Lattice QCD simulation with exact chiral symmetry

--- Not yet at finite temperature ---

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- Introduction
- Lattice fermion actions
- Overlap fermion
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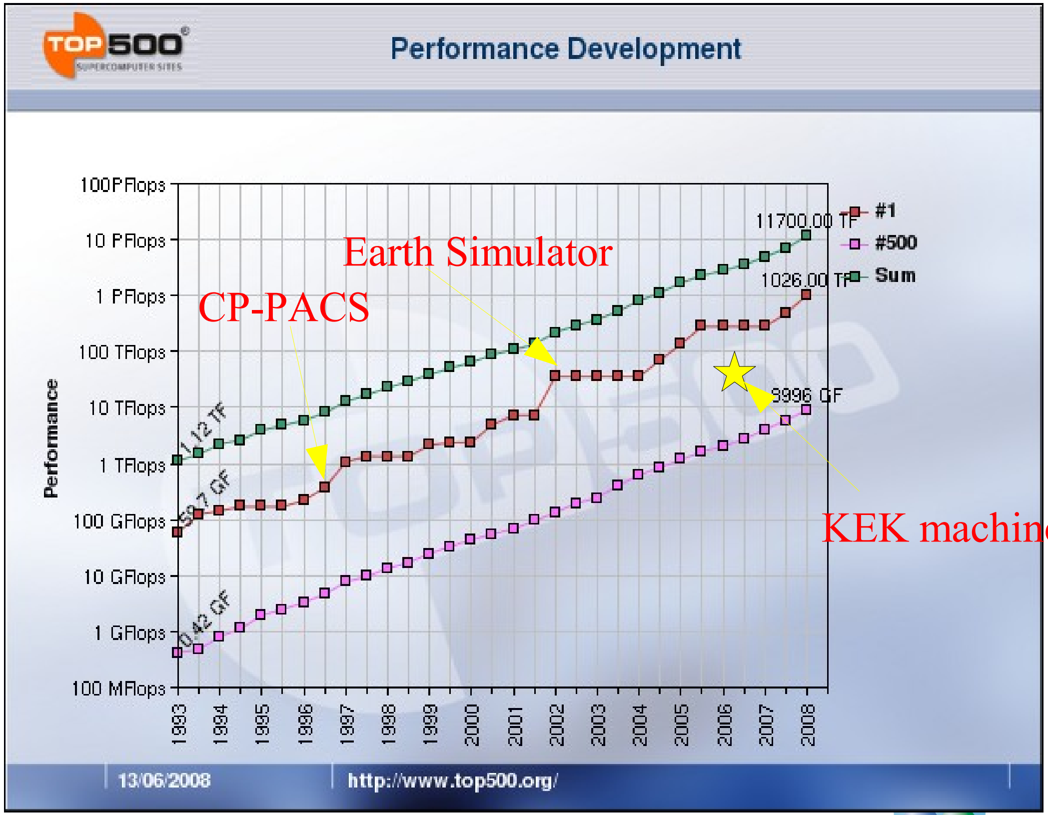
- Summary/outlook

Introduction

- 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
  - Japan: Next generation supercomputer project (10TFlops in 2011)
  - Two projects in USA



Introduction

- 1980's
  - Dawn of lattice simulations
- 1990's
  - Large quenched simulations (w/o dynamical quark effect)
  - Dynamical simulations (exploratory)
  - Matrix elements with 10% accuracy: systematic errors from continuum/chiral limit, quenching
- 2000's
  - Large dynamical simulations
  - Chiral symmetry (domain-wall, overlap,...)
  - Matrix elements with a few % accuracy
- 2010's ?
  - Nuclear physics
  - Thermodynamics

With accuracy!

Introduction

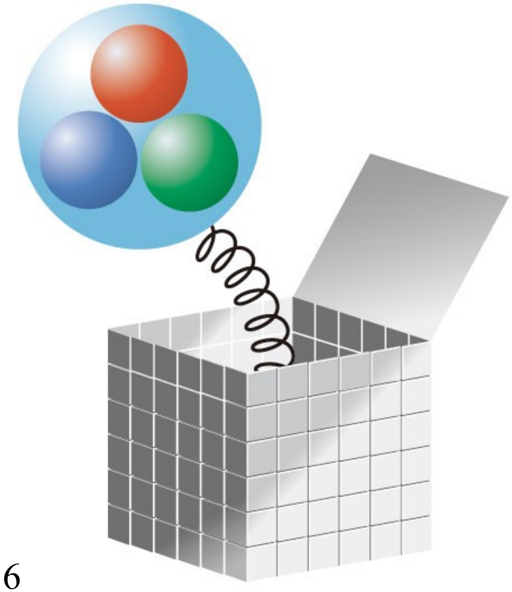
Our choice (JLQCD Collaboration): overlap fermion

- Exact chiral symmetry (theoretically clean)
- Large simulation costs (numerically challenging)
- First large-scale dynamical simulation
- Now rich results are coming

Toward finite temperature (and density) simulation

- What kind of thermal properties to be explored?
- Cost/interest

Lattice fermion actions



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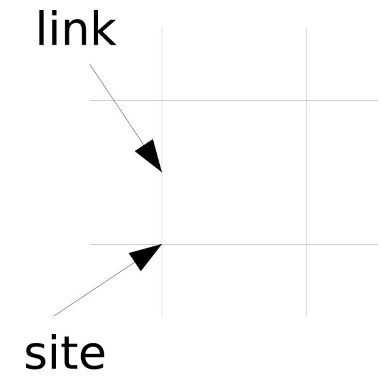
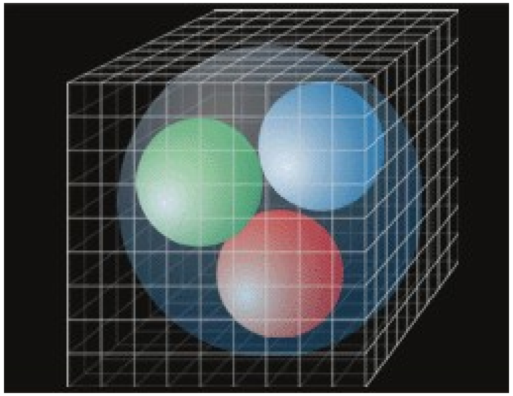
Lattice QCD

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
- Chiral extrapolation is still a source of largest systematic errors!



Femion doubling/Wilson fermion

Fermion doubling

- naïve discretization causes 16-fold doubling
- Nielsen-Ninomiya's No-go theorem
  - Doublers appear unless chiral symmetry is broken

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

- 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

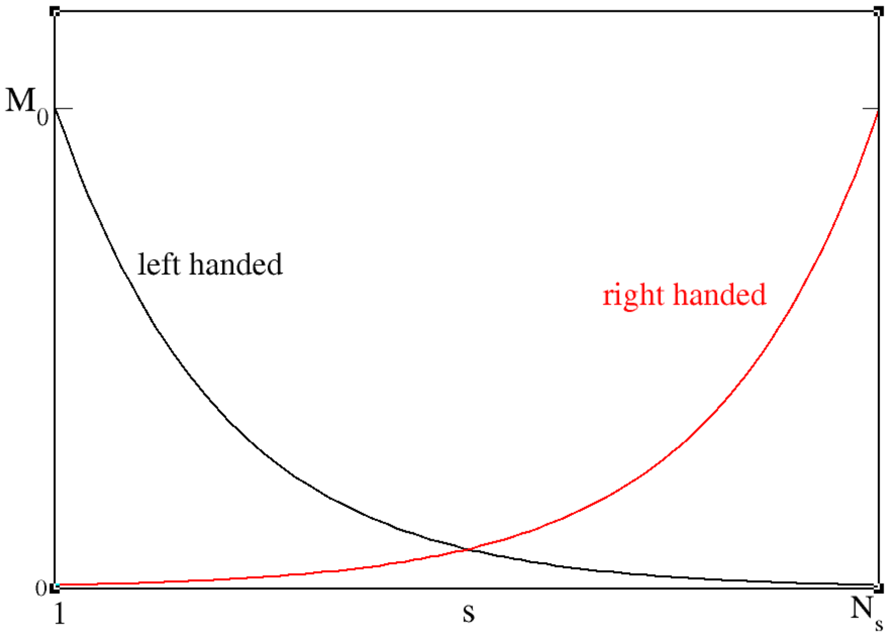
- Staggered fermion
  - 16=4 spinors x 4 flavors ('tastes')
  - Remnant U(1) symmetry
  - Fourth root trick: still debated
  - Numerical cost is low: popular at finite temperature/density

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)

Caution:

Recently Mandula pointed out that Ginsparg-Wilson relation contains infinite number of lattice chiral transformation. What does this cause? [arXiv:0712.0651]

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

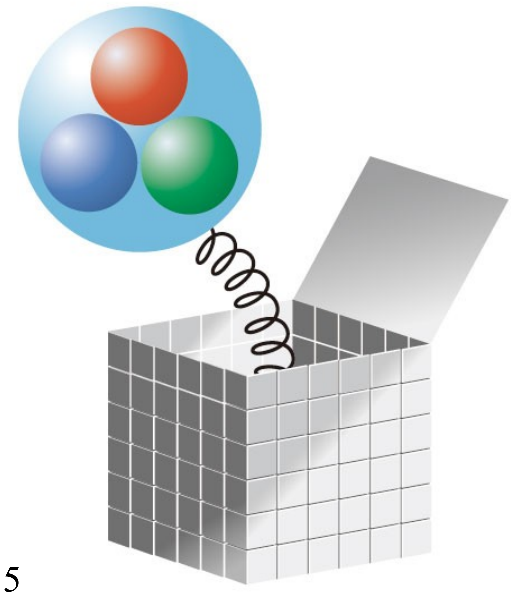
Why overlap fermion?

Exact chiral symmetry

- Exploring the chiral dynamics
  - Confirming the chiral symmetry breaking scenario
  - Epsilon regime
  - Phase transition at $T>0$
- Matrix elements with controlled chiral extrapolation
  - no unwanted operator mixing
- Testing the effective chiral Lagrangian predictions
  - with exact chiral symmetry, continuum ChPT applies

Let us get rid of large cost by large computer power and improved algorithms !

Overlap fermion



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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
    - ex. Chebychev polynomial, partially fractional, etc.

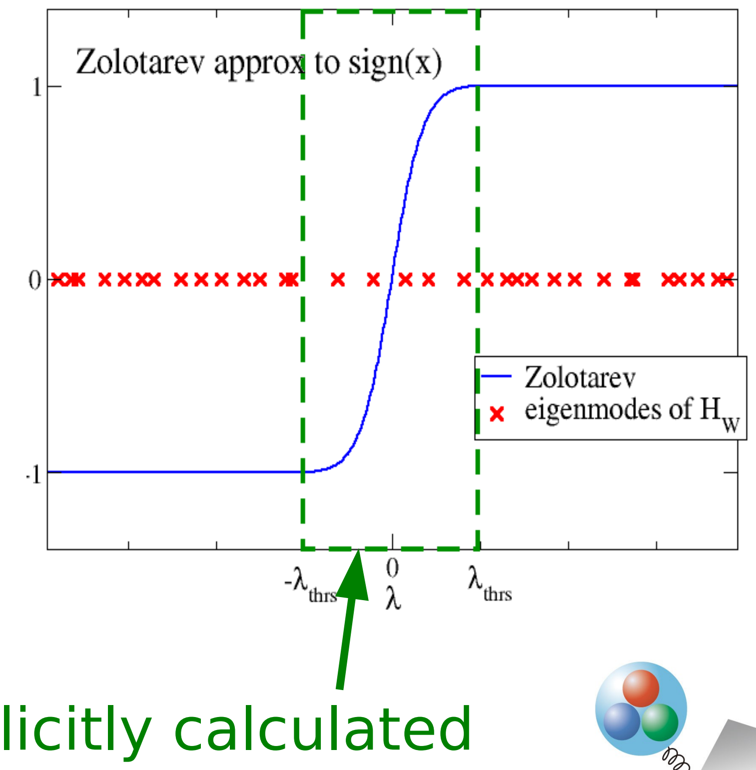
Sign function

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) ∈ $[\lambda_{thrs}, \lambda_{max}]$
- 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)



Locality

Fermion operator should be local

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

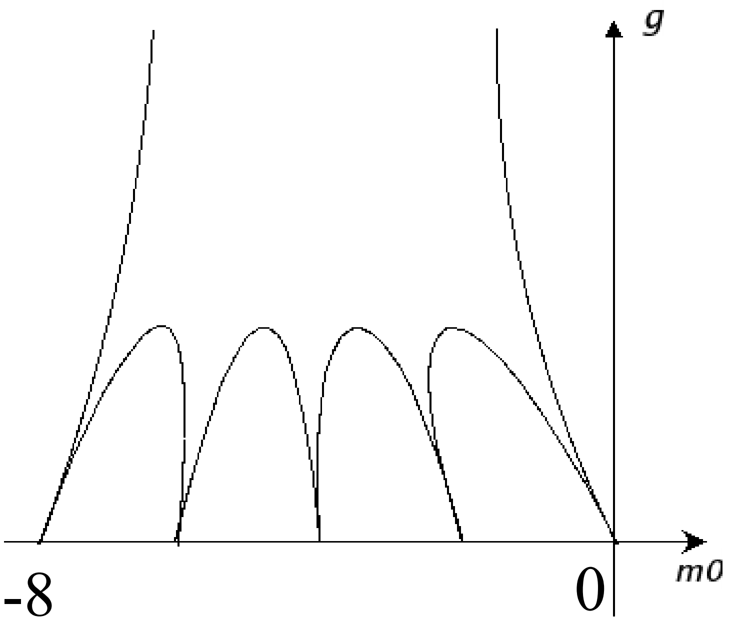
    Hernandez, Jansen, Luscher, 1999

  Near-zero mode is itself exponentially local

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

  ⟺ Out of Aoki phase

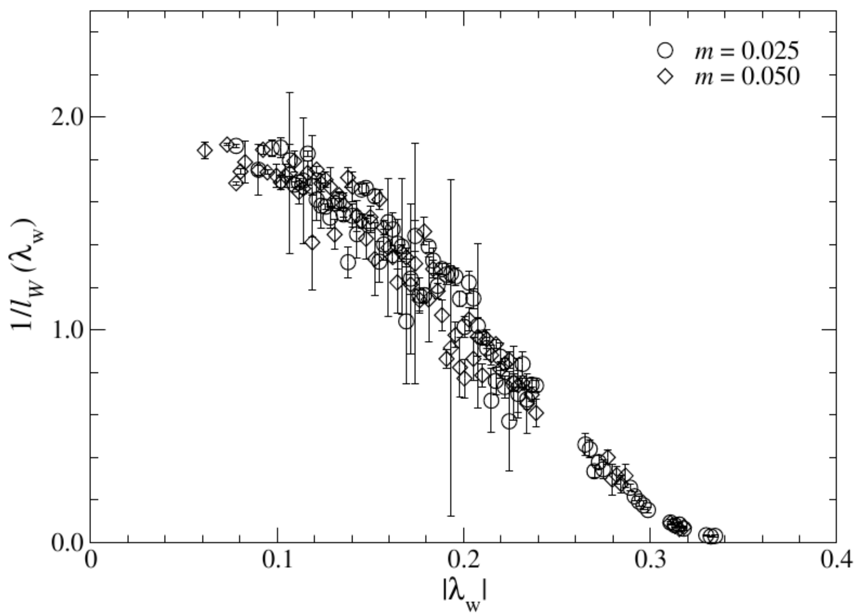
    (parity broken phase



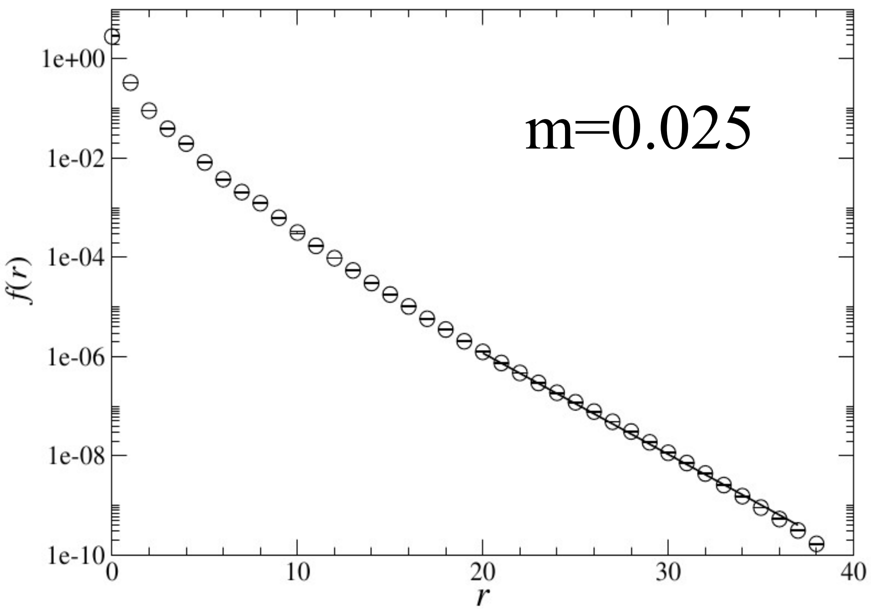
Locality

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

- At beta=2.3 (Nf=2)



Localization length of low eigenmodes of H_W

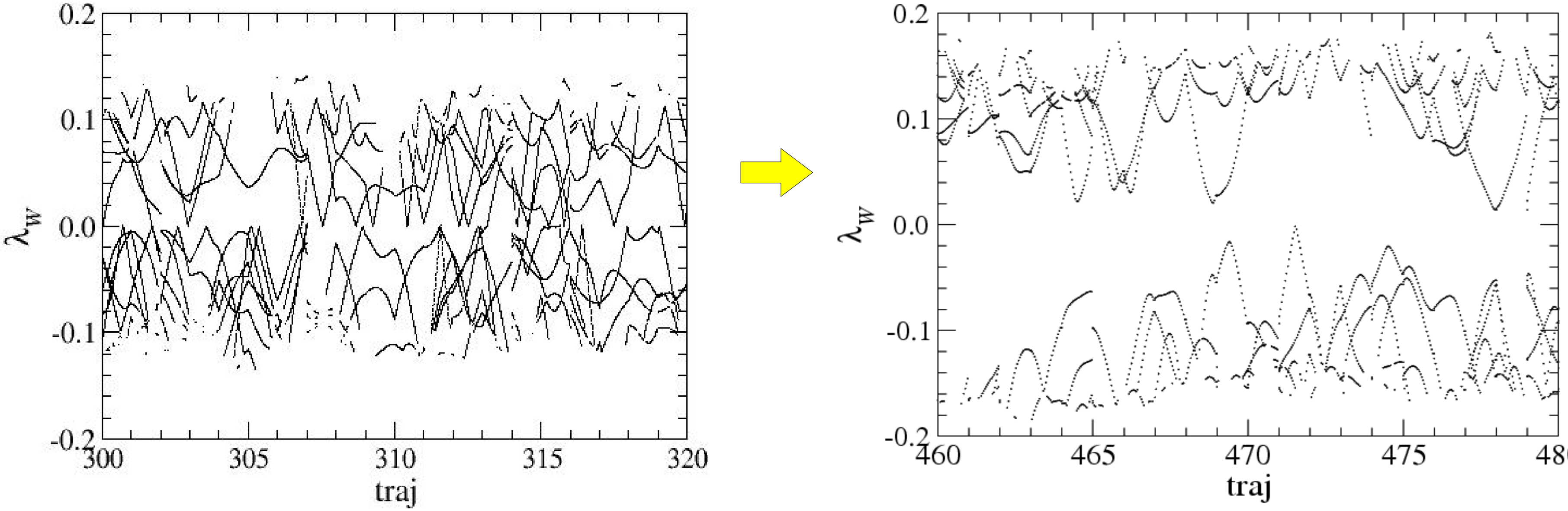


Localization of overlap operator
$l = 0.25$fm ($\sim 2a$)

Simulation at fixed topology

- Suppressing near-zero modes of H_W
  - Locality of overlap operator
  - Cost of dynamical simulation reduced
- Achieved by extra-Wilson fermion term
  - Twisted mass ghost: suppress high mode effect

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



Simulation at fixed topology

Forbidding near-zero mode of H_W ⇔ 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 ⇨ finite V effect
  - θ=0 physics can be reconstructed
    - Finite size correction to fixed Q result (with help of ChPT)
  - Must check local topological fluctuation

    ⇨ 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

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

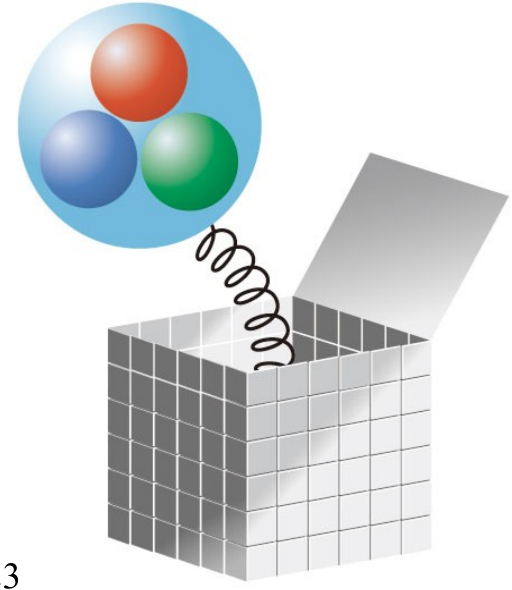
  - For $Q \ll \chi_t V$, Q distribution is Gaussian
- Physical observables
  - Saddle point analysis

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

  - Example: pion mass

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

Large-scale simulation of overlap fermion



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Collaboration

- JLQCD Collaboration
  - S.Hashimoto, T.Kaneko, J.Noaki, E.Shintani, N.Yamada, K.Takeda, H.Ikeda, H.M. (KEK)
  - S.Aoki, K.Kanaya, Y.Kuramashi, Y.Taniguchi, A.Ukawa, T.Yoshie (Tsukuba Univ)
  - H.Fukaya (Niels Bohr Institute)
  - T.Onogi, H.Ohki (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)

Project goals

Dynamical overlap simulations

- Exact chiral symmetry
- Small enough quark masses, ε-regime

- Since 2006 --- on new KEK system (x50 upgraded)
- Let us try new formalism!

Goals:

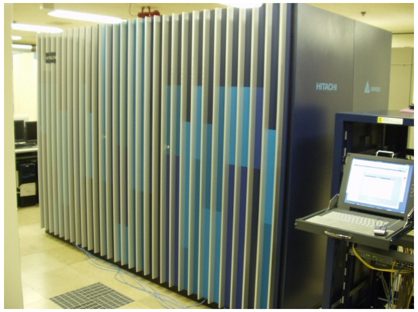
- Exploring the chiral regime
  - Confirming the chiral symmetry breaking scenario
  - Testing the effective chiral Lagrangian predictions
- Matrix elements with controlled chiral extrapolation
  - Without artificial operator mixing
  - Precision computation for flavor physics

Machines

Main machine: IBM Blue Gene/L at KEK

- 57.6 Tflops peak (10 racks)
- 8x8x8(16) torus network

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



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)

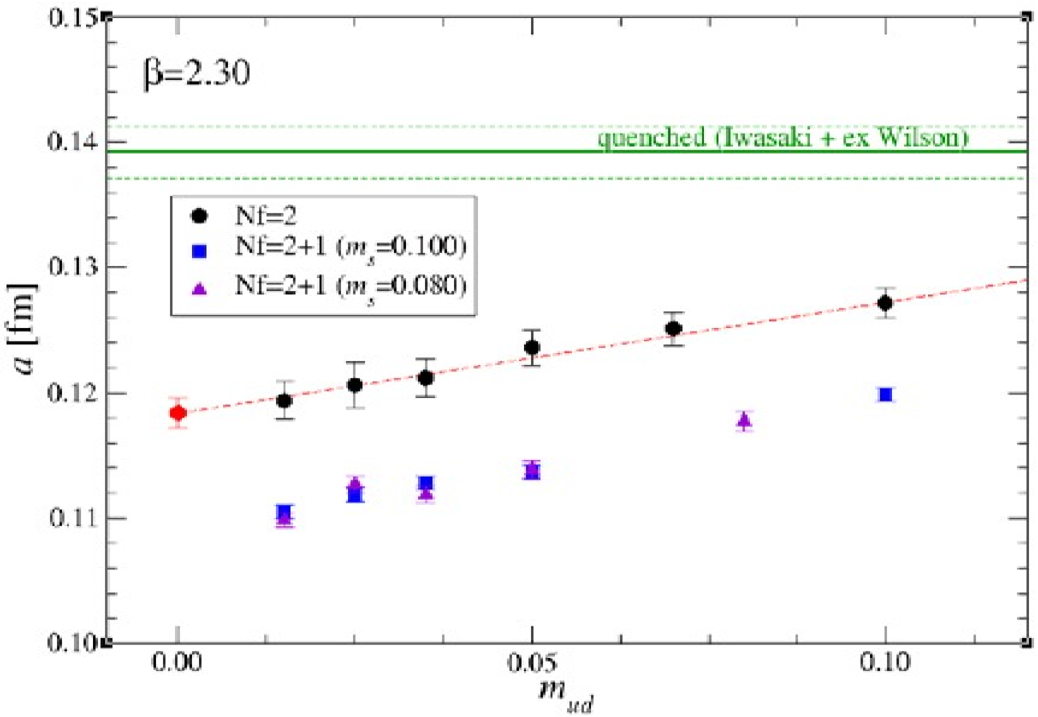
- Nf=2+1 : 16^3x48, a=0.11fm (production run finished)
  - 2 strange quark masses around physical m_s
  - 5 ud quark masses covering (1/6~1)m_s
  - 2500 trajectories with length 1
  - About 2 hours/traj on BG/L 1024 nodes
- Nf=2+1 : 24^3x48 (just started)

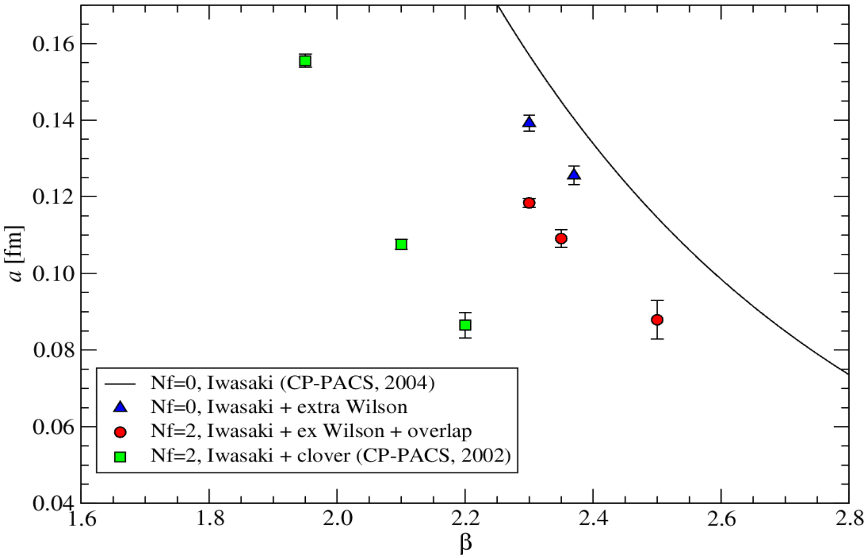
Lattice scale

- 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





Chiral condensate

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

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

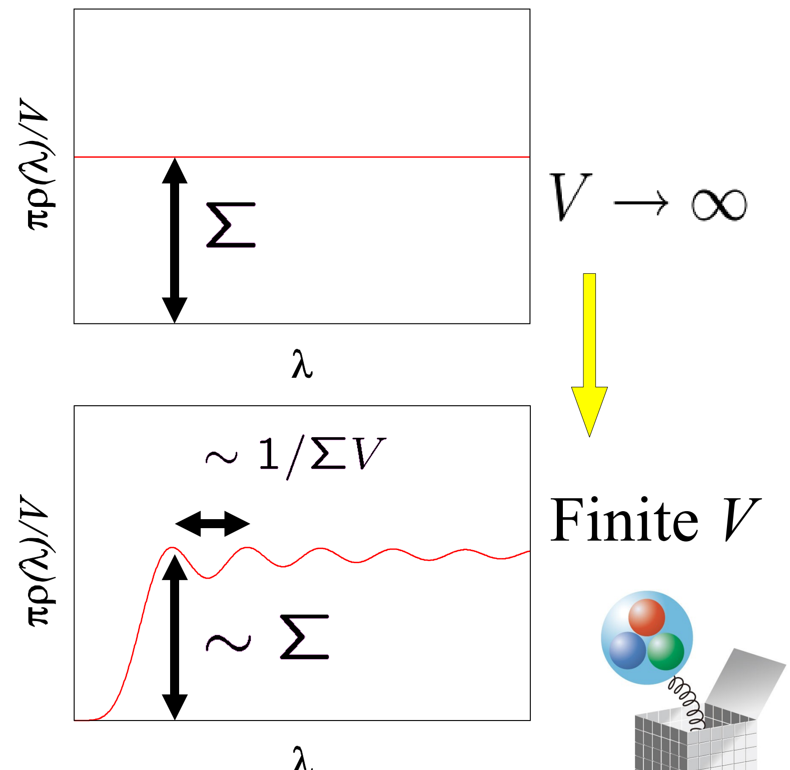
$\rho(\lambda) = \sum_k \langle \delta(\lambda - \lambda_k) \rangle$: spectral density of D

  - 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)



Result in the ε-regime

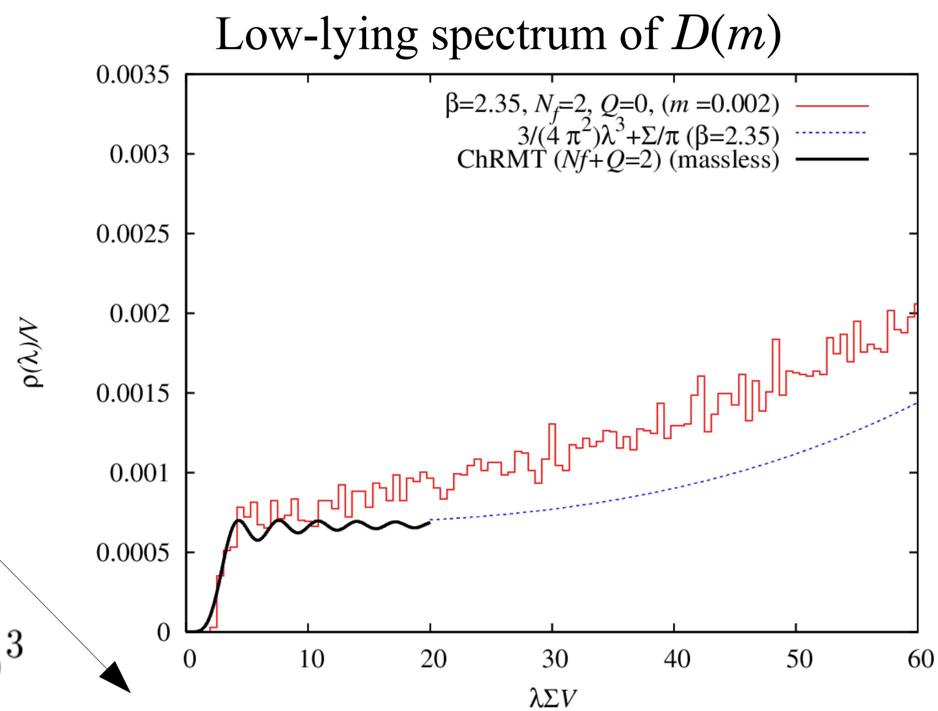
(JLQCD, 2007, JLQCD and TWQCD, 2007)

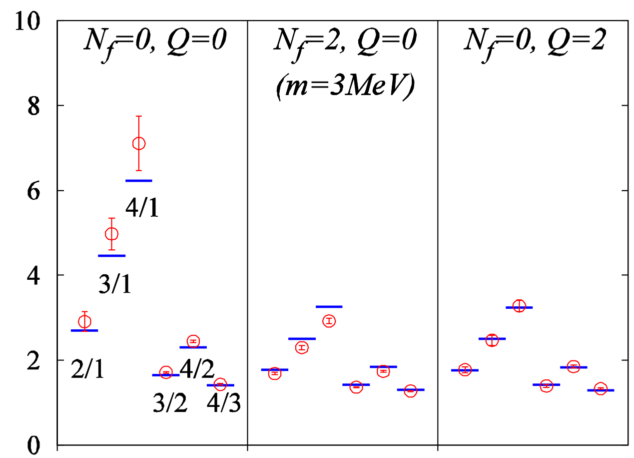
- Nf=2, 16^3x32, a=0.11fm
- m~3MeV

- 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





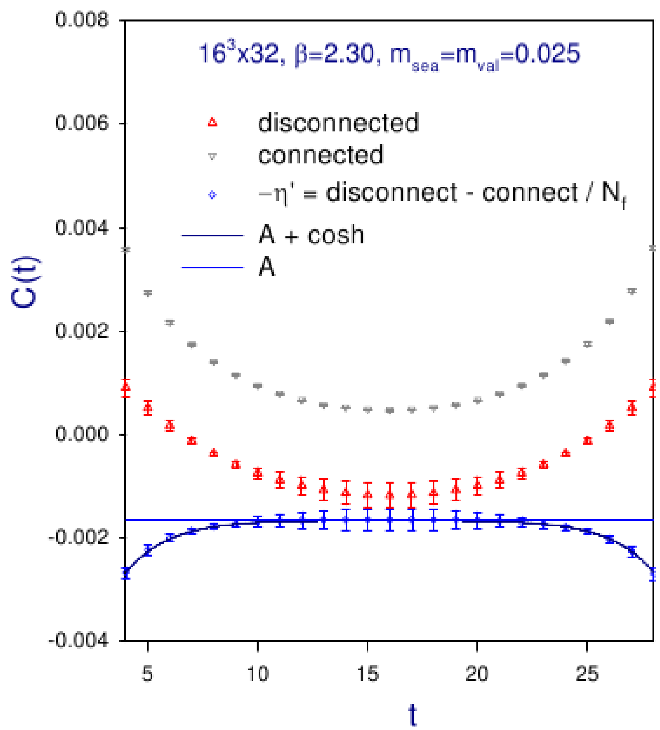
Topological susceptibility

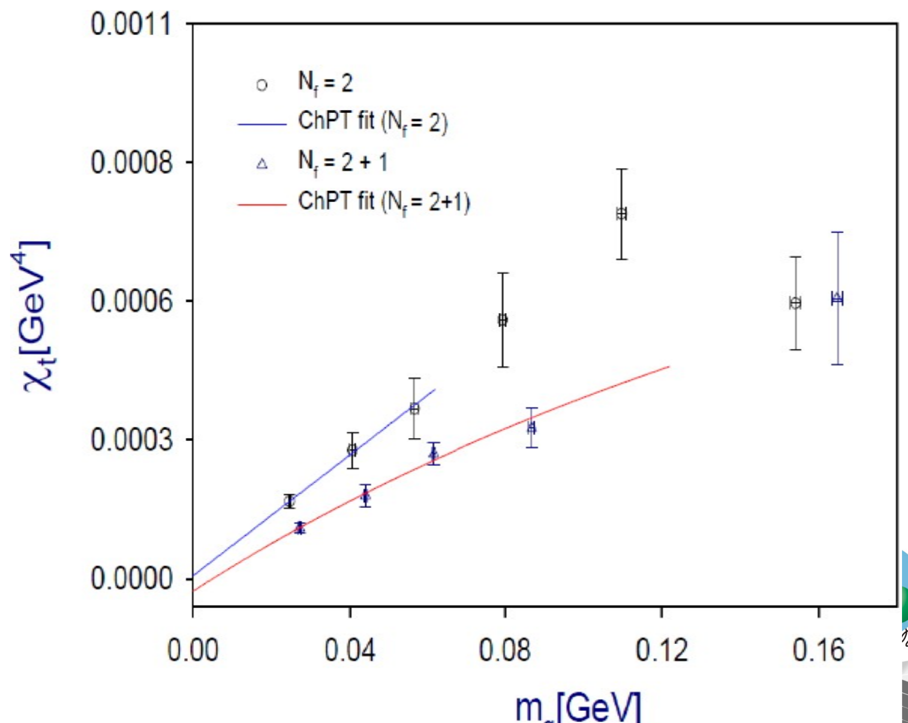
Is local topological fluctuation sufficient ? (JLQCD-TWQCD, 2007)

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





Meson spectrum: finite volume effect

Finite volume correction

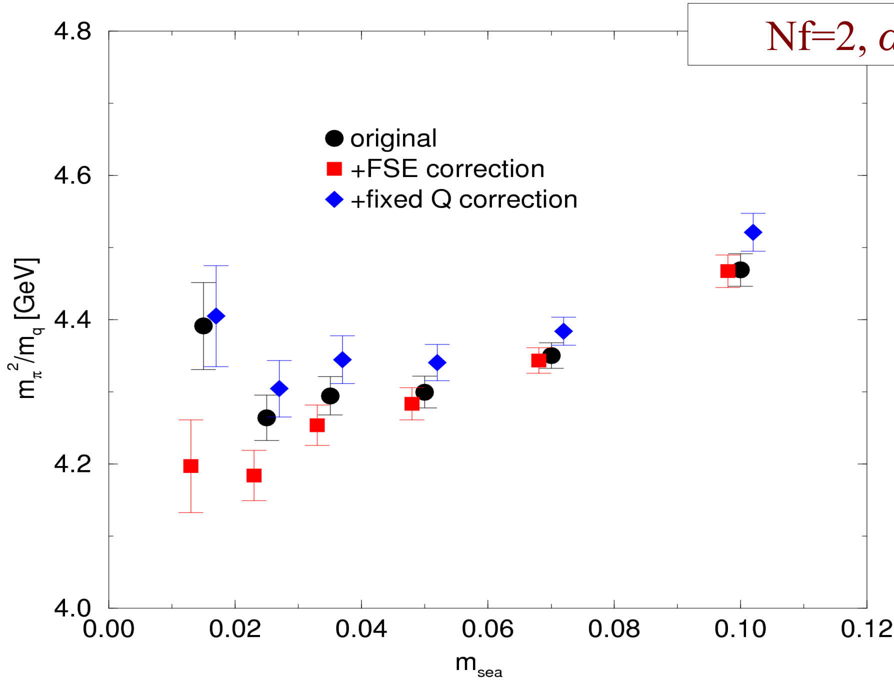
JLQCD, arXiv:0804.0894

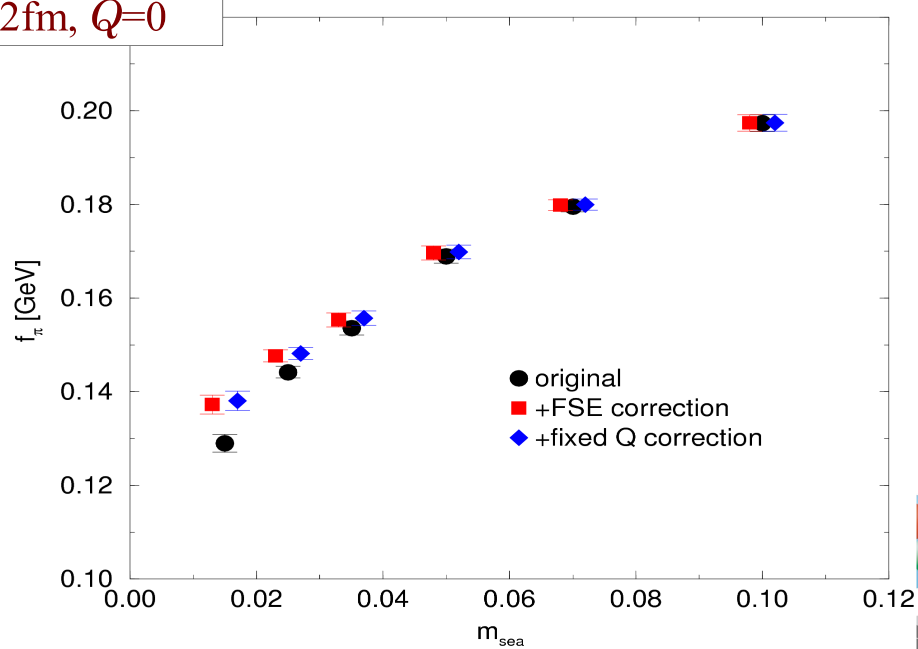
$$\left(m_\pi^2\right)^{\text{corrected}} = \frac{m_\pi^2}{(1+R_m)^2(1+T_m)^2}, \quad (f_\pi)^{\text{corrected}} = \frac{f_\pi}{(1+R_f)(1+T_f)}$$

- 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

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



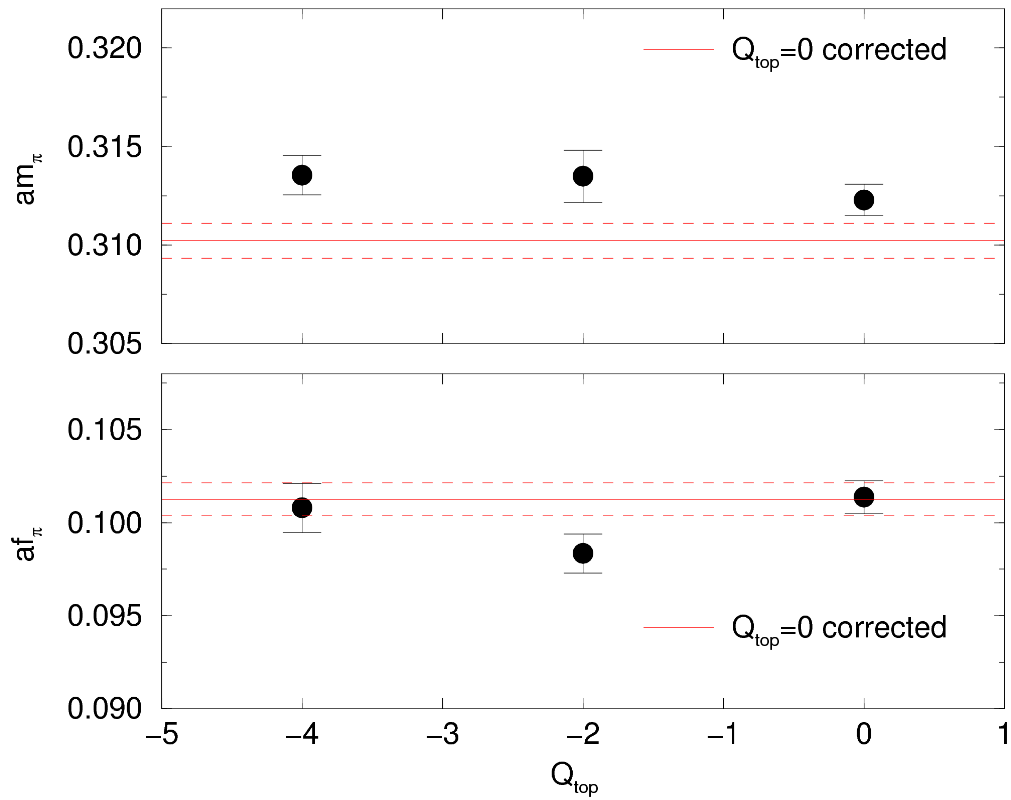


Meson spectrum: Q-dependnece

Nf=2, $m_{sea} = 0.050$

$Q = 0, -2, -4$

- No large Q-dependence
  (consistent with expectation)



Meson spectrum: ChPT test

Chiral expansion

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

JLQCD, arXiv:0804.0894

- Continuum ChPT formula applicable
- The region of convergence

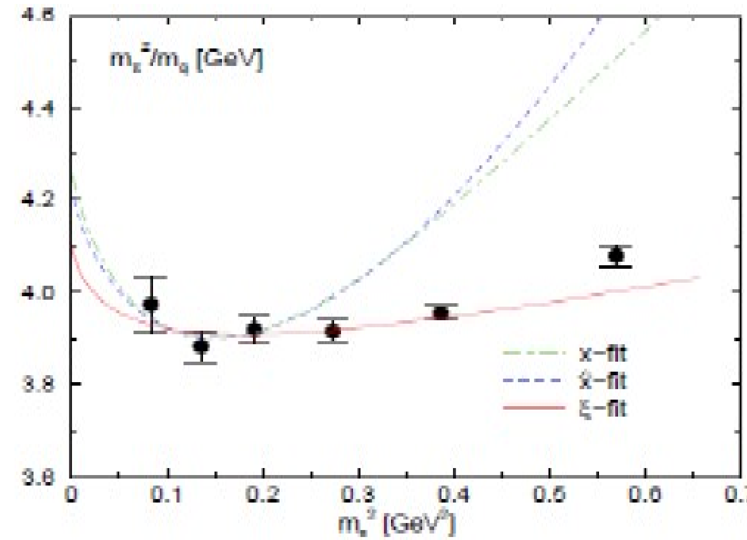
$$\frac{m_\pi^2}{m_q} = 2B[1 + x\ln(x) + c_3 x + O(x^2)]$$

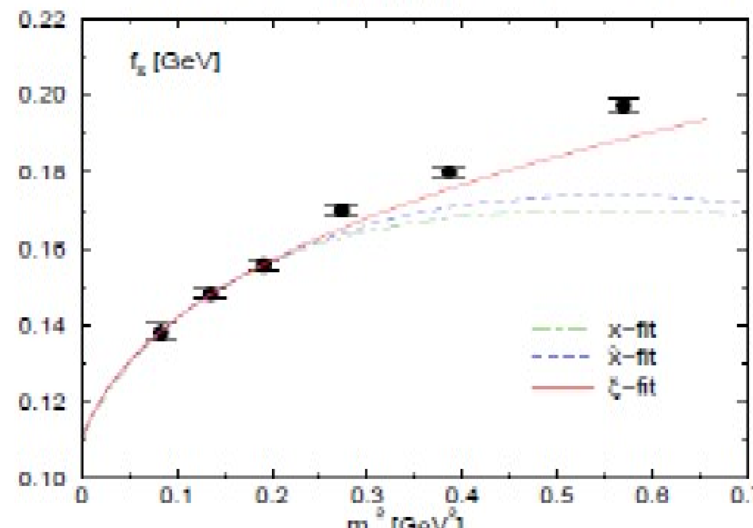
$$f_\pi = f[1 - 2x\ln(x) + c_4 x + O(x^2)]$$

Expand either

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

ξ extends the region significantly



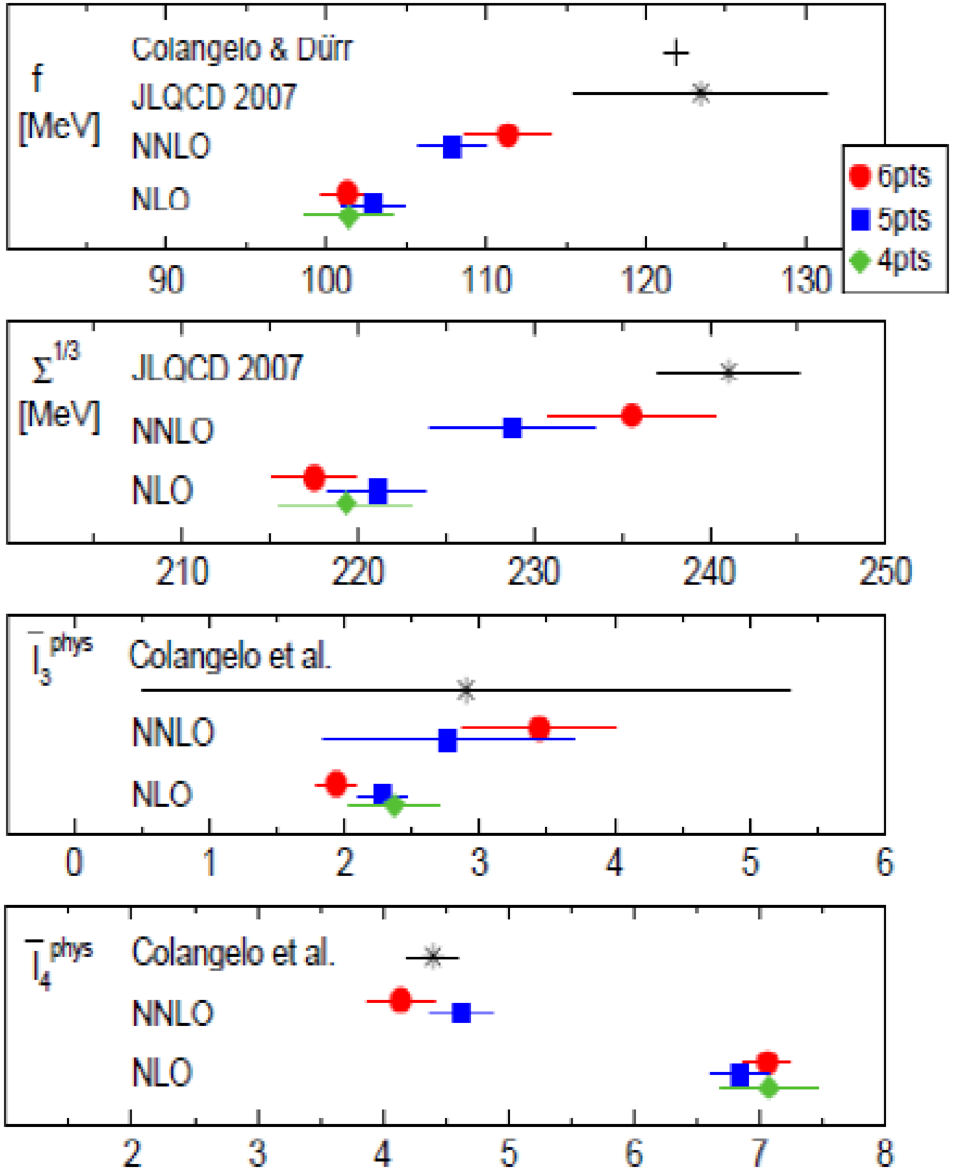


Meson spectrum: low energy consts

Low energy constants

--- NNLO fit with ξ

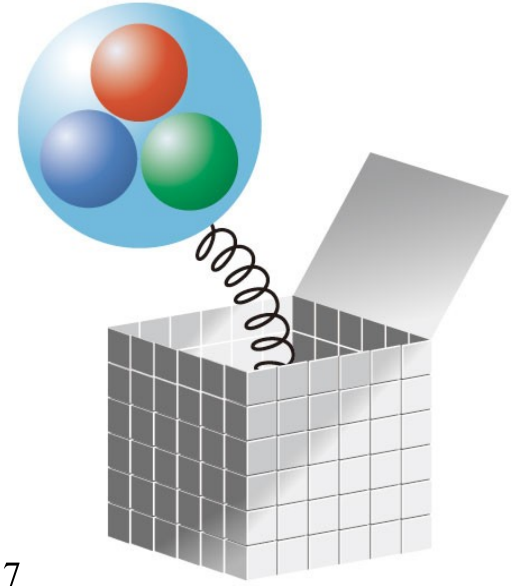
For reliable extraction of low energy constant, NNLO terms are mandatory



Other results

- Physics publication: Cf. http://jlqcd.kek.jp/
  - ε-regime
  - Topological susceptibility
  - Meson spectroscopy and ChPT test
  - π^+-π^0 mass difference
  - Coupling const
  - B_K (Kaon bag parameter)
  - Nucleon sigma term
  - Ps-NG boson mass/S-parameter
  - Pion form factors (in preparation)
  - Nonperturbative renormalization (in preparation)

Toward overlap simulation at finite temperature



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Lattice QCD at T>0

- Phase diagram: still not conclusive
  - Nf=2: expected O(4) scaling not observed in KS
    - All recent works are with KS, Nt=4
    - Work with Wilson fermion is not at enough small quark mass
  - Nf=2+1 (physical point)
    - Recently only with KS fermions, still large uncertainty
- Finite chemical potential
  - various methods proposed, but limited applicability
  - still waiting a breakthrough!
- Thermodynamics (equation of state, etc.)
- Excitation spectrum
- Viscosity

Toward overlap at T>0

Where overlap should be applied ?

- Chiral symmetry is essential
- KS and Wilson (and others) are inconsistent

Phase structure of Nf=2, 2+1

- Vicinity of phase transition --- critical behavior ?
- Observables concerning chiral symmetry and topological charge

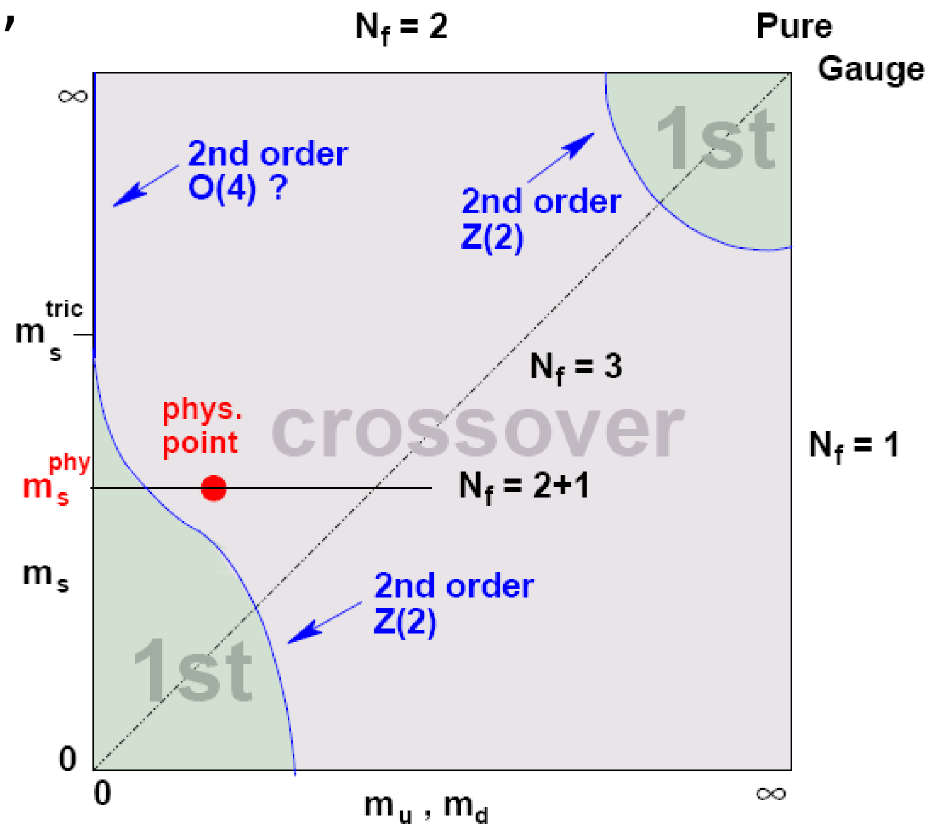
For other topics,

- Overlap costs too much
- Other formulations are sufficient
- Technical development is demanded

Phase diagram

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

Phase diagram

Nf=2 scaling study

- Needs finite size scaling
- Good reference work:

D'Elia, Di Giacomo, Pica, Phys. Rev. D72 (2005) 114510

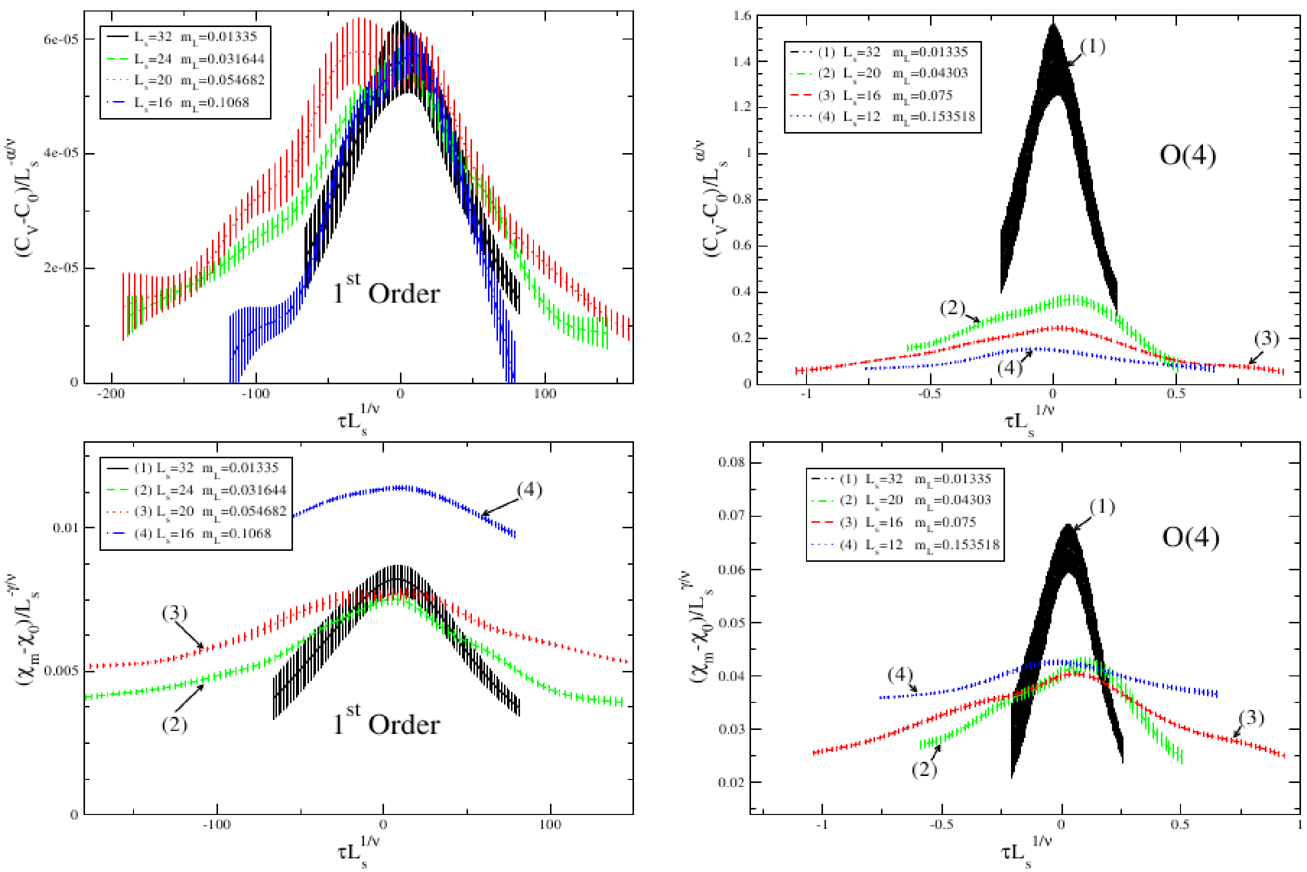
Lattice simulation with

- Staggered (unimproved)
- Lt=4, Ls=12, 16, 20, 24, 32 → finite size scaling
- am=0.01335 – 0.307036
- Measure specific heat, susceptibility
- Comparison with O(4), O(2), 2st order scaling

Nf=2 scaling study

Result (Cossu, D'Elia, Di Giacomo, Pica, PoS(LAT2007) 219):

- Inconsistent with O(4) nor O(2)
- Prefers 1st order (but not all quantities are consistent)



Toward overlap at T>0

To perform the same level of work with overlap fermion,

- Suppose that simulation is possible at Nt=6
  - Locality must be kept
  - Not clear whether possible or not
  - At least, around Ls=32 O(10000) trj x O(20) param. sets
    - → 1-2 years on Blue Gene @KEK (57.3TFlops)
  - Whole project 2-3 years (optimistic estimate)
- At present, not realistic
  - If performance is 5 times improved, may possible
  - Next generation computer? (time passes so fast!)
  - Within a few years, become feasible

Toward overlap at T>0

Preparation should be started

- How 1/a can be reduced keeping locality ?
- Fixed topology effect
  - For matrix elements, finite size effect
  - How about thermodynamic quantities, in particular critical exponent ?
- Survey in parameter space (beta, quark mass, volume)
- Fundamental thermodynamic quantities
- Improved algorithms (always called for!)

Beyond QCD

Motivation:

- What is relation between confinement and chiral symmetry breaking?
- Phase structure of gauge theories
- Advantages of exact chiral symmetry

Beyond QCD applications

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

Summary/outlook

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

Outlook

- Simulation at finite temperature is challenging
- Scaling study ?
- Should start exploratory study
- Beyond QCD simulations are interesting