Dynamical QCD with exact chiral symmetry — from the *p*-regime to the ε-regime

Shoji Hashimoto (KEK)

@ “Domain Wall Fermions at Ten Years”,
BNL, Mar 15, 2007

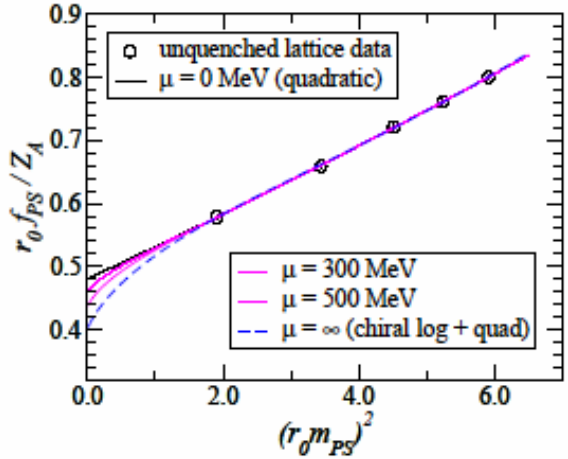
Boston 2002

Panel discussion on chiral extrapolation (chaired by S. Sharpe)

- Chiral log not seen.
- Sea quark masses too large for controlled extrapolation.
  - Introduce a model dependence.
  - Extraction of LECs unreliable.

- Maybe, the standard χPT not applied for Wilson fermion (nor staggered)

JLQCD (2002)
Nf=2 improved Wilson fermion



Motivation for

- much lighter sea quarks
- exact chiral symmetry

Advantages

With the overlap fermion…,

- Standard χPT applicable.
  - No need of "continuum limit before chiral limit"
  - No need of WχPT, SχPT = fitting with many parameters
- Chiral limit exists.
  - Not the case for Wilson-type fermions = unphysical 1st order phase transition before reaching the chiral limit (Sharpe-Singleton).
- ε-regime possible.
  - New frontier. No chiral extrapolation needed..

All at finite a

Why not domain-wall?

Far better than Wilson/staggered. Still…,

- Approximate chiral symmetry
  - The problems we just discussed may persist to some extent (tiny but non-zero).
- Flexibility
  - More opportunity of improvement for overlap; even the 5D solver can be used.

- RBC has already done a tremendous job with domain-wall!

Expensive?

Yes. Cost is the problem. But,

Stag < Wil << DW < ov

naively…, x 4 x L_s x ??

Need continuum extrap.
for controlled chiral extrap.

Chiral/continuum limit
much straightforward

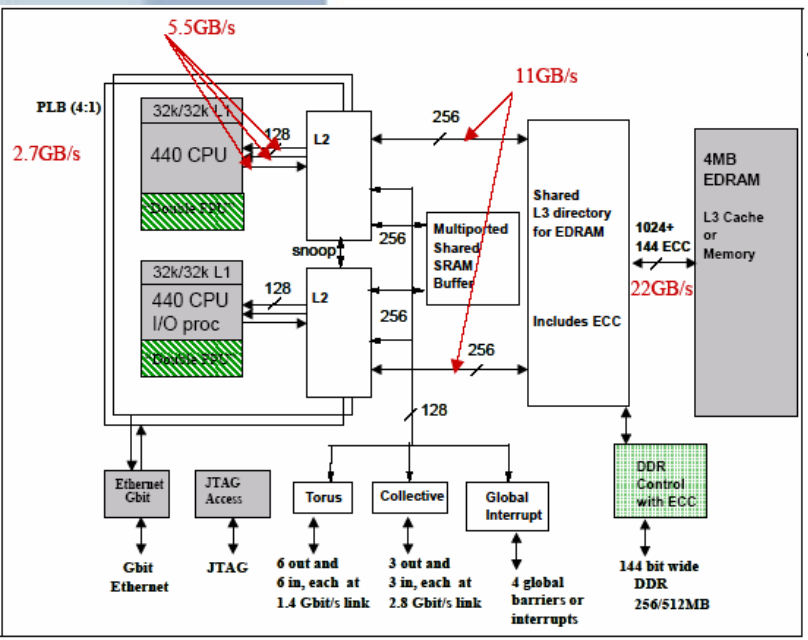
JLQCD collaboration

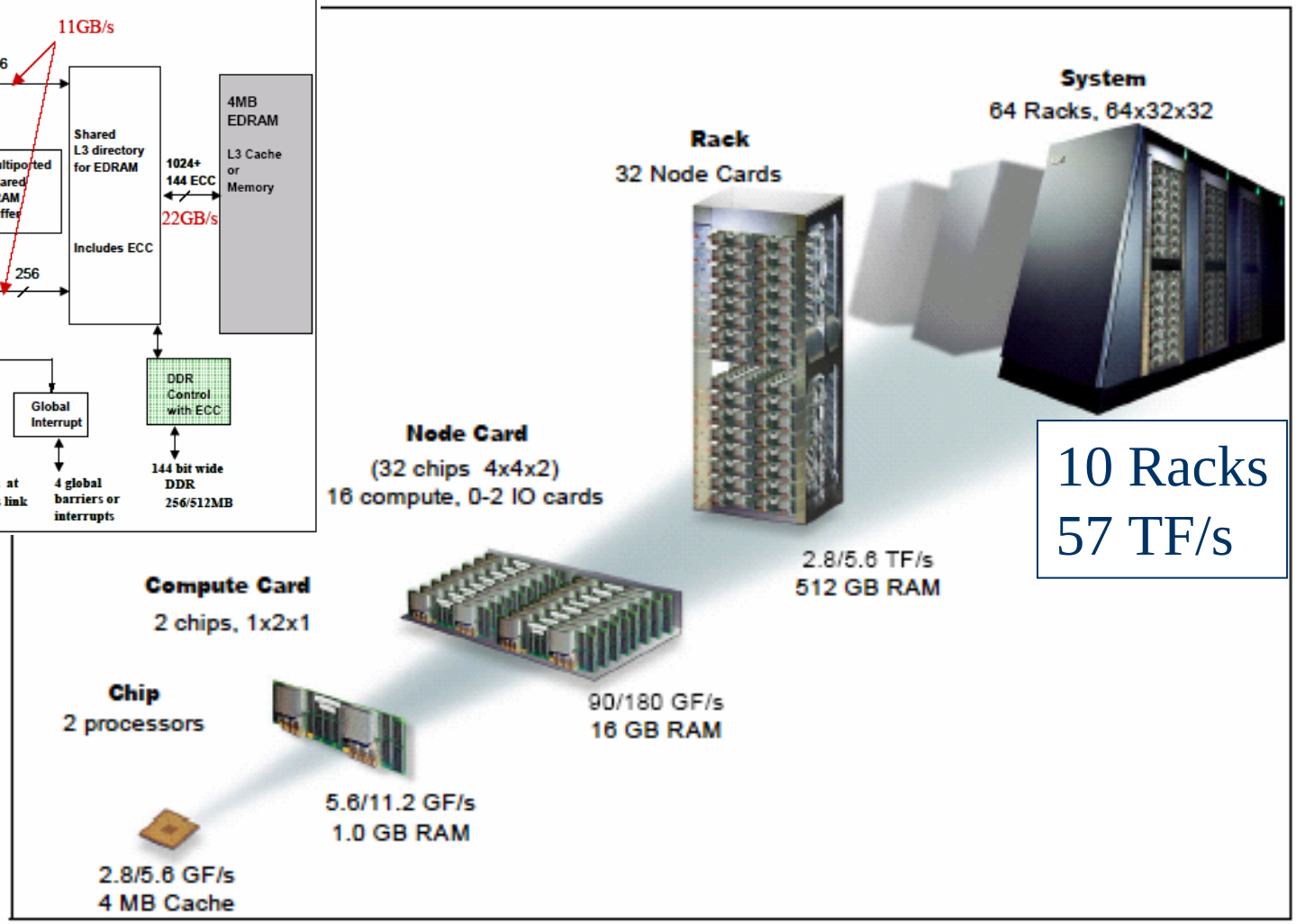
- Members from
  - KEK, Tsukuba, RIKEN, Kyoto
  - Collaboration with TWQCD, Seoul
- New machine at KEK
  - Since March 2006.
  - Hitachi SR11000, 16 nodes, 2.15 TFlops peak.
  - IBM BlueGene/L 10 racks, 57 TFlops peak.

Dynamical overlap

- Two-flavor QCD
  - $a \cong 0.12$ fm, 16^3x32
  - $m_q = m_s/6 \sim m_s$
  - 10,000 HMC traj done at 6 m_q
  - measurements on-going
- ε-regime (two-flavor)
  - $a \cong 0.12$ fm, 16^3x32
  - $m_q = 3$ MeV
  - 4,600 HMC traj. done

IBM BlueGene/L





10 Racks
57 TF/s

Plan of this talk

1. Overlap-Dirac operator
   - Spectrum of H_W
   - Topology conserving action
   - Topology issues
   - Locality
2. Dynamical overlap
   - Implementation/ improvement
3. Pions and Kaons
   - Low-Mode Preconditioning
   - Low-Mode Averaging
   - Chiral log
   - Other targets
4. ε-regime
   - Simulations
   - Eigenvalue spectrum
   - prospects

An overview: Details will be covered by other members.

1. Overlap-Dirac operator

Spectrum of H_W
Topology issues

Neuberger fermion

Neuberger's overlap fermion (1988)

$$D = \frac{1}{a}\left[1 + \gamma_5 \,\mathrm{sgn}(H_W)\right]$$

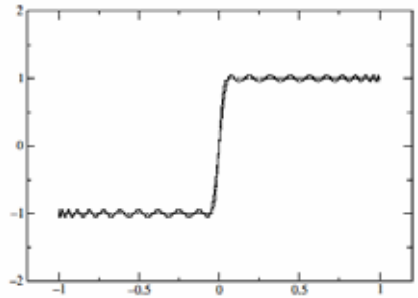
- Exact chiral symmetry through the Ginsparg-Wilson relation.
- Extensively tested in the quenched approximation.

Numerical cost depends on

- Spectrum of H_W
- Approximation of sgn(H_W)

▸ Main issues in the implementation

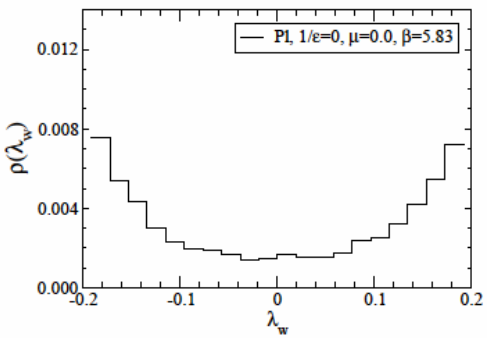
Spectrum of H_W



Non-zero density of near-zero mode (Edwards, Heller, Narayanan, 1998)

$$\rho(\lambda_W) = \frac{1}{V}\left\langle \sum_i \delta(\lambda_i - \lambda_W) \right\rangle$$

Plaquette gauge, β=5.83



- It comes from dislocations (local lumps of gauge field)

- Near-zero modes can be treated *exactly*; the rest may be approximated.
- But, many near-zero modes have to be projected out.
  - Can be reduced by improved actions and/or fat-link, but never become zero.

Serious (practical) problem for overlap

Near-zero mode suppression

Obvious solution = introduce unphysical (heavy negative mass) Wilson fermions (Vranas, JLQCD, 2006)

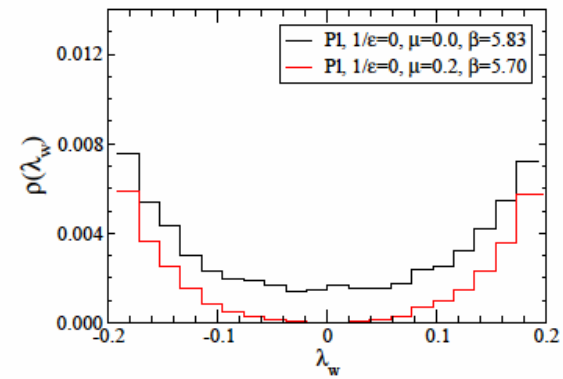
$$\det H_W(-m_0)^2$$

– Our choice

$$\det\left[\frac{H_W(-m_0)^2}{H_W(-m_0)^2+\mu^2}\right]$$

to minimize the effect in UV region.

Plaquette gauge, β=5.83, μ=0; β=5.70, μ=0.2



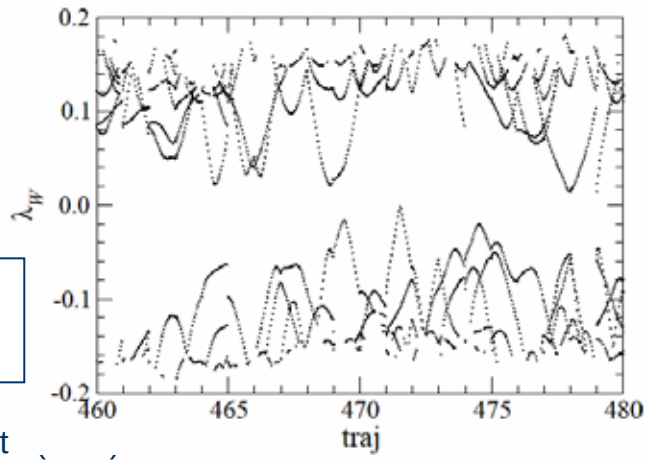
Completely wash-out the near-zero modes. Overlap is much faster.

Topology conserving action

Zero probability to have an exact zero-mode

No chance to tunnel between different topological sectors.

- If the MD-type algorithm is used, the global topology never changes.
  - Provided that the step size is small enough.



History of low-lying eigenvalues

Topology issues

Criticism:

- With the fixed topology simulations, global topology is not correctly sampled. This is not the θ (=0) vacuum.

My answer:

- Exactly. This is the problem for all of us. Topology tunneling is suppressed as one approaches the continuum limit with *any* gauge/fermion action.

= property of continuum gauge theory

How the physics affected?

- Finite volume effect
  - When the volume is large enough, the global topology is irrelevant.
  - Topological charge fluctuate locally, according to χ_t, topological susceptibility.

Theoretical argument:
$\Rightarrow$ Onogi's talk
θ=0 physics can be extracted from the fixed volume simulations.

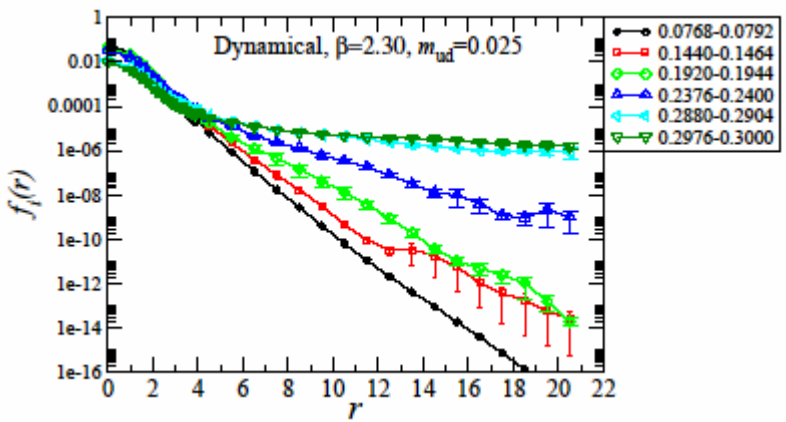
Numerical evidences:
$\Rightarrow$ Chiu's talk
Topological susceptibility can be calculated from local quantities.

Locality

- Overlap operator is not ultralocal, but
  - Exponentially local if there is a lower bound on the spectrum of HW (Hernandez-Jansen-Luscher (1999)).
  - Isolated near-zero modes are okay.
  - Even when $\rho_W(0) \neq 0$, still local if the near-zero modes are localized.

- In our case,
  - $\rho_W(0) = 0$
  - Near-zero modes are localized.

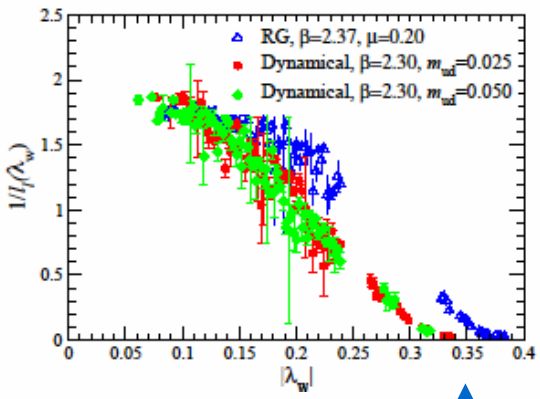
Yamada @ lat06



Mobility edge

Golterman-Shamir-Svetitsky (2003)

the point where the eigenmode becomes extended.

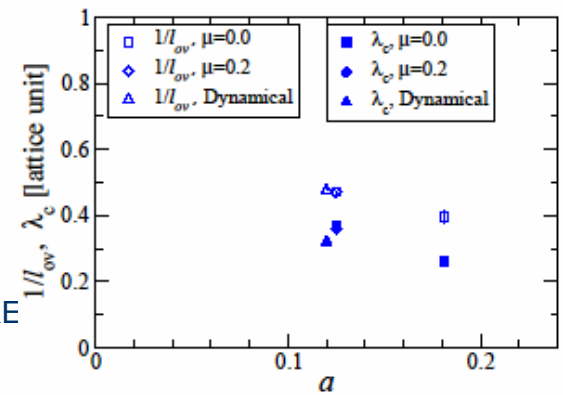


λ_c

- Locality

$$|D_{ov}(x,y)| \sim \bar{\lambda}\rho(\bar{\lambda})\exp\left(-\frac{|x-y|}{2l_l(\lambda)}\right) + O(1)\exp\left(-\lambda_c|x-y|\right)$$

  - D_{ov} is more local than the expectation.
  - Correspondence is non-trivial even in the free case.



2. Dynamical overlap

Implementation / improvement

Dynamical overlap

Recent attempts:

- Fodor-Katz-Szabo (2003)
  - Reflection/refraction trick
- Cundy et al. (2004)
  - Many algorithmic improvements
- DeGrand-Schaefer (2005)
  - Fat-link
  - Some physics results

This work:

- Fixed topology: no reflection/refraction required.
- Large scale simulation with $L \approx 2$ fm, $m_q \sim m_s/6$.
- Pion/kaon physics
- ε-regime

HMC implementation

- Sign function:
  - partial fraction, after projecting out a few near-zero modes
  - N =8-10, $\delta \approx 10^{-(7\text{-}8)}$
  - Multi-shift CG
  - relaxed precition as the outer CG proceeds.

- Mass preconditioning (Hasenbusch)

$$\det\left[D_{ov}(m)^2\right] = \det\left[D_{ov}(m')^2\right]\det\left[\frac{D_{ov}(m)^2}{D_{ov}(m')^2}\right]$$

- Multi-time step
  - Inner-most loop = gauge + extra-Wilson

$\Rightarrow$ Kaneko's talk

5D solver

Significant speed-up by the “5D” solver.

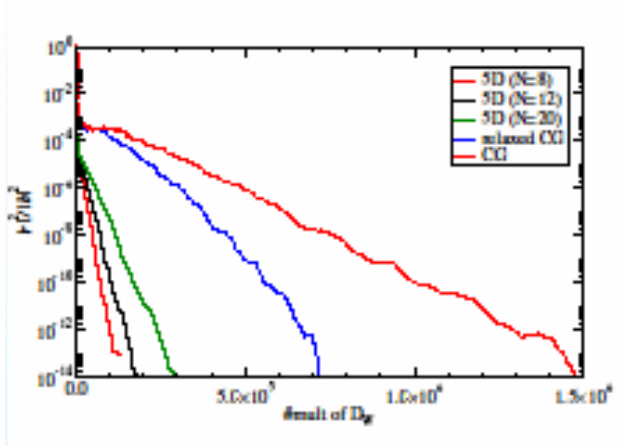
- Inversion of partial fraction

$$R\gamma_5 + p_0 H + H \sum_i \frac{p_i}{H^2 + q_i}$$

- Inversion of 5D matrix

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

Neuberger, Borici, Edwards et al.



- a factor of 5 faster
- the low-mode projection cannot be applied.

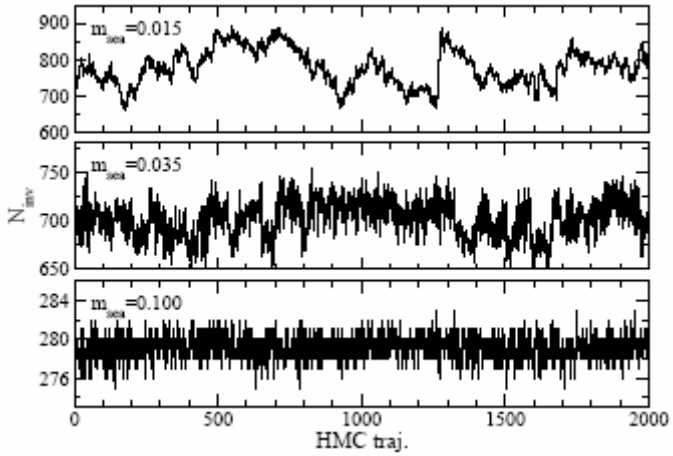
Used with less precise sgn func; corrected later by noisy Metropolis

$\Rightarrow$ Kennedy’s talk

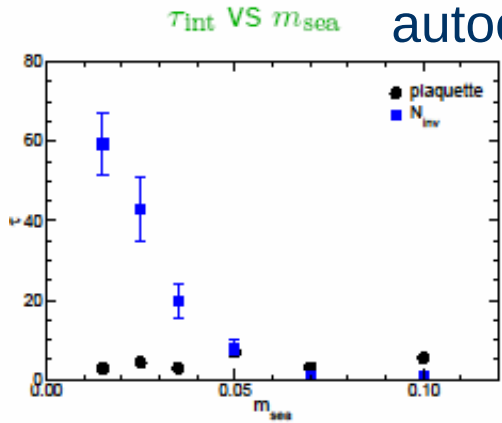
Parameters

- β=2.30, a=0.12 fm, 16^3x32
- 6 sea quark masses m_q = 0.015 … 0.100, covering $m_s/6 \sim m_s$
- 10,000 HMC traj.
  - ~4,000 with 4D solver
  - ~6,000 with 5D solver
- Q=0 sector only, except Q=-2, -4 runs at m_q=0.050

history of N_{inv}



autocorrelation



⇒ Kaneko's talk

3. Pions and kaons

LMP/LMA
Chiral log?

Low mode preconditioning

Time for measurement is not negligible

- At least 12 inversions per conf.
- often done many times for various measurements.

$$\left(1-\sum_k (\lambda_k + m) u_k(x) u_k^\dagger(y)\right) D(m)$$

Another virtue of overlap

- $D^\dagger(m)D(m)$ reduced to ~ $D^\dagger(0)\,D(0)+m^2$
  - multi-shift solver can be used.
- Common eigenvec's
  - once store the eigenvec's of D(0), then use as a preconditioner.

Speed-up by x 8, with 50 eigenpairs.

Low mode averaging

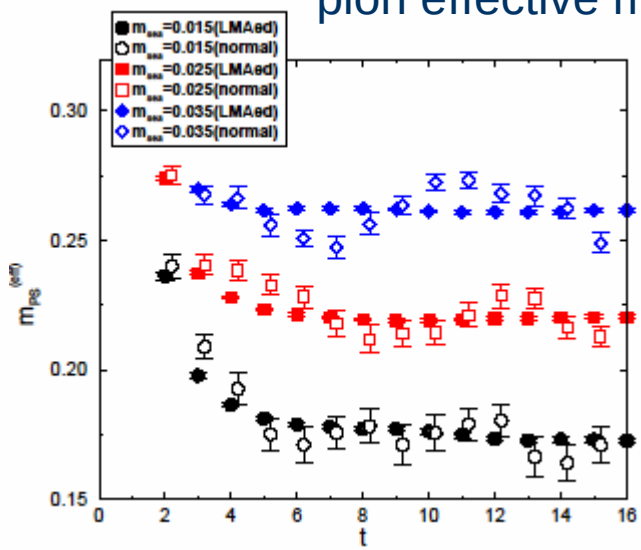
DeGrand-Schaefer (2004), Giusti et al. (2004)

$$D_m^{-1}(x,y) = \sum_{k=1}^{N} (\lambda_k + m)^{-1} u_k(x) u_k^\dagger(y) + D_m^{(h)-1}(x,y)$$

Low modes are all-to-all

$\Rightarrow$ Average over source points

pion effective mass



Meson correlator

$$C(x,y) = \quad + C^{hh}(x,y)$$

$$+ C^{hl}(x,y) + C^{lh}(x,y)$$

This piece can be averaged.

Chiral log?

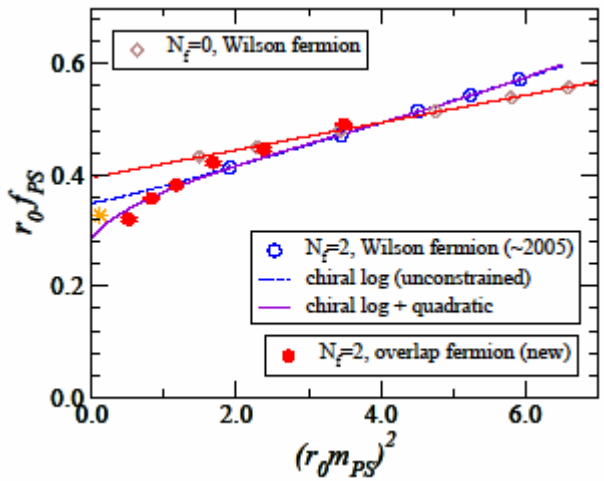
Data points now extended down to $m_s/6$ with exact chiral symmetry.

Is the chiral log seen?

$$\frac{f_\pi}{f} = 1 - \frac{N_f}{2}\frac{m_\pi^2}{(4\pi f)^2}\ln\frac{m_\pi^2}{\Lambda^2} + \cdots$$

Testing with

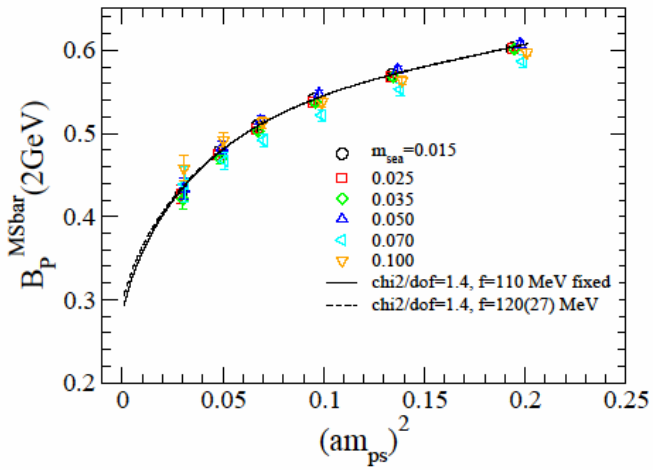
- m_π^2/m_q
- f_π



⇒ Noaki's talk
further tests

Other targets

- B_K
  - measurements/analysis on-going.



⇒ Yamada's talk

- Form factors
  - Pion charge radius
  - Kaon semi-leptonic form factors

planned

- Flavor singlet

planned

- I=2 ππ scattering

measurement/ analysis on-going

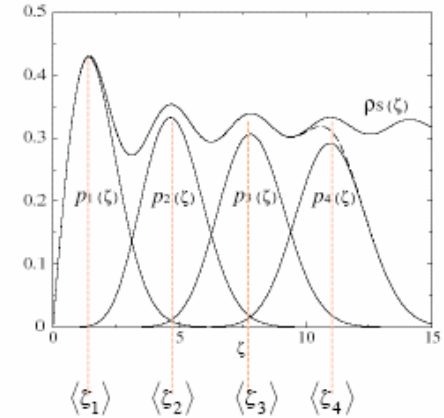
- Heavy quarks
  - Decay constant
  - $B^*B\pi$ coupling

planned

4. ε-regime

Simulations
Eigenvalue spectrum

Near the chiral limit



(Damgaard, Nishigaki, 2001)

Entering the ε-regime:

- Pion is nearly massless.
- Compton wavelength is longer than the lattice extent $m_\pi L \leq 1$
- Finite momentum mode is suppressed.

$$L_{\chi PT} = \Sigma \mathrm{Tr}\left[M(U + U^\dagger)\right]$$

- Dependence on topological charge

- Info on the Dirac operator eigenvalue spectrum through

$$Z_{QCD} = Z_{\chi PT}$$

(Leutwyler-Smilga, 1992)

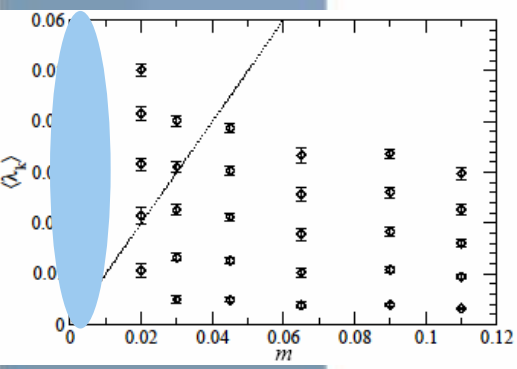
- More detailed analytical info through Chiral Random Matrix Theory (χRMT)

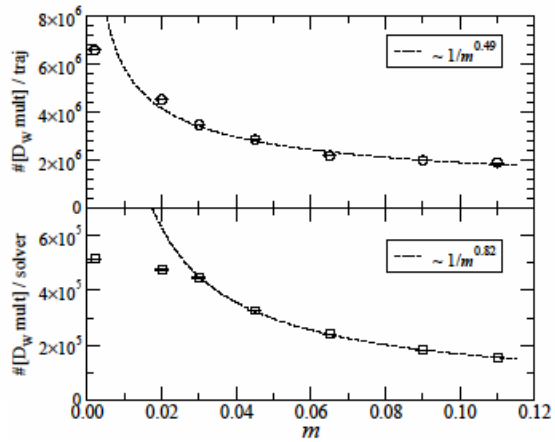
Simulation in the ε-regime

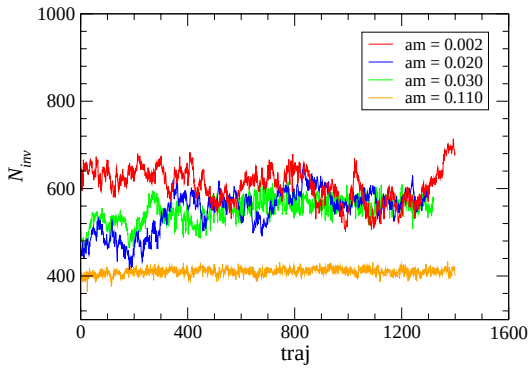
- Harder, but not prohibitive
  - Cost grows rather mildly.
  - Condition number is governed by the first eigenvalue, not m
  - First eigenvalue is lifted by the fermion determinant.

$$\prod_k \left(|\lambda_k|^2 + m^2 \right)$$

  - Auto-correlation is longer.





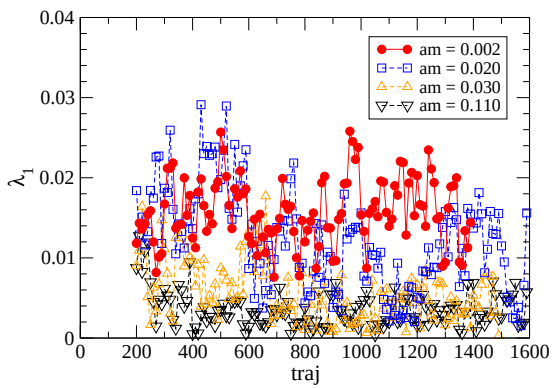


Eigenvalue spectrum

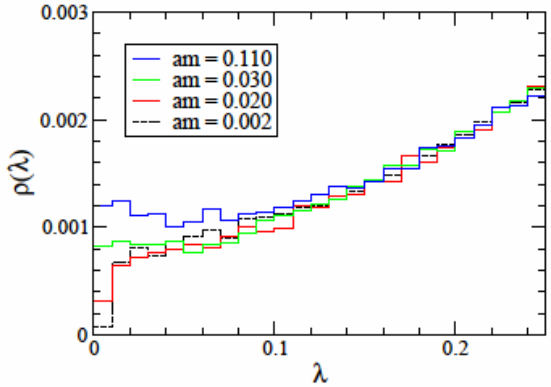
Simulation parameters:

- β=2.35, a = 0.11 fm, 16^3x32, 6 m_q + 1
- m_q = 3 MeV reached. $m_\pi L \approx 1$
- 4,600 HMC traj.
- 50 pairs of eigenvalues

.0 traj.



Spectral densiry



Banks-Casher relation

$$-\langle \bar{\psi}\psi \rangle = \pi \rho(0)$$

- Chiral symmetry restored in the massless limit (fixed V)

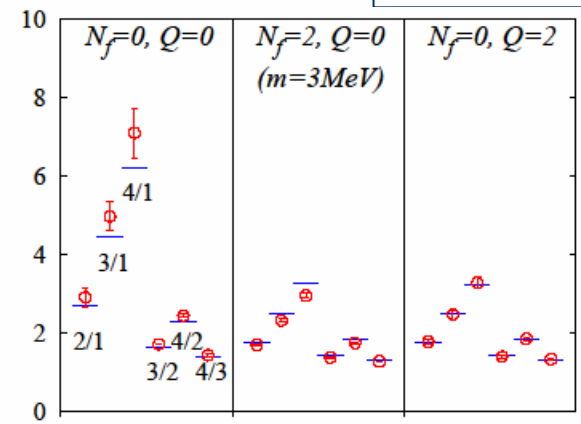
Comparison with χRMT

χRMT

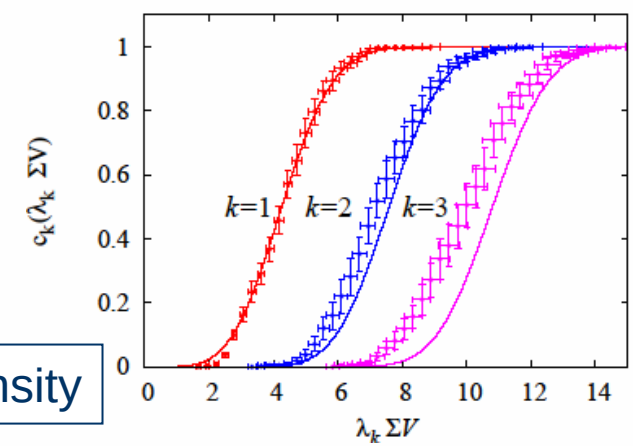
- Equivalent to χPT at the LO in the ε-expansion.
- Predicts eigenvalues of D in unit of $\lambda\Sigma V$.
  - $\langle\lambda_1\rangle\Sigma V = 4.30$
  - $\langle\lambda_2\rangle\Sigma V = 7.62$
  - …

  for N_f=2, Q=0.
- Σ may be extracted from average eigenvalues.

eigenvalue ratios



flavor-topology duality observed.



cumulative density

Extraction of Σ

- The lowest eigenvalue is most reliable: less contaminated by bulk modes.

$$\Sigma = \frac{4.30}{\langle \lambda_1 \rangle V}$$

- NLO in the ε-expansion for chiral condensate:

$$\Sigma\left[1+\frac{N_f^2-1}{N_f}\frac{\beta_1}{(FL)^2}\right]$$

about 13%. But not known for individual eigenvalues.

- Z-factor calculated using the NPR technique.

$$Z_S^{\overline{MS}}(2\,\mathrm{GeV}) = 1.14(2)$$

- Final result:

$$\Sigma^{\overline{MS}}(2\,\mathrm{GeV}) = \left[251(7)(11)\ \mathrm{MeV}\right]^3$$

  – Final error is our estimate of the higher order effects in ε.

Other applications

- Meson correlators
  (Damgaard et al., 2002)
  - in the ε-regime
  - can extract f_π
  - NLO calculation possible/available.

measurement/ analysis on-going

- 3-pt functions
  (Hernandez-Laine, 2006)
  - Several B parameters

- Eigenvalue correlations
  (Damgaard et al., 2006)
  - with imaginary chemical potential
  - can extract f_π

measurement/ analysis on-going

Wide variety of applications, all without chiral extrapolations.

$\Rightarrow$ Hernandez's talk

Plans

Current plans

- Two-flavor simulation has done.
  - At a single lattice spacing a=0.12 fm
  - On a 16^3x32 lattice
  - 6 m_q x 10,000 traj.
- Possible directions of improvement
  - Smaller a
  - Larger L

  on a 24^3x48 lattice.

- 2+1-flavor simulation
  - Necessary extension
  - Easier with overlap

    (det H^2 factorizes to det H_L^2 and det H_R^2)

- Right now, running
  - 2+1-flavor at a=0.12 fm.
  - 16^3x48 lattice

- And, many physics measurements…

Summary

- Dynamical QCD with exact chiral symmetry is feasible and promising.
  - No restriction in the light quark mass. Much better control of chiral extrapolation.
  - The ε-regime is within reach.
  - Many new techniques, new applications

New frontier of lattice QCD simulations