MILC Physics Program: Now and in the Teraflops/s Era

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Collaborators

MILC Collaboration: E. Gregory, C. Aubin, R. Sugar, U. Heller, J. Hetrick, S. G., C. Bernard, C. DeTar, J. Osborn, D. Toussaint, B. Billeter

$+$ HPQCD & UKQCD Collaborations (for m_s, $\hat{m}$, $m_s/\hat{m}$): C. Davies, A. Gray, J. Hein, G. P. Lepage, Q. Mason, J. Shigemitsu, H. Trottier, M. Wingate

Outline

- Outline of MILC Projects
- Ensemble of Configurations
- Ratio Plot
- Recent Results
- Teraflops/s Era

Outline of MILC Projects

MILC's physics interests are varied:

- Light quarks
  - π, K decay constants
  - quark masses
  - spectrum, including exotics
- Heavy quarks
  - leptonic decay constants
  - semi-leptonic decays
- Topology
- High temperature QCD

Ensemble of Configurations

To carry out a simulation we must select certain physical parameters:

- lattice spacing (a) or gauge coupling (β)
- fix grid size ($N_s^3 \times N_t$)
- quark masses ($m_{u,d}$, m_s)

To control systematic error we must

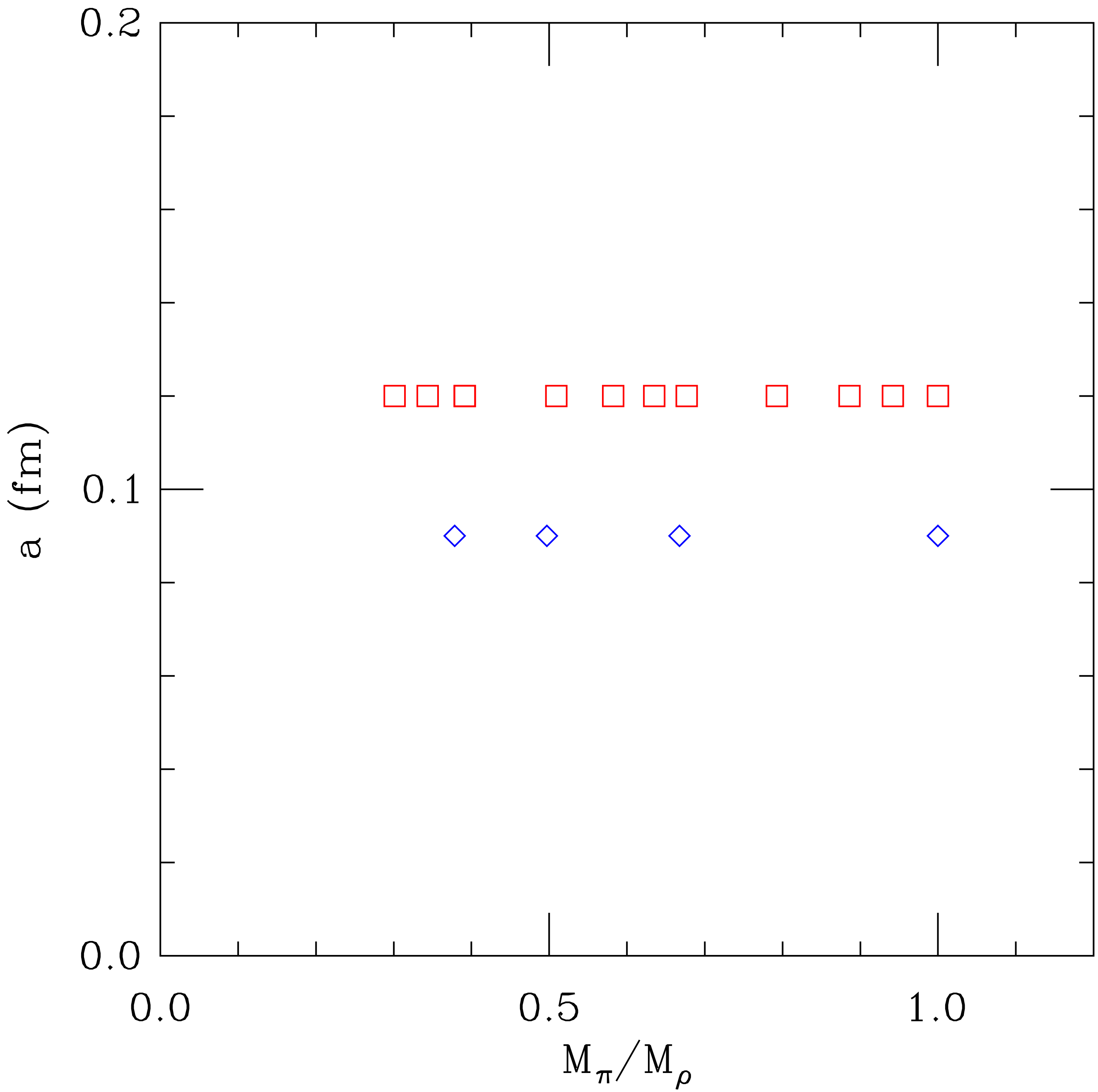
- take continuum limit
- take infinite volume limit
- extrapolate to light quark mass; can work at physical s quark mass

MILC has been generating three flavor configurations to allow control of these errors. Many configurations are available to others through NERSC Gauge Connection. Some new configurations generated via SciDAC

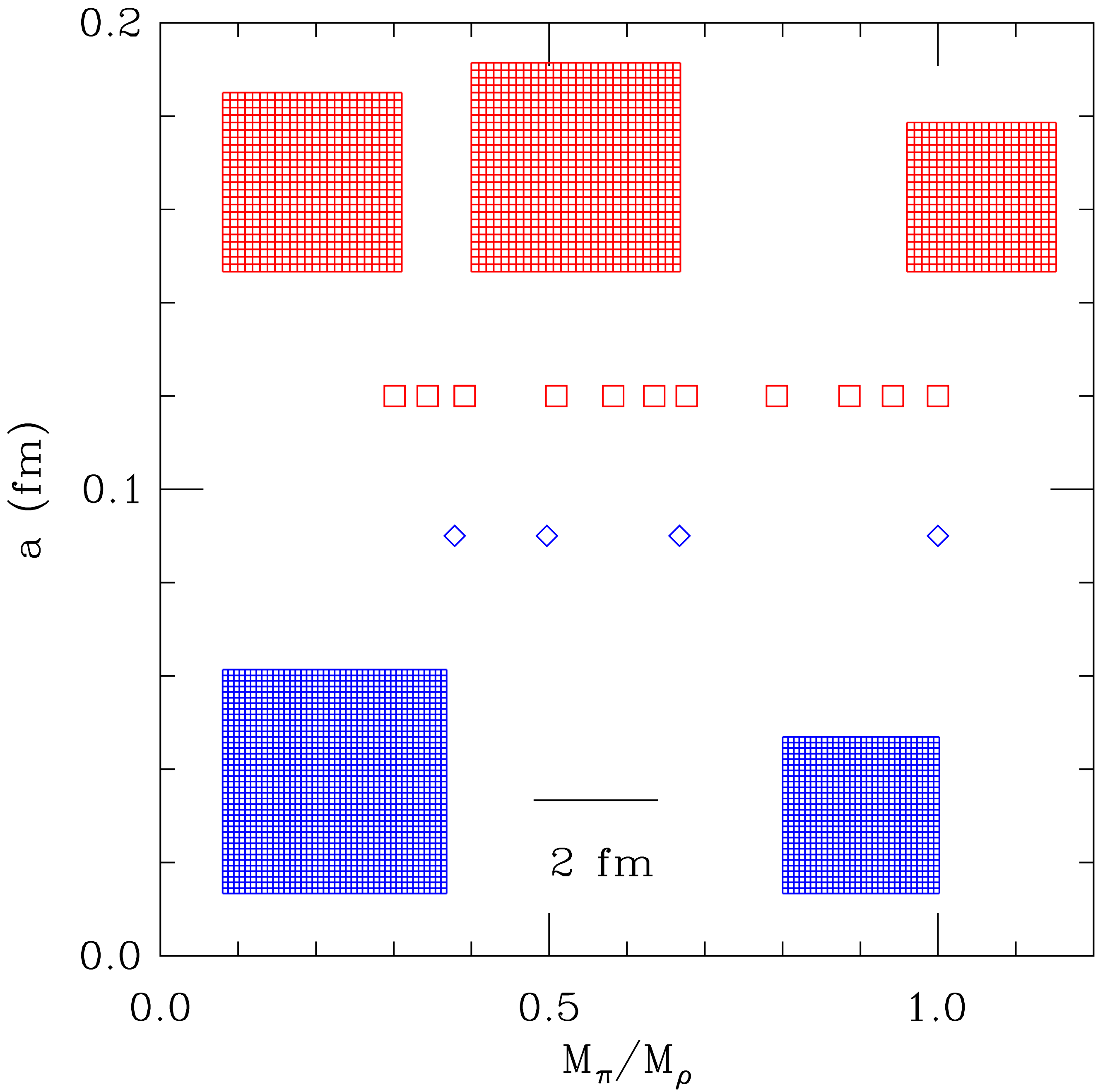
$a = 0.09$ fm; $28^3 \times 96$		
$am_{u,d}$ / am_s	$10/g^2$	# config.
0.031 / 0.031	7.18	496
0.0124 / 0.031	7.11	527
0.0062 / 0.031	7.09	592
$a = 0.09$ fm; $40^3 \times 96$		
0.0031 / 0.031	7.08	≈ 100

$a = 0.12$ fm; $20^3 \times 64$		
$am_{u,d}$ / am_s	$10/g^2$	# config.
0.40 /0.40	7.35	332
0.20 /0.20	7.15	341
0.10 /0.10	6.96	339
0.05 /0.05	6.85	425
0.04 /0.05	6.83	351
0.03 /0.05	6.81	564
0.02 /0.05	6.79	484
0.01 /0.05	6.76	658
0.007/0.05	6.76	493
$a = 0.12$ fm; $24^3 \times 64$		
0.005/0.05	6.76	≈ 375

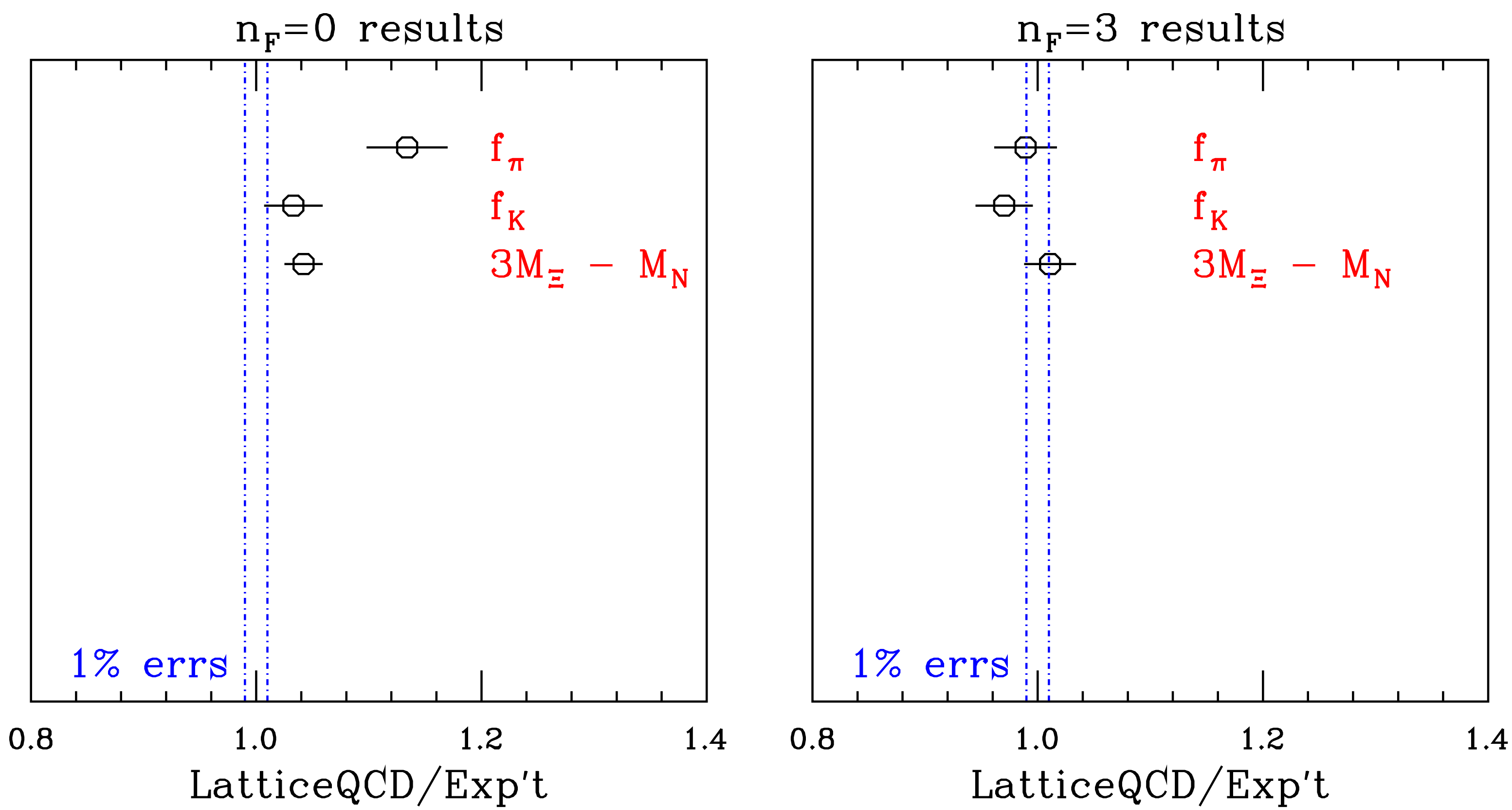
MILC Ensembles



MILC Ensembles

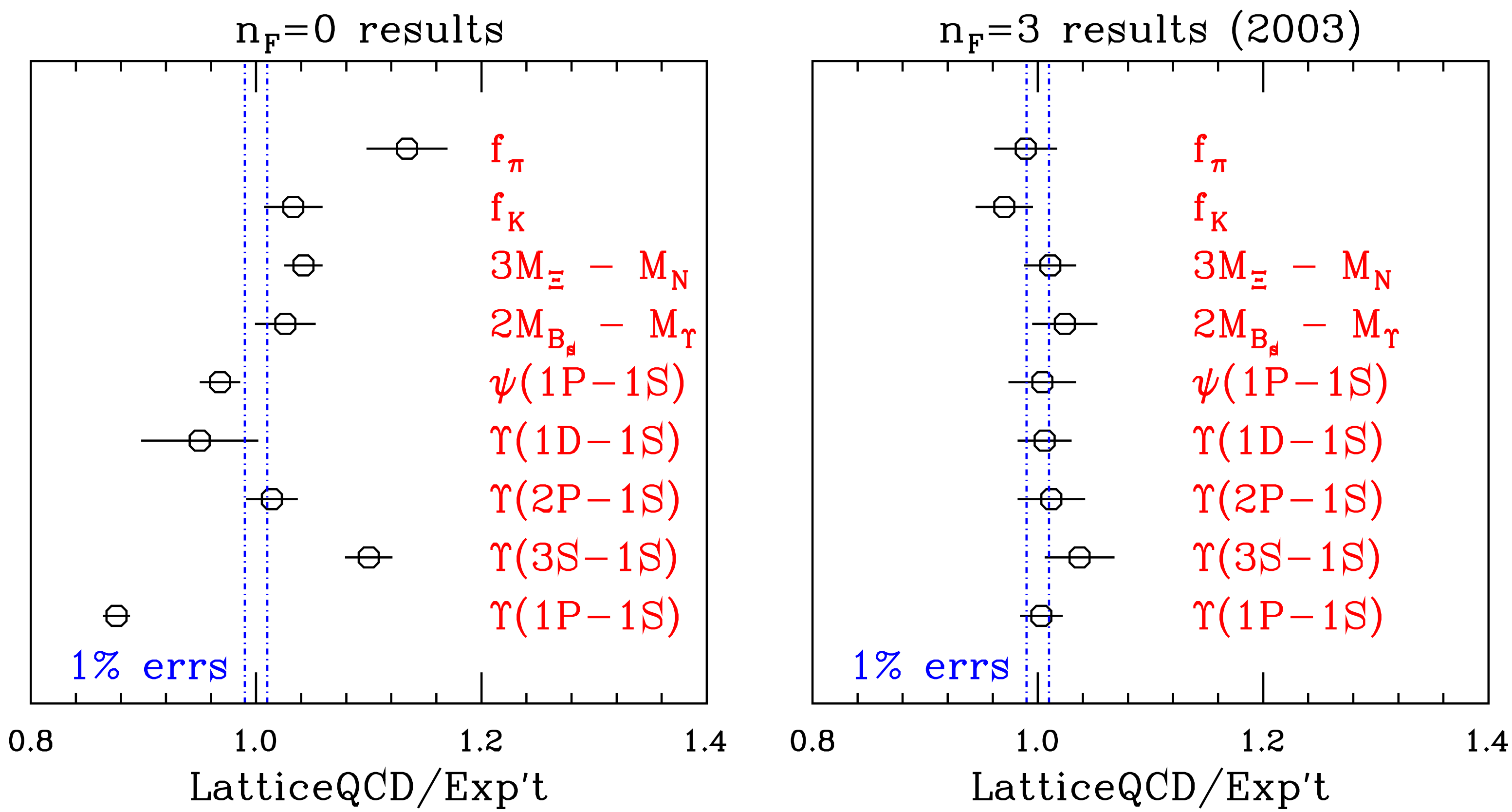


Ratio Plot



n_F=0 results
f_π
f_K
$3M_\Xi - M_N$
1% errs
0.8
1.0
1.2
1.4
LatticeQCD/Exp't
n_F=3 results
f_π
f_K
$3M_\Xi - M_N$
1% errs
0.8
1.0
1.2
1.4
LatticeQCD/Exp't

Ratio Plot



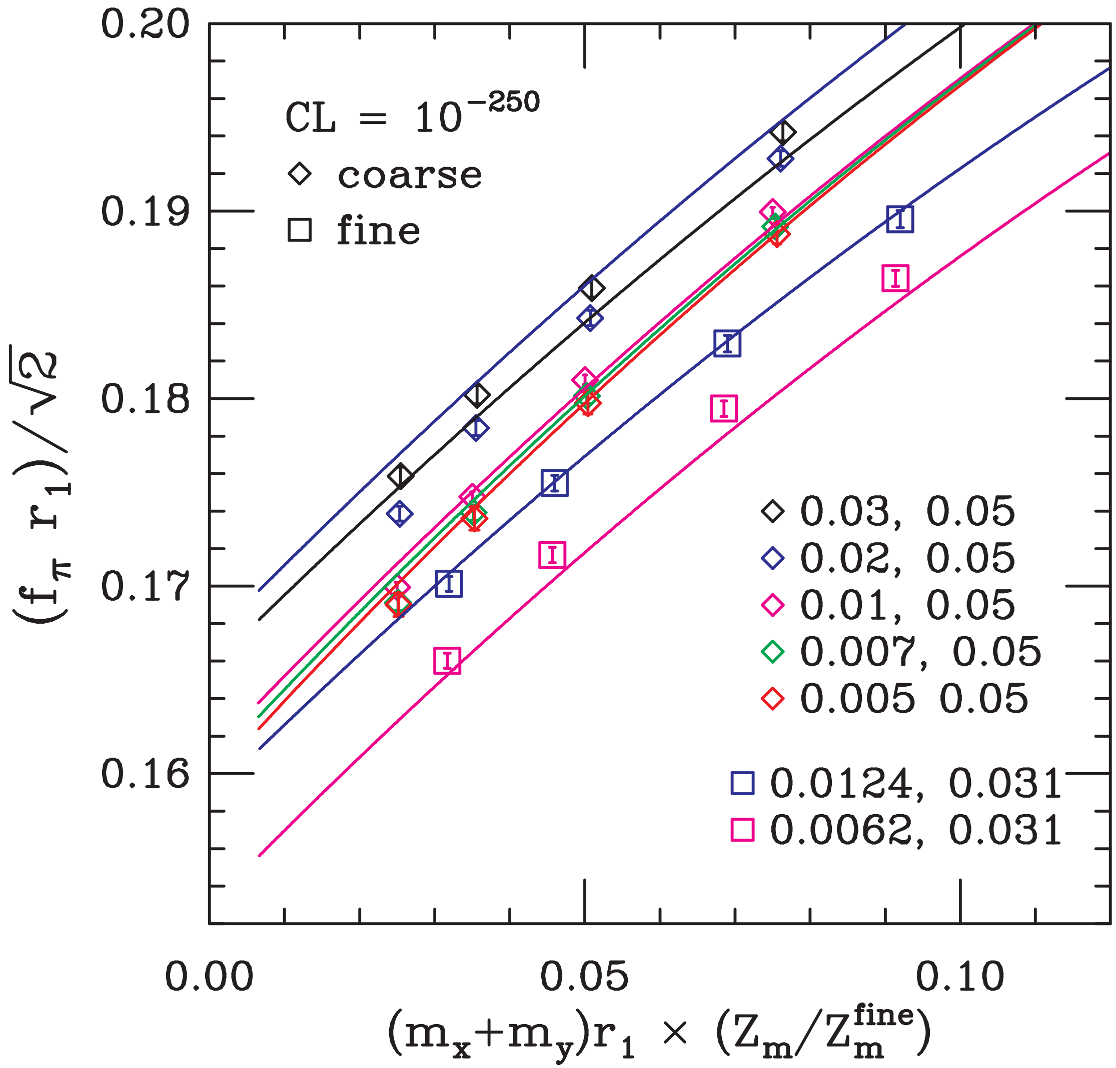
By sharing with FNAL, HPQCD and UKQCD

Who uses MILC configurations

M. Alford (Washington U)	T. Blum (Connecticut U)	F.D.R. Bonnet (Regina U)
R.C. Brower (Boston U)	C. Davies (Glasgow U)	M. Di Pierro (DePaul U)
A. Dougall (Glasgow U)	P. Dreher (MIT)	A. El-Khadra (U Illinois)
R. Edwards (Jefferson Lab)	G. Fleming (Jefferson Lab)	K. Foley (Cornell U)
E. Follana (Glasgow U)	E. Gamiz (Glasgow U)	A. Gray (Ohio State U)
E. Gulez (Ohio State U)	P. Hagler (MIT)	J. Hein (Edinburgh U)
G.P. Lepage (Cornell U)	R. Lewis (Regina U)	Q. Mason (Cornell U)
M. Nobes (Simon Fraser U)	A.S. Kronfeld (Fermilab)	T. Lippert (Wuppertal U)
J.W. Negele (MIT)	P.B. Mackenzie (Fermilab)	D. Menscher (Fermilab)
M. Okamoto (Fermilab)	M. Oktay (U Illinois)	K. Orginos (MIT)
P. Petreczky (BNL)	K. Petrov (Columbia U)	A.V. Pochinsky (MIT)
D.B. Renner (MIT)	D. Richards (William & Mary U)	K. Schilling (Wuppertal U)
W. Schroers (MIT)	J. Shigemitsu (Ohio State U)	J. Simone (Fermilab)
H. Trottier (Simon Fraser U)	M. Wingate (Washington U)	

π, K decay constants

continuum χPT fit to both f_π and m_π

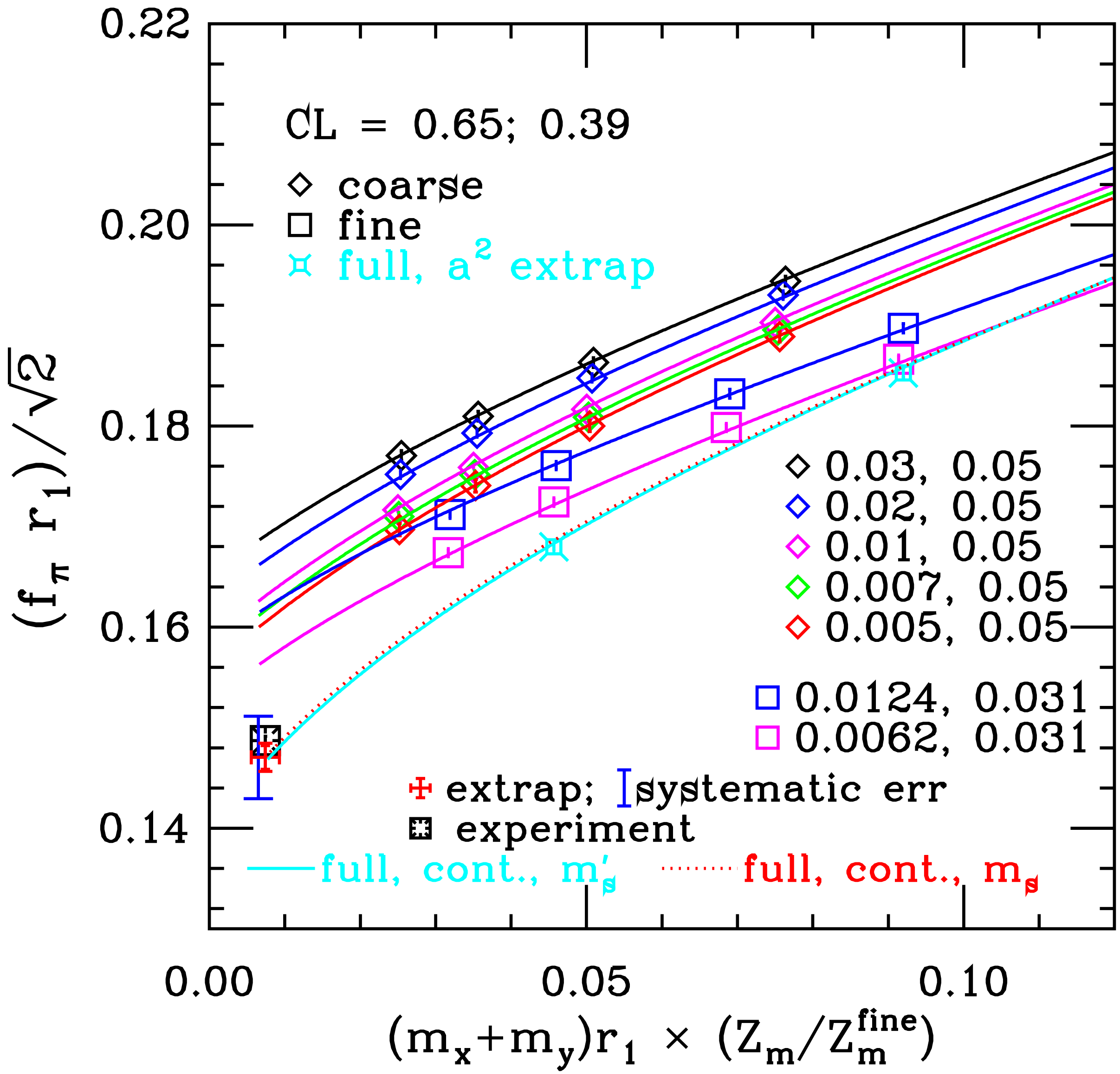


Next two slides show improved fit:

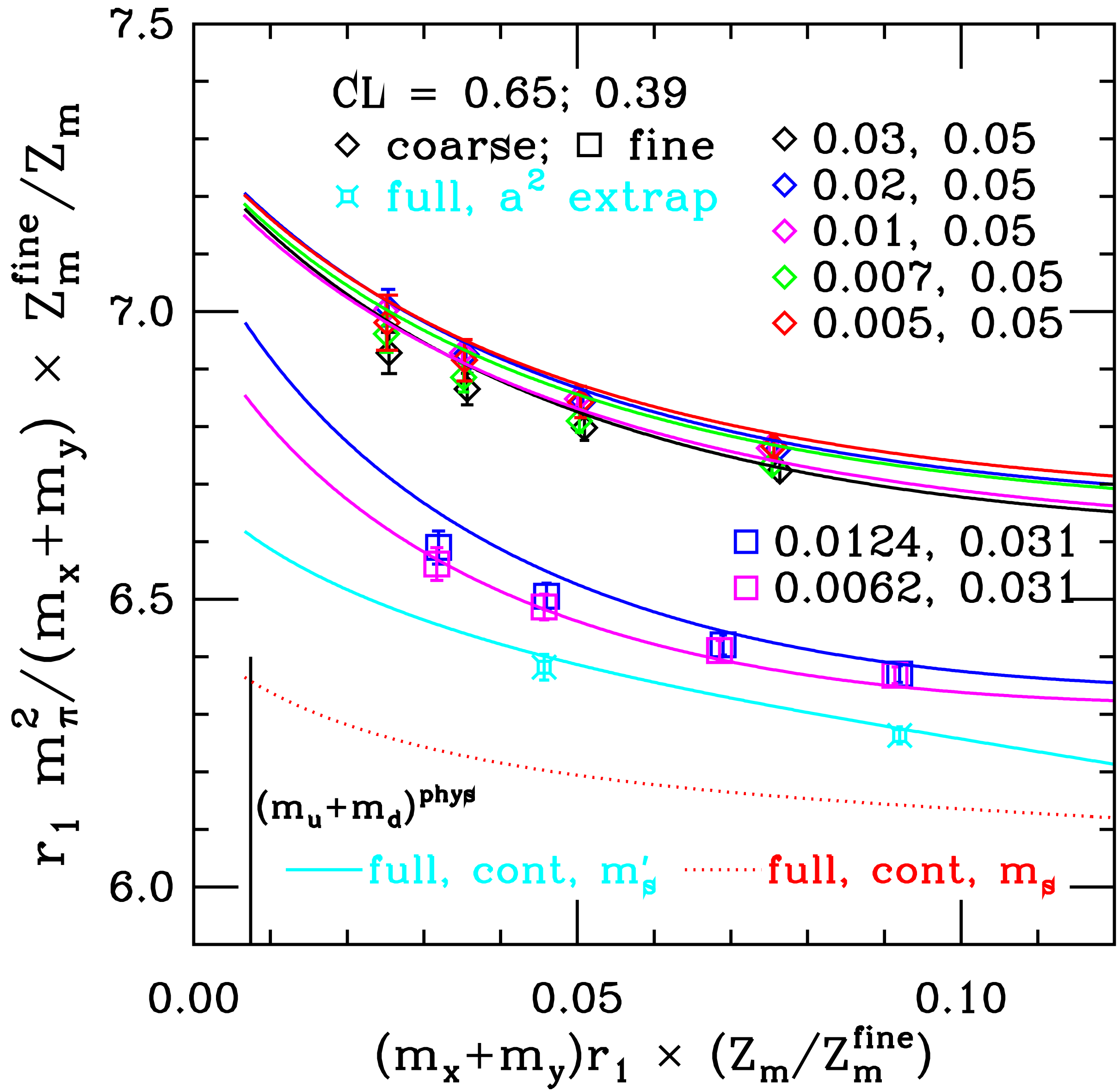
- Use SχPT(Aubin & Bernard) with NNLO corrections
- Points plotted after finite volume correction

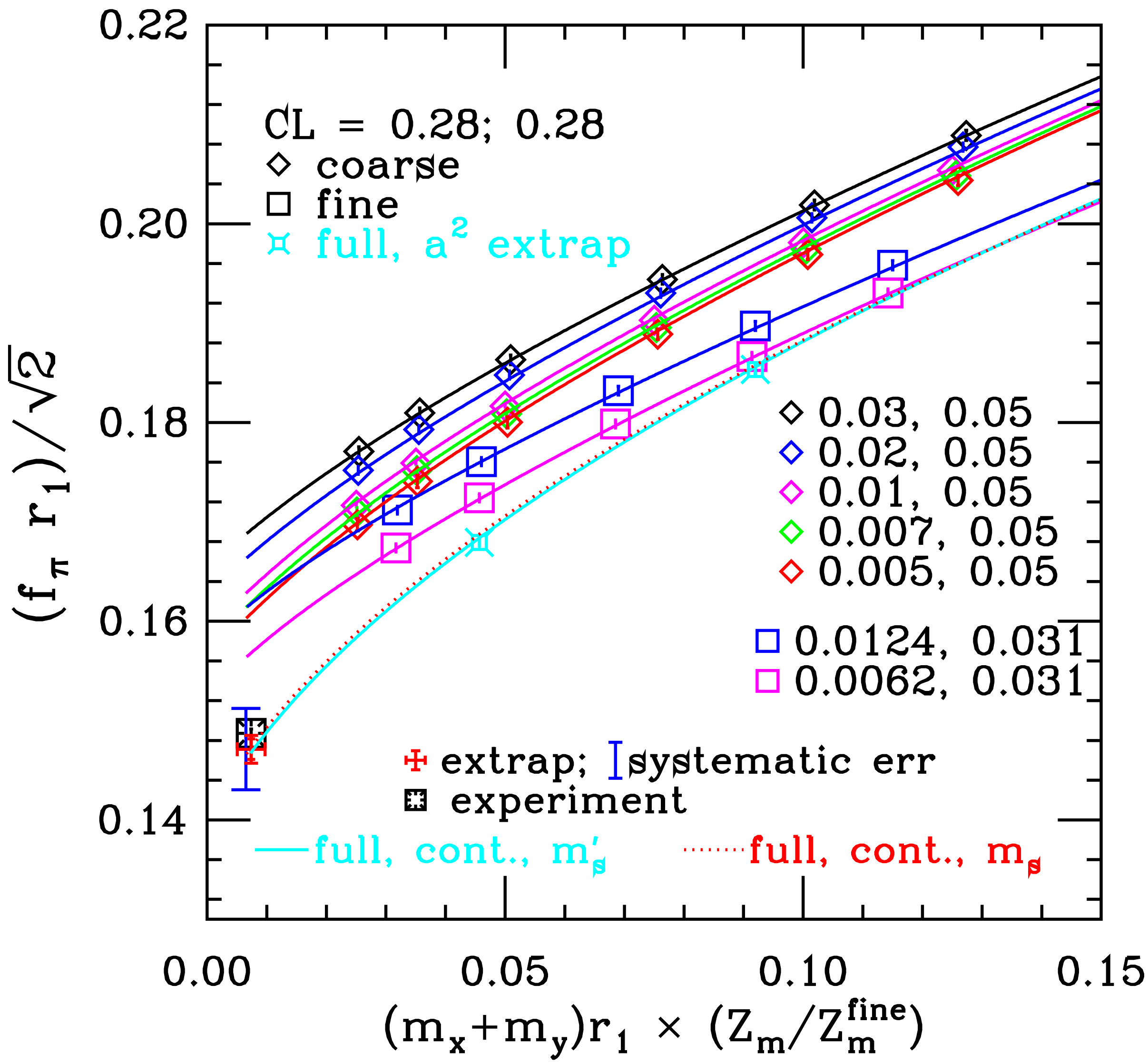
After fit, we:

- Extrapolate fit parameters to continuum
- Show difference between m_s' (simulation strange mass) and m_s (correct value)
- Details in hep-lat/0407028

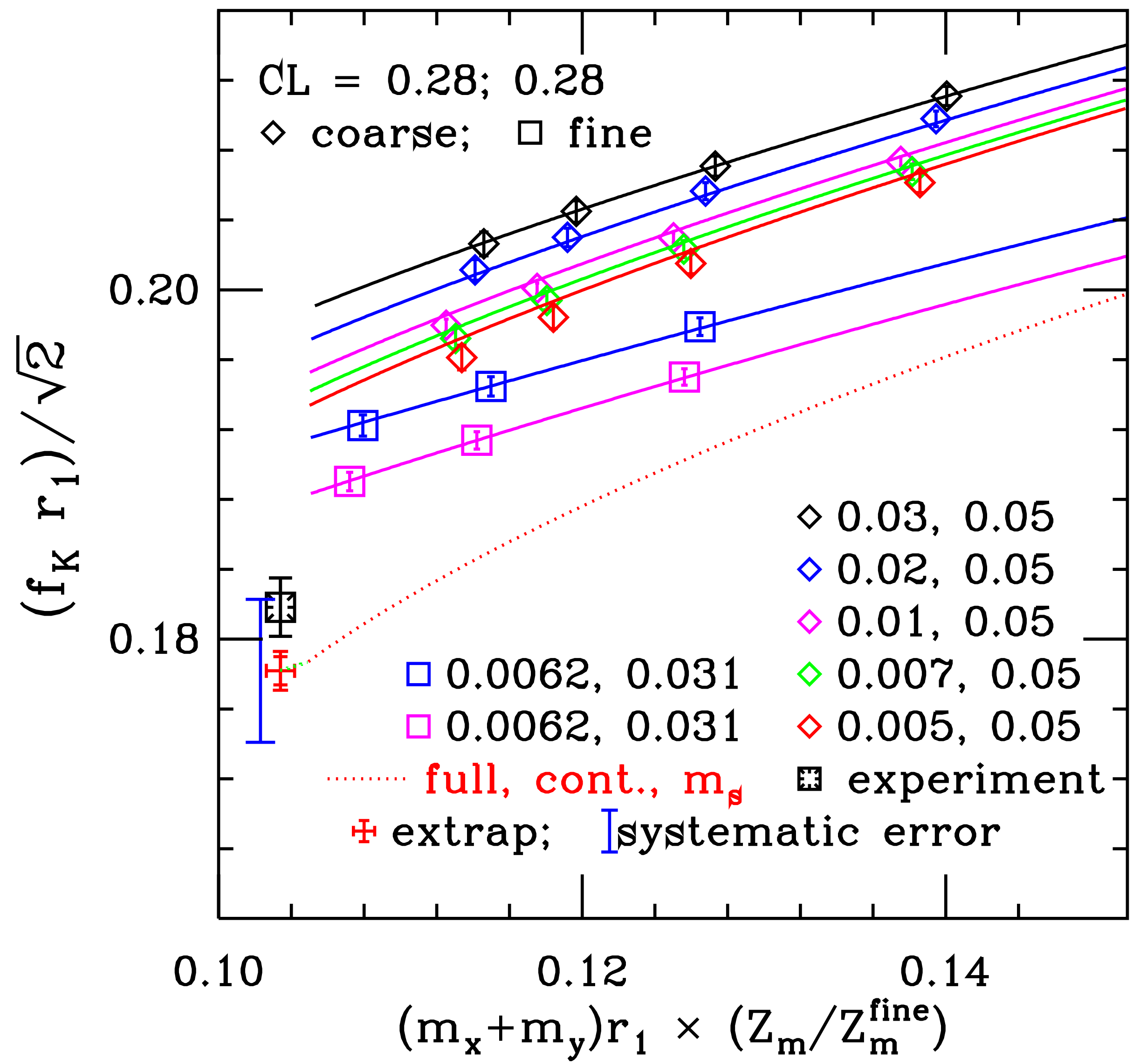


CL = 0.65; 0.39
coarse
fine
full, a² extrap
0.03, 0.05
0.02, 0.05
0.01, 0.05
0.007, 0.05
0.005, 0.05
0.0124, 0.031
0.0062, 0.031
extrap; systematic err
experiment
full, cont., m′s
full, cont., ms
0.22
0.20
0.18
0.16
0.14
0.00
0.05
0.10
(fπ r1)/√2
(mx+my)r1 × (Zm/Zm^fine)


CL = 0.65; 0.39
◇ coarse; □ fine
full, a² extrap
◇ 0.03, 0.05
◇ 0.02, 0.05
◇ 0.01, 0.05
◇ 0.007, 0.05
◇ 0.005, 0.05
□ 0.0124, 0.031
□ 0.0062, 0.031
$(m_u+m_d)^{phys}$
full, cont, m_s'
full, cont, m_s
7.5
7.0
6.5
6.0
0.00
0.05
0.10
$r_1\ m_\pi^2/(m_x+m_y) \times Z_m^{fine}/Z_m$
$(m_x+m_y)r_1 \times (Z_m/Z_m^{fine})$

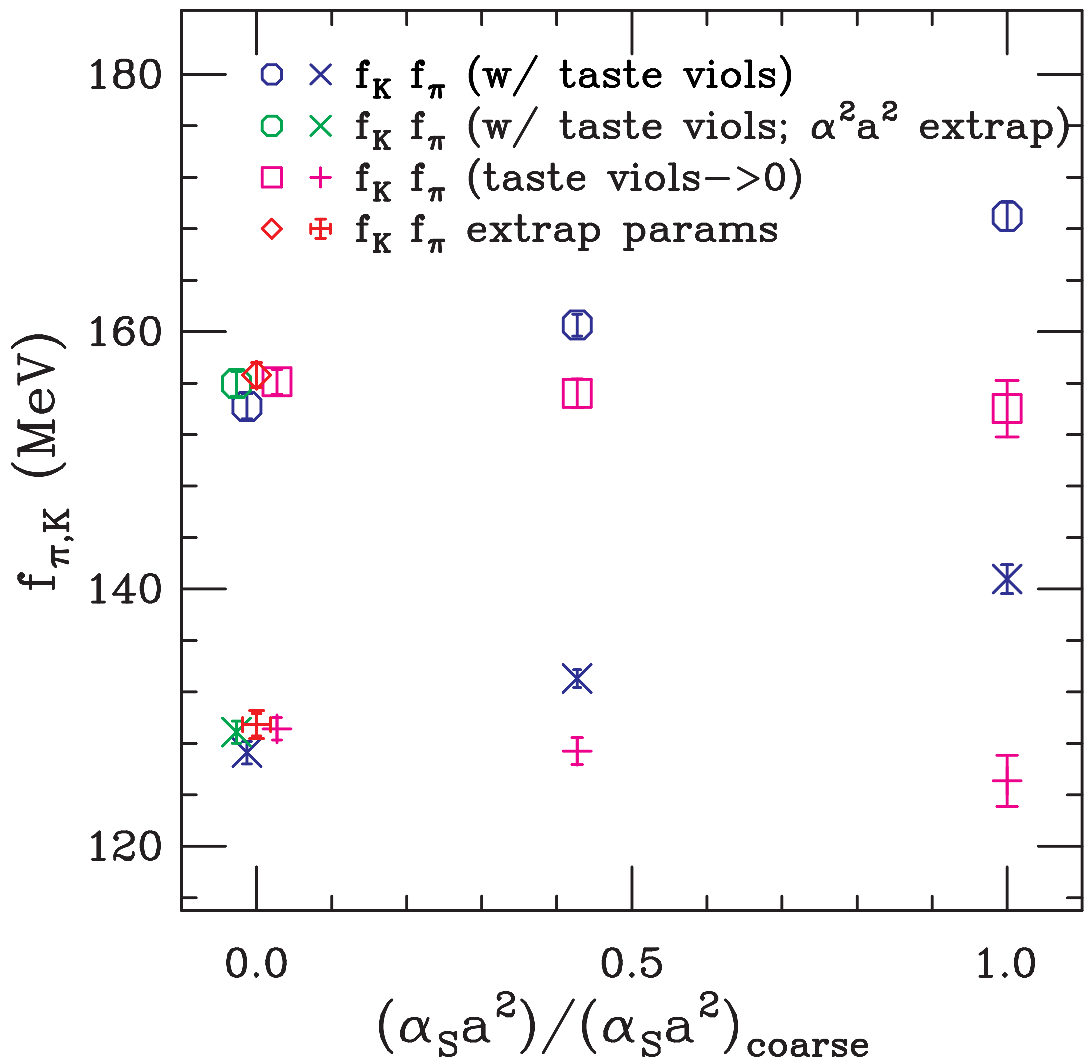


CL = 0.28; 0.28
coarse
fine
full, a² extrap
0.03, 0.05
0.02, 0.05
0.01, 0.05
0.007, 0.05
0.005, 0.05
0.0124, 0.031
0.0062, 0.031
extrap; systematic err
experiment
full, cont., m′s
full, cont., ms
0.22
0.20
0.18
0.16
0.14
0.00
0.05
0.10
0.15
(fπ r1)/√2
(mx+my)r1 × (Zm/Zm^fine)

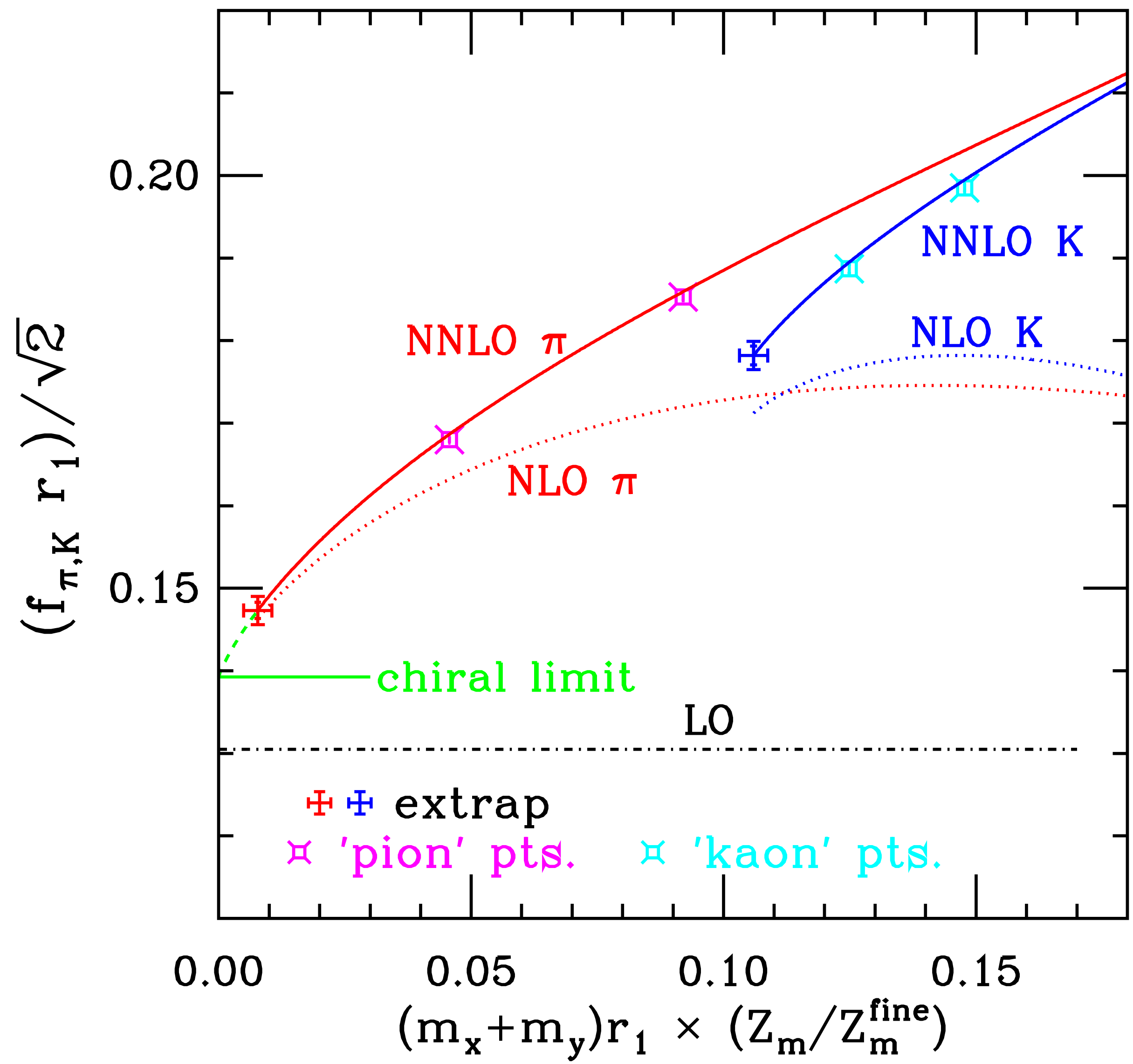


CL = 0.28; 0.28
◇ coarse; □ fine
0.03, 0.05
0.02, 0.05
0.01, 0.05
0.007, 0.05
0.005, 0.05
0.0062, 0.031
0.0062, 0.031
full, cont., m_s
experiment
extrap; systematic error
0.20
0.18
0.10
0.12
0.14
$(f_K\ r_1)/\sqrt{2}$
$(m_x+m_y)r_1 \times (Z_m/Z_m^{fine})$

Alternate continuum extrapolations



Convergence of $SU(3)_L \times SU(3)_R$ χPT



Results for light decay constants

$$
\begin{aligned}
f_\pi &= 129.5 \pm 0.9 \pm 3.5 \text{ MeV} \\
f_K &= 156.6 \pm 1.0 \pm 3.6 \text{ MeV} \\
f_K/f_\pi &= 1.210(4)(13) \ ,
\end{aligned}
$$

Experiments find: $f_\pi = 130.7 \pm 0.4\,\text{MeV}$, $f_K = 159.8 \pm 1.5\,\text{MeV}$, $f_K/f_\pi = 1.223(12)$.

- Large error in f_K from error in V_{us}
- Using our $f_K/f_\pi \Rightarrow V_{us} = 0.2219(26)$
- PDG value = 0.2196(26)
- Recent KTeV = 0.2252(8)(21)
- Our error identical to PDG, so with a reduced error, lattice calculation will be best method to determine V_{us}

Unitarity

$$|V_{ud}|^2 + |V_{us}|^2 = 0.9979(15)$$

The 2σ violation that comes from using the PDG value $|V_{us}| = 0.2196(26)$ becomes a 1.4σ effect here.

Light Quark Masses

To find quark masses, must extrapolate to the physical meson masses
Electromagnetic and isospin-violating effects are important

- Experimental masses:
  $m_{\pi^0}^{\text{expt}}$, $m_{\pi^+}^{\text{expt}}$, $m_{K^0}^{\text{expt}}$, $m_{K^+}^{\text{expt}}$
- Masses with EM effects turned off:
  $m_{\pi^0}^{\text{QCD}}$, $m_{\pi^+}^{\text{QCD}}$, $m_{K^0}^{\text{QCD}}$, $m_{K^+}^{\text{QCD}}$
- Masses with EM effects turned off and $m_u = m_d = \hat{m}$:
  $m_{\hat{\pi}}$, $m_{\hat{K}}$

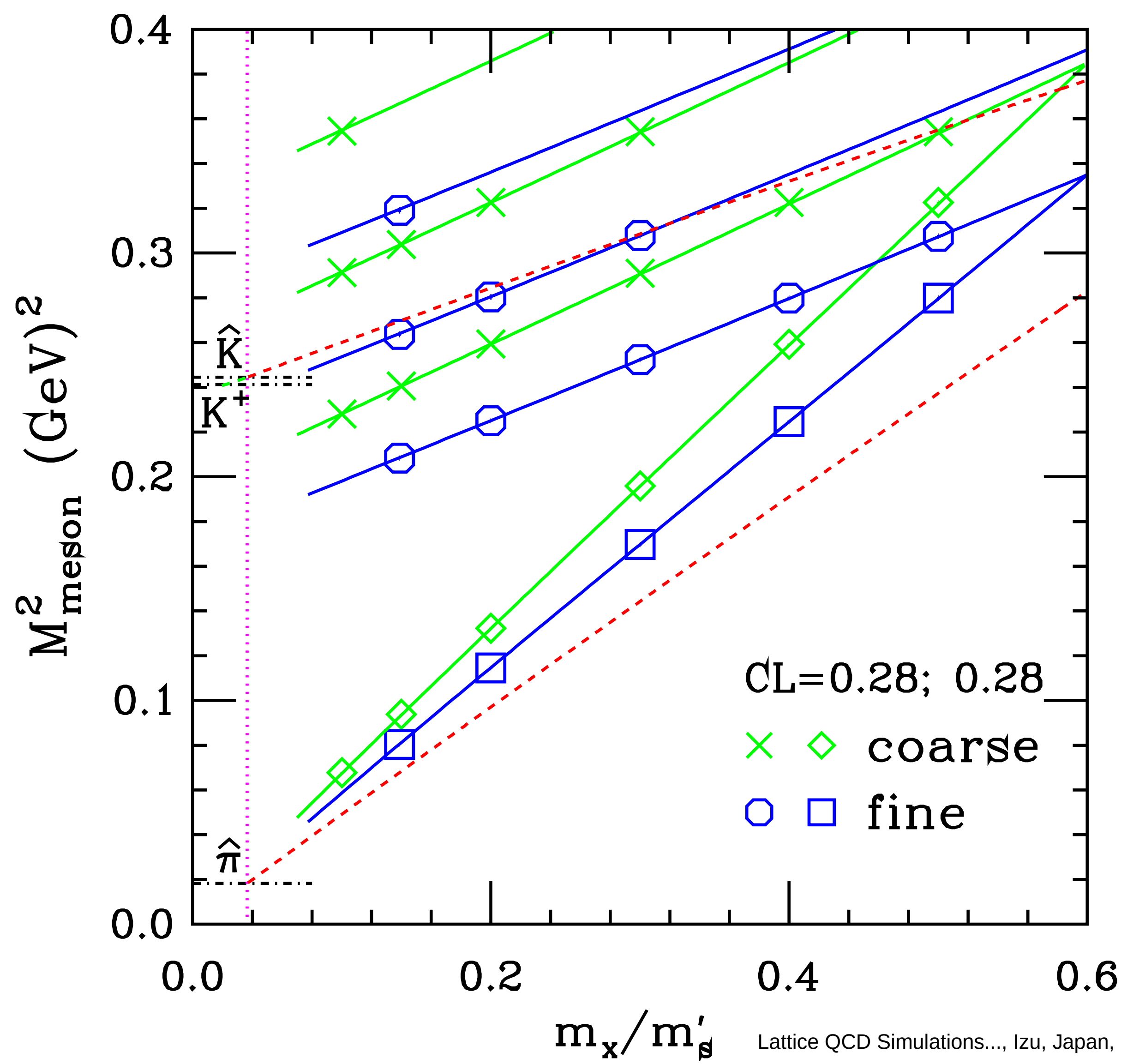
EM & Isospin Violation

$$
\begin{aligned}
m_{\hat{\pi}}^2 &\approx (m_{\pi^0}^{\mathrm{QCD}})^2 \approx (m_{\pi^0}^{\mathrm{expt}})^2 \\
m_{\hat{K}}^2 &\approx \frac{(m_{K^0}^{\mathrm{QCD}})^2 + (m_{K^+}^{\mathrm{QCD}})^2}{2} \\
(m_{K^0}^{\mathrm{QCD}})^2 &\approx (m_{K^0}^{\mathrm{expt}})^2 \\
(m_{K^+}^{\mathrm{QCD}})^2 &\approx (m_{K^+}^{\mathrm{expt}})^2 - (1+\Delta_E)\left((m_{\pi^+}^{\mathrm{expt}})^2 - (m_{\pi^0}^{\mathrm{expt}})^2\right)
\end{aligned}
$$

- $\Delta_E = 0$ is “Dashen’s theorem.”
- Continuum suggests: $\Delta_E \approx 1$.
- We use $0 < \Delta_E < 2$

Fit for $\hat{m}$, m_s

Red lines are continuum extrapolated full QCD fits with m_s adjusted so that both $\hat{\pi}$ and $\hat{K}$ are fit

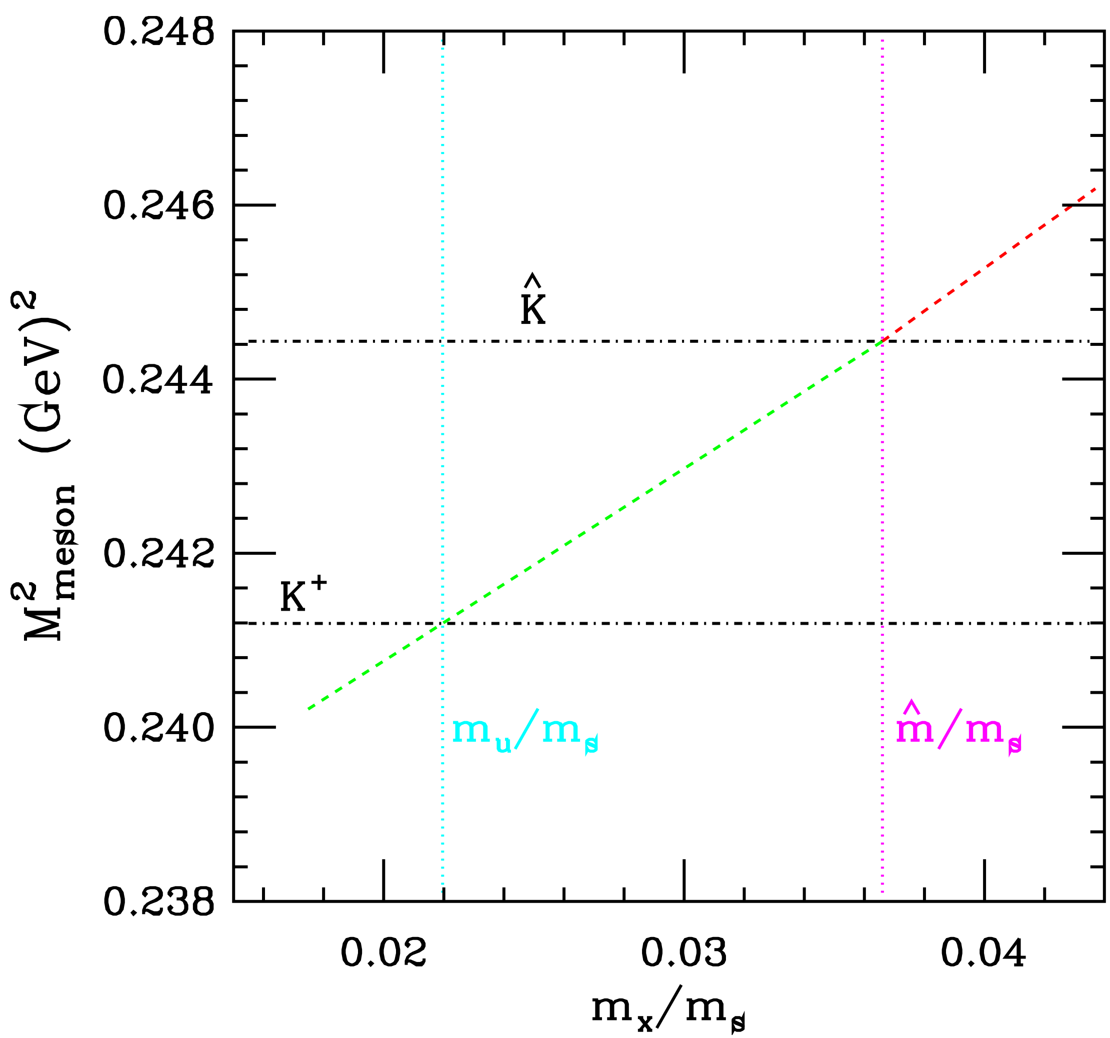


Using a perturbative evaluation of the mass renormalzation constant allows us to obtain absolute values of quark masses.
In collaboration with the HPQCD and UKQCD groups, we find (hep-lat/0405022):

$$\begin{aligned} m_s^{\overline{\mathsf{MS}}} &= 76(0)(3)(7)(0)\ \mathrm{MeV}\ , \\ m_{u,d}^{\overline{\mathsf{MS}}} &= 2.8(0)(1)(3)(0)\ \mathrm{MeV}\ , \\ m_s/m_{u,d} &= 27.4(1)(4)(0)(1) \end{aligned}$$

where the errors are from statistics, simulation, perturbation theory, and electromagnetic effects, respectively. The renormalization scale of the masses is $2\,\mathrm{GeV}$.

Next estimate m_u by extrapolating in quark mass to K^+ mass.
Below $\hat{m}$ only valence mass changes. There is a small isospin violation because $m_u = m_d = \hat{m}$.



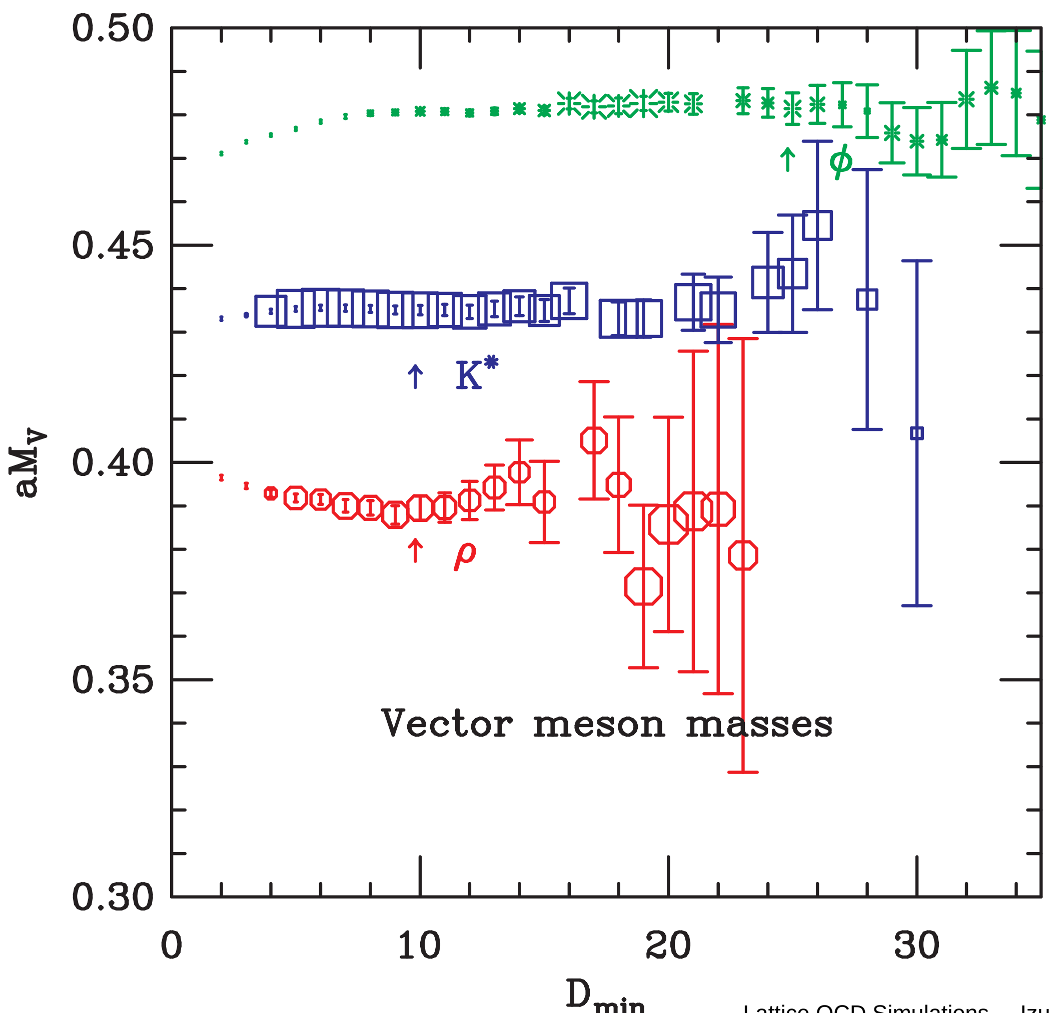
$$m_u/m_d = 0.43(0)(2)(8)\ ,$$

where the errors are statistical (rounded down to 0), lattice systematics, and a conservative estimate of the effects of electromagnetism, which have not been included in the simulation.
Using instead a phenomenological evaluation of the electromagnetic effects from Bijnens and Prades we would obtain $m_u/m_d = 0.44(0)(1)(2)$.

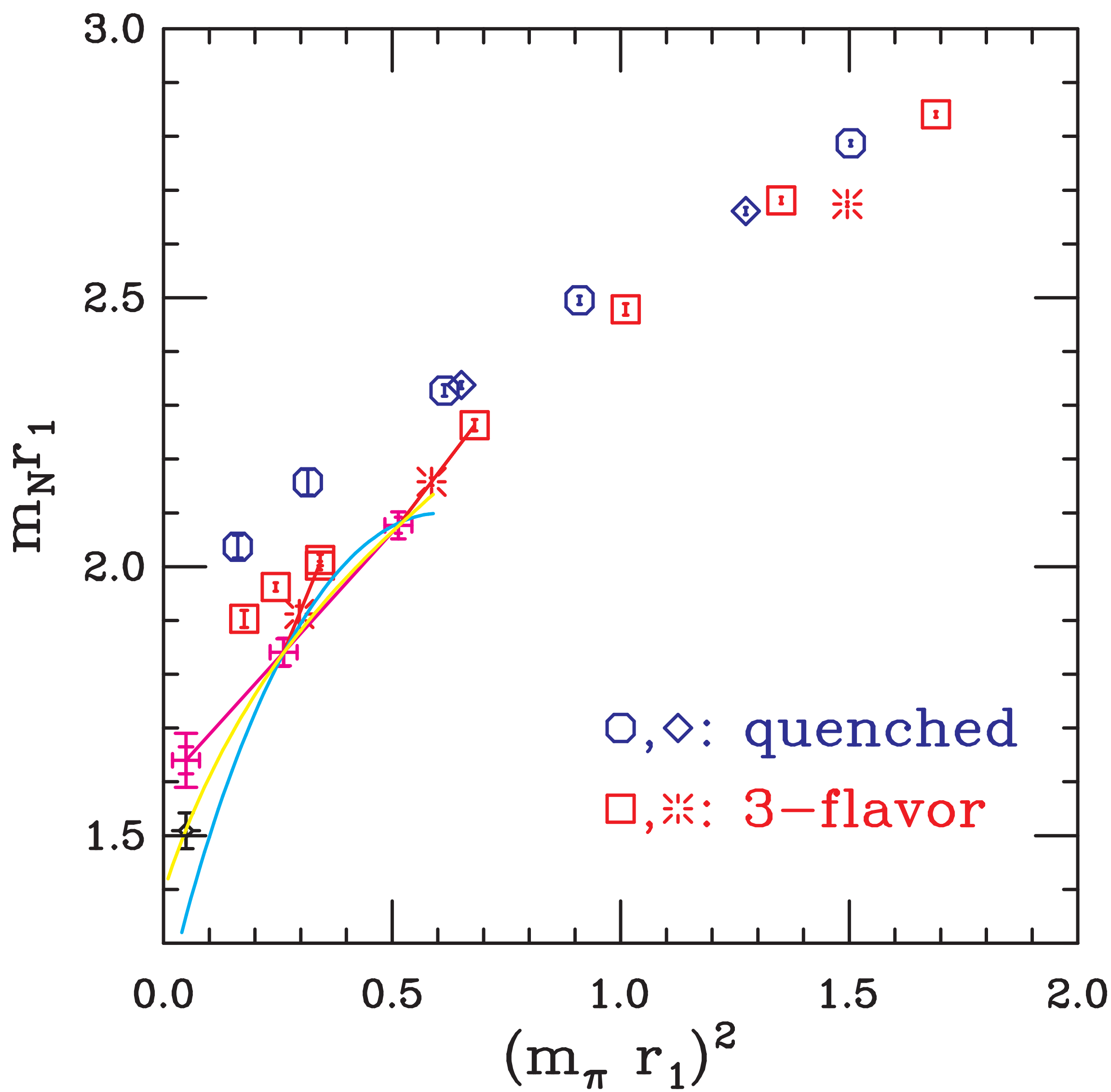
Spectrum

hep-lat/0402030

Vector meson mass fits: $10/g^2 = 7.09$ and $am_{l/s} = 0.0062/0.031$

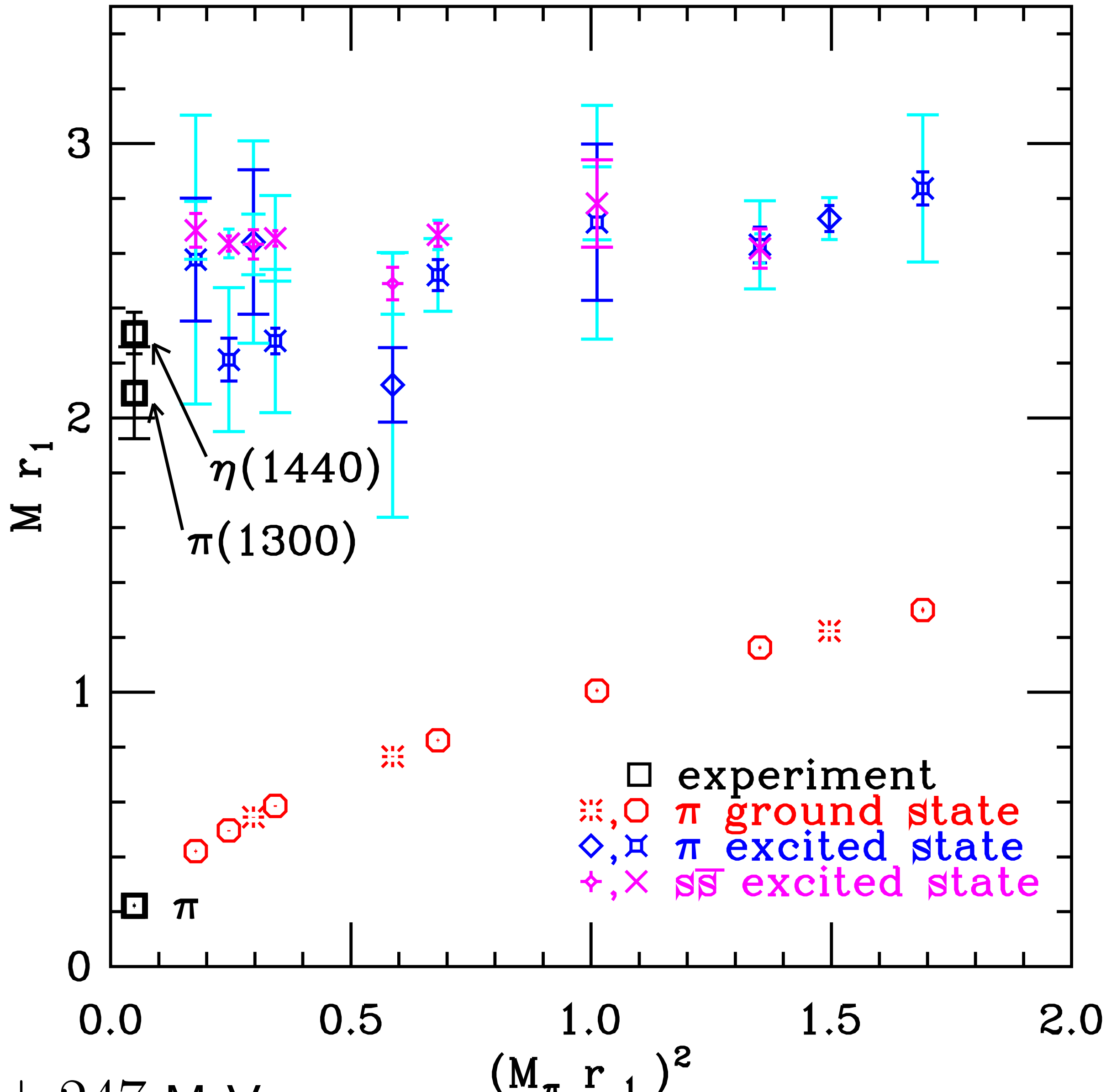


Nucleon continuum chiral extrapolation



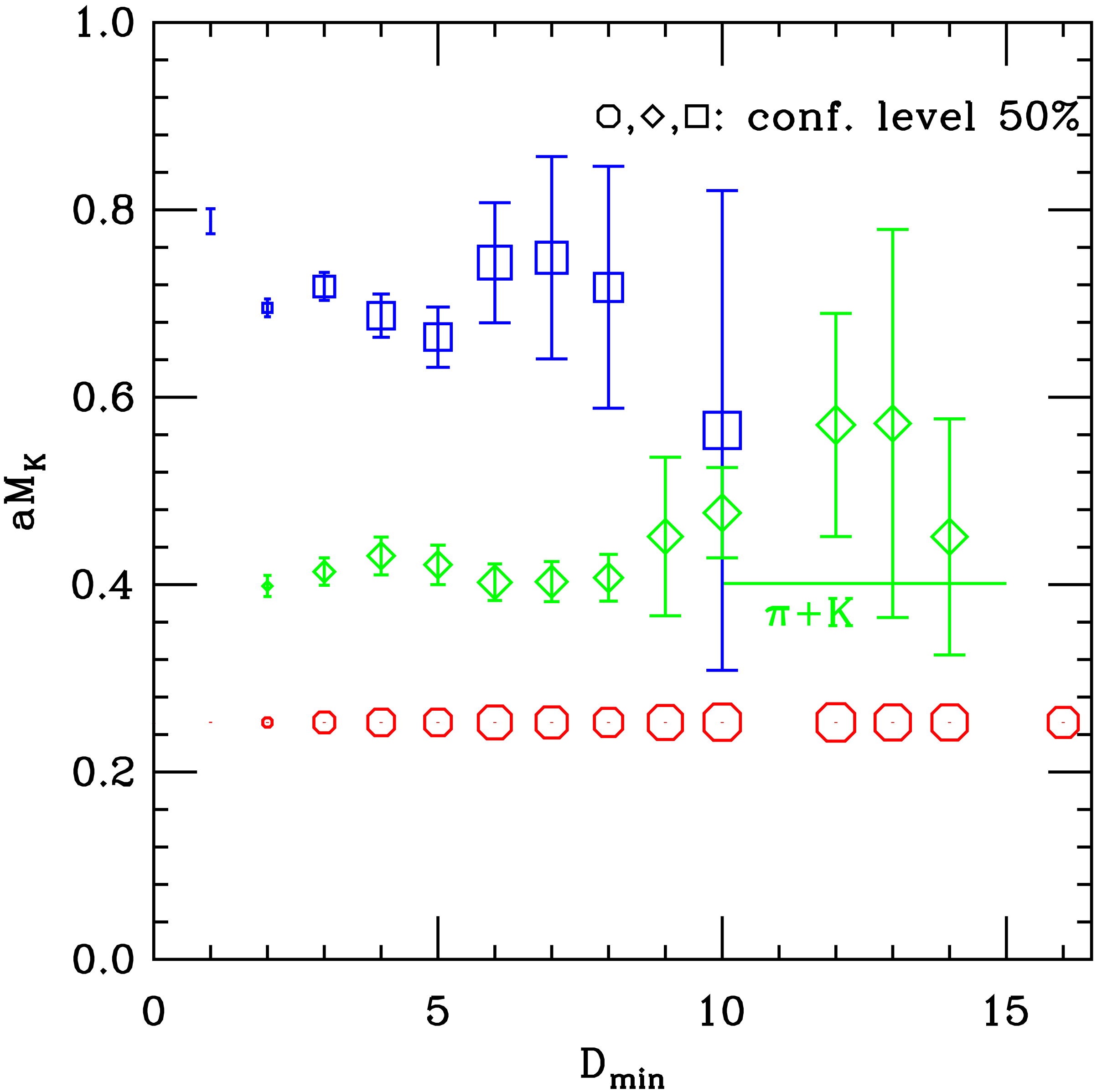
Curves come from two theories containing two parameters

Excited State 0^{-+} Masses

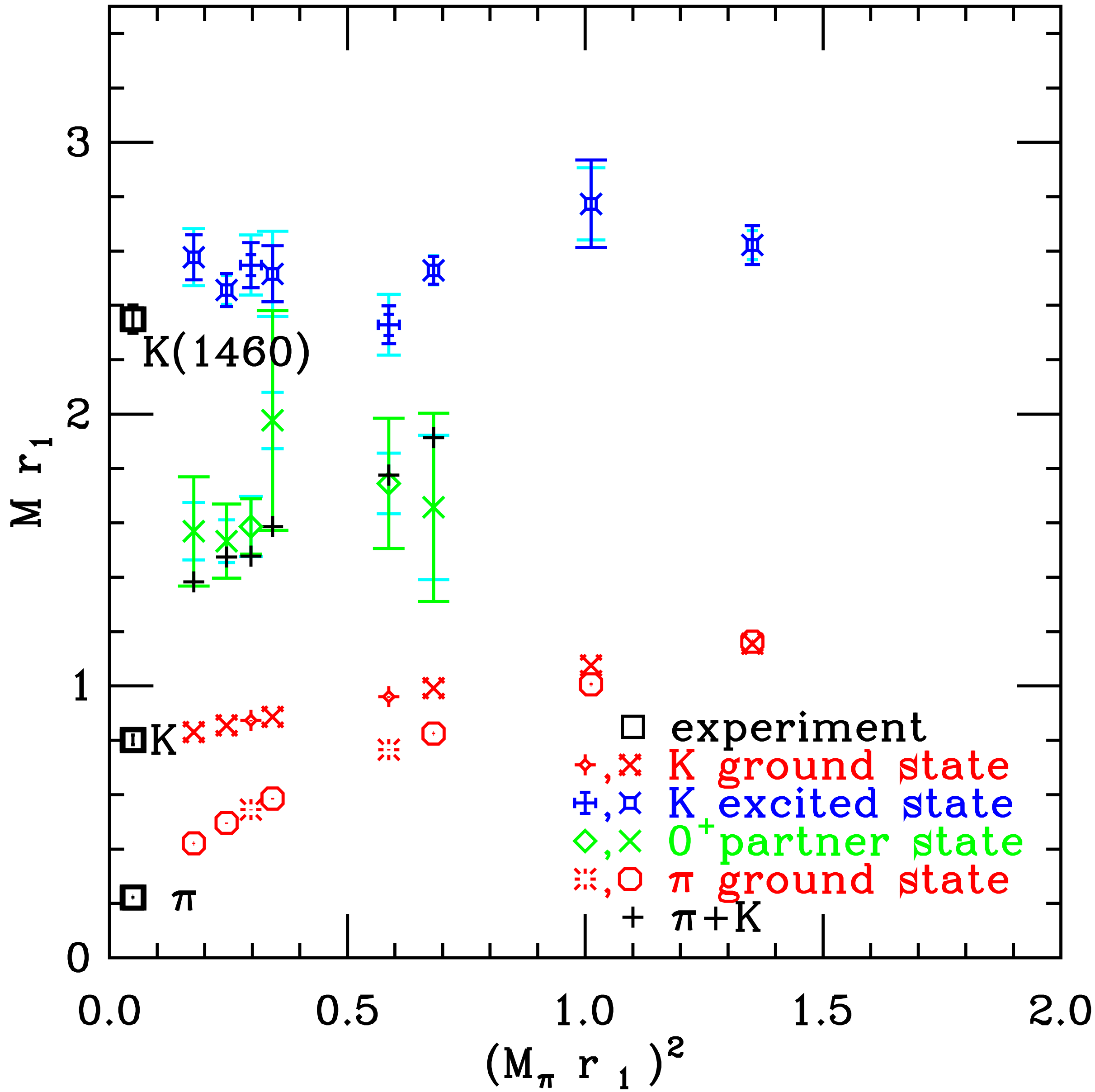


$1362 \pm 41 \pm 247$ MeV

Diamond is opposite parity; square excited state

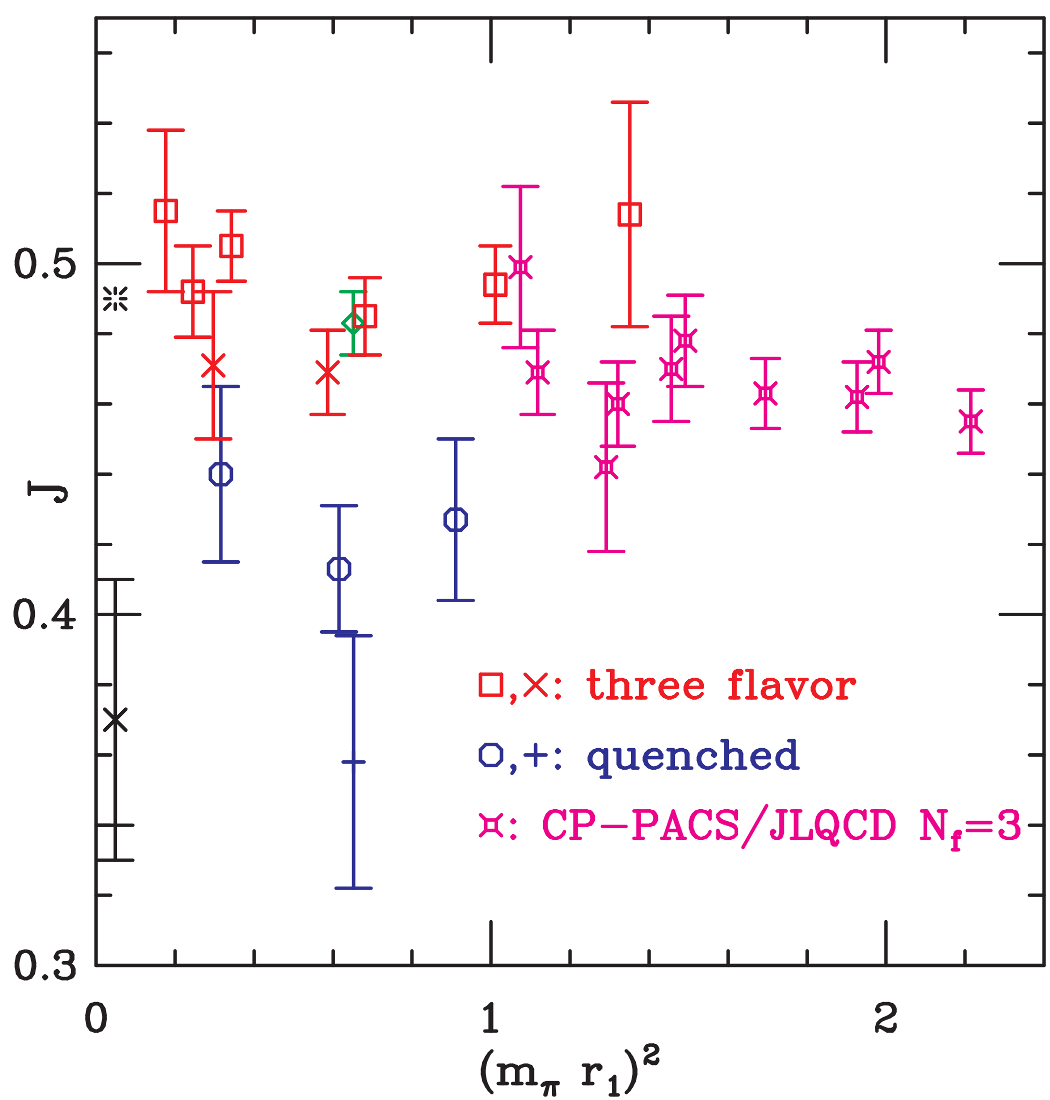


K and excited K state

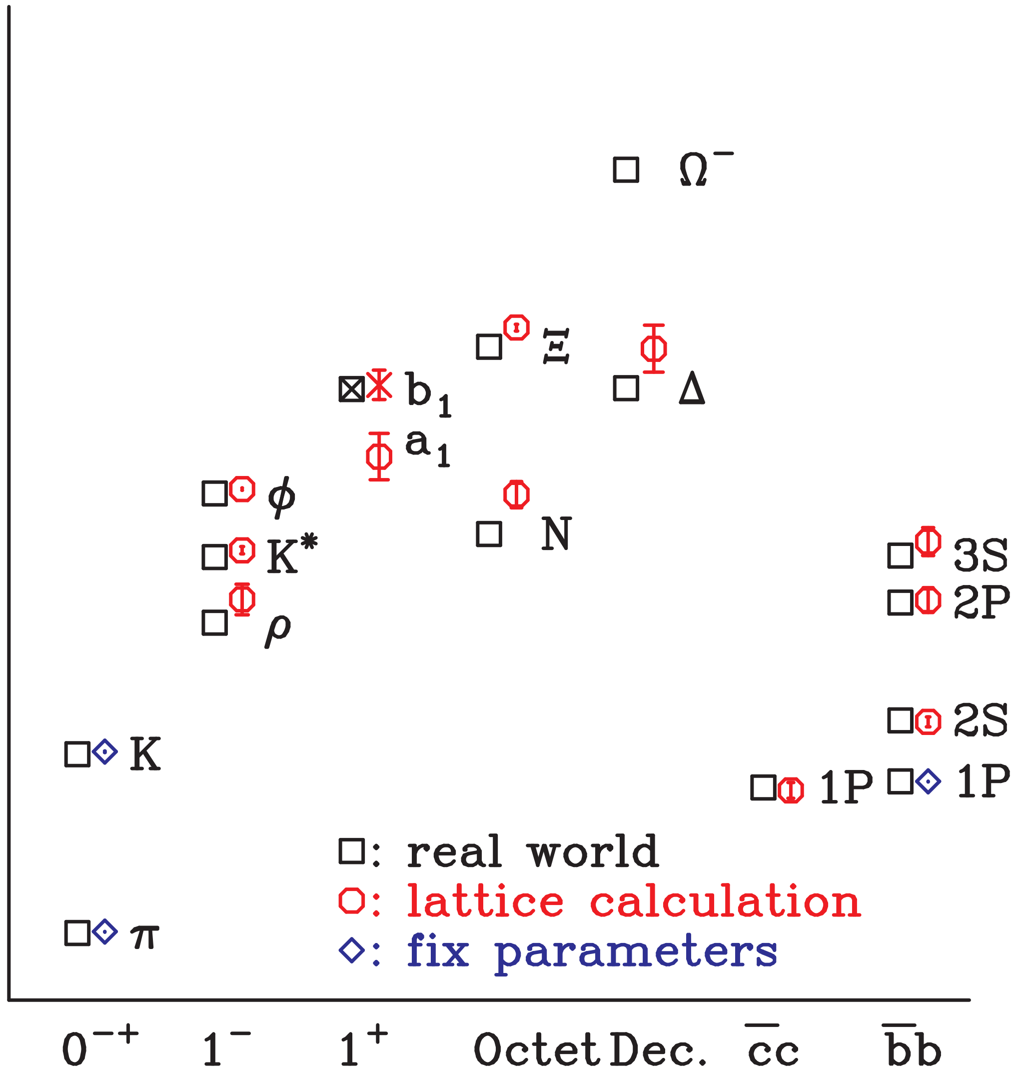


$1527 \pm 46 \pm 68$ MeV, *cf.* K(1460)

J Parameter



Big Picture



Ω⁻
Ξ
b₁
Δ
a₁
φ
N
K*
3S
2P
ρ
2S
K
1P
1P
□: real world
○: lattice calculation
◇: fix parameters
π
0⁻⁺
1⁻
1⁺
Octet
Dec.
c̄c
b̄b

Heavy quarks

- MILC has been doing Clover-light, Clover-heavy calculations for some time using $N_f = 3$ ensembles
- Using same ensembles, now using Asqtad light quarks in collaboration with Fermilab group
  - This allows better control of chiral extrapolation (D, B)
  - Techniques may be comparable for D_s and B_s
  - See later talk by Paul Mackenzie

Topology

(Lee and Sharpe; Aubin and Bernard)

$$\begin{aligned}\mathcal{L} &= \frac{f^2}{8}\mathrm{Tr}\left(\partial_\mu U^\dagger \partial_\mu U\right) - \frac{\mu f^2}{4}\mathrm{Tr}[\mathcal{M}(U^\dagger + U)] \\ &+ \frac{m_0^2}{2}\phi_{0I}^2 + a^2\mathcal{V}(U)\end{aligned}$$

Billeter, DeTar and Osborn (hep-lat/0406032) find:

$$\chi = \left\langle \nu^2 \right\rangle / V = \frac{f^2/16}{\sum_{i=1} n_i(1/m_{iI}^2 + 1/m_0^2)}$$

where the bare flavor-neutral, taste-singlet pseudoscalar masses are

$$m_{iI}^2 = 2\mu m_i + a^2\Delta_I$$

For our $N_f = 3$ simulations:

$$\chi = \frac{f^2 m_{\pi,I}^2/8}{1 + m_{\pi,I}^2/2m_{ss,I}^2 + 3m_{\pi,I}^2/2m_0^2}$$

Identical to continuum result, except taste single meson mass appears

A variance reduction technique is crucial:

$$\left\langle \nu^2 \right\rangle /V = \sum_r C_{\mathrm{meas}}(r),$$

where the measured topological charge density correlation function, is

$$C_{\mathrm{meas}}(r) = \langle \rho(0)\rho(r) \rangle$$

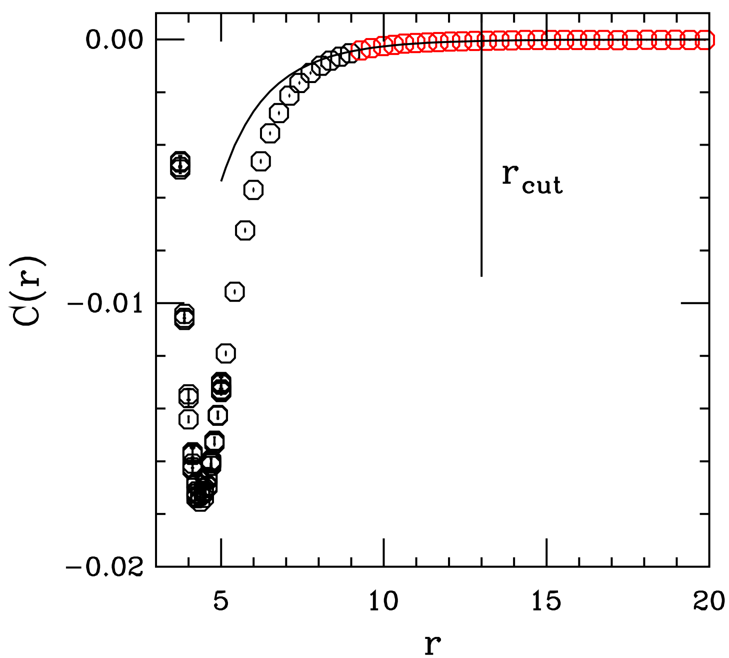
and ρ is the topological charge density operator.

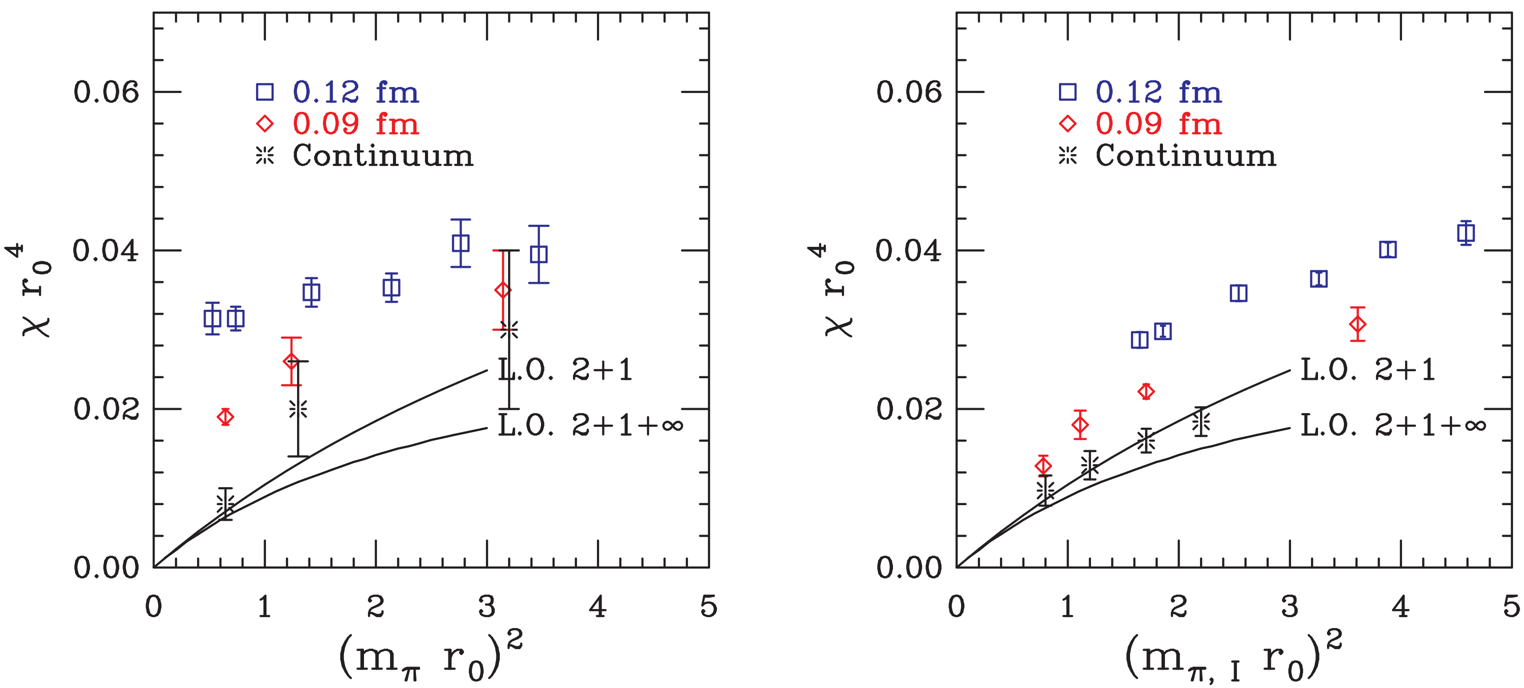
The correlator has the asymptotic form (Shuryak, Verbaarschot):

$$C_{\rm fit}(r) = b_\eta D(m_\eta, r) + b_{\eta'} D(m_{\eta'}, r) + \ldots$$

To reduce the variance, we use:

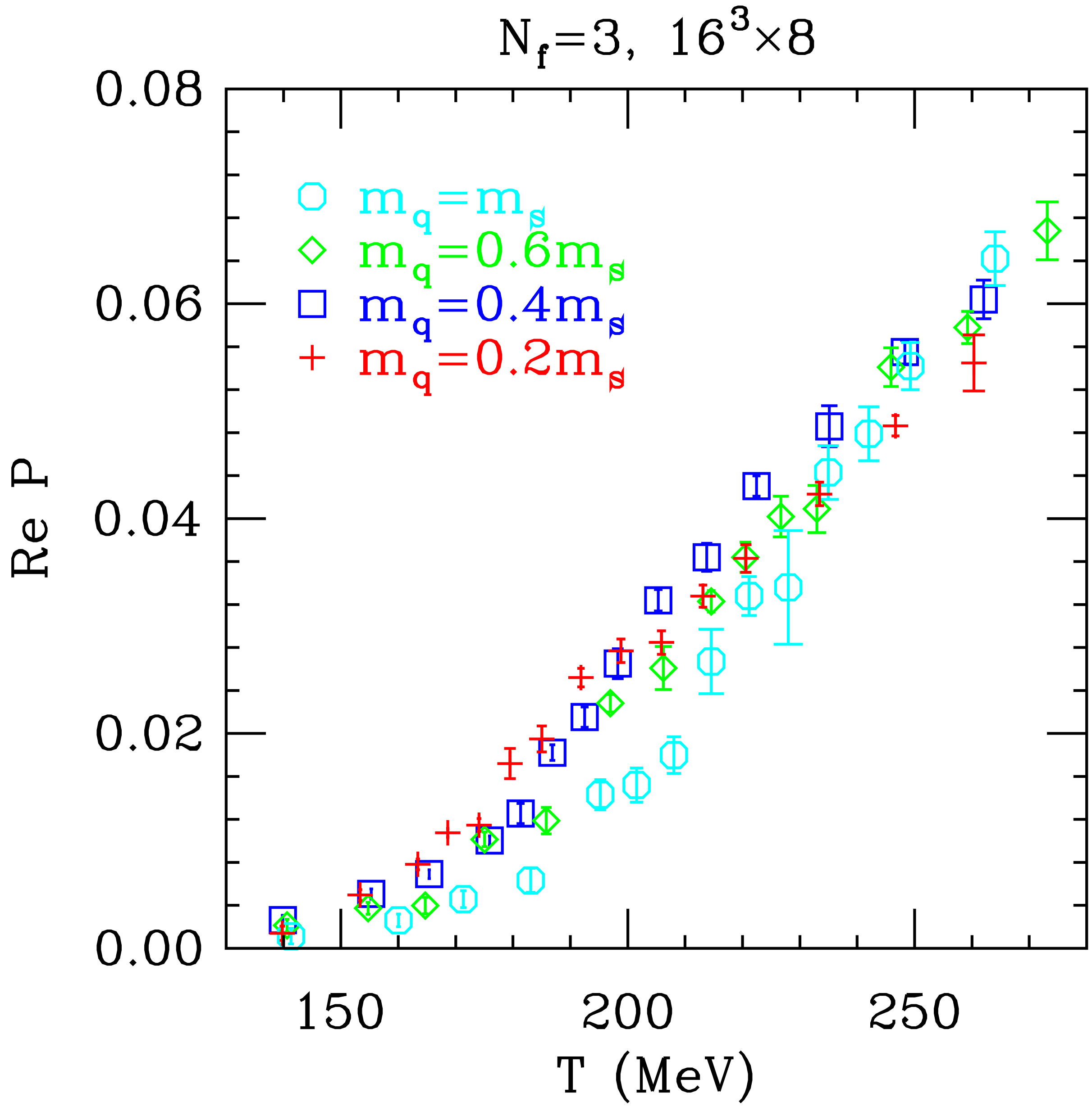
$$\left\langle \nu^2 \right\rangle / V = \sum_{|r| \le |r_{\rm cut}|} C_{\rm meas}(r) + \sum_{|r| > |r_{\rm cut}|} C_{\rm fit}(r).$$

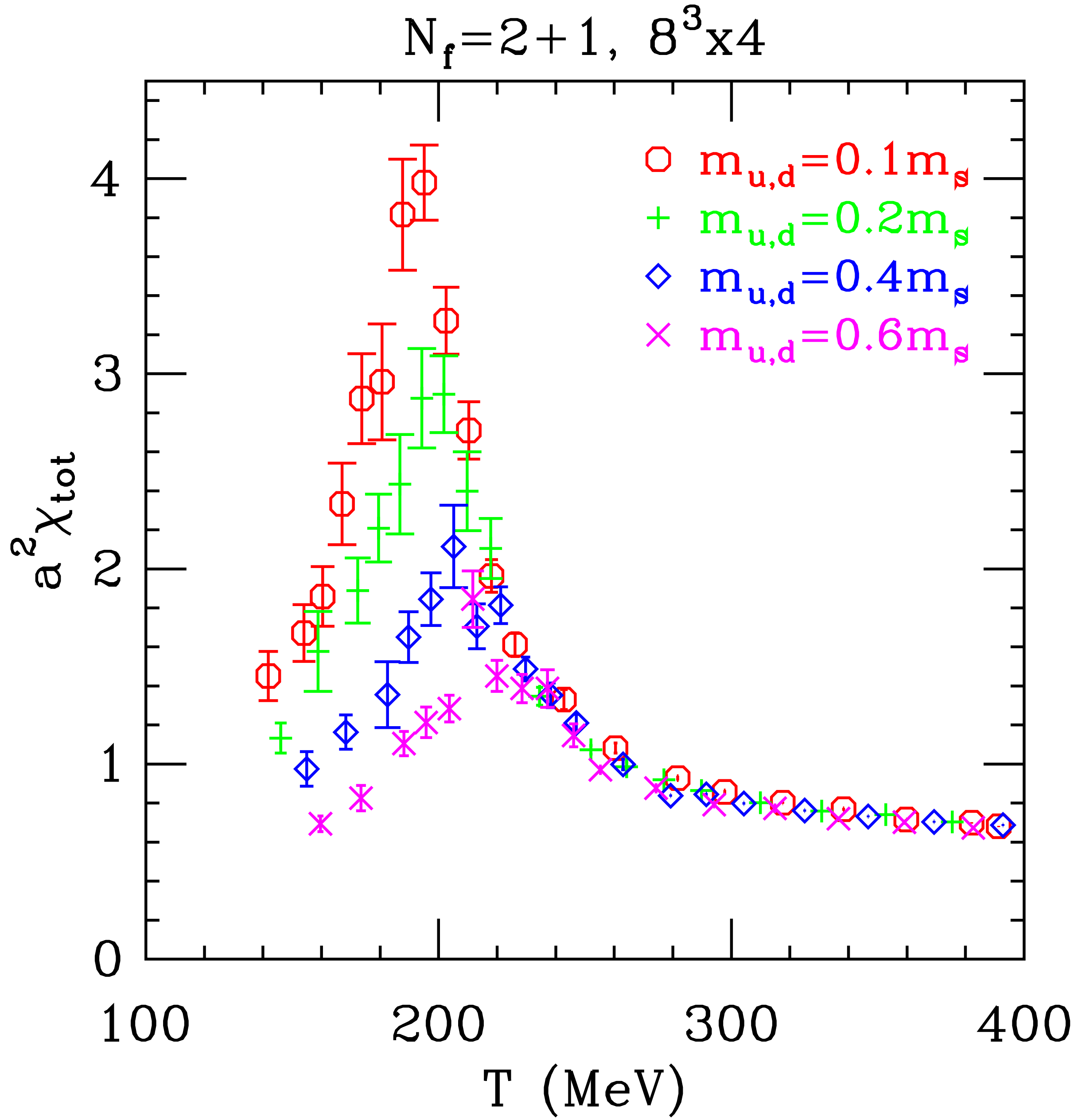




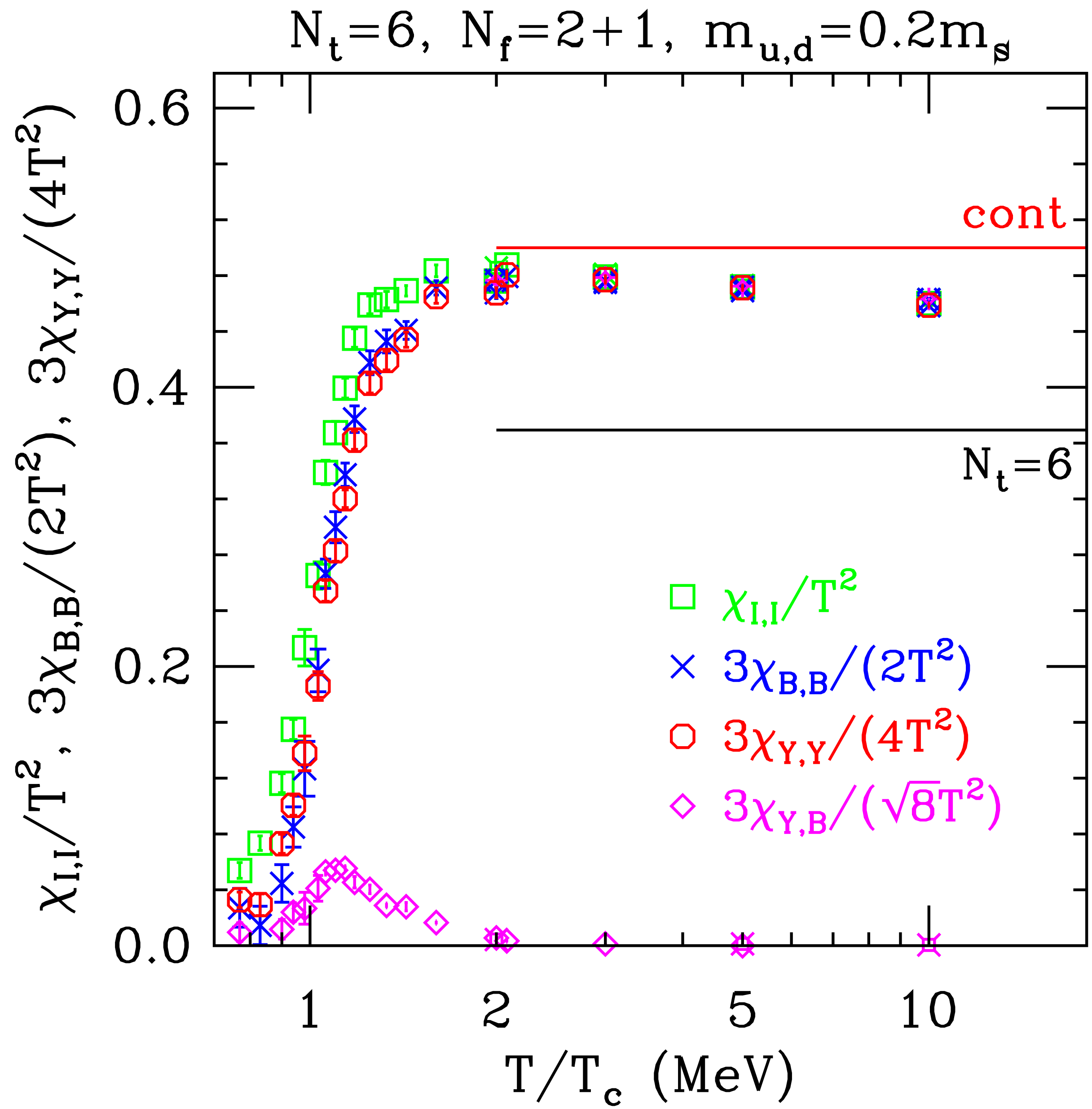
0.12 fm
0.09 fm
Continuum
L.O. 2+1
L.O. 2+1+∞
$\chi\, r_0^4$
$(m_\pi\, r_0)^2$
$(m_{\pi,\,I}\, r_0)^2$
0.00
0.02
0.04
0.06
0
1
2
3
4
5

High Temperature QCD





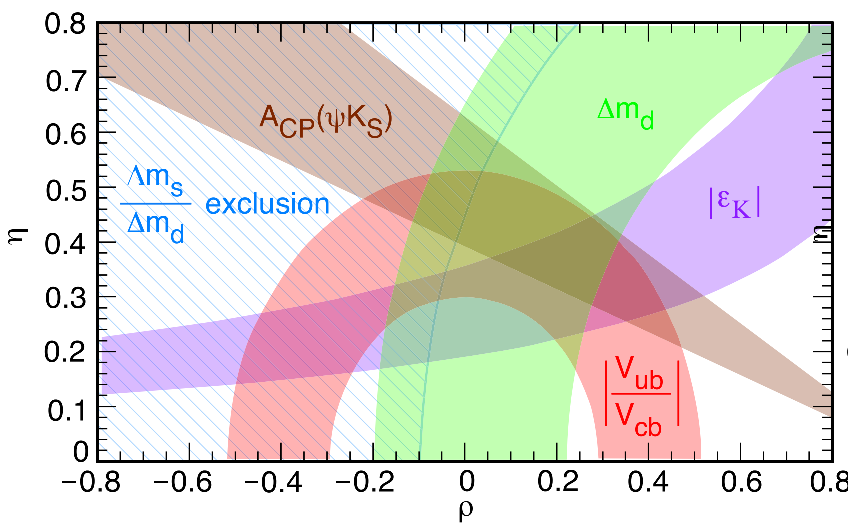
$N_f=2+1,\ 8^3x4$
$m_{u,d}=0.1m_s$
$m_{u,d}=0.2m_s$
$m_{u,d}=0.4m_s$
$m_{u,d}=0.6m_s$
$a^2\chi_{tot}$
0
1
2
3
4
100
200
300
400
T (MeV)

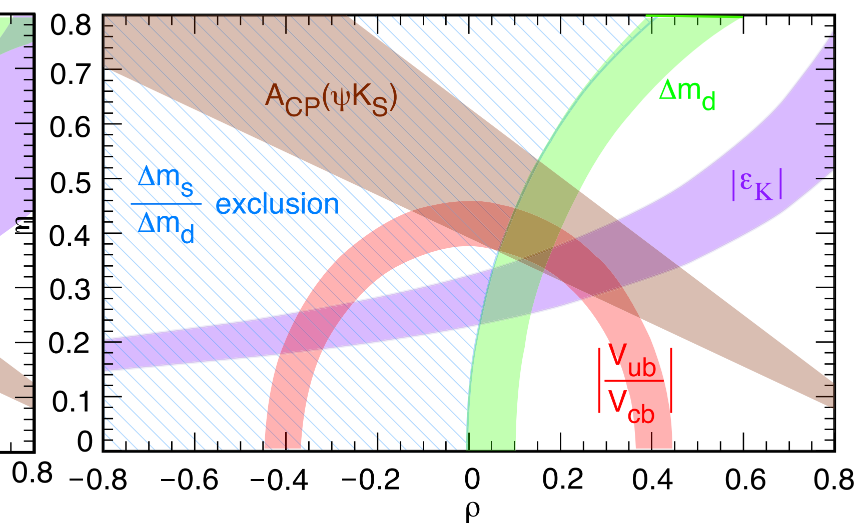


N_t=6, N_f=2+1, m_u,d=0.2m_s
0.0
0.2
0.4
0.6
1
2
5
10
T/T_c (MeV)
χ_I,I/T², 3χ_B,B/(2T²), 3χ_Y,Y/(4T²)
cont
N_t=6
χ_I,I/T²
3χ_B,B/(2T²)
3χ_Y,Y/(4T²)
3χ_Y,B/(√8T²)

Teraflops/s Era

- To go closer to the chiral and continuum limits will be expensive
- However, it is important to reduce systematic errors
- RH graph shows improvement with reduction of lattice errors to 3%





m-light	m-heavy	beta	N-s	N-t	CG-l	CG-h	steps	trajecs	Tf-yr
0.005	0.05	6.76	24	64	893	143	333	3000	0.057
0.0124	0.031	7.11	28	96	352	189	125	2000	0.024
0.0062	0.031	7.09	28	96	687	190	250	2500	0.077
0.0031	0.031	7.08	40	96	700	189	500	3000	0.541
0.0031	0.031	7.08	40	96	700	189	500	4200	0.757
0.0031	0.031	7.08	40	96	1400	189	500	4200	1.097
		a(fm)							
0.00155	0.031	0.09	56	96	1400	200	1000	4200	6.049
0.00155	0.031	0.09	56	96	2800	200	1000	4200	9.781
0.008	0.02	0.06	42	144	355	300	188	3000	0.300
0.004	0.02	0.06	42	144	1030	300	375	3750	1.129
0.002	0.02	0.06	60	144	1050	300	750	4500	7.979
0.001	0.02	0.06	84	144	2100	300	1500	6300	93.188
0.006	0.015	0.045	56	192	700	400	250	4000	2.246
0.003	0.015	0.045	56	192	1300	400	500	5000	7.518
0.0015	0.015	0.045	80	192	1400	400	1000	6000	54.824