
Lattice QCD with dynamical fermions

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Recent progress in lattice QCD

Major advances in simulations of fermions on the lattice

- algorithmic developments
[Hasenbusch 01, Luscher03f, Urbach et al 05, Clark & Kennedy 06]
- program efficiency & faster computers
[PC clusters, APE, QCDOC → BG]

Numerical studies can now access the chiral regime of QCD, at large volumes and small lattice spacing, with different discretizations.

- taming systematic errors
- quantitative tool for non-perturbative QFT
- revised cost estimates in more detail...

New scope for lattice QCD

Cost formula for 100 cnfg: eg $N_f = 2$, $O(a)$ improved, Wilson quarks, $2L \times L$ lattice

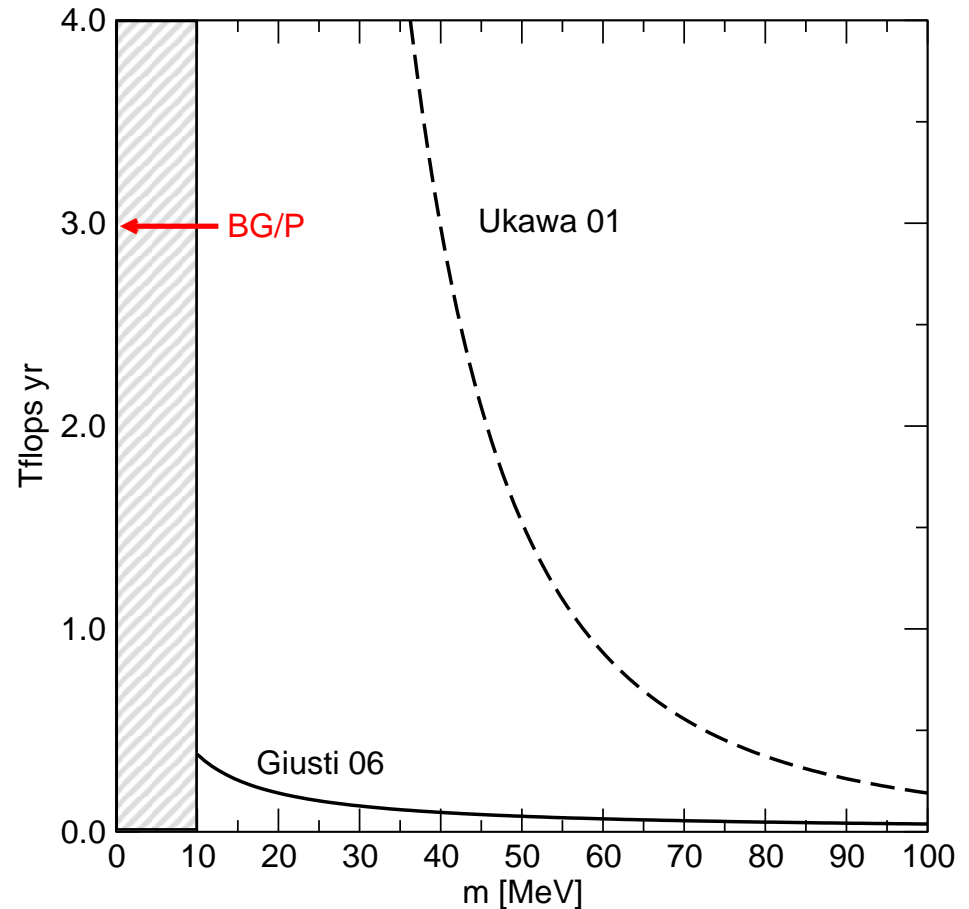
Ukawa lat01

$$5 \left[\frac{20 \text{ MeV}}{m} \right]^3 \left[\frac{L}{5 \text{ fm}} \right]^5 \left[\frac{0.1 \text{ fm}}{a} \right]^7$$

Giusti lat06

$$0.05 \left[\frac{20 \text{ MeV}}{m} \right]^1 \left[\frac{L}{5 \text{ fm}} \right]^5 \left[\frac{0.1 \text{ fm}}{a} \right]^6$$

64×32^3 lattice, $L \approx 2.5 \text{ fm}$, $a \approx 0.09 \text{ fm}$



Chiral regime of (full) QCD

- SU(2) chiral perturbation theory predicts:

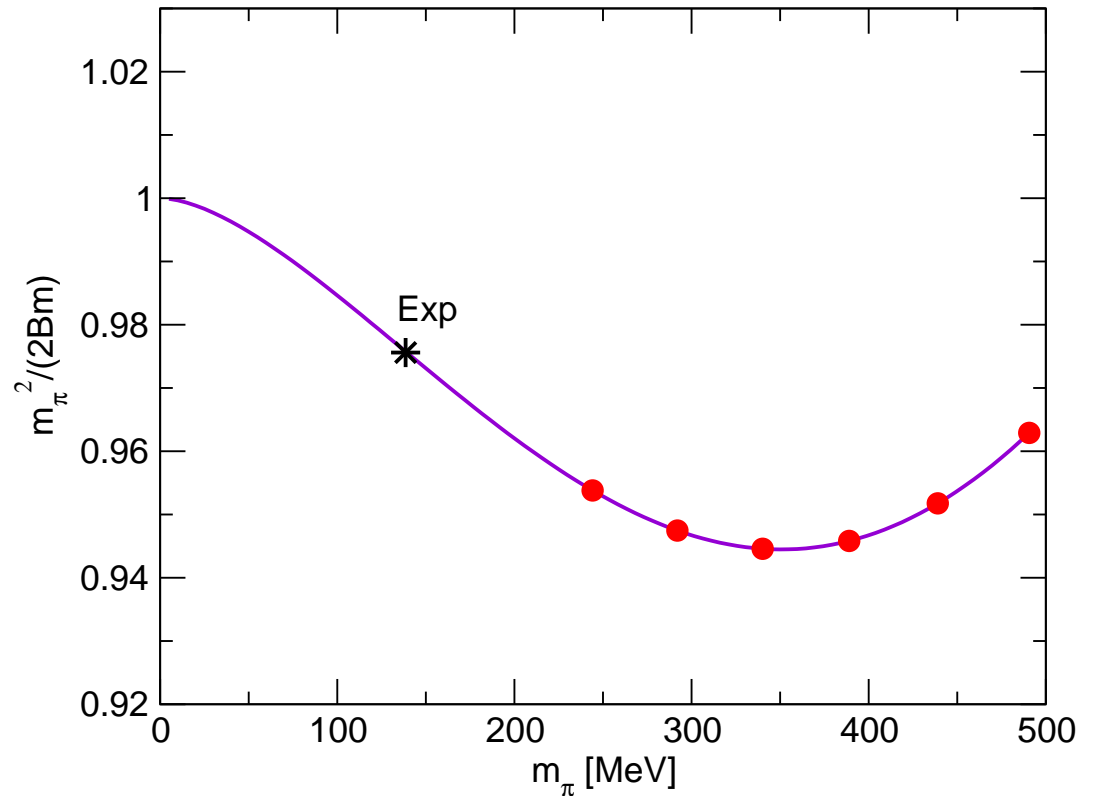
$$m_\pi^2 = M^2 \left[1 + \frac{M^2}{32\pi^2 F^2} \log(M^2/\Lambda_3^2) + \dots \right], \quad M^2 = 2Bm$$

$$f_\pi = F - \frac{M^2}{16\pi^2 F^2} \log(M^2/\Lambda_4^2) + \dots$$

LEC determined from
phenomenological studies

small masses and $\approx 1\%$ precision

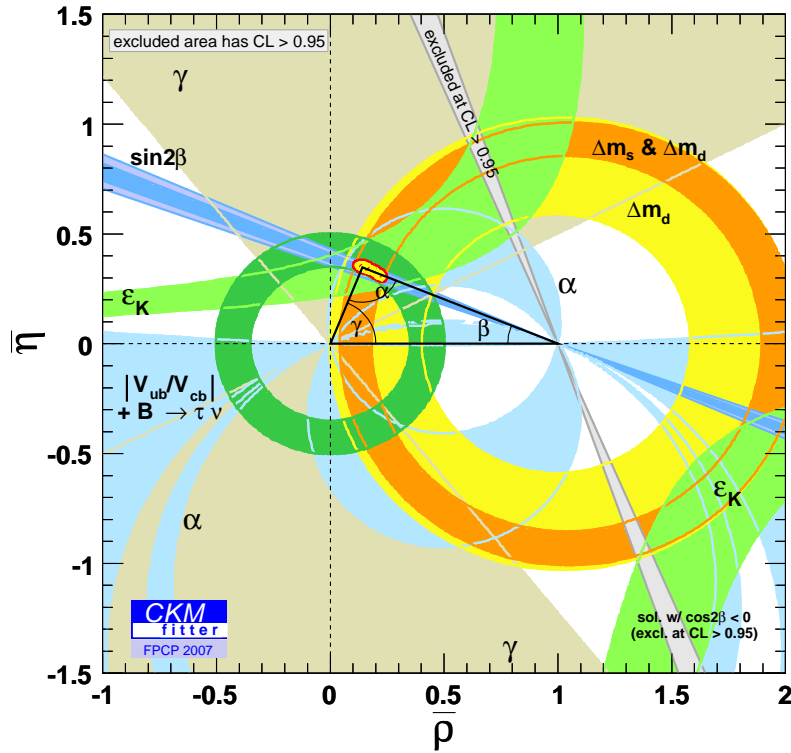
- $\rho \rightarrow \pi\pi$ decays
- flavour-singlet phenomenology



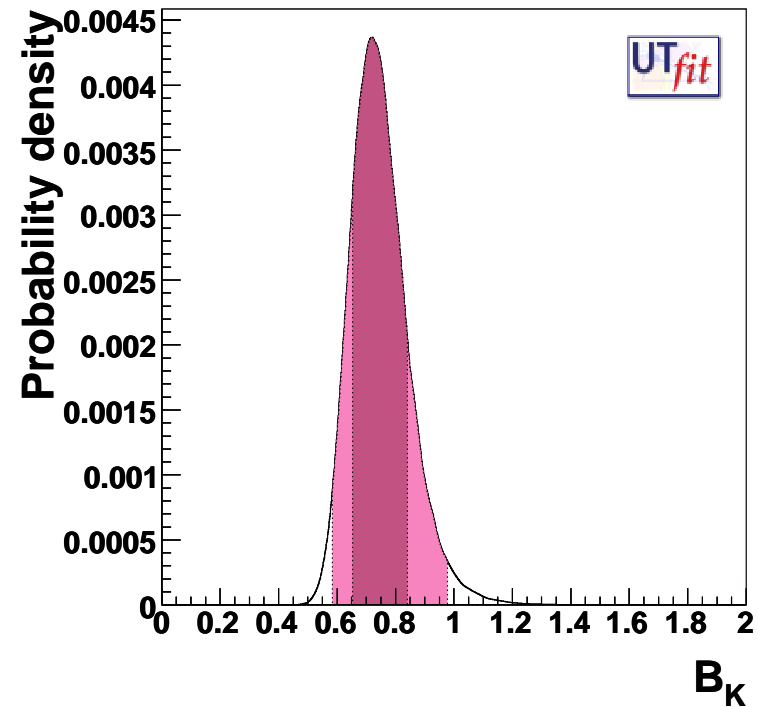
UT phenomenology

Lattice input [CKMfitter,UTfit]:

- K_{l3} form factor [Zanotti, EPS07]
- semileptonic B decays form factors
- f_B, B_B, ξ for B mixing [Papinutto, EPS07]
- B_K for kaon mixing



$$\hat{B}_K = 0.75 \pm 0.09$$



Non Perturbative New Physics?

Growing interest for BSM strong dynamics:

- five-dimensional gauge theories

[Knechtli, EPS07]

- novel models of technicolor

[Sannino et al 04f]

- orientifold planar equivalence

[Armoni, Shifman, Veneziano 04f]

- susy on the lattice

[eg Giedt, lat06]

Dynamical fermions play a crucial role in (almost all) these models.

Explore space of theories as N_c , N_f , and the fermion representation is varied.

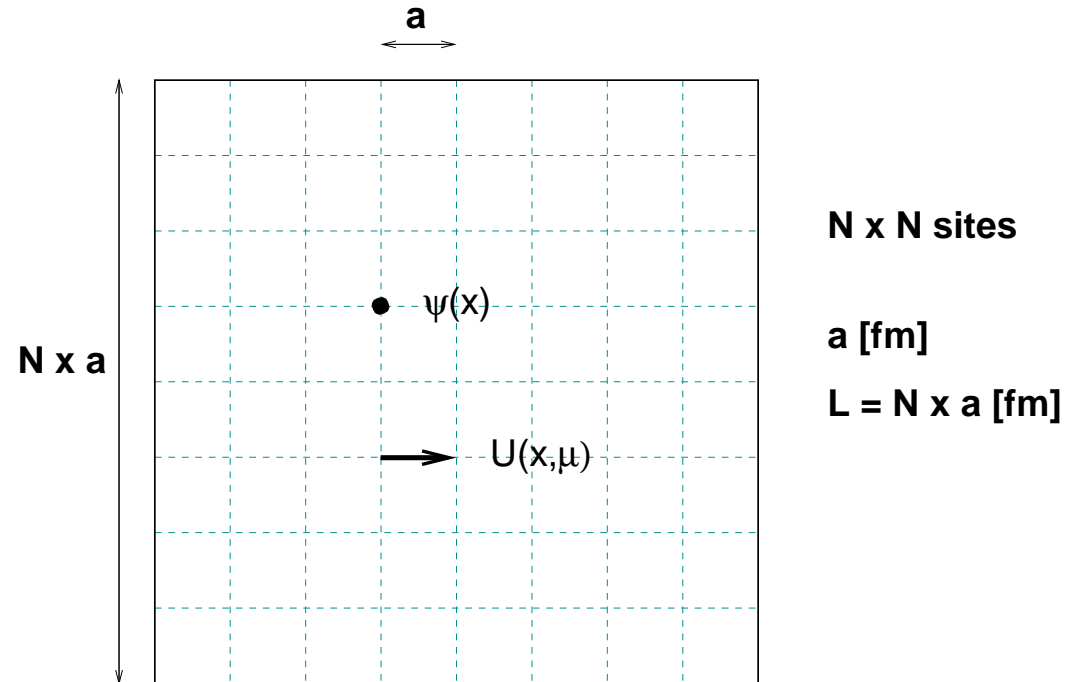
When all are one...

Different actions for lattice QCD:

- precision computations
- affordable cost
- clean theoretical grounds

Control of systematics:

- light masses: $m_\pi \approx 300$ MeV
- large volume: $m_\pi L \geq 3$, ie $L \geq 2 \div 3$ fm
- lattice artefacts: $O(a)$ improved theories
- NP renormalization
- sampling of topology
- $U(1)_A$ sector



$$\begin{aligned} Z &= \int dU d\psi d\bar{\psi} \exp [-S(U, \psi, \bar{\psi})] \\ &= \int dU d\phi d\phi^* \exp [-S_G - |D^{-1}\phi|^2] \end{aligned}$$

Lattice Dirac operator

For massless fermions:

$$S_F = a^4 \sum_{x,y} \bar{\psi}(x) D(x,y) \psi(y)$$

Naive continuum limit suggests:

- (a) $D(x,y)$ is local
- (b) $D(p) = i\gamma_\mu p_\mu + O(ap^2)$
- (c) $D(p)$ invertible for $p \neq 0$
- (d) $\{\gamma_5, D\} = 0$

Nielsen-Ninomiya thm: (a)–(d) can not hold simultaneously

↪ **doublers:** anomaly–cancelling spectrum

Wilson: explicit breaking of chiral symmetry

Staggered: left with four species (“tastes”), rooting [Sharpe lat06, Kronfeld lat07]

Ginsparg–Wilson: relax (d) $\longrightarrow \{\gamma_5, D\} = aD\gamma_5D$ [Ginsparg & Wilson 82]

Wilson fermions

$$D = \frac{1}{2} \sum_{\mu} \{ \gamma_{\mu} (\nabla_{\mu} + \nabla_{\mu}^{*}) - \nabla_{\mu}^{*} \nabla_{\mu} \} + m$$

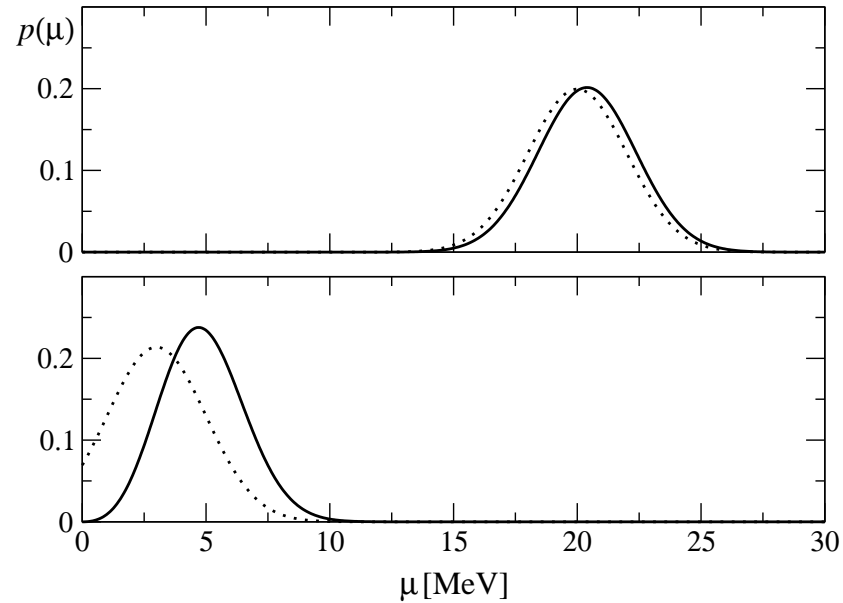
- doublers removed by adding **irrelevant operator**
- explicit breaking of axial symmetry at $m = 0$
- NP renormalization [ALPHA]
- NP $O(a)$ improvement [ALPHA]
- $N_f = 2$ CERN–TOV, QCDSF (UKQCD, CP–PACS)
- $N_f = 2 + 1$ PACS–CS

breaking of axial symmetry \implies non–trivial approach to the chiral limit...

Eigenvalues of the Dirac operator

- continuum theory: $\{\gamma_5, D\} = 0$
 \implies the massive Dirac operator is protected from small e.v.
- Wilson fermions break chiral symmetry
 \implies no protection for $D_m = D_w + m_0$
- for particular gauge fields: **exceptionally small e.v.**
 \implies instabilities / more expensive computations
- CERN-TOV observed smooth runs: can NOT be a property of the algorithm
distribution of the **spectral gap** is a property of D_m
- scaling as $a \rightarrow 0$
 $m \rightarrow 0$
 $V \rightarrow \infty$
- analytical control: PQChPt/RMT, $O(a^2)$ effects, finite volume [Sharpe 06]

Gap distribution - 1



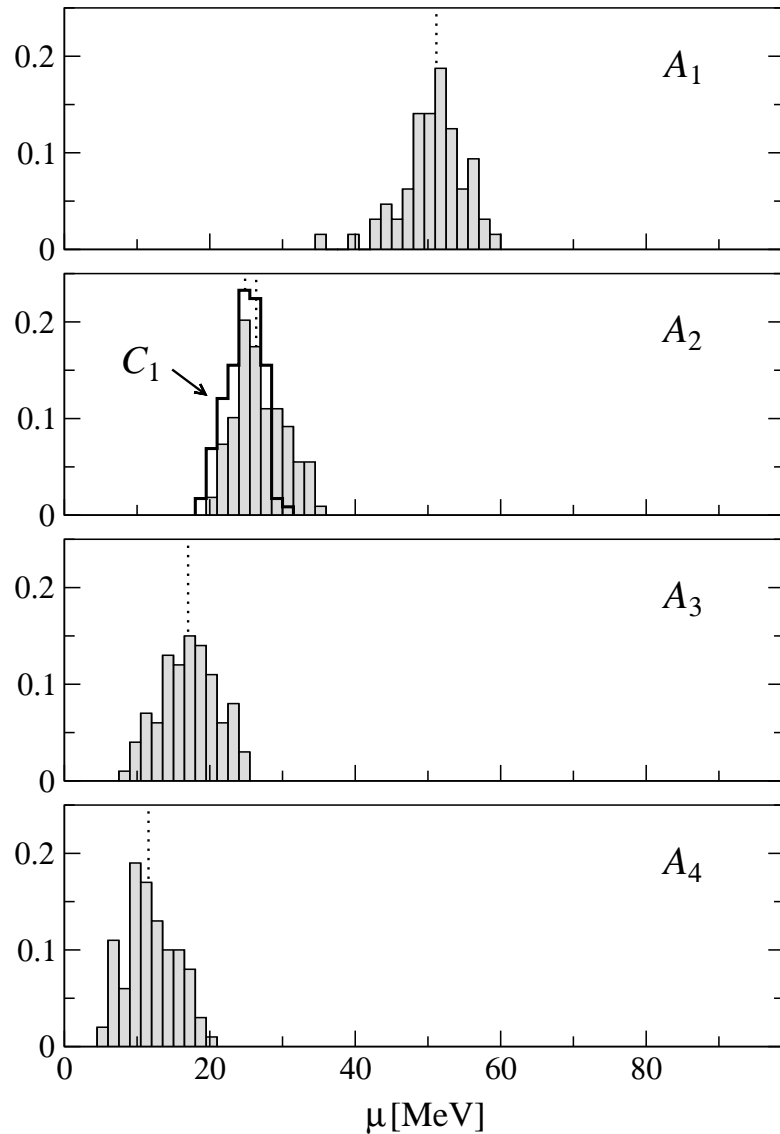
- μ lowest eigenvalue of D_m
- integration instabilities / reversibility
- ergodicity problem
- sampling of observables: $p(\mu)/\mu^2$

difficult regime for simulations:

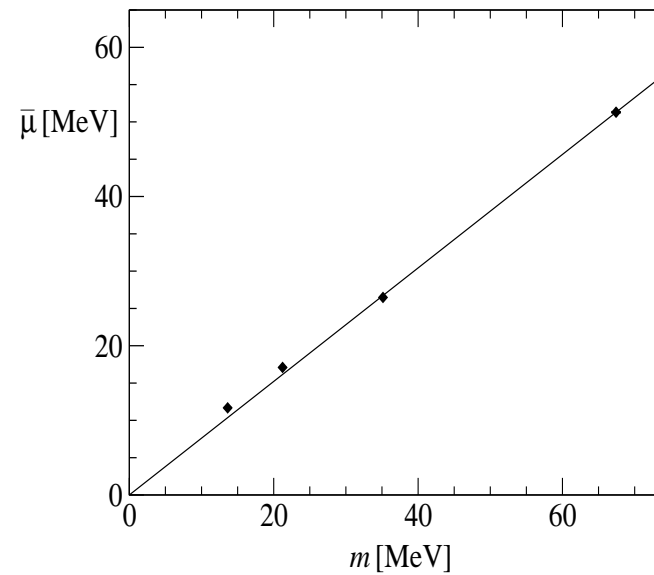
$$m \rightarrow 0$$
$$a, V \text{ fixed}$$

\hookrightarrow is there a safe regime?

Gap distribution - 2



- stability is related to the width of the distribution
- $\bar{\mu}$ shifts linearly with m
- width independent of the mass
- scaling with a and V : $\sigma \propto aV^{-1/2}$



[Idd et al 05]

Safety distance

To avoid instabilities:

$$\bar{\mu} \geq 3\sigma$$

which yields:

$$m \geq \frac{3a}{Z_A \sqrt{V}}$$

Introducing $B = m_\pi^2/2m$ and lattice with geometry $2L \times L^3$:

$$(m_\pi L)^2 \geq 3\sqrt{2}B/Z_A a$$

From our numerical study:

$$m_\pi L \geq \begin{cases} 2.8 & \text{at } a = 0.07 \text{ fm,} \\ 2.3 & \text{at } a = 0.05 \text{ fm} \end{cases}$$

↔ chiral symmetry and continuum limit entangled

tmQCD

$$D = \frac{1}{2} \sum_{\mu} \{ \gamma_{\mu} (\nabla_{\mu} + \nabla_{\mu}^*) - \nabla_{\mu}^* \nabla_{\mu} \} + (m + i\gamma_5 \tau_3 \mu)$$

Tune $m = m_{\text{crit}}(\mu)$ to achieve *maximal twist*:

$$m_{\text{pcac}} = \frac{\sum_{\mathbf{x}} \langle \partial_0 A_0^a(t, \mathbf{x}) P^a(0) \rangle}{\sum_{\mathbf{x}} \langle P^a(t, \mathbf{x}) P^a(0) \rangle} = 0$$

- breaking of vector symmetry and parity - π^{\pm}, π^0 splitting
- NP renormalization
- at maximal twist: NP $O(a)$ improvement automatic for parity-even operators
- tuning only one parameter to achieve maximal twist
- $N_f = 2$ ETMC [Urbach lat07]

Ginsparg–Wilson fermions

- Ginsparg-Wilson relation (82)

$$\{\gamma_5, D\} = \bar{a}D\gamma_5D$$

- Neuberger overlap operator (97)

$$D = \frac{1}{\bar{a}} [1 + \gamma_5 \epsilon(H_w)]$$
$$H_w = \gamma_5 [aD_w - (1 + s)]$$

where $\bar{a} = a/(1 + s)$, and $s \in [0, 2]$

- lattice chiral symmetry [Lüscher 98]

$$\delta\psi = \hat{\gamma}_5\psi, \quad \hat{\gamma}_5 = \gamma_5(1 - \bar{a}D)$$
$$\delta\bar{\psi} = \bar{\psi}\gamma_5$$

- anomaly and index theorem on the lattice [Hasenfratz et al 97]

$$a^4Q(x) = \frac{\bar{a}}{2} \text{Tr} [\gamma_5 D(x, x)]$$

Domain-wall fermions

[Shamir & Furman 93]

- Introduce extra dimension L_S
- Dirac operator: $D_{x,s;x',s'} = \delta_{s,s'} D_{x,y}^{\parallel}(-M) + \delta_{x,y} D_{s,s'}^{\perp}(m)$
- at finite L_S , partial decoupling of chiral modes:

$$\partial_{\mu} A_{\mu}^a = 2m J_5^a + 2J_{5q}^a$$

- for $m = 0$, $L_S \rightarrow \infty$: chiral symmetry restored
- residual chiral symmetry breaking parameterized by the **residual mass**
- (almost) automatic $O(a)$ improvement
- extra computational cost
- chiral limit is **decoupled** from the continuum one
- AWI on the lattice
- $N_f = 2 + 1$ RBC/UKQCD collaboration [Boyle lat07]

First results

[lat07]

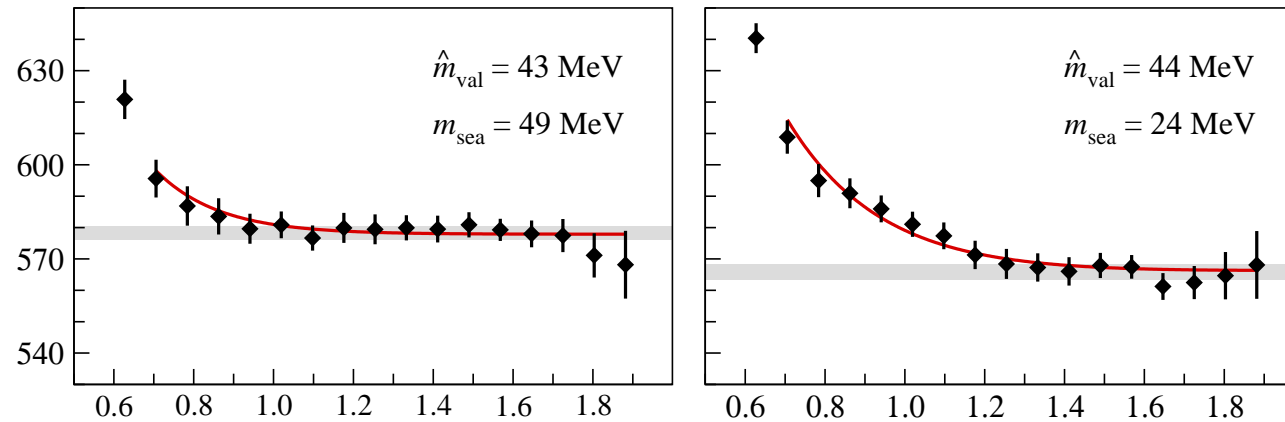
Several collaborations worldwide:

- ALPHA $N_f = 2$, $O(a)$ improved Wilson
- CERN-TOV $N_f = 2$, $O(a)$ improved Wilson
- JLQCD $N_f = 2$, overlap
- QCDSF $N_f = 2$, $O(a)$ improved Wilson, baryon physics
- ETMC $N_f = 2$, tmQCD

- BGR $N_f = 2 + 1$, perfect action
- HPQCD, MILC $N_f = 2 + 1$, staggered
- PACS-CS $N_f = 2 + 1$ $O(a)$, improved Wilson
- NPLQCD mixed action
- RBC/UKQCD $N_f = 2 + 1$, Domain Wall Fermions

Effects of dynamical fermions

CERN-TOV, $a = 0.078$ fm, $[M_V/M_{PS}]$, $L \approx 2$ fm [Idd et al 05]



Pseudoscalar two-pt function - coupling to multi-particle states:

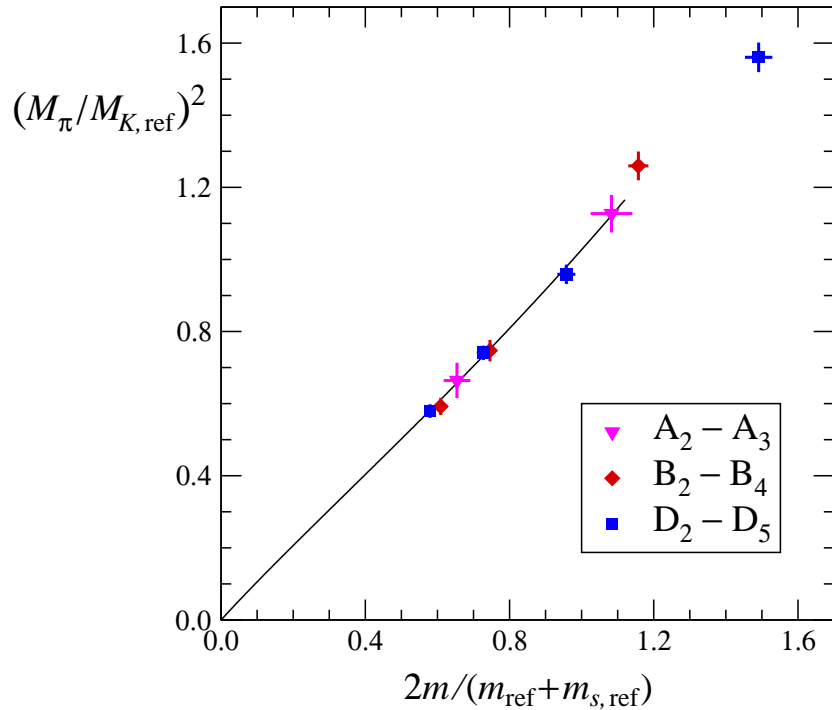
$$f_{\text{PP}}(t) = c_0 e^{-M_0 t} + c_1 e^{-M_1 t} + \dots$$

In the full theory: $M_1 = M_0 + 2M_\pi$, ie. three meson state at rest

$$M_{\text{eff}}(t) = -\frac{d}{dt} \log f_2(t) = M_0 + C e^{-(M_1 - M_0)t} + \dots$$

Chiral extrapolations

[Idd et al. 06]



$$x = \frac{2m}{m_{\text{ref}} + m_{s,\text{ref}}}, \quad C = \frac{M_{K,\text{ref}}^2}{32_\pi^2 F_{K,\text{ref}}^2}$$

$$\hat{F} = \frac{F}{F_{K,\text{ref}}}, \quad \hat{B} = \frac{m_{\text{ref}} + m_{s,\text{ref}}}{M_{K,\text{ref}}^2} B$$

$$\hat{l}_3 = \log(\Lambda_3^2/M_{K,\text{ref}}^2)$$

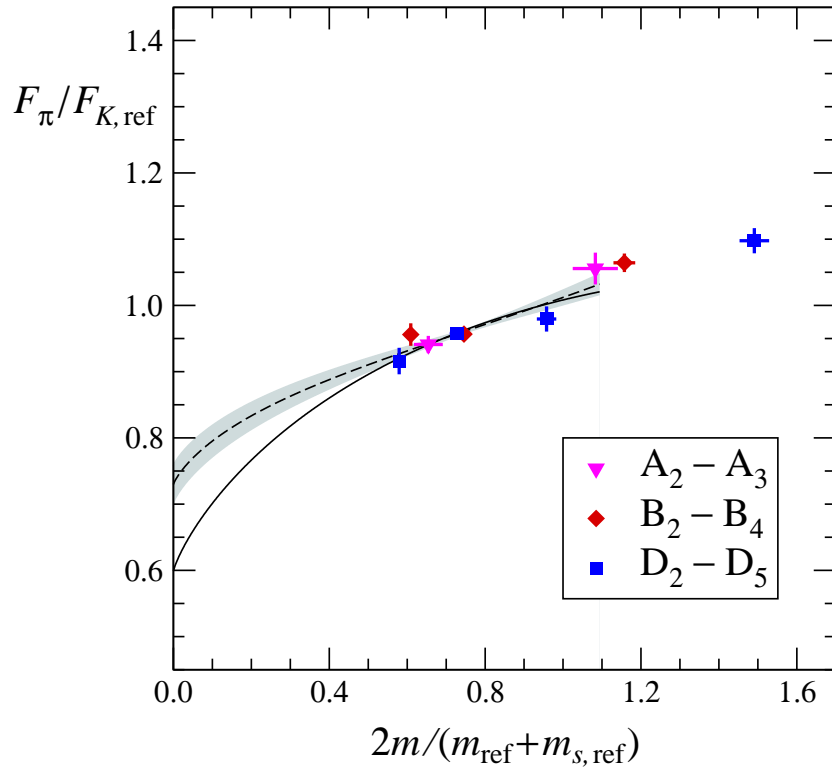
$$\frac{M_\pi^2}{M_{K,\text{ref}}^2} = \hat{B}x + C \frac{\hat{B}^2 x^2}{\hat{F}^2} \left[\log(\hat{B}x) - \hat{l}_3 \right]$$

$$\hat{B} = 1.11(6)(3), \quad \hat{l}_3 = 0.5(5)(1)$$

lightest pion: $m_\pi \approx 377 \text{ MeV}$

Chiral extrapolations

[Idd et al. 06]



$$x = \frac{2m}{m_{\text{ref}} + m_{s,\text{ref}}}, \quad C = \frac{M_{K,\text{ref}}^2}{32^2 \pi^2 F_{K,\text{ref}}^2}$$

$$\hat{F} = \frac{F}{F_{K,\text{ref}}}, \quad \hat{B} = \frac{m_{\text{ref}} + m_{s,\text{ref}}}{M_{K,\text{ref}}^2} B$$

$$\hat{l}_4 = \log(\Lambda_4^2 / M_{K,\text{ref}}^2)$$

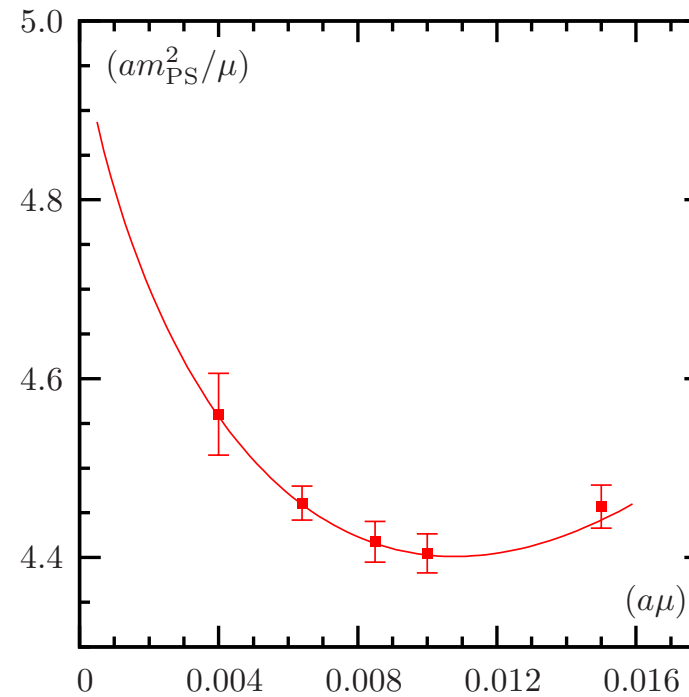
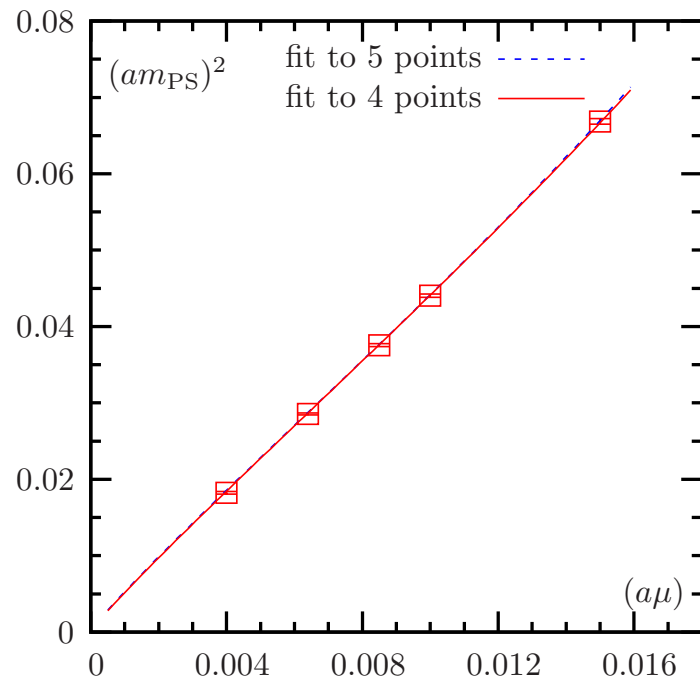
$$\frac{F_\pi}{F_{K,\text{ref}}} = \hat{F} - 2C \frac{\hat{B}x}{\hat{F}} \left[\log(\hat{B}x) - \hat{l}_4 \right]$$

$$\hat{F} = 0.60(4), \quad \hat{l}_4 = 1.6(1)$$

Chiral extrapolations

ETMC, $a = 0.087$ fm, [chiral fit], $L \geq 2$ fm

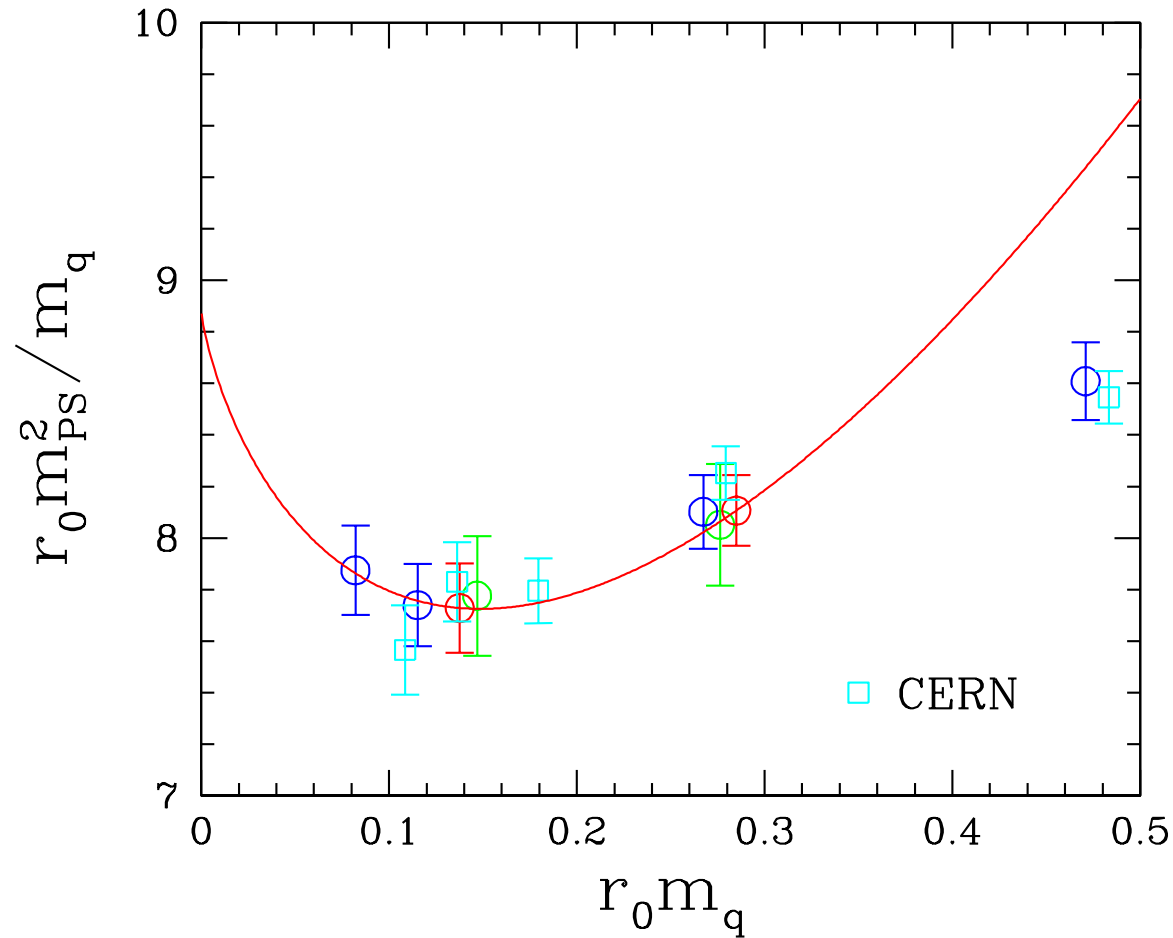
[Boucaud et al 07]



combined chiral fit to m_π and f_π , lightest pion $m_\pi \approx 309$ MeV

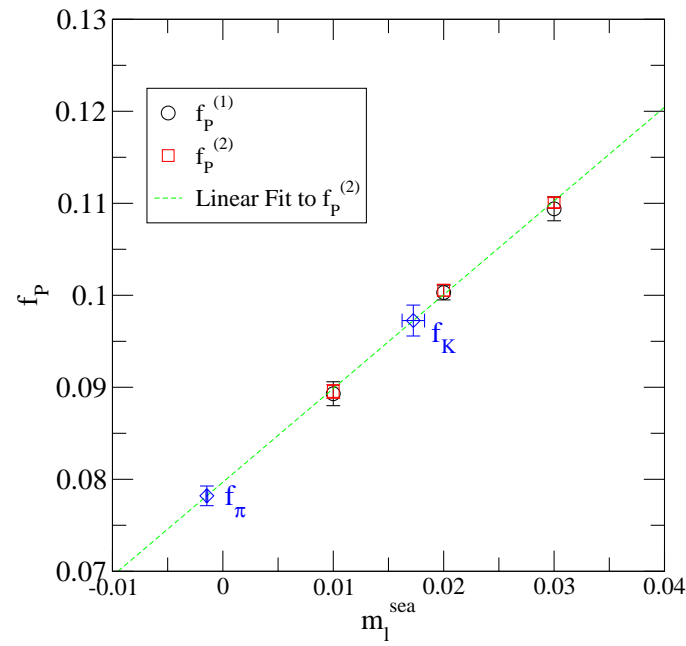
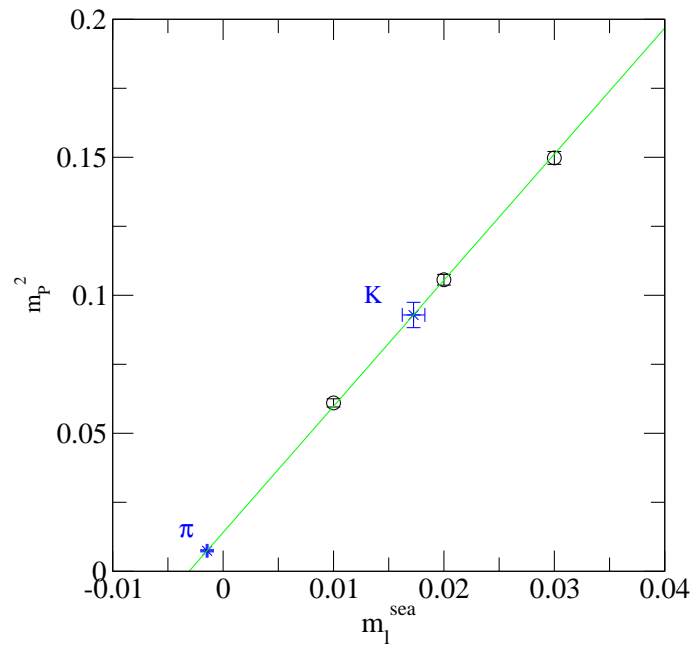
Chiral extrapolations

QCDSF, $a = 0.07$ fm, [chiral fit], $L \geq 2$ fm, lightest pion $m_\pi \approx 313$ MeV



Chiral extrapolations

RBC/UKQCD, $a = 0.123$ fm, $[M_V/M_{PS}]$, $L \geq 2$ fm

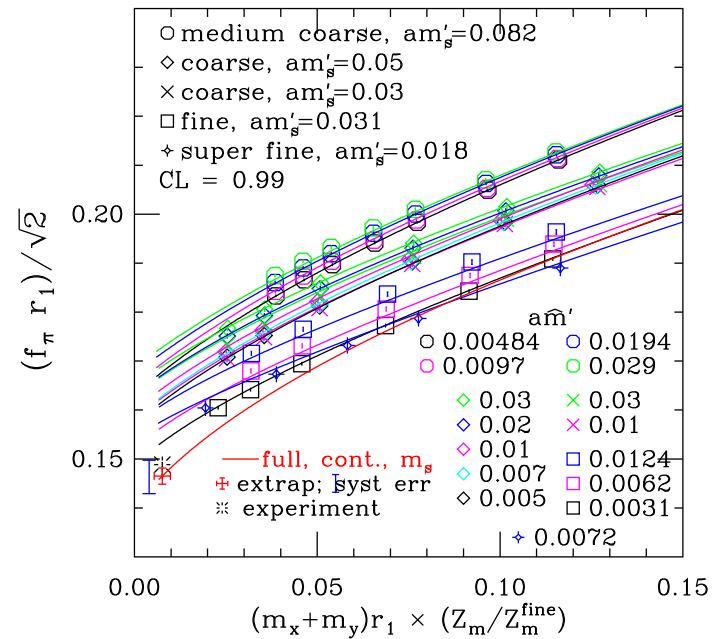
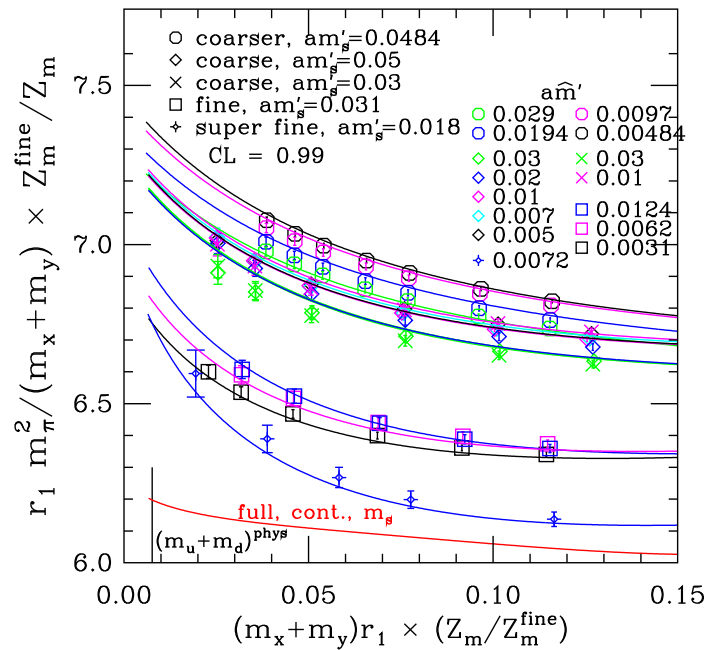


16^3 lattice, lightest pion $m_\pi \approx 390$ MeV

new data on a larger volume and lighter mass available soon

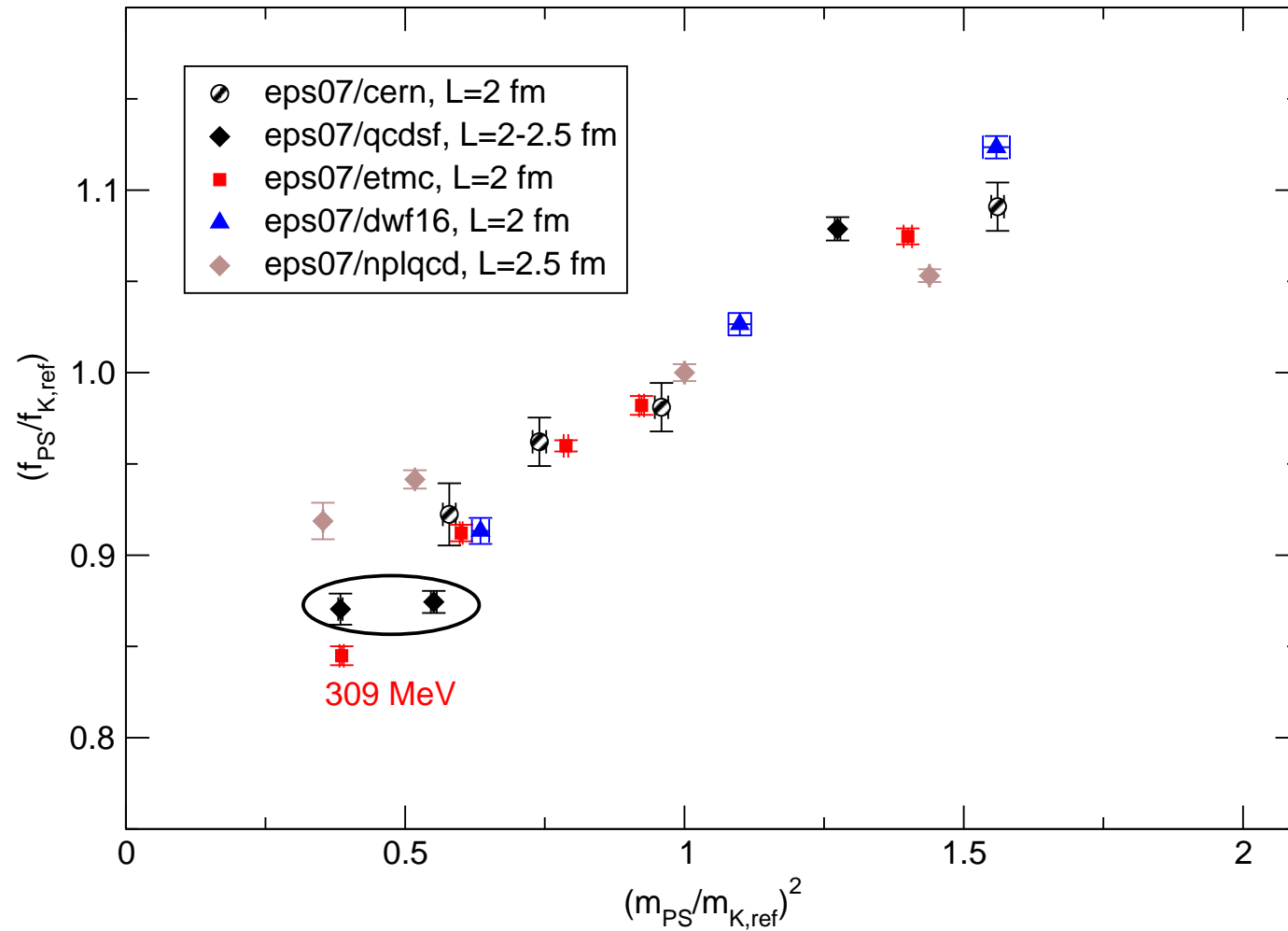
Chiral extrapolations

MILC, $a = 0.06 \div 0.015$ fm, $L = 2.4 \div 3.4$ fm



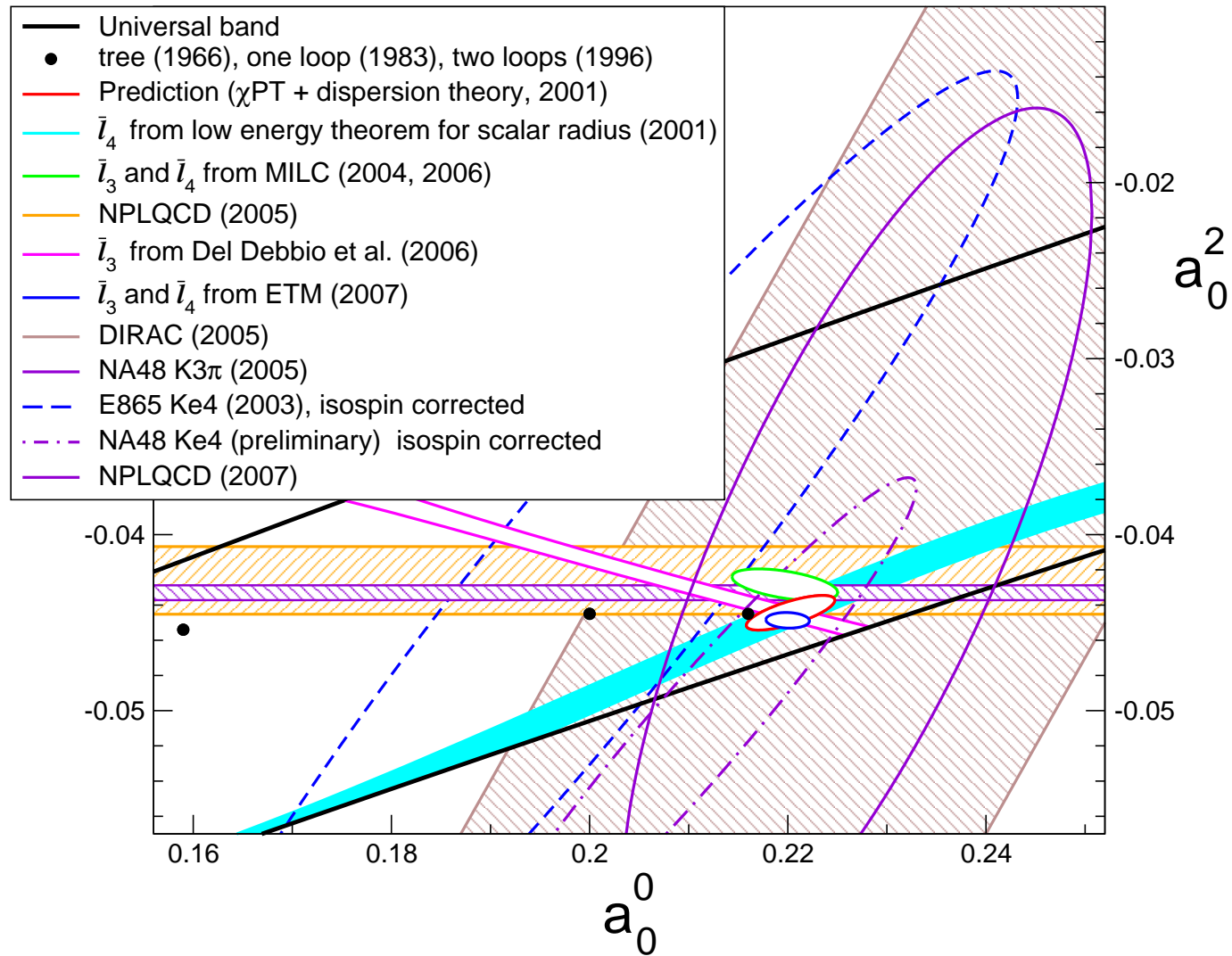
26-parameter combined fit to NLO (S)ChPT using the lighter masses [Sugar lat06]

Chiral extrapolations - summary



precision data at light quark masses is within reach!! see [lat07] for new data

Chiral extrapolations - impact



[Leutwyler Moriond07]

Kaon mixing – DWF

non-perturbative contribution encoded in:

$$B_K = \frac{\langle K^0 | \mathcal{O}_{VV+AA} | \bar{K}^0 \rangle}{\frac{8}{3} f_K^2 M_K^2}$$

RI-MOM multiplicative renormalization:

$$B_K^{\overline{\text{MS}}} = Z_{B_K}^{\overline{\text{MS}}} B_K^{\text{lat}}$$

no chirality mixing, $O(a^2)$ lattice artefacts

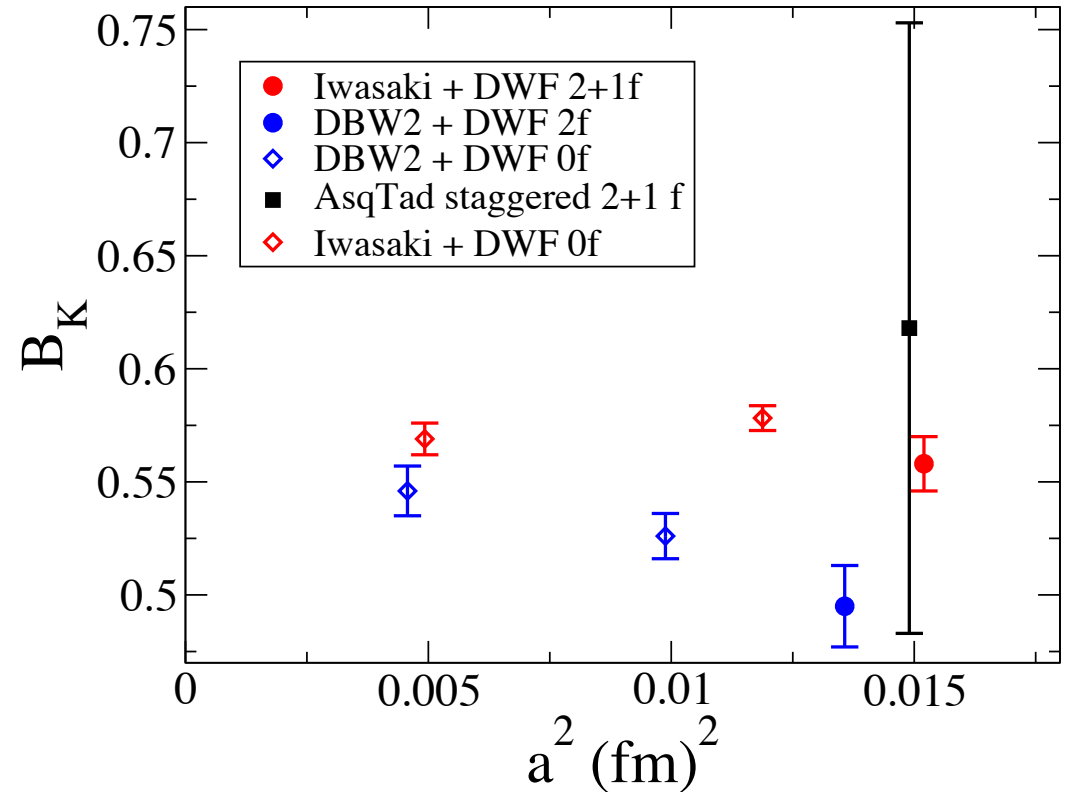
cfr. Wilson fermions:

$$\mathcal{O}_{VV+AA}^R = Z(g_0) \left[\mathcal{O}_{VV+AA} + \sum_i c_i(g_0) \mathcal{O}_i \right]^{\text{lat}}$$

$$\hat{B}_K = 0.77(2)(4)$$

[Antonio et al 07]

$$[\hat{B}_K = 0.79(2)(9)]$$



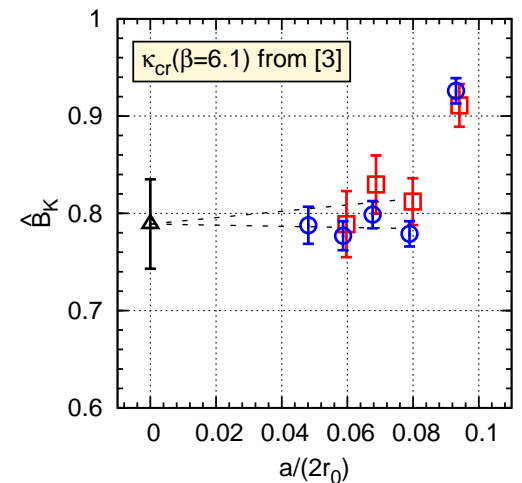
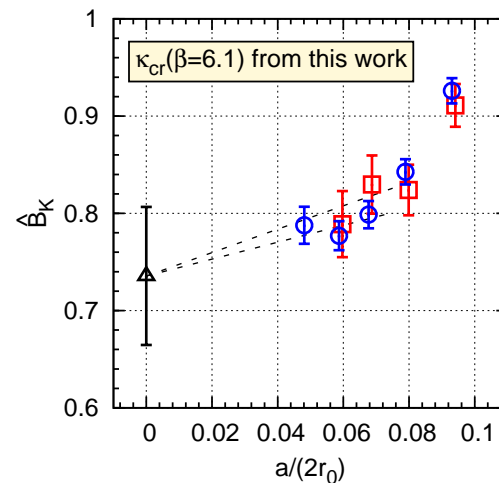
Kaon mixing – tmQCD

$$\langle K^0 | \mathcal{O}_{VA+AV} | \bar{K}^0 \rangle_{\text{tmQCD}} = i \langle K^0 | \mathcal{O}_{VA+AV} | \bar{K}^0 \rangle_{\text{QCD}}$$

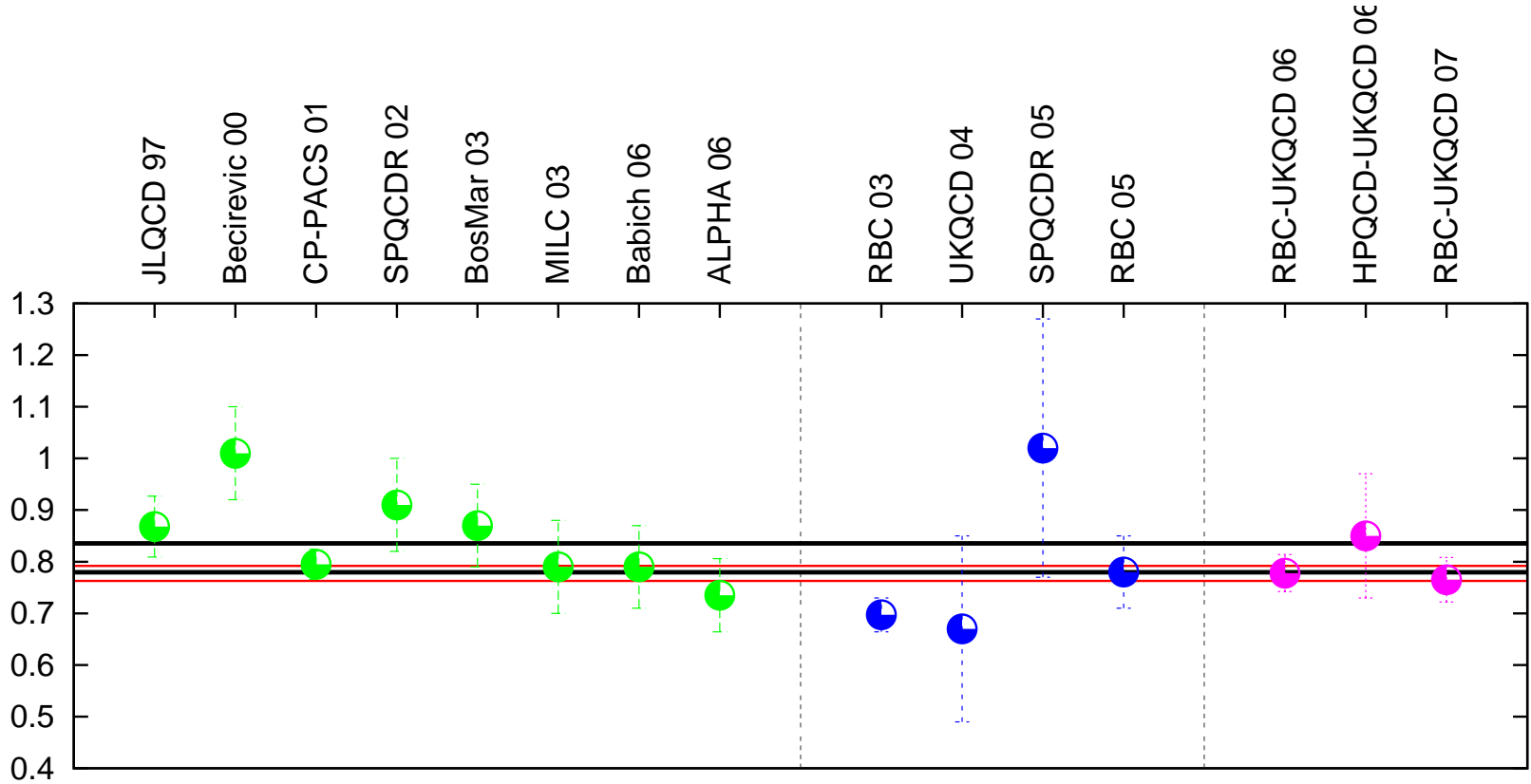
- \mathcal{O}_{VA+AV} protected from mixing
- WME is not improved $\Rightarrow O(a)$ artefacts
- tuning of the mixing angle: m_{crit}
- quenched result!!

$$\hat{B}_K = 0.74(7)$$

[Dimopoulos et al 07]



Kaon mixing – summary



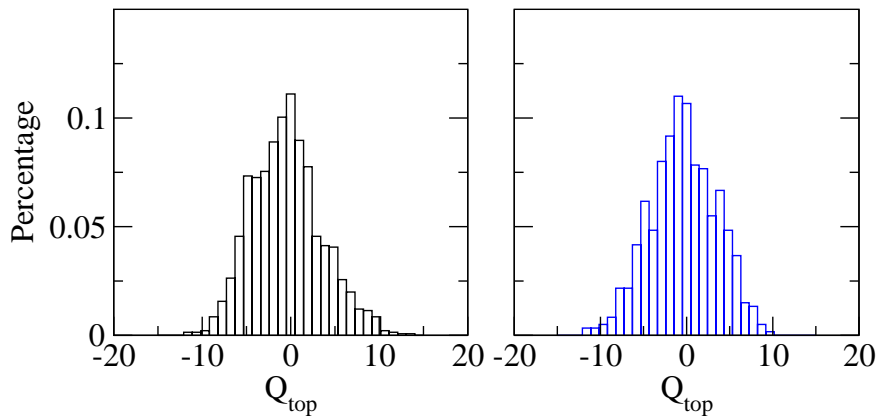
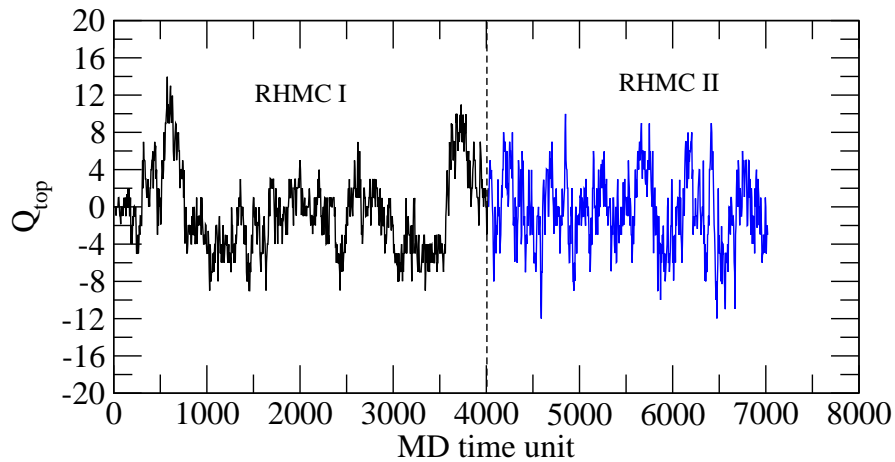
updated from [Tantalo CKM06]

Theta dependence

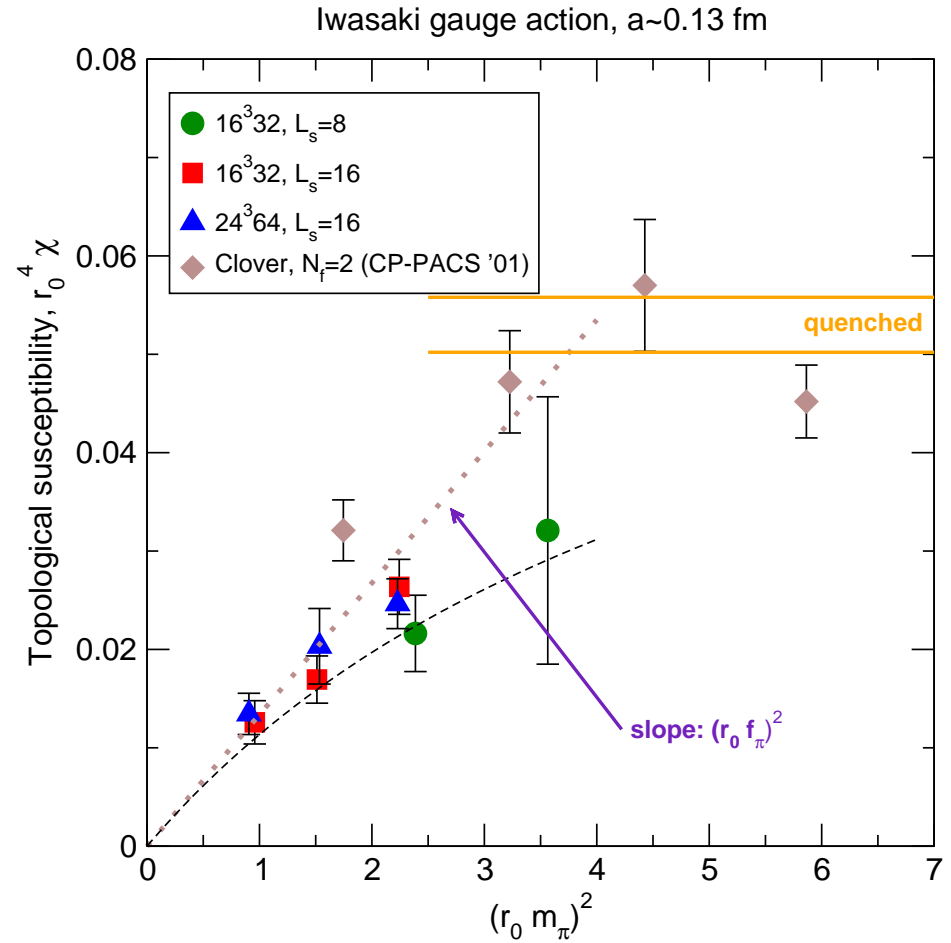
$$\begin{aligned} Z(\theta) &= \int [dA] \exp \left[- \left(\int \frac{1}{4g^2} G^2 + i \theta \nu \right) \right], & \nu &= \int Q(x) = \frac{1}{32\pi^2} \int G\tilde{G} \\ &= \exp [-VF(\theta)] \\ f(\theta) &= r_0^4 F(\theta) \\ &= \frac{1}{2} (r_0^4 \chi) \theta^2 [1 + b_2 \theta^2 + \dots] \end{aligned}$$

- complex weight in Euclidean path integral
- anomaly connects the flavour and gauge sectors
- θ dependence cancels for $m = 0$: $\chi = f_\pi^2 m_\pi^2 + \dots$
- axial Ward Identities: WV formula, $U(1)_A$ sector phenomenology
- lattice AWIs using GW... [Luscher 98, Giusti et al 02f]
- ...if fermionic estimators are used; heuristic studies with bosonic estimators
[Teper, Di Giacomo et al 90f, Idd et al 02f, Giusti et al 07, RBC/UKQCD 06f, ...]

Topology sampling



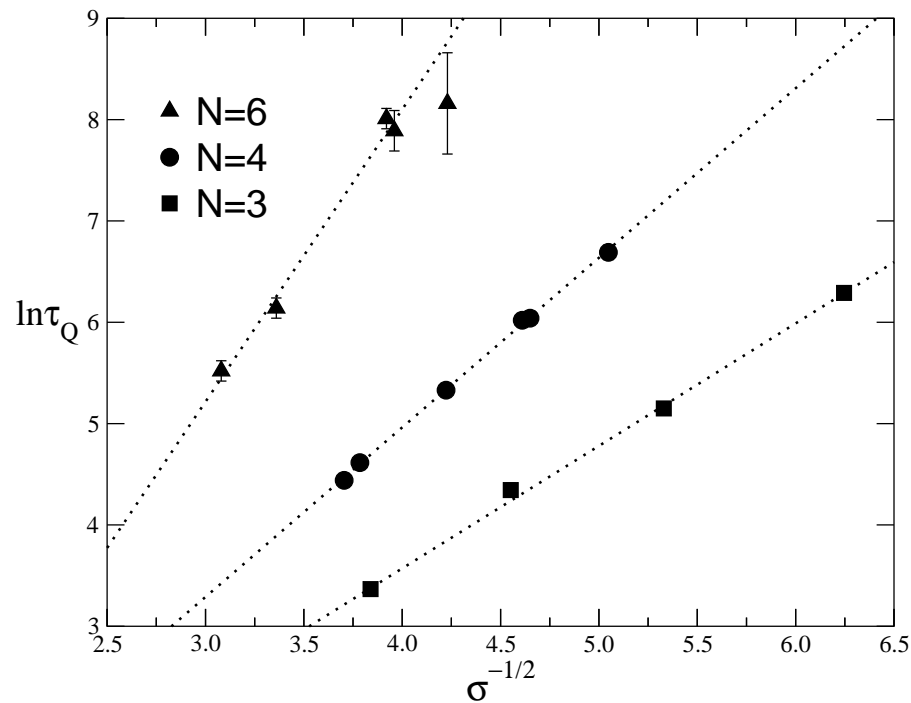
[Allton et al 07]



[Hart, Idd]

Fixed topology

Severe critical slowing down



[Idd et al 02]

- work at fixed topology – violates cluster property

$$\langle O \rangle_Q = \langle O \rangle_\theta + O(1/V)$$

exact formula can be worked out for each correlator at fixed Q

[Aoki et al 07]

- improve the tunneling of the HMC
still needs to be explored in detail – acceptance
[Golterman & Shamir 07]

Conclusions

- lattice QCD has entered the era of dynamical simulations
- many interesting effects of light sea quark will be seen
- taming of systematics is crucial for precision physics

- faster machines will be available
- next two/three years: lighter masses, bigger volumes
- study of the continuum limit
- precision to impact on SM phenomenology