Exploring chiral regime with dynamical overlap fermions

- Introduction
- Overlap fermion
- Algorithms
- Simulation
- e-regime
- Fixed topology
- Pion mass/decay const
- Summary/outlook

http://jlqcd.kek.jp/

Hideo Matsufuru for the JLQCD Collaboration

High Energy Accerelator Research Organization (KEK)

Collaboration

- JLQCD Collaboration
  - S.Hashimoto, T.Kaneko, J.Noaki, E.Shintani, N.Yamada, H.M. (KEK)
  - S.Aoki, K.Kanaya, A.Ukawa, T.Yoshie (Tsukuba Univ)
  - H.Fukaya (RIKEN)
  - T.Onogi (YITP, Kyoto Univ)
  - K-I.Ishikawa, M.Okawa (Hiroshima Univ)
- TWQCD Collaboration
  - T-W.Chiu, K.Ogawa (Natl.Taiwan Univ)
  - T-H.Hsieh (RCAS, Academia Sinica)

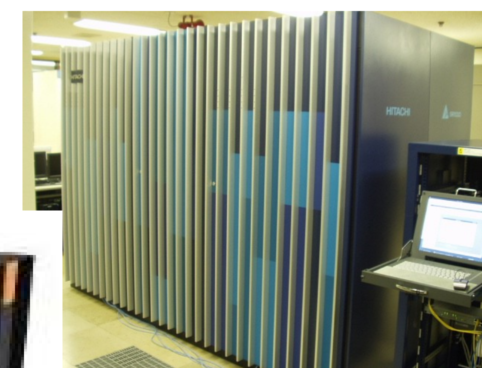
Machines

Main machine: IBM Blue Gene/L at KEK

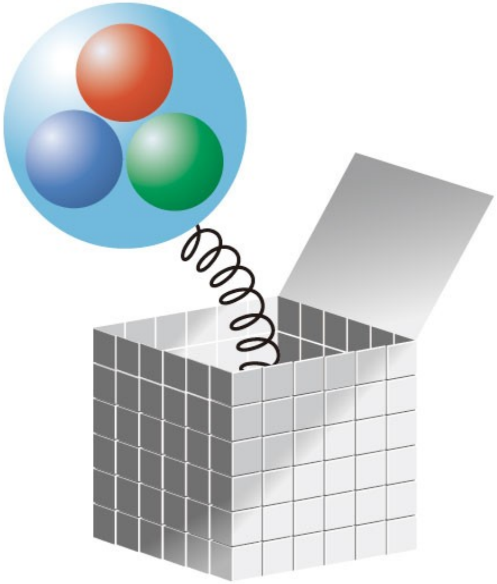
- 57.6 Tflops peak (10 racks)
- 0.5TB memory/rack
- 8x8x8(16) torus network
- ~30% performance for Wilson kernel
  (Doi and Samukawa, IBM Japan)
- Overlap HMC: 10~15% on one rack

Also using

- Hitachi SR11000 (KEK)
  - 2.15TFlops/0.5TB memory
- NEC SX8 (YITP, Kyoto)
  - 0.77TFlops/0.77TB memory



Introduction



Physics goals

- Approaching/exploring the chiral regime
  - Confirming the chiral symmetry breaking scenario with exact chiral symmetry
  - Testing the effective chiral Lagrangian predictions
- Matrix elements with controlled chiral extrapolation
  - f_π, f_K
  - Pion form factor, K_{l3}
  - B_K
  - $\pi\pi$ scattering
  - π^+-π^0 mass difference
  - Heavy flavor physics

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})
- Numerically costs highly
  - Calculation of sign function
  - Discontinuity at zero eigenvalue of H_W
- Has become feasible with
  - Improvement of algorithms
  - Large computational resources

Project

Nf =2, 2+1 dynamical overlap fermions

- Small enough quark masses: $m_s/6$--m_s, ε-regime
- Iwasaki gauge action
- Extra Wilson fermion/ghost to suppress near-zero modes of H_W
- Fixed Q at 0, 2, 4
- Large statistics

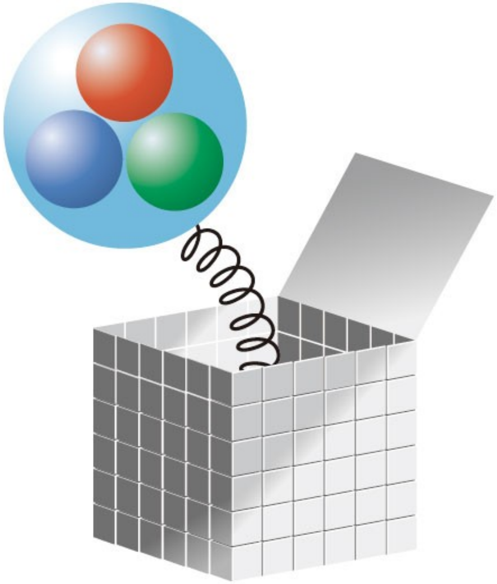
Present status

- Nf=2: 16^3x32, a=0.12fm

  --- Production done, physics measurement on-going
- Nf=2+1: 16^3x48, a=0.11fm

  --- Production in progress

Overlap fermion



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Overlap operator

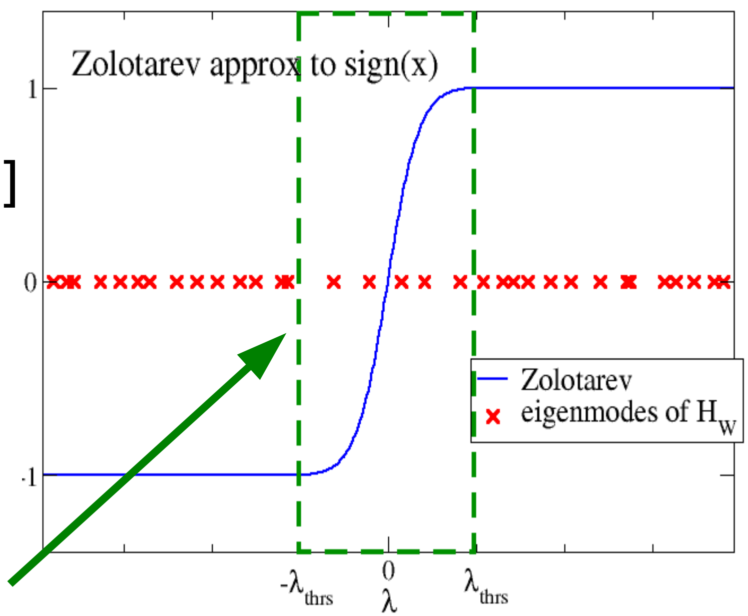
$$D(m) = \left(M_0 + \frac{m}{2}\right) + \left(M_0 - \frac{m}{2}\right) \gamma_5 \mathrm{sign}(H_W)$$

Zolotarev's Rational approximation

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

- $(H_W^2 + q_l)^{-1}$: calculated by multishift CG simultaneously
- Valid for |λ| (eigenmode of H_W) ∈ $[\lambda_{thrs}, \lambda_{max}]$
- Smaller λ_{thrs}, larger N is needed for accuracy: ~exp(-$\lambda_{thrs} N$)
- Projecting out low-modes of H_W below λ_{thrs}

$\rightarrow$ $\mathrm{sign}(\lambda)$ $(\lambda < \lambda_{thrs})$ explicitly determined



--- Cost depends on the low-mode density

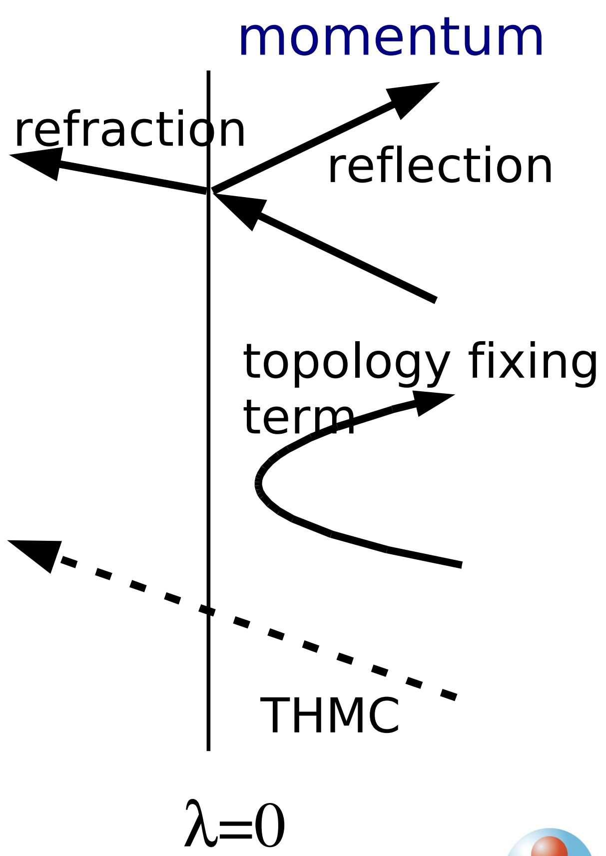
(λ_{thrs}=0.045, N=10 in this work)

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)
  - $\lambda \sim 0$ 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

Topology fixing term: extra Wilson fermion/ghost

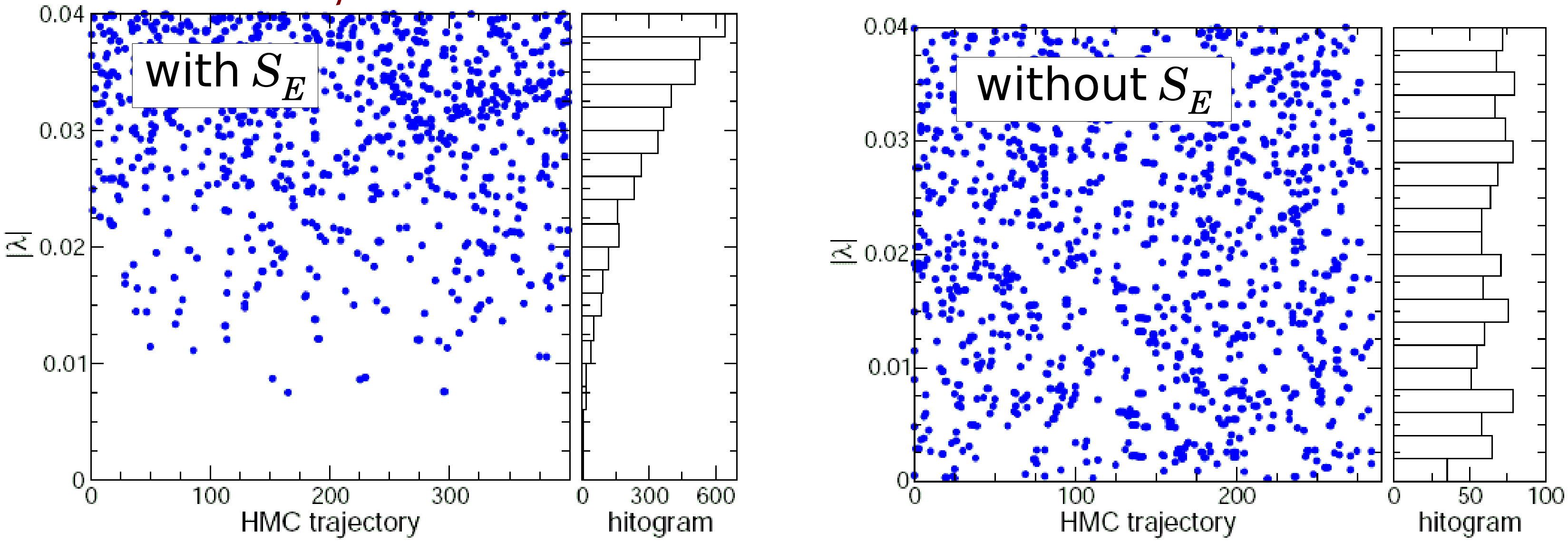
(Vranas, 2000, Fukaya, 2006, JLQCD, 2006)

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

--- avoids $\lambda\sim 0$ during MD evolution

- No need of reflection/refraction
- Cheeper sign function

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



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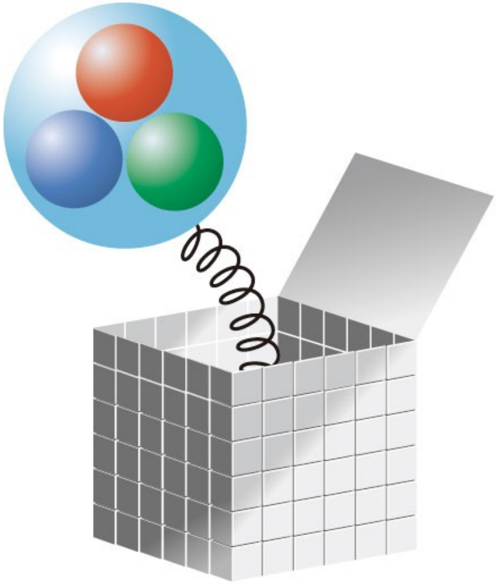
Algorithm



Algorithm

Improvement of HMC

- Mass preconditioning (Hasenbusch, 2001)
- Multi-time step (Sexton-Weingarten, 1992)

- Nf=2 (JLQCD, Proc. Lattice 2006)
  - Noisy Metropolis (Kennedy and Kuti, 1985)
  - 5D solver without projection of low-modes of H_W
  - At an early stage, 4D solver w/o noisy Metropolis (twice slower)
- Nf=2+1 (poster by S.Hashimoto)
  - Nf=1 part: one chirality sector

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

    $H^2 = D^\dagger(m)D(m)$ commutes with γ_5

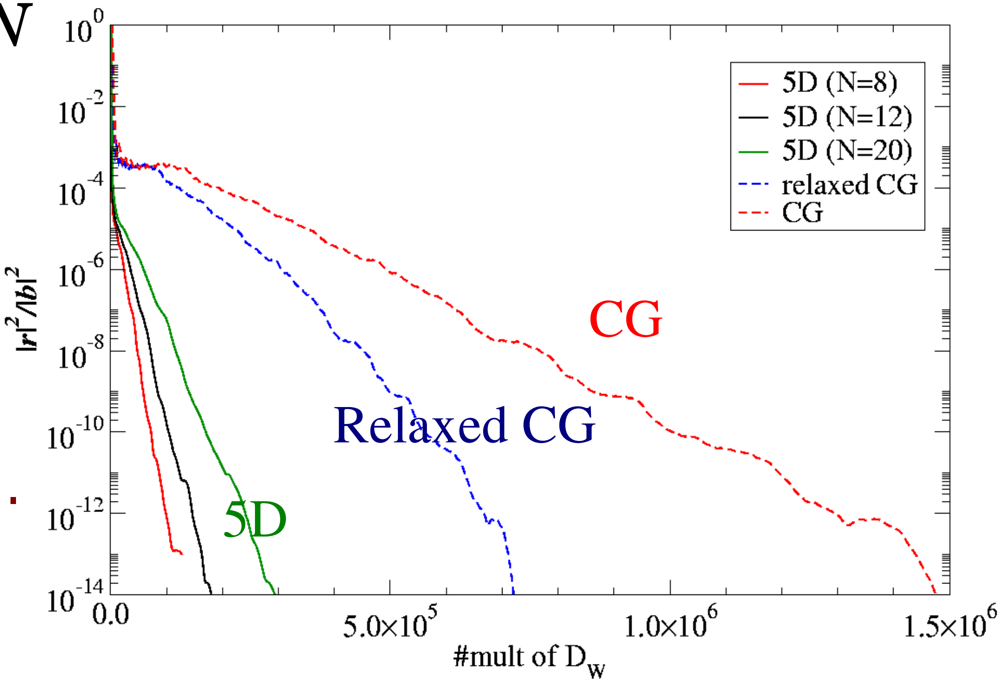
    $$H^2 = P_+H^2P_+ + P_-H^2P_- \Rightarrow \det H^2 = \det(P_+H^2P_+) \cdot \det(P_-H^2P_-)$$
  - 5D solver (with low-mode projection)

Overlap solver

Solver algorithm for overlap operator

- Most time-consuming part of HMC
- Two algorithms used: Nested (4D) CG and 5D CG

- 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

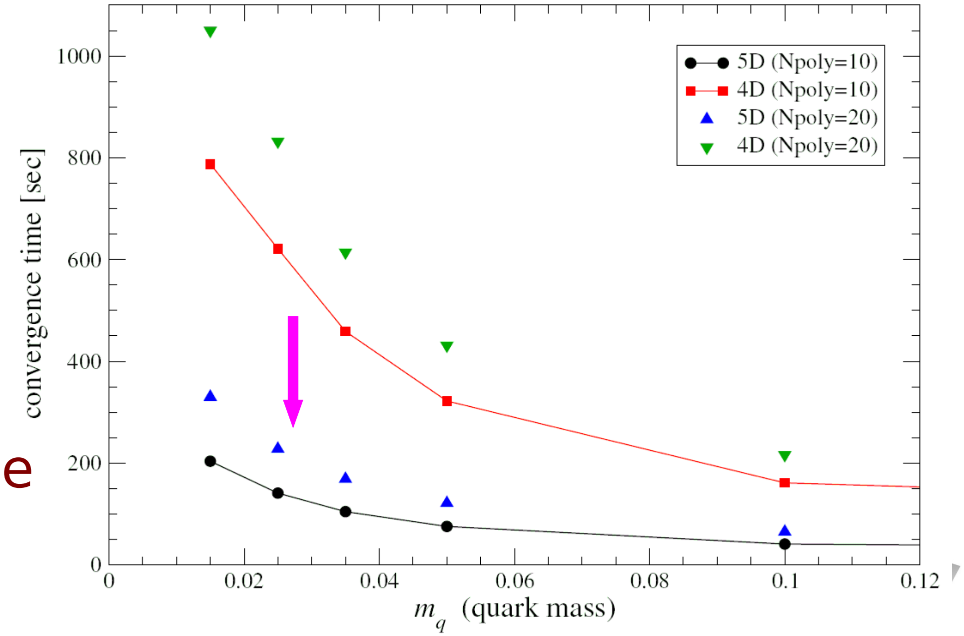
5D solver

- 5-dimensional CG (Borici, 2004, Edwards et al., 2006)
  - One can solve $S\psi_4 = \chi_4$ by solving (example: N=2 case)

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

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

  - Even-odd preconditioning
  - Projection of low-mode of H_W
  - O(3-4) times faster than 4DCG



Nf=2+1 HMC on BG/L 1024-node

$|r|/|b| < 10^{-10}$ (N_{sbt}=8)

Comparison with Domain-wall

Rough comparison of cost of CG solver

- 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)

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

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

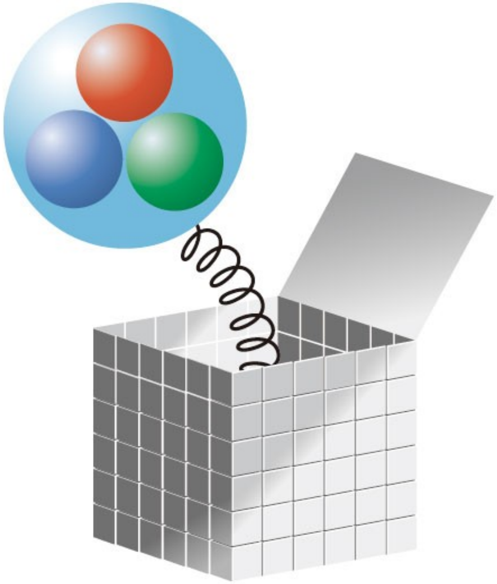
At $m=m_s/2$, a^{-1}=0.17GeV, 16^3x32/48, up to residual 10^{-10}:

- 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)

- Currently factor ~2.5 difference

Simulation



Runs

- 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)

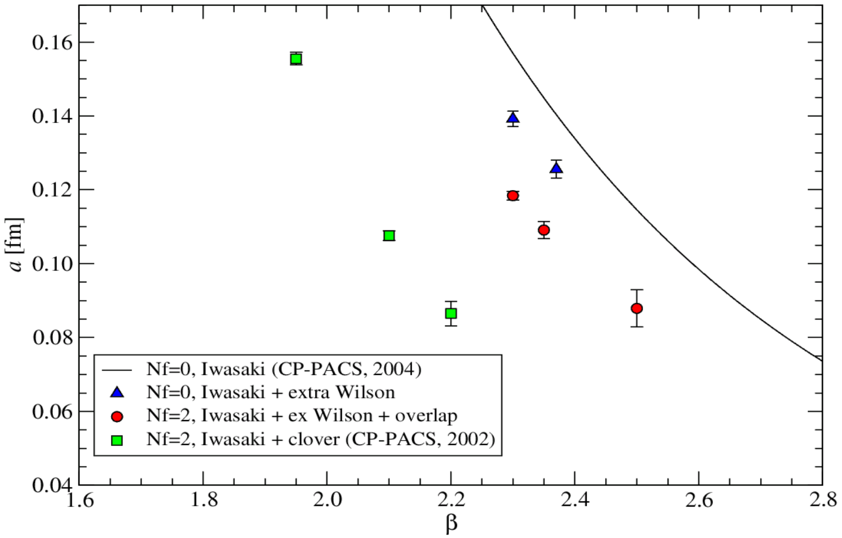
- Nf=2+1 : 16^3x48, a=0.11fm (in progress)
  - 2 strange quark masses around physical m_s
  - 5 ud quark masses covering (1/6~1)m_s
  - Trajectory length = 1
  - About 2 hours/traj on BG/L 1024 nodes

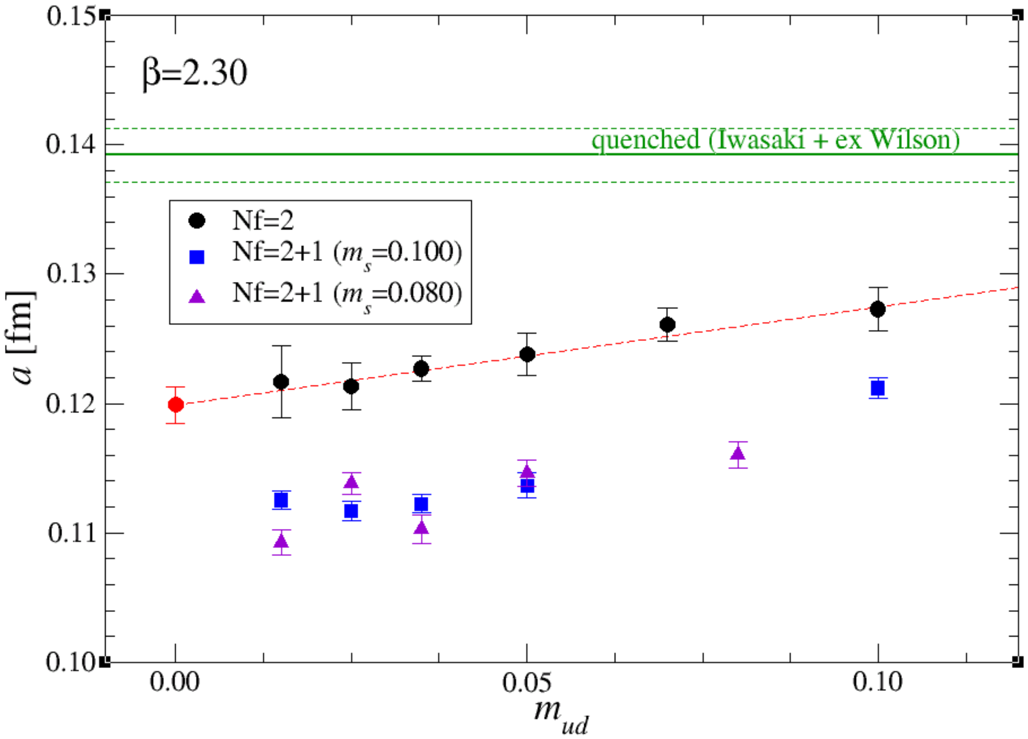
Lattice scale

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

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

  - Milder β-shift than Wilson-type fermion

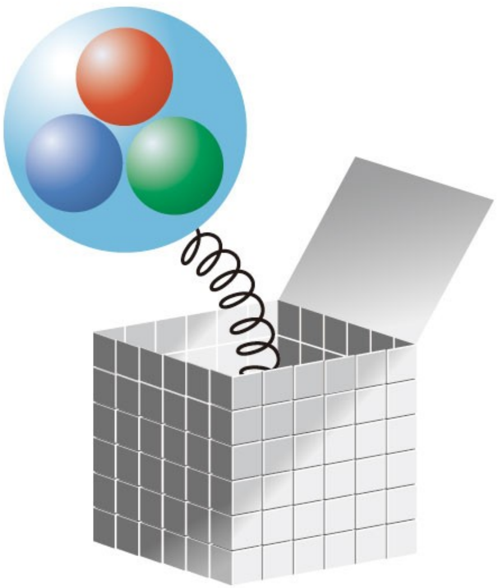




Results

- Physics measurements: in progress on Nf=2 lattices
  - ε-regime --- talk by H. Fukaya (Thu,pm)
  - Topological susceptibility --- talk by T.-W. Chiu (Tue,pm)
  - Meson spectroscopy --- talk by J. Noaki (Mon,pm)
  - π^{+}-π^{0} mass difference --- talk by E. Shintani (Tue,pm)
  - B_K --- talk by N. Yamada (Thu,pm)
  - Pion form factors --- talk by T. Kaneko (Wed,am)
  - Pion scattering length --- talk by T. Yagi (Thu,pm)
- Study on Nf=2+1 lattice has been started
  - Status --- poster by S.Hashimoto

ε-regime



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Chiral condensate

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

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

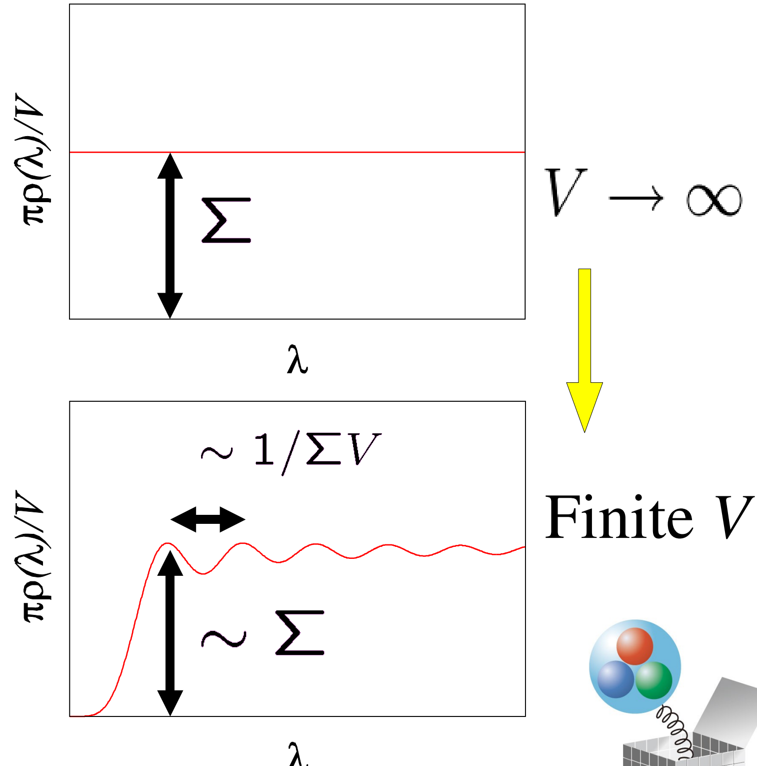
$\rho(\lambda) = \sum_k \langle \delta(\lambda - \lambda_k) \rangle$: spectral density of D

  - Accumulation of low modes ⟺ Chiral SSB
  - $V \to \infty, \text{ then } m \to 0$

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

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

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



Result in the ε-regime

(JLQCD, 2007, JLQCD and TWQCD, 2007)

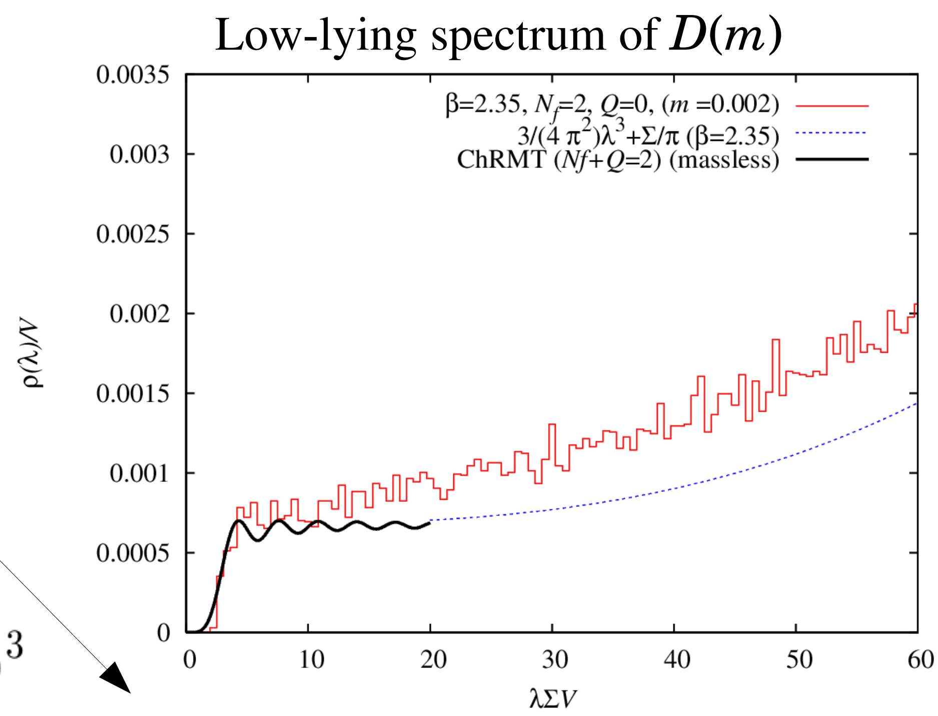
- Nf=2, 16^3x32, a=0.11fm
- m~3MeV

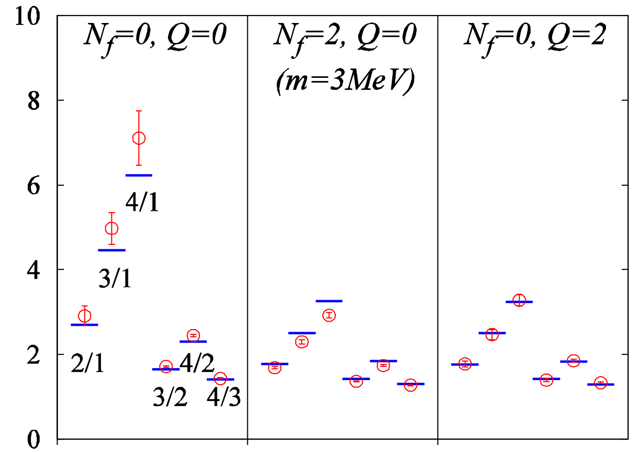
- Good agreement with RMT
  - lowest level distrib. $\longrightarrow \Sigma$
  - Flavor-topology duality
- Chiral condensate:
  - Nonperturbative renorm.

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

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

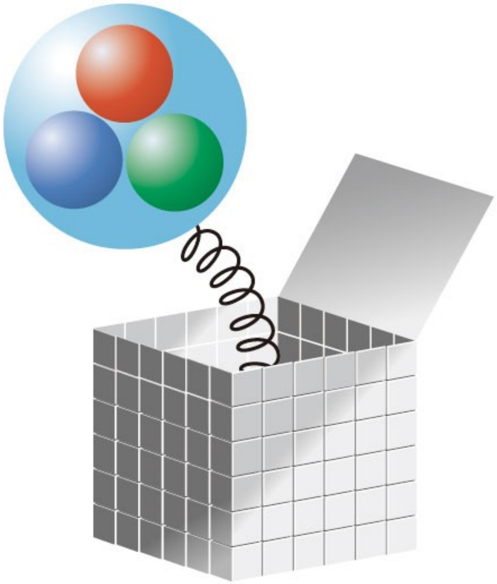
--- talk by H.Fukaya (Thu,pm)





Fixed topology

-- problem or benefit ?



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Simulation at fixed topology

Talk by T.Onogi (Tue,pm)

Out of the ε-regime, fixing topology could be a problem

- In the infinite V limit,
  - Fixing topology is irrelevant
  - Local fluctuation of topology is active
- In practice, V is finite
  - Topology fixing ⇨ finite V effect
  - $\theta=0$ physics can be reconstructed (see below)
  - Must check local topological fluctuation
    ⇨ topological susceptibility, η' mass
  - Questions: Ergodicity ?

Physics at fixed topology

Talk by T.Onogi (Tue,pm)

One can reconstruct fixed θ physics from fixed Q physics

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

- Partition function at fixed topology

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

  - For $Q \ll \chi_t V$, Q distribution is Gaussian
- Physical observables
  - Saddle point analysis

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

  - Example: pion mass

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

Topological susceptibility

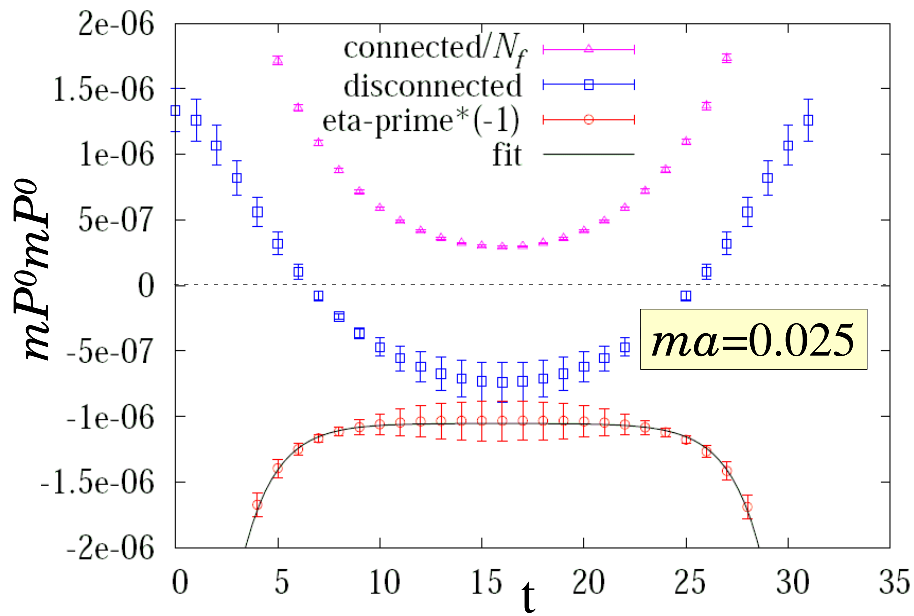
Talk by T-W. Chiu (Tue,pm)

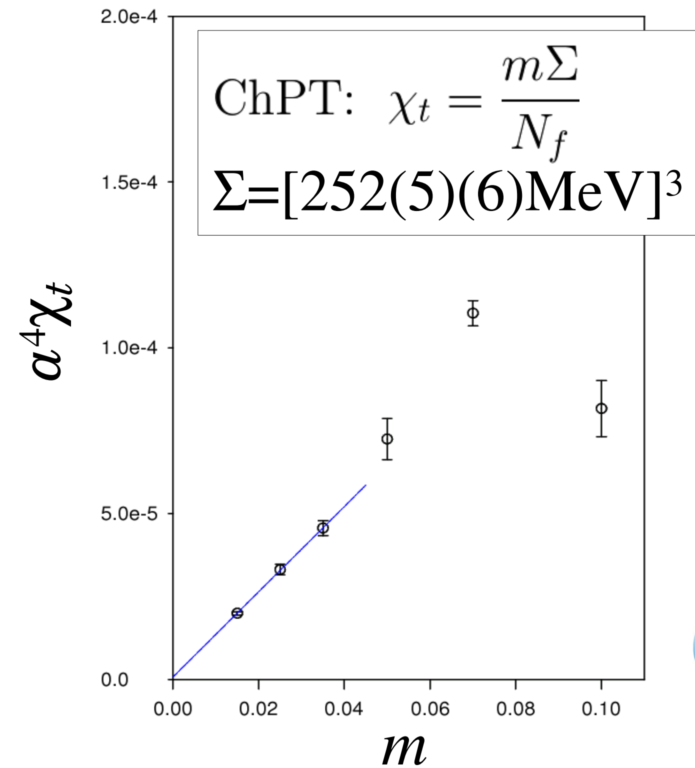
- Topological susceptibility χ_t can be extracted from correlation functions (Aoki et al., 2007)

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

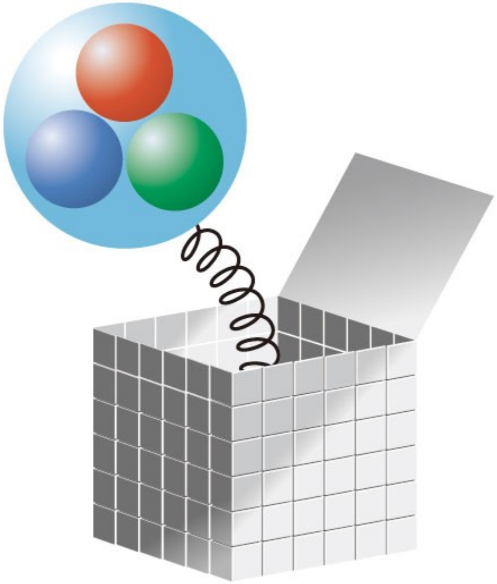
where $$P^0 \equiv \frac{1}{N_f}\sum_{f=1}^{N_f}\bar{q}_f\gamma_5\left(1-\frac{D}{2m_0}\right)q_f$$

Numerical result at Nf=2, a=0.12fm





Pion mass/decay const
Others



Low-mode averaging

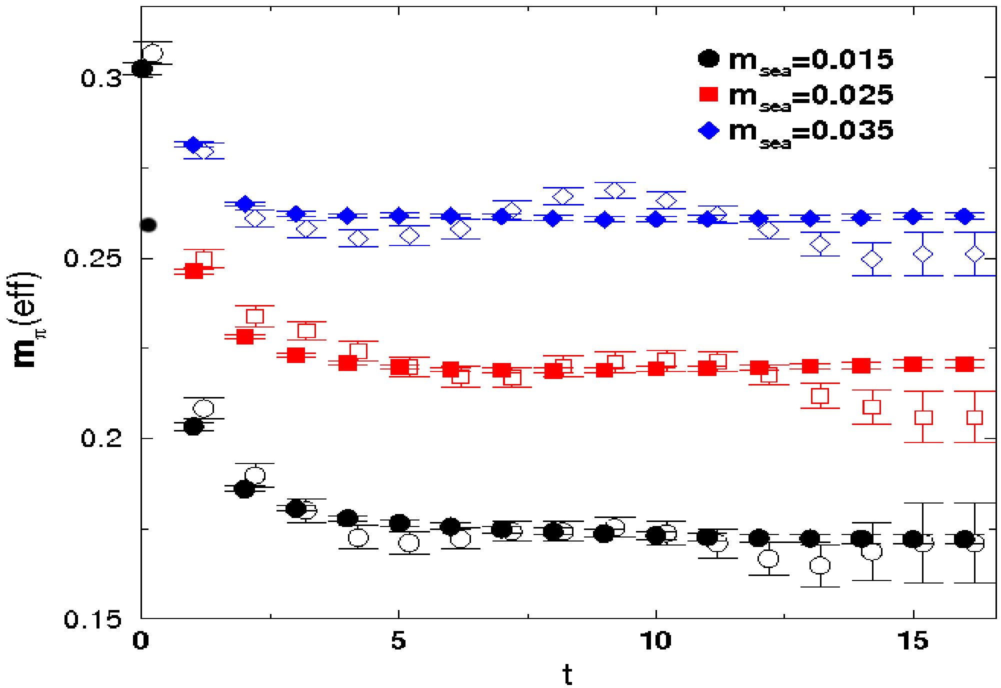
Talk by J.Noaki (Mon,pm)

Technical improvement:

- 50 pairs of eigenmodes of D predetermined
- Solver with low mode projection (8 times faster)
- Low-mode averaging (DeGrand, 2004, Giusti et al., 2004)
  - Averaging over source points only for low mode contrib.

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

3 smallest m_{sea}=$m_{val.}$



Two-loop ChPT test

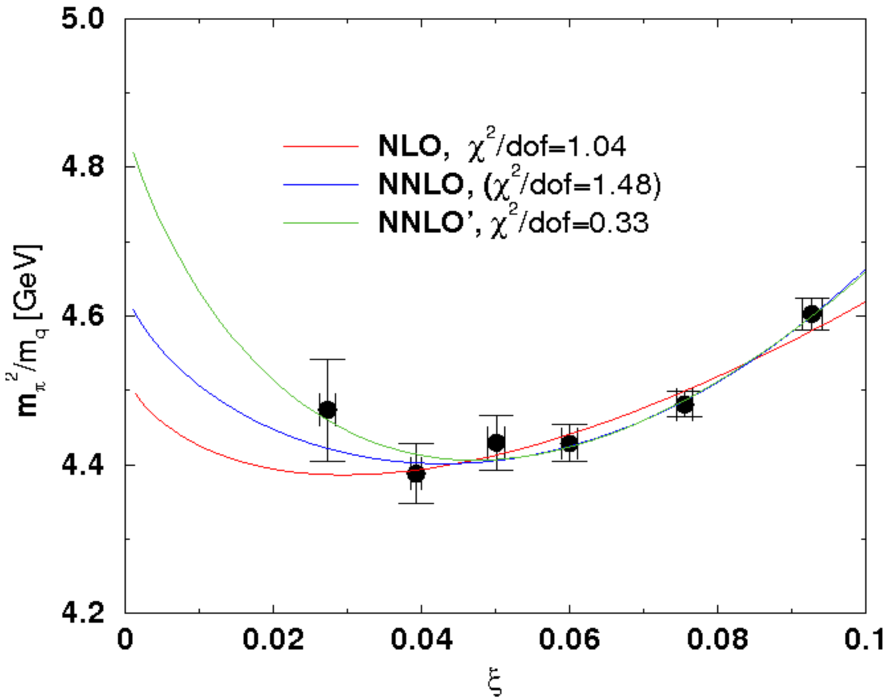
Talk by J.Noaki (Mon,pm)

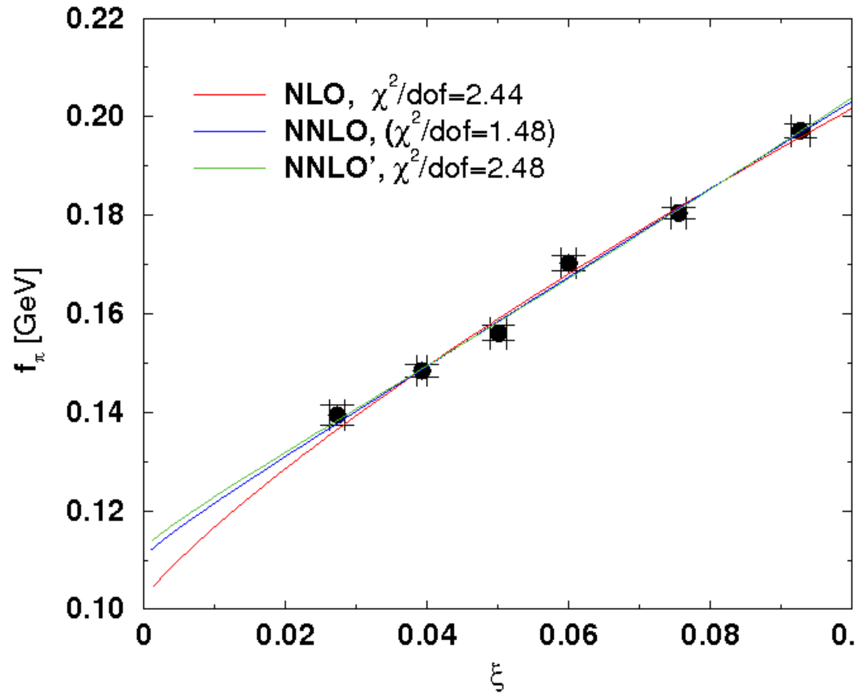
Chiral extrapolation

- Fit parameter: $\xi \equiv \left(\frac{m_\pi}{4\pi f_\pi}\right)^2$ (f_π is mass dependent)
- NLO vs NNLO of ChPT
  --- NLO tends to fail; NNLO successful
- Low energy constants:

$$f = 111(4)(2) \text{ MeV}, \quad \sigma^{1/3} = 242(6)(6) \text{ MeV},$$
$$\bar{l}_3^{\text{phys}} = 2.9(4)(1.6), \quad \bar{l}_4^{\text{phys}} = 4.3(5)(2).$$

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



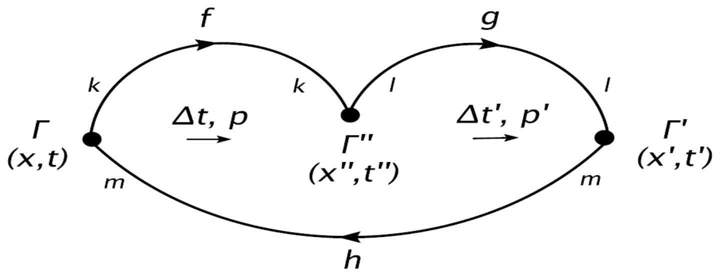


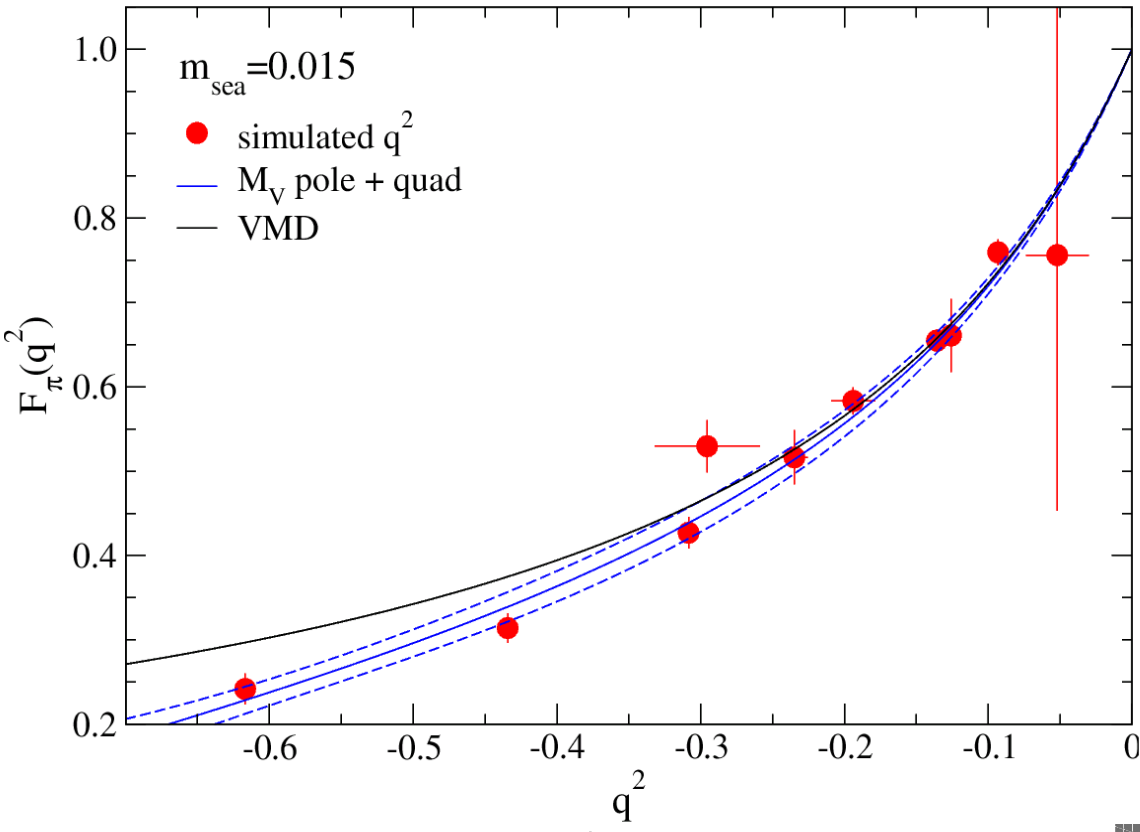
Pion form factor

Talk by T.Kaneko (Wed,am)

- Precisely calculated with the all-to-all technique
  (J.Foley et al., 2001)
- Pion charge radius

Nf=2, a=0.12fm, preliminary result:





π^+-π^0 mass difference

Talk by E.Shintani (Tue,pm)

- Das-Guralnik-Mathur-Low-Young sum rule (1967)

$$\Delta m_\pi^2 = -\frac{3\alpha_{\mathrm{EM}}}{4\pi f_\pi^2}\int_0^\infty dQ^2\, Q^2\left[\Pi_V^{(1+0)}(Q^2) - \Pi_A^{(1+0)}(Q^2)\right]$$

  – Vacuum polarization

$$\langle J_\mu J_\nu\rangle(p^2) = (\delta_{\mu\nu}p^2 - p_\mu p_\nu)\Pi_J^{(1)}(p^2) - p_\mu p_\nu \Pi_J^{(0)}(p^2) + (\text{lattice artifact})$$

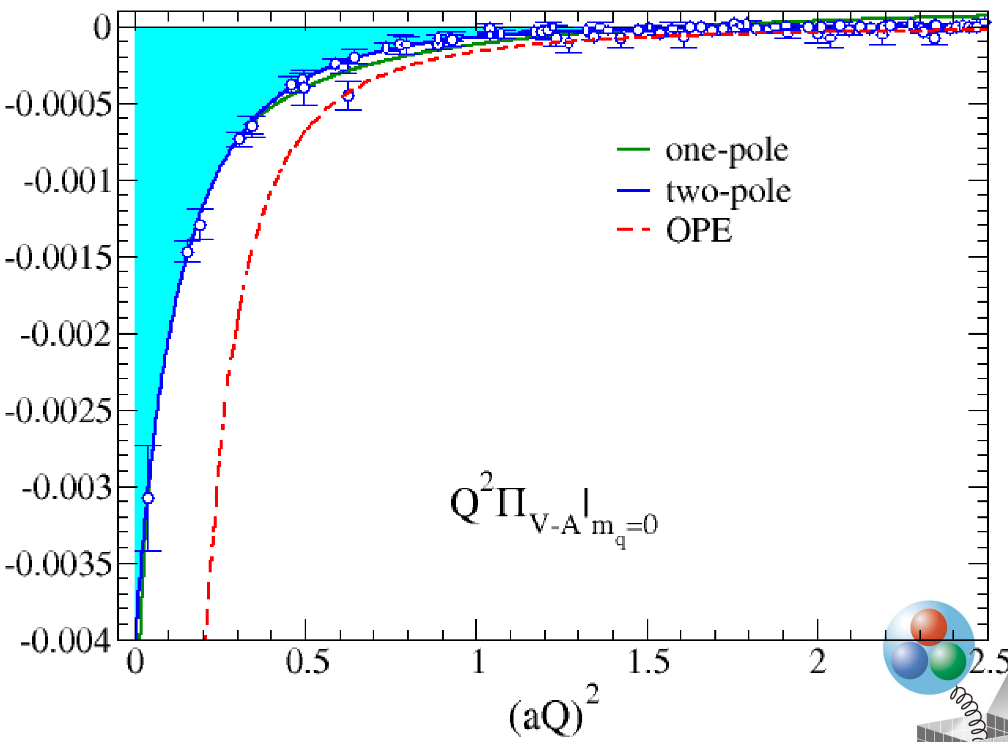
    - Low Q^2: pole dominance
    - High Q^2: OPE

Nf=2, a=0.12fm

$$\Delta m_\pi^2 = 1044\,(94)_{\mathrm{stat}}\,(44)_{\mathrm{syst}}\ \mathrm{MeV}^2$$

Cf. exp. 1242 MeV^2

Exact chiral symmetry plays essential role !



B_K

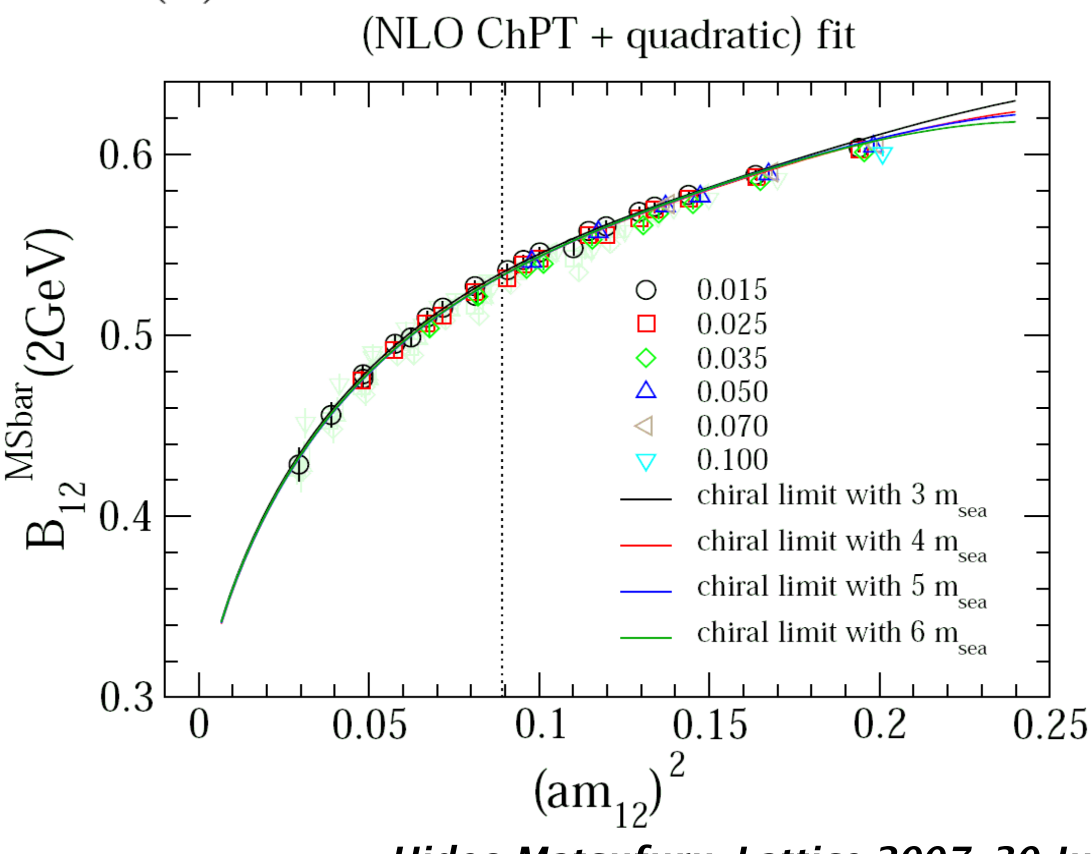
Talk by N.Yamada (Thu,pm)

Kaon bag parameter

- Nonperturbative renorm. with RI-MOM scheme
- NLO of PQChPT

Nf=2, a=0.12fm, preliminary result:

$$B_K^{\overline{MS}}(2\,\mathrm{GeV}) = 0.533\,(7)_{\mathrm{stat}}$$



Summary/Outlook

We are performing dynamical overlap project at fixed topological charge

- Nf=2 on 16^3x32, a~0.12fm: producing rich physics results
- Nf=2+1 on 16^3x48, a~0.11fm: in progress

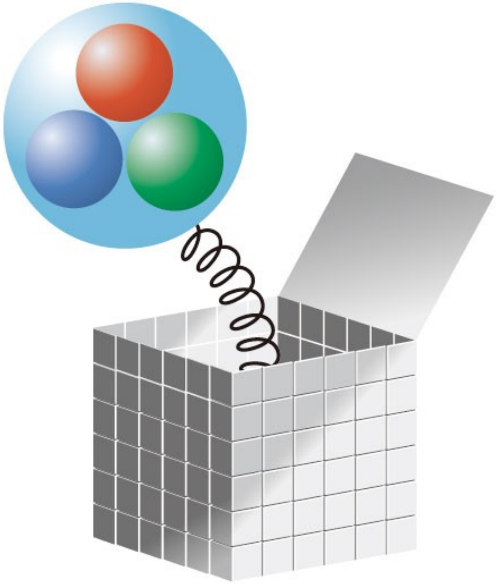
- Understanding chiral dynamics with exact chiral symmetry
- Application to matrix elements in progress
- Configurations will be supplied to ILDG

  (After first publication of spectrum paper)

Outlook

- More measurements planned
- Larger lattices 24^3x48: need further improved algorithms

Backup



Finite volume effect

Finite volume correction

Talk by J.Noaki

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

- R: ordinary finite size effect

  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

– No Q-dependence (consistent with expectation)