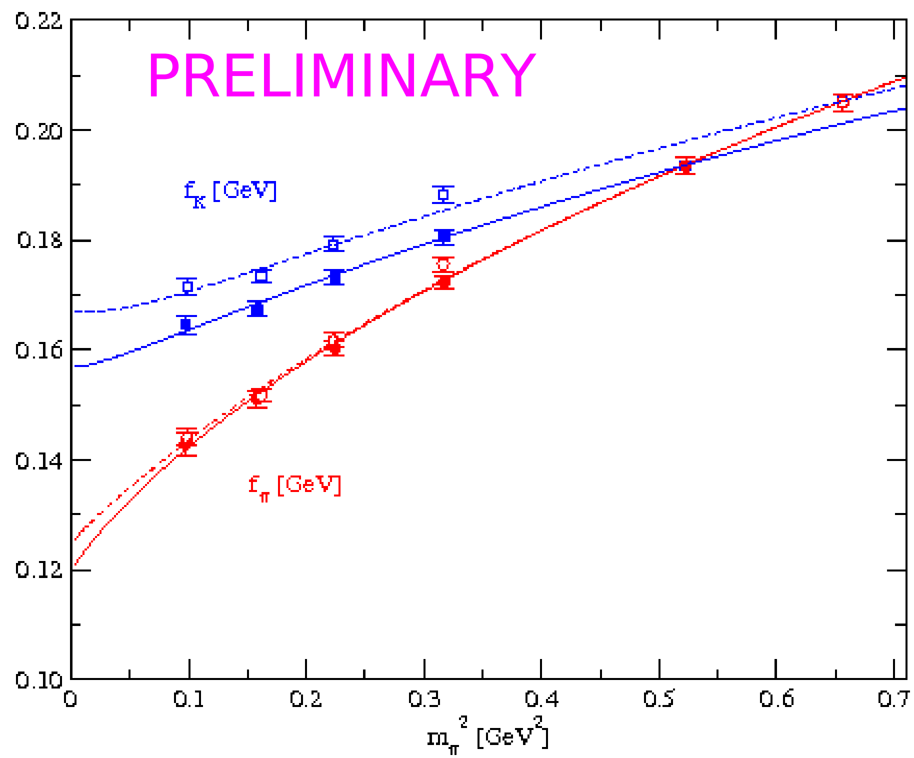
    Gasser *et al.*, 2007; RBC+UKQCD, 2008; PACS-CS, 2008

- Our meson spectroscopy at 2+1 flavors:
  - 2 values of m_s
  - 5 ud masses for each m_s: 310 MeV < m_π < 800 MeV
  - L=1.8 fm, 1/a=1.83GeV, 16^3x48 lattice
  - 80 conjugate pairs of eigenmodes
  - Nonperturbative renormalization
  - Finite volume effects (Luscher's formula/fixed topology)

Nf =2+1, NNLO SU(3) ChPT

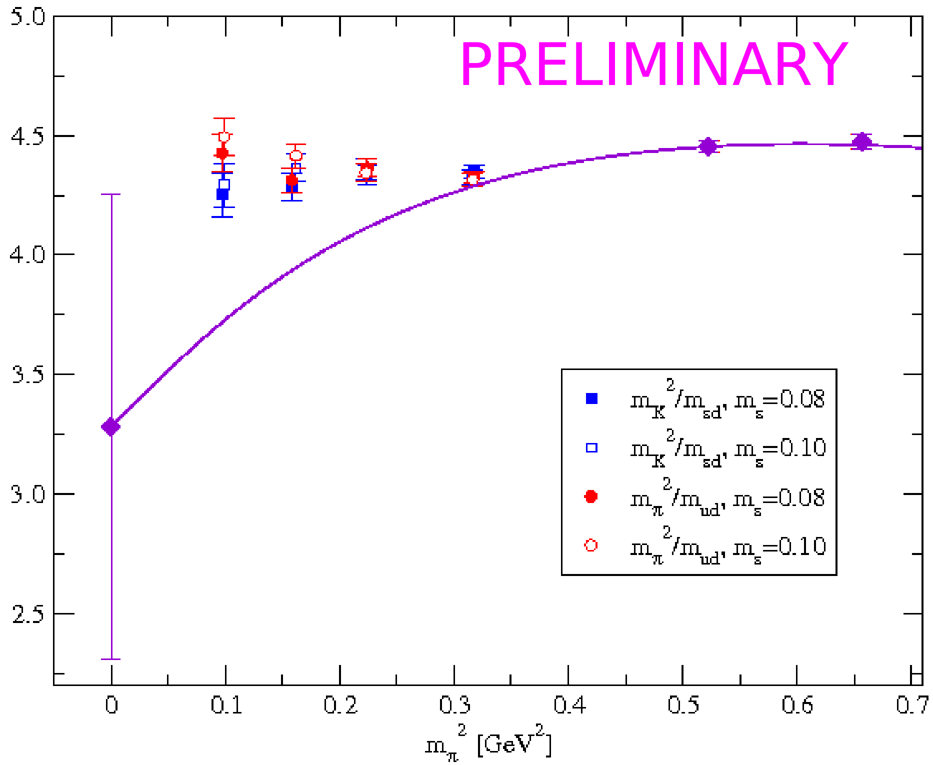
- 2-loop + analytic terms Amoros et al., 2000
  - input: $L^r{}_1, L^r{}_2, L^r{}_3, L^r{}_7$ -- uncertainty gives small syst. errors
  - 4x10–4 = 36 data points, 16 parameters
  - Expansion in $\xi_\pi=(m_\pi/(4\pi f_\pi))^2$, $\xi_K=(m_K/(4\pi f_\pi))^2$
  - Correlated simultaneous fit: χ^2/dof = 1.58

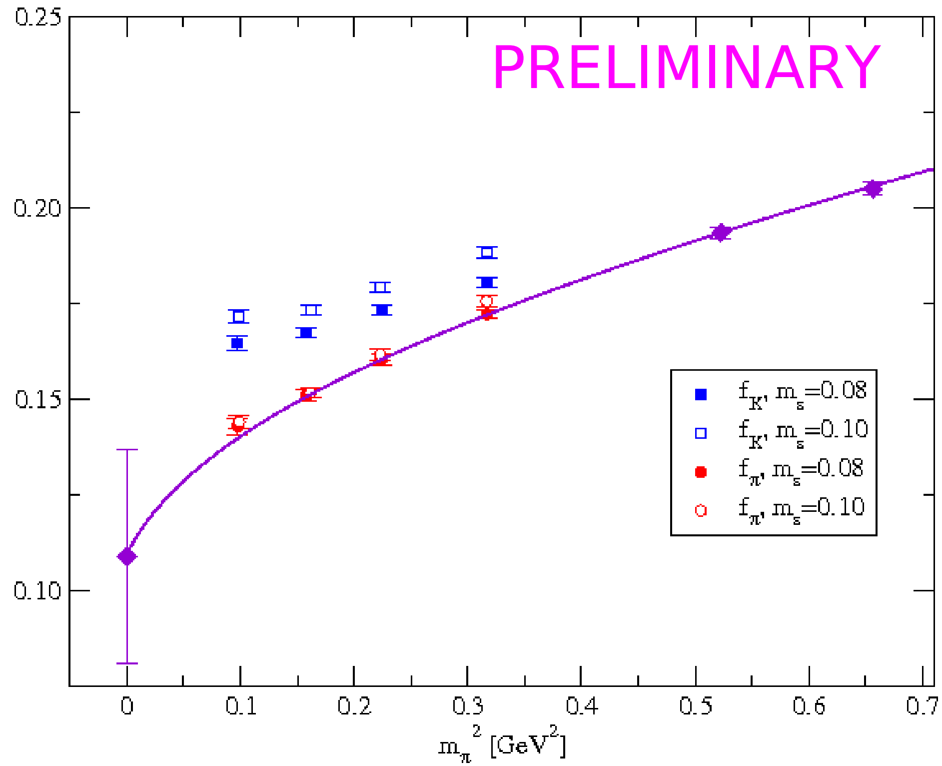




Ambiguity in SU(3) limit

- By putting $m_{ud}=m_s$





- Lowest order low energy constants B_0, f_0 are not determined
  (Lack of data for strange mass dependence)
- Can be solved only by other simulations at degenerate masses

2+1 fit results

- Preliminary results

f_0 = 109(28) MeV
Σ_0 = [213.5(6.9) MeV]^3
$L^r_4(m_\rho)$ = -1.09(19) x 10^{-3}
$L^r_5(m_\rho)$ = -9.00(97) x 10^{-4}
$L^r_6(m_\rho)$ = -3.64(75) x 10^{-4}
$L^r_8(m_\rho)$ = 6.23(92) x 10^{-4}

m_{ud}(2GeV) = 4.05(27) MeV
m_s(2GeV) = 109.8(2.4) MeV
f_π = 124.8(2.8) MeV
f_K = 156.0(2.7) MeV
f_K/f_π = 1.249(17)

  - Only way to determine LEC in SU(3) ChPT
  - So far no other lattice calculation including NNLO
- Reduced SU(2) ChPT
  - Reduced SU(2) $\Rightarrow$ LECs in SU(2) ChPT
  - Roughly consistent with previous analysis in Nf=2
- $24^3 \times 48$ lattice will confirm finite size effect

Other results

Cf. http://jlqcd.kek.jp/

- Nonperturbative renormalization
- Kaon bag parameter B_K
- Vacuum polarization function
  - π^+-π^0 mass difference
  - Strong coupling const
  - S-parameter
- Nucleon structure
  - Nucleon sigma term
  - S-quark content (y-parameter)
- Pion form factors

Summary/outlook

- Overlap fermion has elegant chiral structure
- Numerical cost is high, but can be simulated
- JLQCD is performing large dynamical overlap project at Nf=2 and 2+1
- Rich physics results are being produced

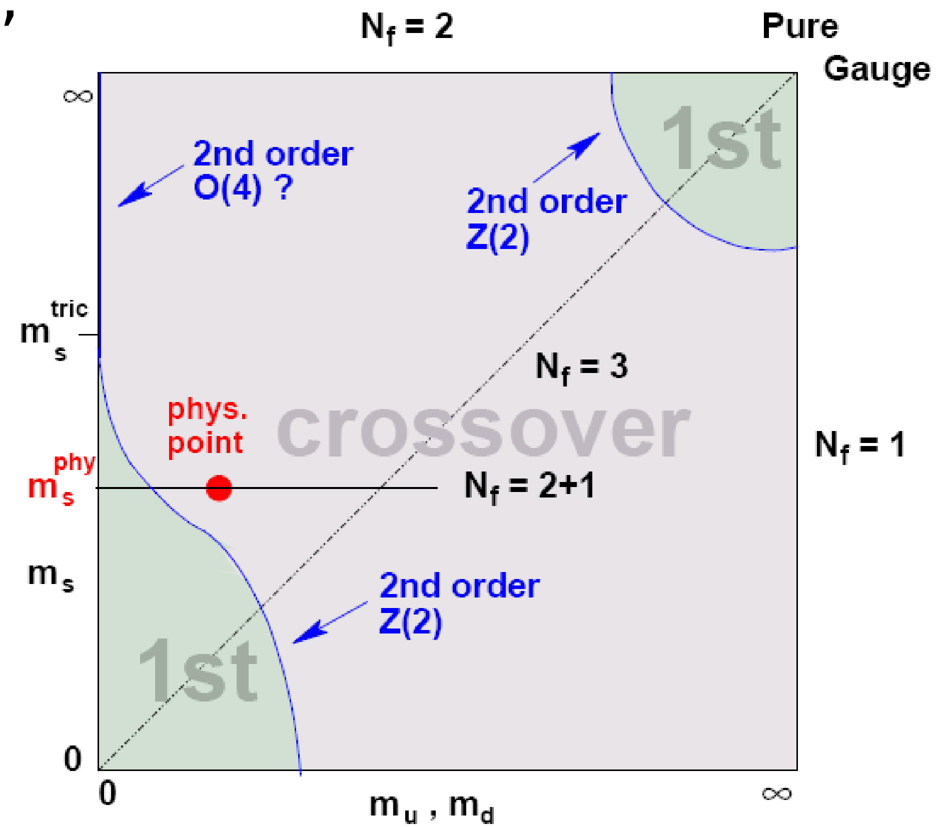
Outlook

- Run on larger lattice (L=24) in progress
- Simulation at finite temperature is challenging
- Beyond QCD simulations are interesting

Lattice QCD at T>0 (μ>0)

Now popular phase diagram, but;

- How reliable?
- Consistency check enough?



(DeTar, Lattice 2008)

Nf=2

- KS fermion does not exhibit expected O(4) scaling
- Wilson quark shows O(4), but at rather heavy masses
- Most recent works are by KS, Nt=4.

Nf=2+1 (physical point)

- Really crossover ? [(old) Wilson result is of 1st order]
- Recently only with KS fermions, still large uncertainty

Beyond QCD

Motivation:

- Technicolor ?
- Phase structure of (lattice) gauge theories
- Advantages of exact chiral symmetry

Beyond QCD applications

- Large Nf
- Non-fundamental representations (adjoint, etc.)
- Nc not 3
- Are confinement and broken chiral symmetry occur simultaneously ?

Machine prospect

- Lattice QCD has been an application which requires most large computational resources
- Growth of computational power → new era of lattice simulations
- Around 2010, ~10PFlops expected
  - Next generation supercomputer project (10TFlops in 2011?)
  - Two projects in USA
- Other architecture
  - GPGPU (NVIDIA, etc)
  - CELL
  - Other arithmetic accelerators
  - Needs better algorithms