Actions for dynamical fermion simulations: are we ready to go?

Karl Jansen

- Conceptual questions
- Algorithmic questions
- questions in (chiral) perturbation theory
- Practical questions
- some results
- Con(cl)(f)usions


DANGER
MINEFIELD

Actions

- **Wilson fermions**
  - non-perturbatively improved fermion action
  - various gauge actions (Plaquette, Symanzik, RG-improved)
- **Staggered fermions**
  - improved fermion action (Asqtad)
  - various gauge actions
- **Domain wall and overlap fermions**
  - RG improved gauge actions
  - fermion actions with eigenvalue projection
- **Designer actions**
  - FLIC, Hypercube (various versions) + many more

$\longrightarrow$ have to agree in continuum limit: provide valuable cross check

$\longrightarrow$ don't waste resources

rigorous actions

- **reflection positivity, Osterwalder-Schrader positivity, positive transfer matrix $\Rightarrow$ reconstruction theorem**
  - Wilson action

    Lüscher, Commun.Math.Phys.54:283,1977; for $r = 1$, $\kappa < 1/6$

    (– tmQCD)
  - (naive) staggered fermions:

    Sharatchandra, Thun, Weisz,Nucl.Phys.B192:205,1981; Smit, Nucl.Phys.Proc.Suppl.20:542-545,1991 ; Palumbi, hep-lat/0208005

    positive transfer matrix for 2 lattice spacings not rigorous but local actions

- **no proof of reflection positivity or construction of positive transfer matrix**
- **ultra local actions**
  - Designer actions, I will take as example FLIC*
  - Symanzik improved actions
  - truncated perfect action
- **exponentially localized**
  - overlap
  - domain wall
  - perfect action

* *Fat Link Irrelevant Clover fermions*

$$D_{\mathrm{FLIC}} = \frac{1}{u_0}\nabla_\mu\gamma_\mu + \frac{1}{2u_0^{(fl)}}\left(\Delta^{(fl)} - \frac{1}{2u_0^{3(fl)}}\sigma\cdot\mathcal{F}^{(fl)}\right)$$

Non-local actions?

candidate: taking square root of staggered fermion matrix

test following Hernández, Lüscher, K.J.

Source point

$$\eta_\alpha(x) = 1 \ \text{ for } \ x = 1, \alpha = 1 \quad \eta_\alpha(x) = 0 \ \text{ else}$$

compute for some operator $A^\dagger A$

$$\Psi(x) = \sqrt{A^\dagger A}\eta(x)$$

test whether couplings of the operator decay exponential

$$f(r) = \max\{\|\Psi(x)\|; \|x - y\|_{\mathrm{taxi}} = r\}$$

test for fixed value of lattice spacing a; positive outcome:

$$f(r) = e^{-r/r_{\mathrm{local}}}$$

locality in continuum limit?

possibility I

$$r_{\mathrm{local}} \cdot m_\pi = \mathrm{constant};\ \mathrm{for}\ \ a \rightarrow 0,\ m_\pi\ \ \mathrm{fixed}$$

$\Rightarrow$ obtain a continuum theory with $r_{\mathrm{local}} \propto \xi_\pi$ non-local theory on the scale of pion Compton wave length $\Rightarrow$ unacceptable

possibility II

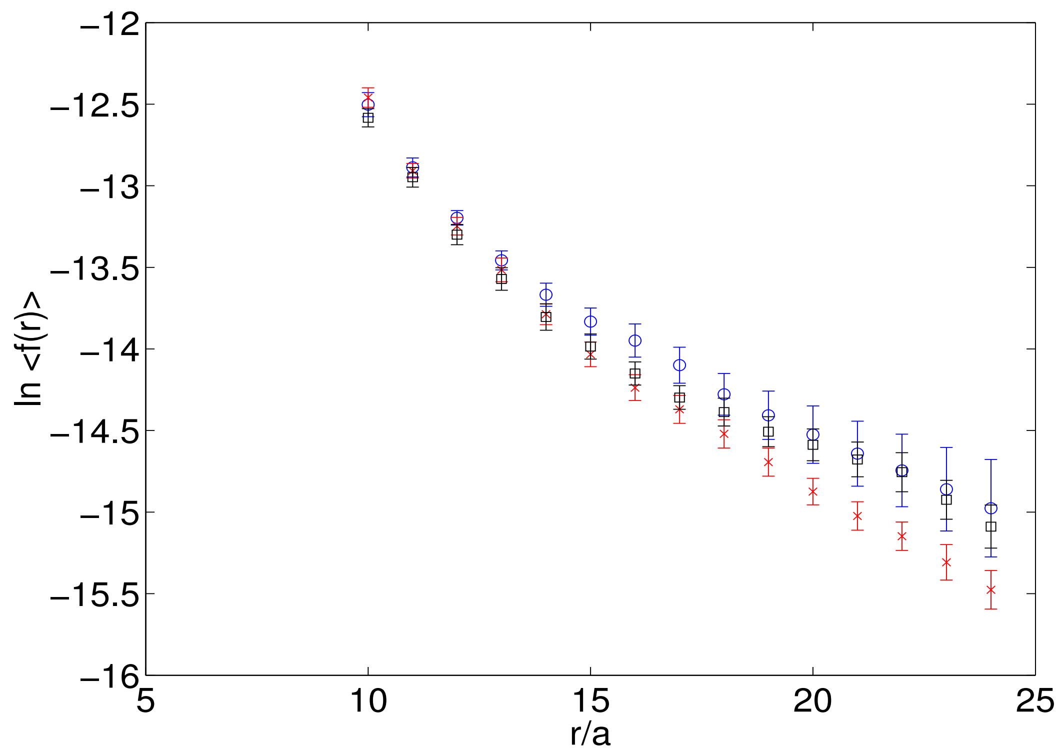
$$r_{\mathrm{local}} \cdot m_\pi \rightarrow 0\ \mathrm{for}\ \ a \rightarrow 0,\ m_\pi\ \ \mathrm{fixed}$$

$\Rightarrow$ $r_{\mathrm{local}}/a = const$ obtain a point local continuum theory

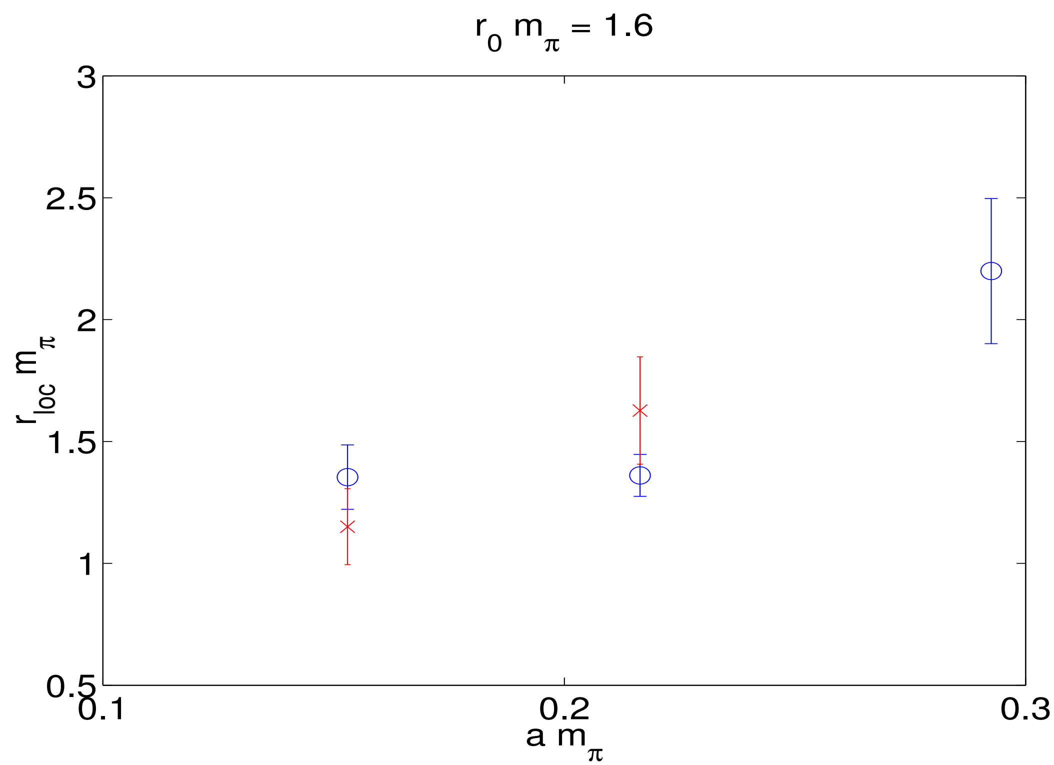
A first look

use (F. Knechtli, K.J.): $A =$ Wilson operator, $\sqrt{A^\dagger A} = P_{n,\epsilon}(A^\dagger A)$

fix $r_0 \cdot m_\pi = 1.6$, various $\beta = 6, 6.2, 6.45$



$$r_{\mathrm{local}} \cdot m_\pi$$



red crosses: take r_{local} at $\beta = 6.0$ and scale it according to change of lattice spacing

My personal wishlist I

precise check for localization of staggered fermions

work in progress, Della Morte, Knechtli, K.J.

C, P & T

A warning from M. Creutz

spontaneous CP violation might be possible for $m_u \rightarrow 0$ tuning it negative

$\leftarrow$ miss this possibility when taking square roots?
$\leftarrow$ miss interesting part of physics?

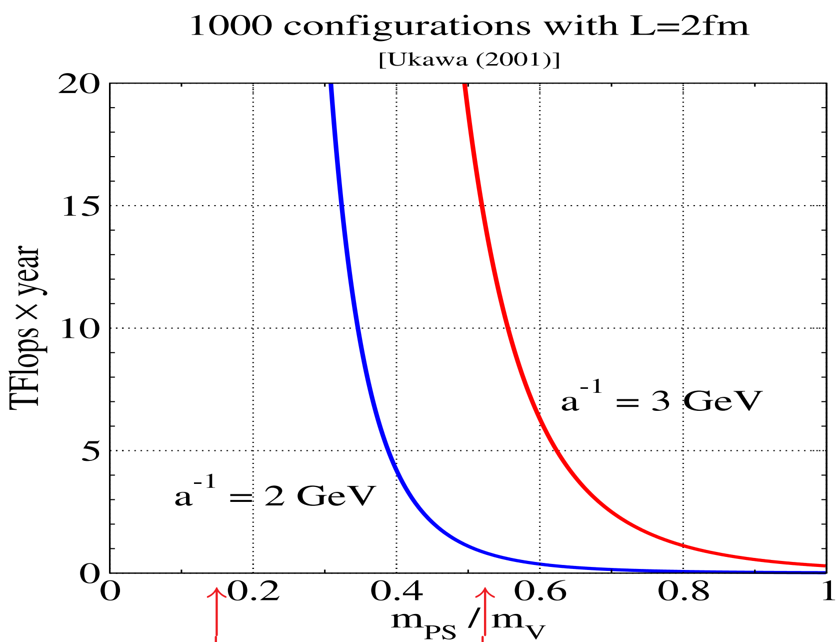
A warning from Klinkhamer and J. Schilling

for a special class of gauge fields $(U_4(\mathbf{x}, x_4) = 1, U_m(\mathbf{x}, x_4) = U_m(\mathbf{x}))$ *chiral gauge theories* from overlap fermions not CPT invariant

$\leftarrow$ violation of reflection positivity? Consequences?
see also Fujukawa, Ishibashi, Suzuki

Costs of dynamical fermions simulations

see panel discussion in Lattice2001, Berlin, 2001



formula $C \propto \left(\frac{m_\pi}{m_\rho}\right)^{-z_\pi} (L)^{z_L} (a)^{-z_a}$

$$z_\pi = 6$$

$$z_L = 5$$

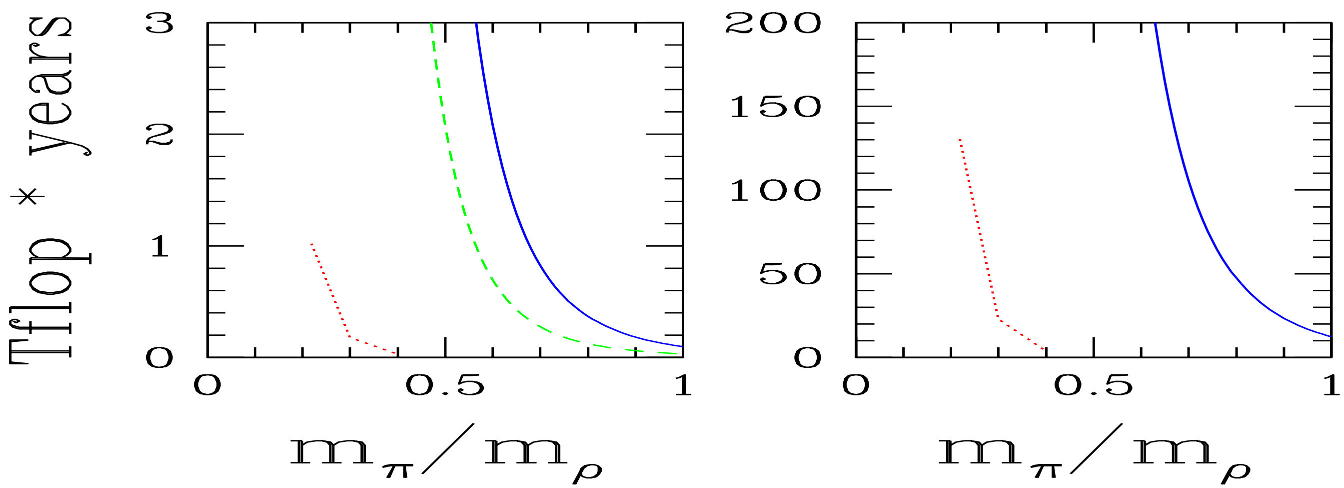
$$z_a = 7$$

physical point

contact to χPT (?)

$\Rightarrow$ use chiral perturbation theory (χPT) to extrapolate to physical point

Wilson versus staggered at fixed box length $L = 2.5$ fm



$a = 0.09$ fm
staggered: measured

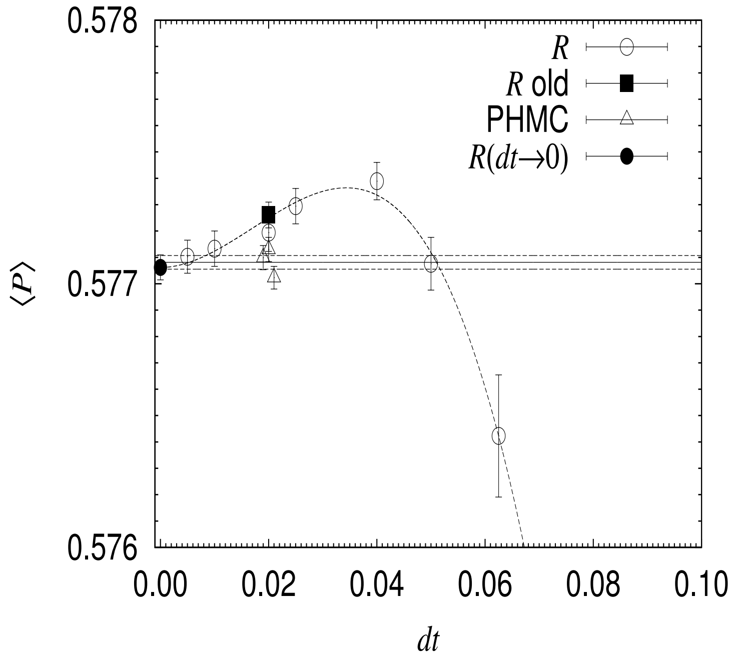
$a = 0.045$ fm
staggered: extrapolated

full line: Wilson; dashed line: staggered; dashed line: Wilson/3

MILC data, thanks to S. Gottlieb

Exact vs. inexact: why inexact?

Exact algorithm PHMC algorithm for $N_f = 3$ Aoki et.al. (JLQCD) hep-lat/0208058
(see also T. Kennedy)



→ extraplation to $\delta\tau = 0$ difficult

→ treat $(A^\dagger A)^{1/n}$ by polynomial

→ noisy Metropolis step or correction factor
inversion of $(A^\dagger A)^{1/n}$ by Lancsoz method

→ cost of exact algorithm ≈ in-exact

My personal wishlist II
Use and test exact odd flavour algorithms
fair comparison of exact algorithms, continuum approach

How to simulate a designer action

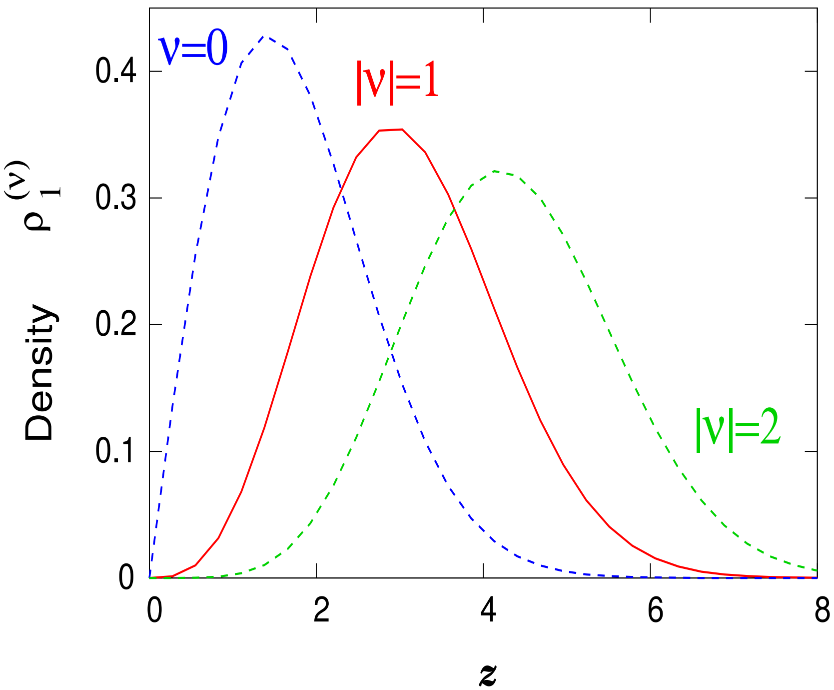
$\longrightarrow$ complicated interactions, fattening

- first way a la Hasenbusch; Hasenfratz and Knechtli + many others

  i) $U \longrightarrow U'$ according to gauge field action
  ii) $\det(A'^{\dagger}A')/\det(A^{\dagger}A) \longrightarrow$ accept/reject; correction factor
  iii) needs smearing/fattening
  improvements: break up of determinant, ultraviolett filtering, $\cdots$

- second way a la W. Kamleh
  re-unitarization through $X/\sqrt{X^{\dagger}X}$
  expand $1/\sqrt{X^{\dagger}X}$
  use chain rule to go from fattended link $U^{(n)}$ to original link $U^{(0)}$

A problem of principle: the eigenvalue distribution from Random matrix Theory



⇒ small eigenvalues have to appear, checks in quenched simulations
Bietenholz, Shcheredin, K.J., QCDSF, Weisz et.al.

⇒ can lead to large statistical fluctuations or difficulties in the simulations when approaching the physical point

Perturbation theory
(review Capitani, hep-lat/0211036)

Analysis for Wilson fermions Bochicchio, Maiani, Martinelli, Rossi, Testa

Analysis for staggered Sharatchandra, Thun, Weisz; Goltermann, Smit, Vink

Designer actions

more links of course more complicated but doable

fattening/smearing/blocking $\longrightarrow$

$$\int \frac{d^4q}{(2\pi)^4} I(q) \to \int \frac{d^4q}{(2\pi)^4} \left(1 - \frac{c}{6}\hat{q}^2\right)^{2N} I(q)$$

$c < 1$ smearing coefficient, N number of smearing steps

tadpole contribution substantially reduced:
$12.23 g_0^2/(16\pi^2) C_F \to 0.35 g_0^2/(16\pi^2) C_F$

Reisz Power Counting Theorem

(Reisz, Lüscher)

statement is that the lattice integral

$$I = \int_{-\pi/a}^{\pi/a} \frac{d^4k}{(2\pi)^4} \frac{V(k,m,a)}{C(k,m,a)}$$

exists in the continuum limit, if (among others) the condition

$$|C(l,m,a)| \geq A(\hat{l}^2 + m^2)$$

is fulfilled for a small enough and some positive value of A

$$\text{Wilson}(r=1) \quad C = (1+am)\hat{p}^2 + m^2 + \tfrac{1}{2}a^2 \textstyle\sum_{\mu<\nu} \hat{p}_\mu^2 \hat{p}_\nu^2$$

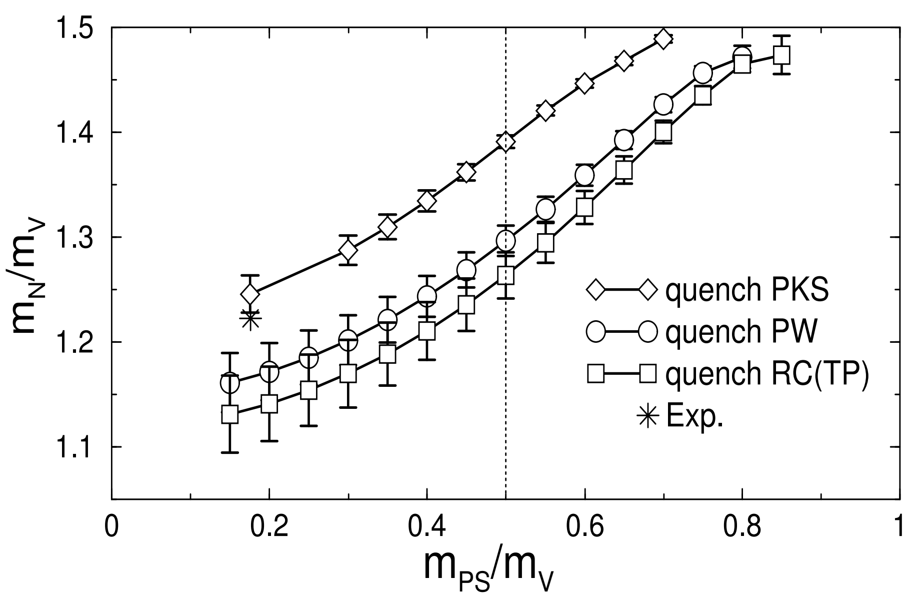
$$\text{Staggered} \quad C = \textstyle\sum_\mu \sin^2 k_\mu + m^2 = \sum_\mu \hat{k}^2 - \frac{a^2}{4} \sum_\mu \hat{k}^4 + m^2$$

My personal wishlist III
construct a "Reisz theorem" for staggered fermions

Inconsistencies?

S. Aoki, hep-lat/0011074, Lattice2000 review

PKS:	plaquette action, staggered fermions
PW:	plaquette action, Wilson fermions
RC(TP):	RG gauge action, tadpole improved Wilson

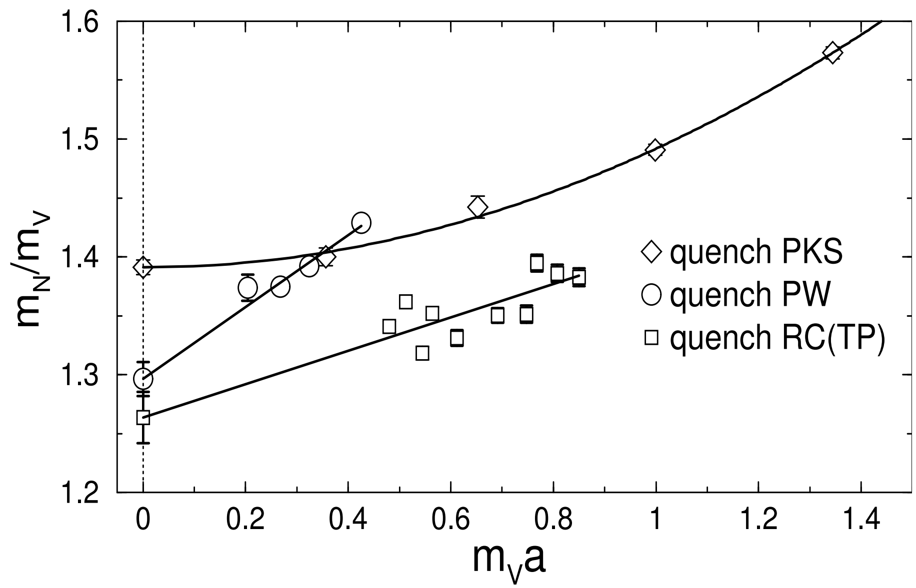


$\longrightarrow$ different continuum results even at large masses!

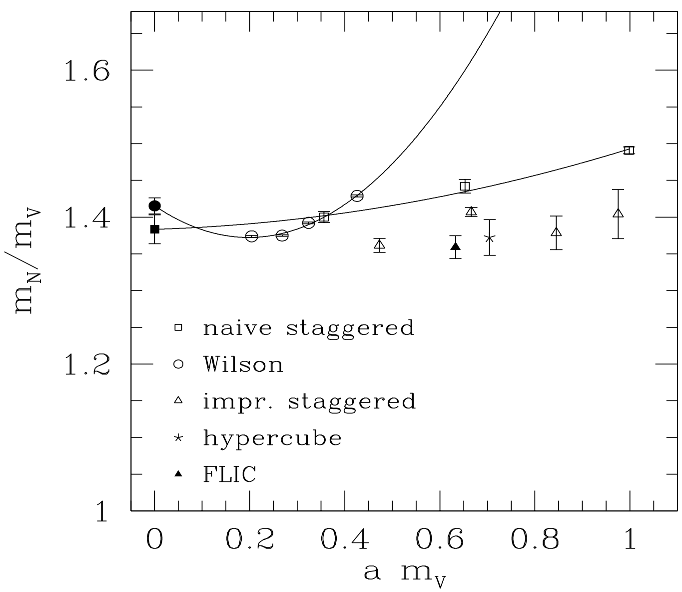
The continuum extrapolation

S. Aoki, hep-lat/0011074, Lattice review

$m_\pi/m_\rho = 0.5$



Large lattice artefacts/alternative fits?



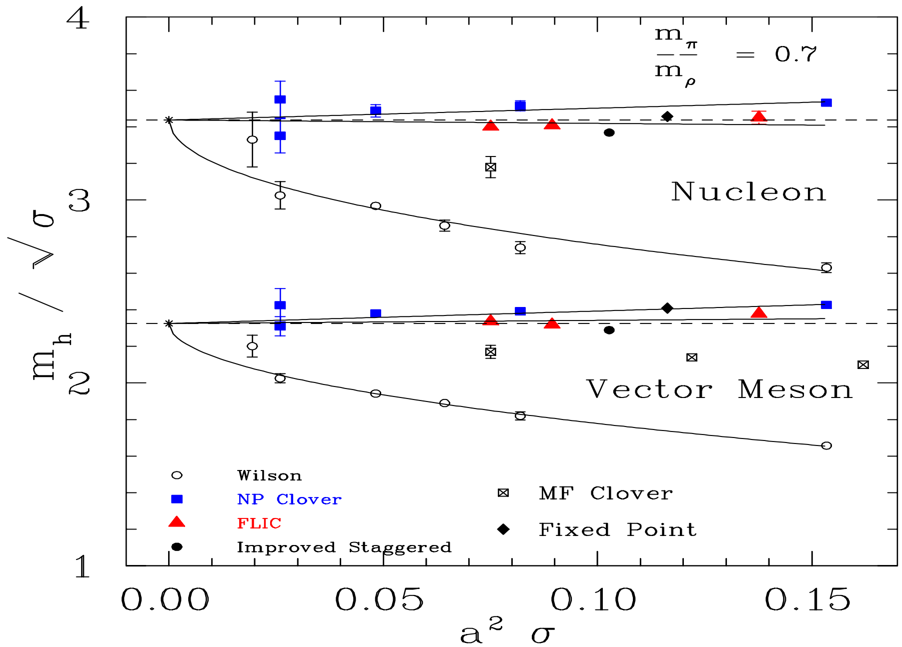
K.J. and J. Zanotti

fit may not not be the final one, but it is a possibility

My personal wishlist IV

precise scaling analysis for various fermion actions in the quenched approximation

A scaling plot



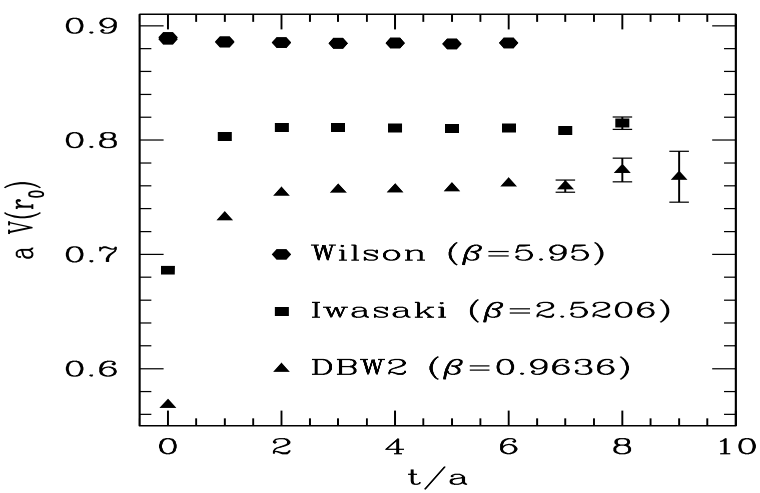
thanks to J. Zanotti

(talks by A. & P. Hasenfratz for scaling tests of Hyp, Asqtad, CI and TP)

Problems in practical dynamical simulations:
Gauge actions

I: RG action $\longrightarrow$ not reflection positive

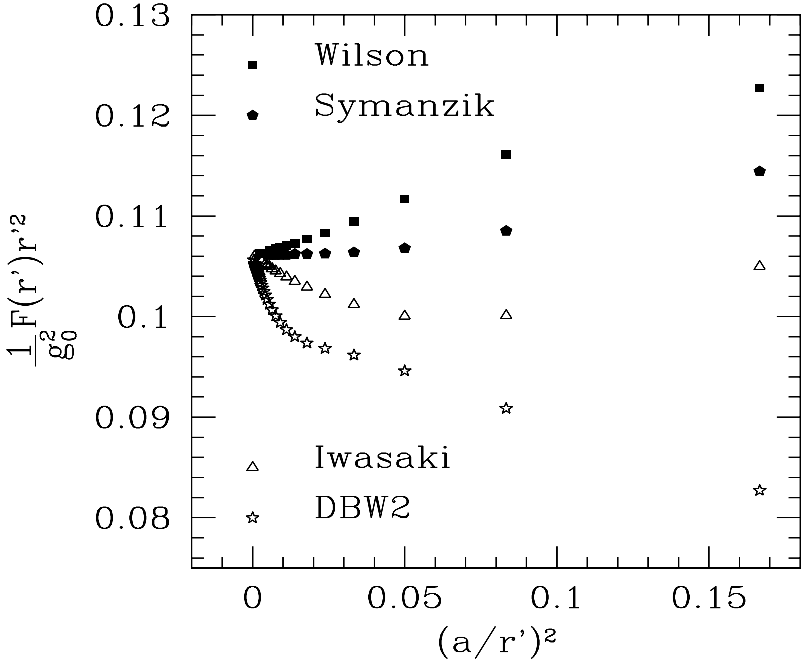
$\Rightarrow$ complex energies



Necco, Sommer

free field analysis: $t \gg t_{\text{min}} = \begin{cases} 0.5 & \text{Symanzik} \\ 0.9 & \text{Iwasaki} \\ 1.7 & \text{DBW2} \end{cases}$

II: large lattice artefacts possible

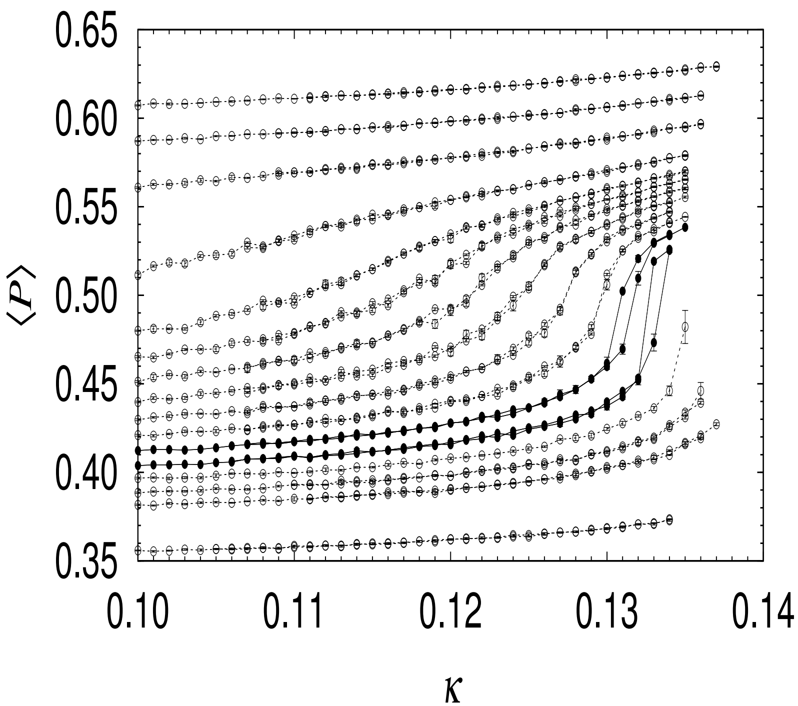


$\Rightarrow$ two action method?

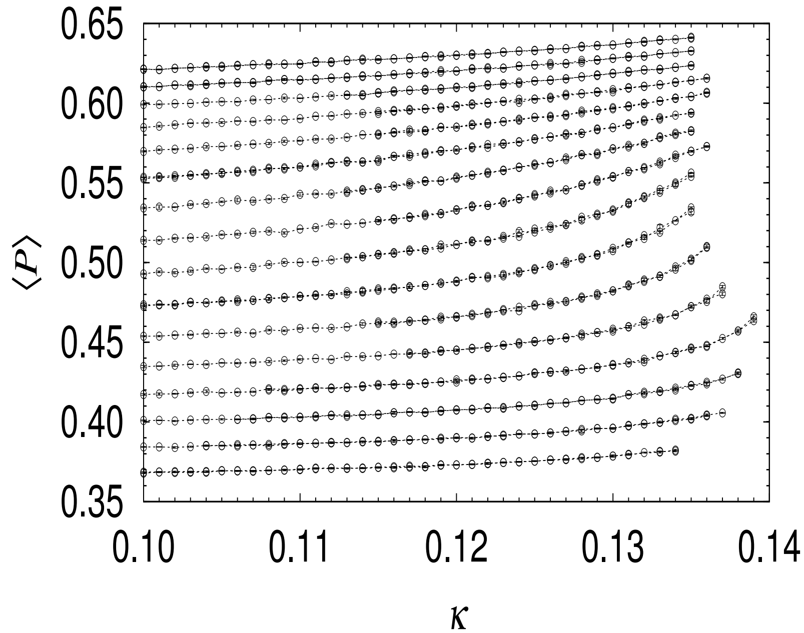
III: difficulty of sampling topological charge sectors

Problems in practical dynamical simulations: Wilson

Simulations with $N_f = 3$ improved fermions CP-PACS

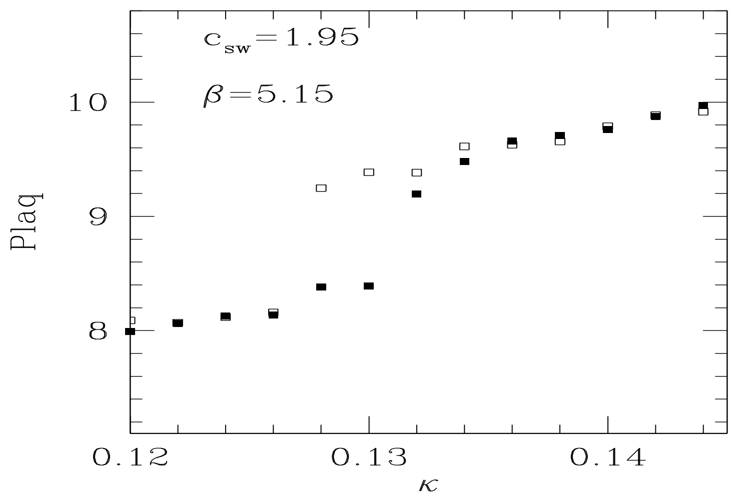


Wilson gauge



RG improved action

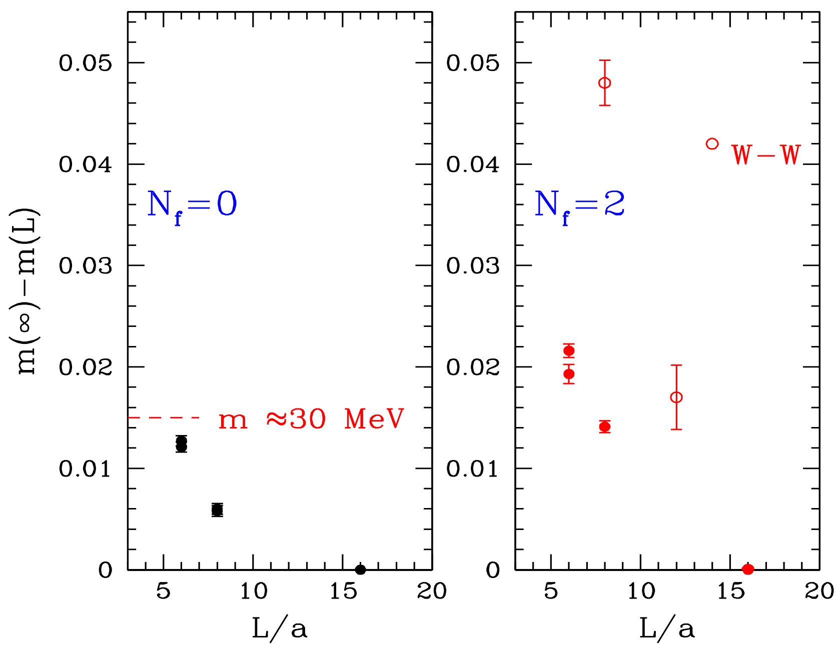
Simulations with $N_f = 2$ Wilson gauge non-perturbatively improved fermions (K.J.)



- hysteresis effect
- effects almost independent from values $1 < c_{\rm sw} < 2$
- small lattice simulations

(unexpected) large lattice artefacts in quark mass

Wilson gauge, non-perturbatively improved Wilson fermions



Non-perturbatively improved Wilson

$m(\infty) = m(16)$, W-W: Wilson action

My personal wishlist VI

Study and understand $T = 0$ phase diagram of QCD

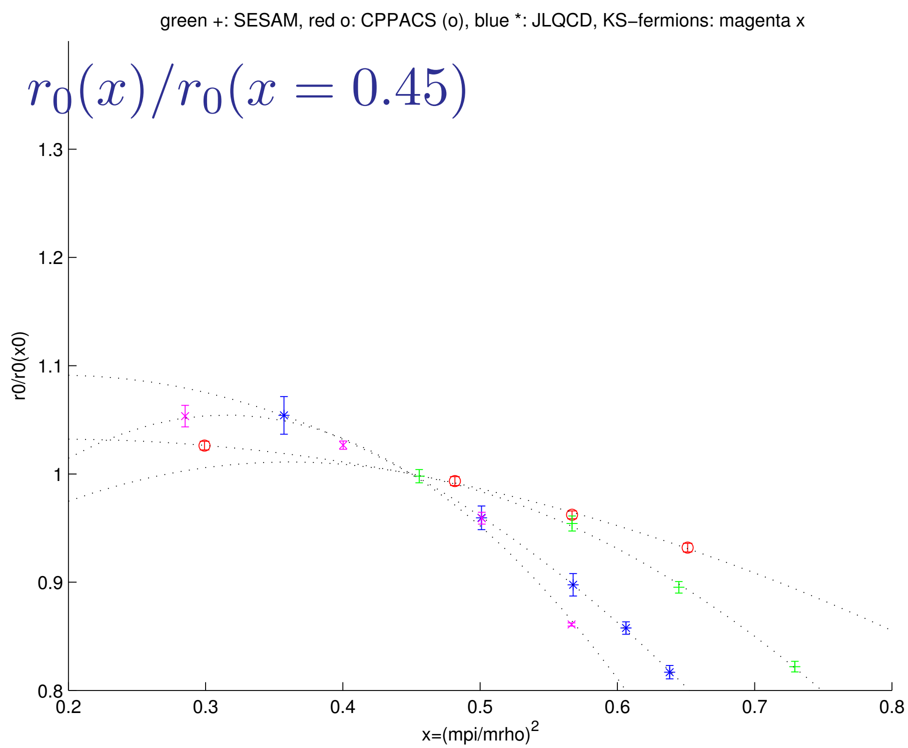
Investigate different gauge actions

understand nature of phase transition

W-KS: x W-W: + I-SW: o W-SWimpr: $*$

$R(y)$ for $y_{\rm ref} = 0.45$, $a \approx 0.1$ fm

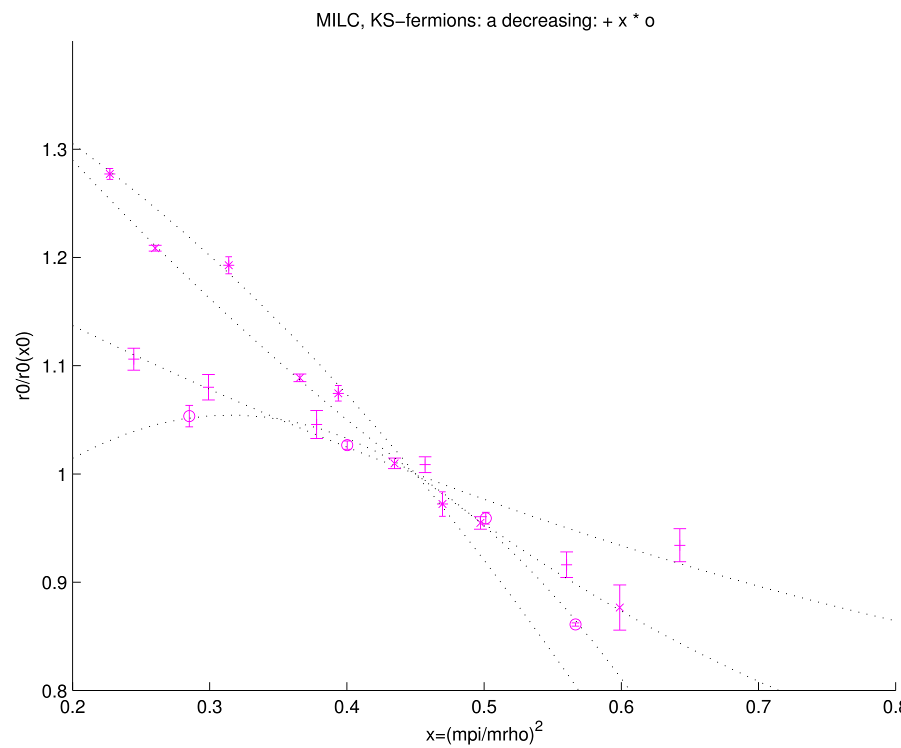
$r_0(x)/r_0(x=0.45)$



x$=(m_\pi/m_\rho)^2$

Large effects?

KS-fermions various $a \geq 0.1$ fm

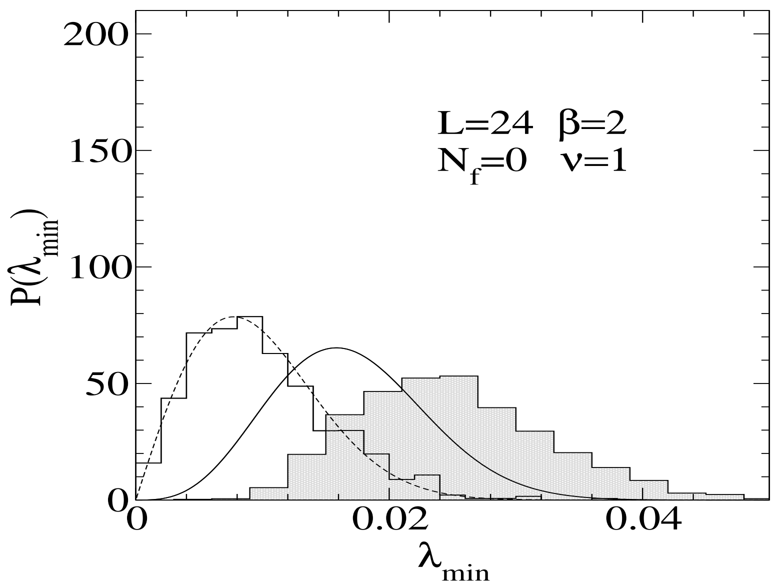


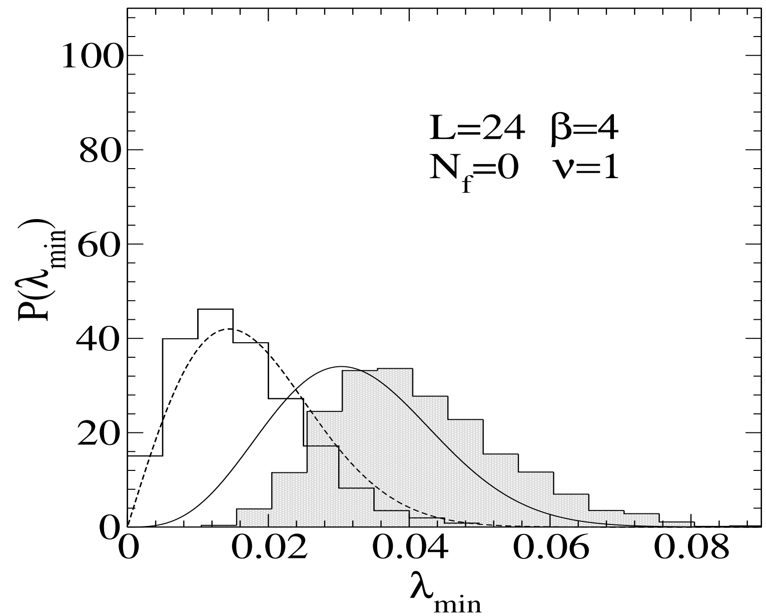
Large cutoff effects!

R. Sommer

Problems in practical dynamical simulations: Staggered

Eigenvalue distribution of staggered operator in comparison to Random matrix theory





Farchioni, Hip, Lang

see also: Damgaard, Heller, Niclasen, Rummukainen, Berg, Markum, Pullirsch, Wettig

does problem disapear for $a \ll 1$? How do improved actions behave?

Results (nevertheless) Wilson

- comparison to chiral perturbation theory
- finite size effects
- status of running quark mass
- towards $N_f = 3$
- meson spectrum

Chiral Perturbation theory

two strategies:

1.) *extrapolate to continuum limit and fit then to predictions of* χPT

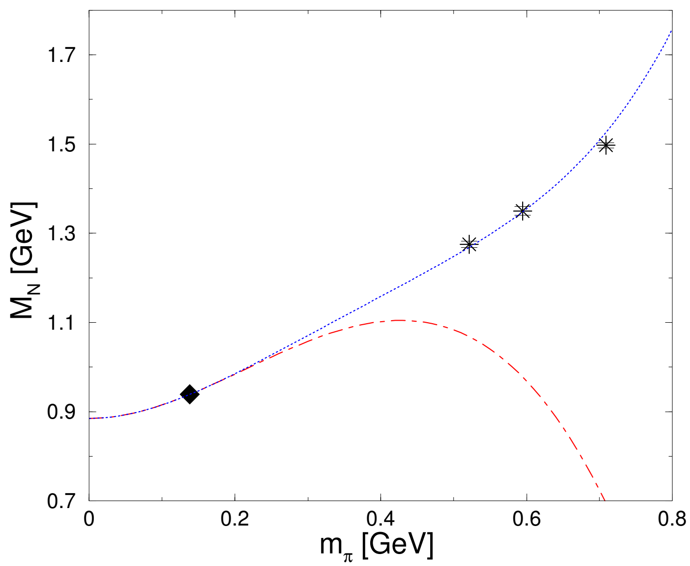
advantages/disadvantages

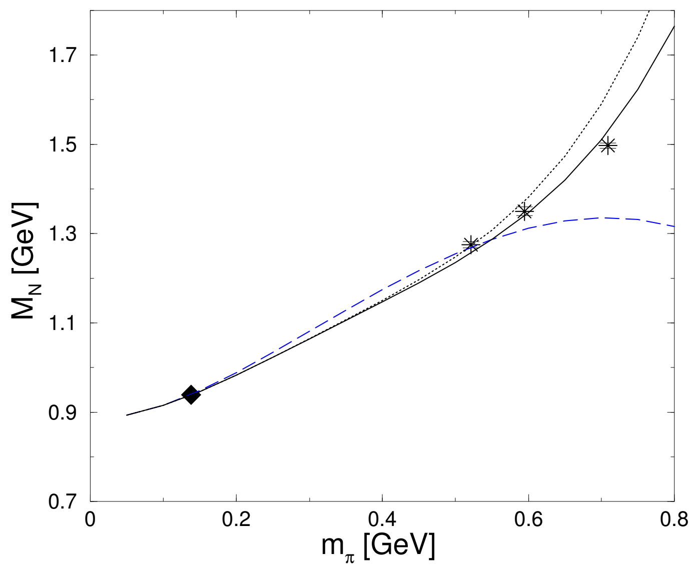
- chiral invariance ensured
- direct comparison possible
- computationally demanding

in practise (χPT practitioners): lattice data at non-vanishing lattice spacing are compared to continuum formulae

lattice data from chirally non-invariant lattice formulations

Example Bernard, Hemmert, Meissner

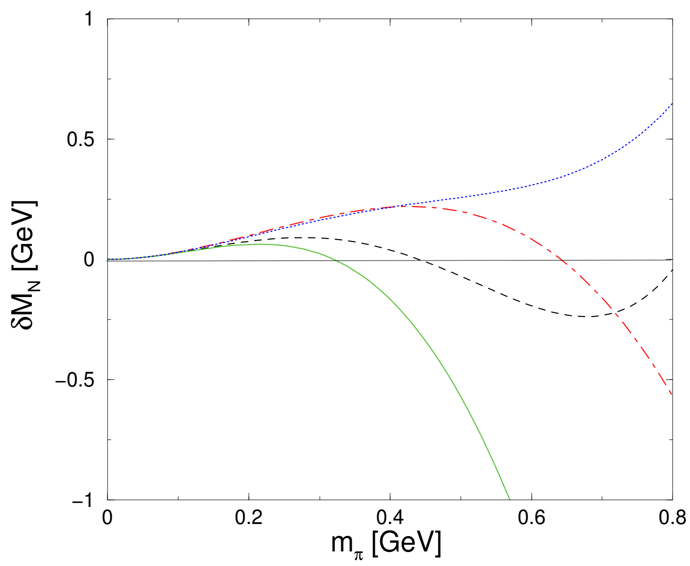


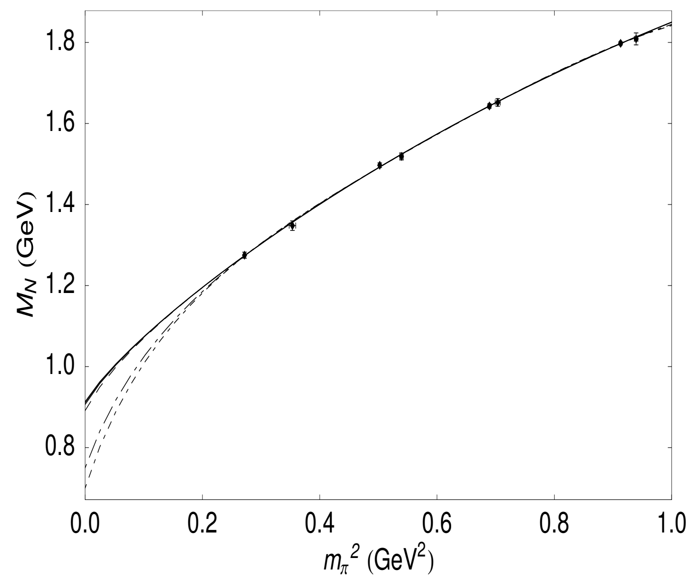


dimensional

cut-off

- 4-loop results (quadratic in quark mass) keeping consistently chiral symmetry
- parameters of chiral lagrangian *fixed* at physical point
- "improvement term" added but only one!!
- data (CP-PACS) at smallest values of a availabe: close enough to the continuum? (see later)





size of 4-loop corrections

Leinweber, Thomas, Young ("pion cloud")

BHM: *We stress again that applying the expressions to pion masses above 600 MeV is only done for illustrative purposes, for a realistic chiral extrapolation smaller pion masses are mandatory*

- it is possible to model lattice data
- clearly want, however, pure chiral perturbation theory

Chiral Perturbation theory

2.) *take discretization effects into account* Sharpe

Wilson fermions Baer, Rupak, Shoresh; Aoki

$\Rightarrow$ duplication of low energy constants

$\rightarrow$ physical LEC $l_4, \cdots, l_8 \leftrightarrow w_4, \cdots, w_8$

Staggered fermions Aubin, Bernard, Goltermann, Lee, Sharpe $+ \cdots$

start with Lee-Sharpe lagrangian

$$L = \frac{f^2}{8}\mathrm{tr}(\partial_\mu \Sigma \partial_\mu \Sigma^\dagger) - \frac{1}{4}\mu m f^2 \mathrm{tr}(\Sigma + \Sigma^\dagger) + \frac{2m_0^2}{3}(\Phi_I)^2 + a^2 V$$

$\Sigma = \exp(i\phi/f),$, $\phi = \sum_a^{16} \phi_a T_a$

Φ_I singlet field

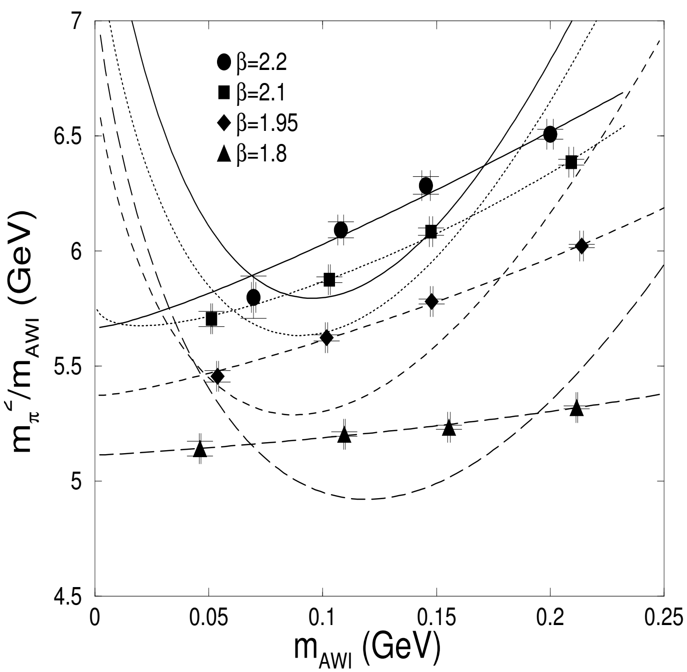
V staggered flavor breaking potoential $\rightarrow$ six terms with coefficients $C_1, \cdots, C_6$

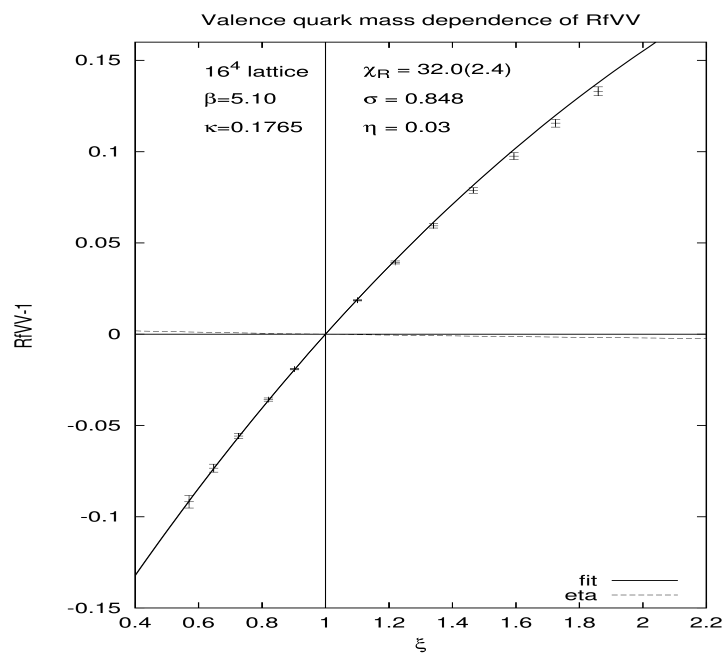
Chiral Perturbation theory

advantages/disadvantages

- lattice discretization effects can be (partly) absorbed
- allows for hybrid simulations such as improved fermions dynamical, overlap quenched
- (many) new parameters
- dependence of new fit parameters on g_0

Wilson examples





M_π^2/m_q (Aoki)

double ratio (Farchioni,Gebert, Montvay,Scholz,Scorzato)

$$Rf_{VV} = \frac{M_\pi^2(\text{sea})/m_q(\text{sea})}{M_\pi^2(\text{valence})/m_q(\text{valence})}$$

$\rightarrow$ amazing cut-off cancelations in double ratios $a = 0.28$fm (!)

Chiral Perturbation theory

remarks: it would be important to disentangle

- sea quark effects: plot only sea quark dependence
- a effects: de-double double ratios

a problem for universal LEC: assume

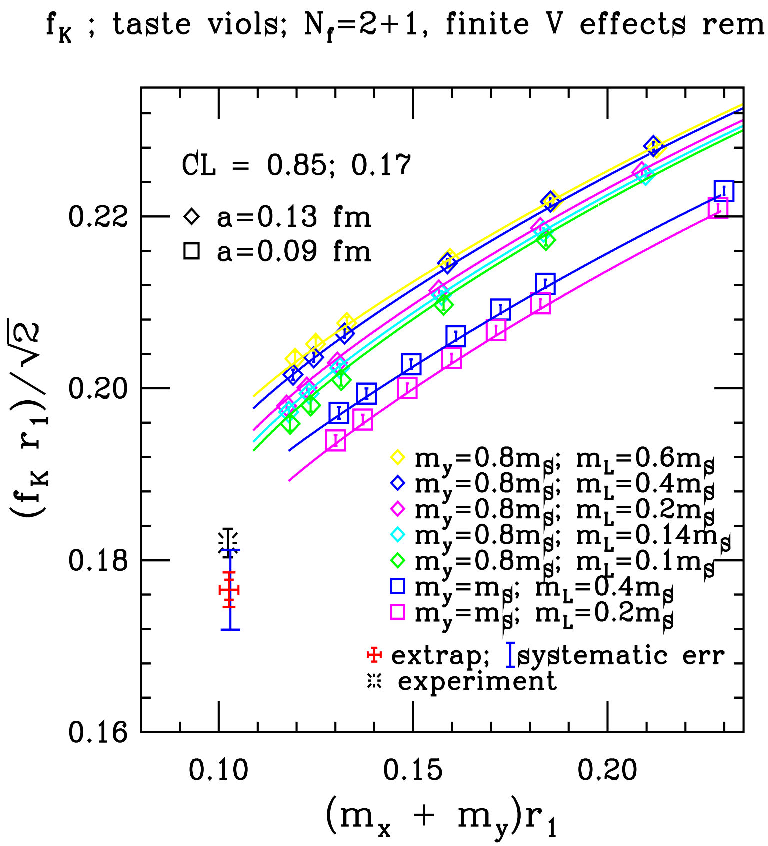
Aoki: shifting $\beta = 2.1 \rightarrow \beta = 2.2$, $\Lambda = 0.694(20) \rightarrow \Lambda = 0.128(88)$

DESY group: different definitions of lattice spacing a :
$\Lambda_3/f_0 = 30.4(2.9)$ or $\Lambda_3/f_0 = 6.51(57)$

results are a warning that more studies are needed

Chiral Perturbation theory

A staggered example (thanks to C. Bernard)



f_π, f_K agree with experiment

combinaton of GL coefficients seem to rule out $m_u = 0$ scenario

Two notes:

First: taking $\sqrt{\det}$ amounts in SχPT to a partially quenched situation with 2 quenched fermions Bernard, Golternman

$\det^{1/4}$ with u,d,s quarks means in 1-loop of SχPT

- do SχPT with $N_f = 4$ flavours; correct by hand: multiply loops by $1/4$

generalizable to all orders of SχPT? Bernard

- replica trick: computation with arbitary N_u, N_d, N_s of u,d,s quarks
- correct/tune by hand: set $N_u = N_d = N_s = 1/4$

Second: nice example of application of χPT (Chandrasekharan, Jiang)
$\longrightarrow$ very precise computation of condensate and susceptibility using meron cluster alorithm in strong coupling limit

My personal wishlist V
Need to discuss all these issues of chiral perturbation theory
$\longrightarrow$ workshop

Finite size effects

generally $M(L) - M = -\frac{3}{16\pi^2 ML}\int_{-\infty}^{\infty} F(iy)e^{\sqrt{M_\pi^2+y^2}L}$

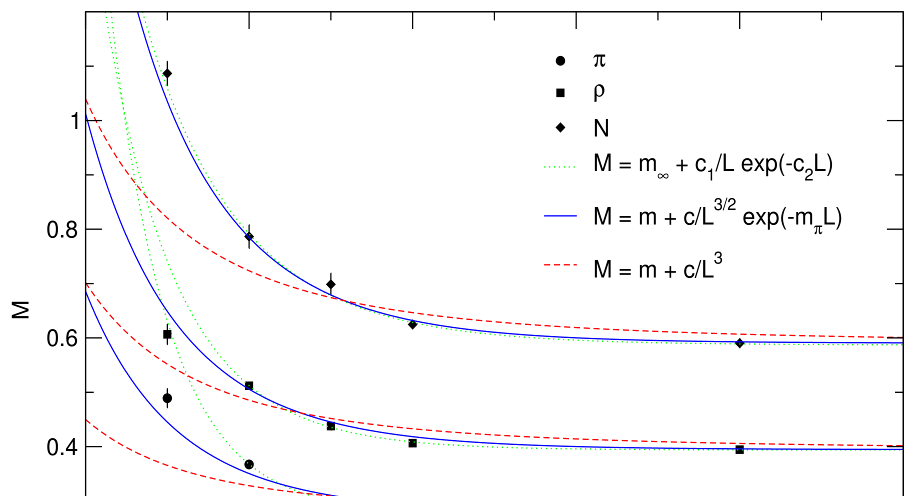
F: $\pi - \pi$ forward scattering amplitude in infinite volume

Lüscher's formula $L^{-3/2}e^{-m_\pi L}$: leading order of F

corrections: Colangelo, Dürr, Sommer

$\frac{1}{2}L^{-3/2}e^{-m_\pi L} + \frac{1}{\sqrt{2}L^{-3/2}}e^{-\sqrt{2}m_\pi L} + \frac{1}{\sqrt{3}L^{-3/2}}e^{-\sqrt{3}m_\pi L}$

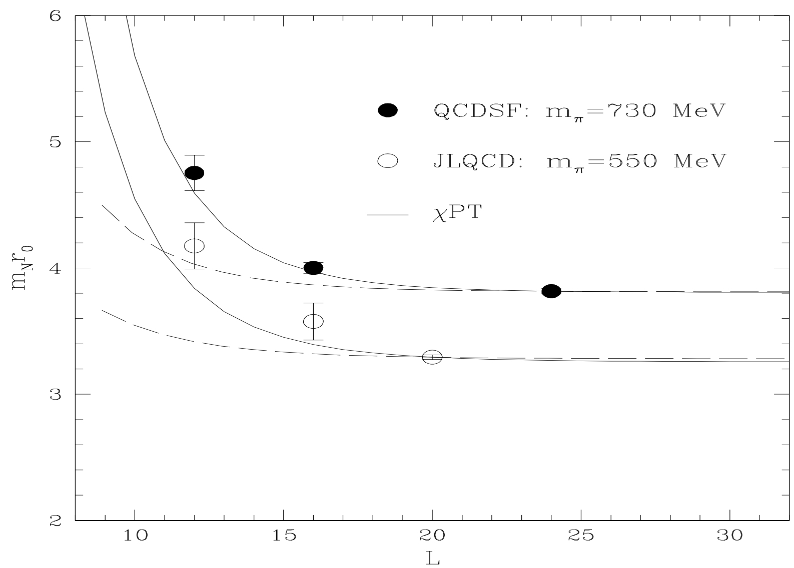
find (found) in practise $M = m_\infty + c/L^3$ (Fukugita, Mino, Okawa, Parisi, Ukawa)



Lippert, Orth, Schilling

$\longrightarrow$ claim: find expected exponential finite size effects coeff. of exp. fitted

Finite size effects from chiral perturbation theory



QCDSF collaboration

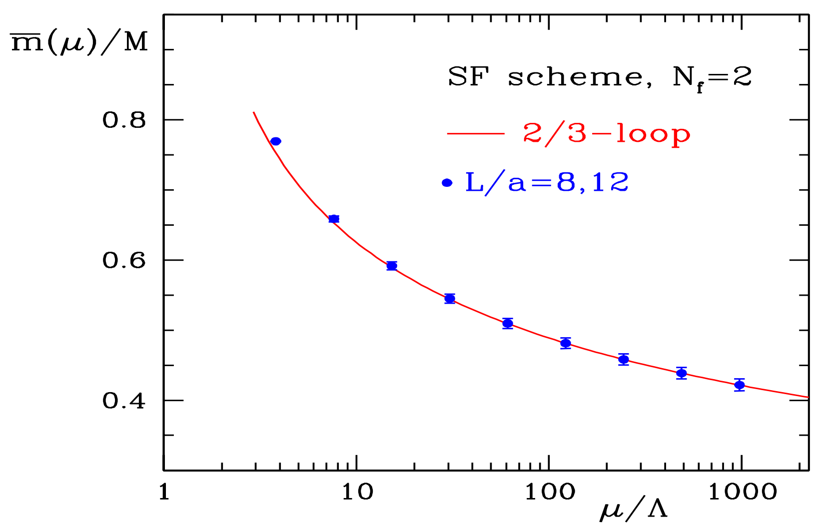
chiral perturbation theory result:

$$\delta = \frac{3g_A^2 m_\pi^2}{16\pi^2 F^2} \int dx \sum_n K_0(Ln\sqrt{m_{N_0}^2 x^2 + m_\pi^2(1-x)})$$

m_{N_0} Nucleon mass in chiral limit

no free parameter! Leading order agrees with Lüscher formula

Running quark mass: status



ALPHA Collaboration

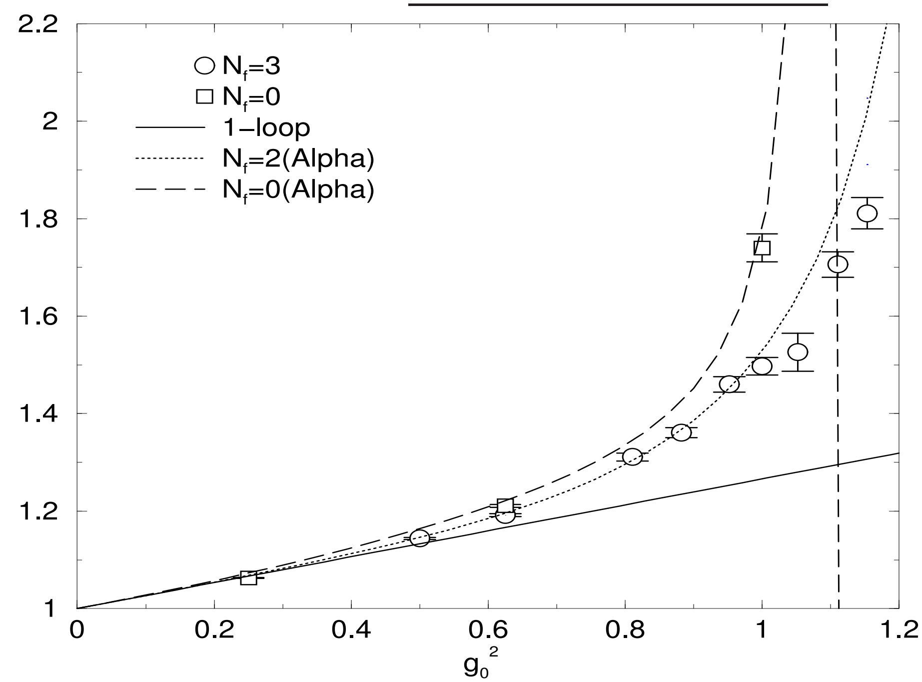
- $\rightarrow$ averagered over $L = 8 \rightarrow L = 16$ and $L = 12 \rightarrow L = 24$
- perturbation theory works well (unfortunately!?)
- point for smallest μ/Λ corresponds to large value of coupling $(L = \max)$
- scale still missing

Towards $N_f = 3$ dynamical Wilson simulations

→ joint japaneses forces of CP-PACS and JLQCD collaborations

→ RG improved gauge and $\mathrm{O}(a)$ improved Wilson fermion action
⇐ phase transition

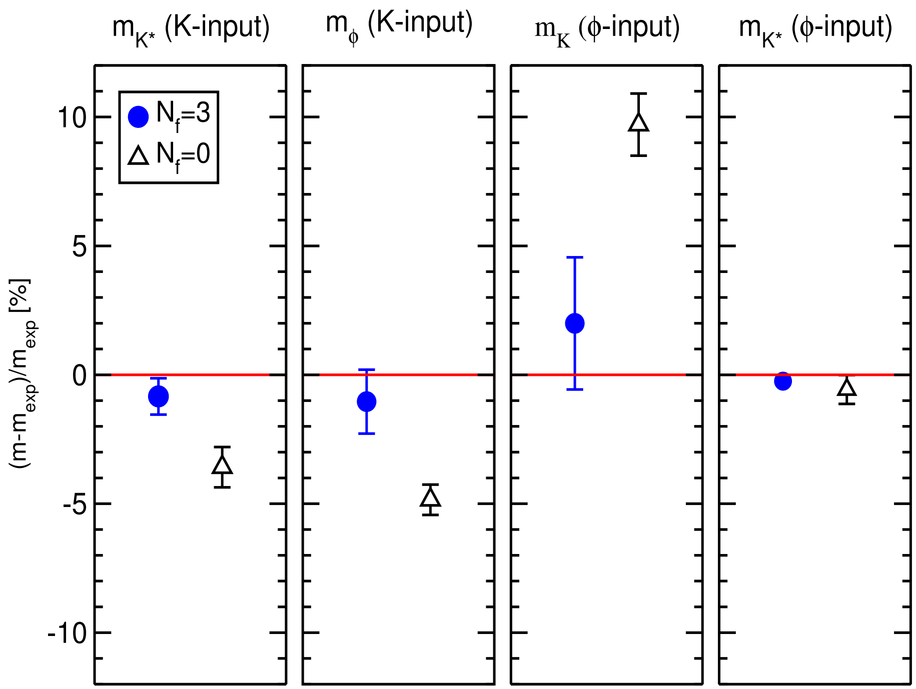
→ determination of c_{sw} non-perturbatively



→ Schrödinger functional

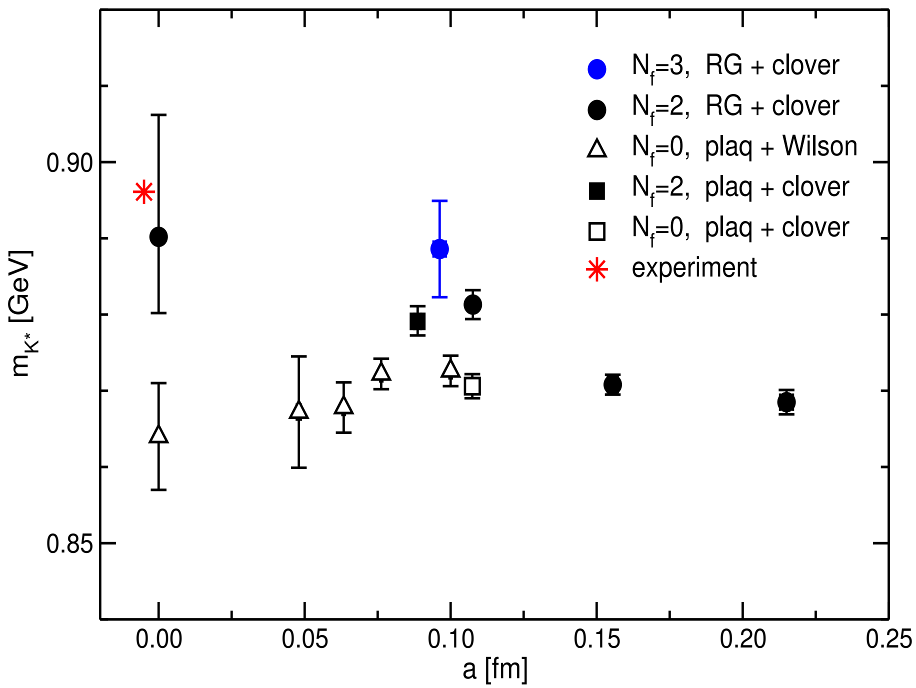
Towards $N_f = 3$ dynamical Wilson simulations: physical input

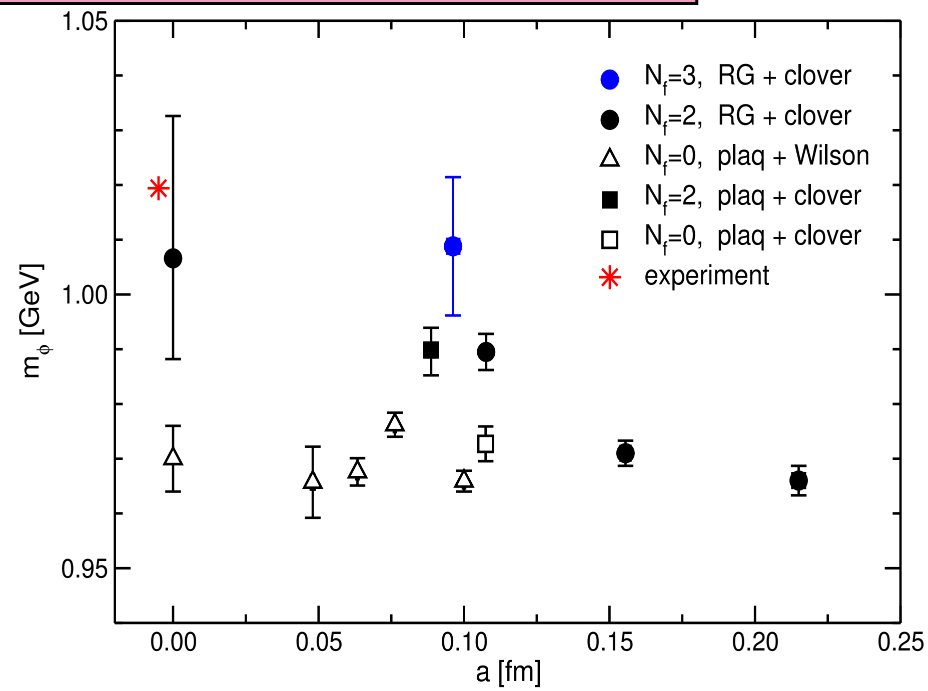
$L \approx 1.6$fm



$\longrightarrow$ re-assuring: dynamical results can eliminate systematic uncertainty

Towards $N_f = 3$ dynamical Wilson simulations: meson spectrum





My personal wishlist VII

Add improved staggered results

What was left out, with all my apologies

- domainwall fermions RBC
- localization in QCD Golterman, Shamir
- structure functions MIT, SESAM, QCDSF
- topological susceptibility Hart et.al.
- η' from low-lying eigenmodes SESAM, MIT

Conclusion

New powerful computers (apeNEXT, QCDOC, PC cluster, comm. supercomputers)

★ allow transition to serious dynamical fermion simulations

★ they are expensive machines that should be used wisely

- $\longrightarrow$ check that your lattice formulation of continuum theory is okay
- $\longrightarrow$ support and participate in ILDG to share configurations/propagators
- $\longrightarrow$ work hard on algorithmic improvements

what do we answer somebody coming with a really big machine and asks

– what action to choose

– what algorithm to employ

Conclusion

there are dangerous animals on the lattice that lurk in the dark
$\longleftarrow$ found surprises in dynamical simulations

$\Longrightarrow$ try to use always <u>two</u> actions, depending on your question

baryon spectrum, decay constants etc. (heavier quarks):
improved staggred $\leftrightarrow$ improved Wilson with (carefully selected) gauge action

very light quarks: chirally improved actions
(truncated fixed point, domain wall with $L_s \ll 1$, hypercude,FLIC)
$\leftrightarrow$ actions with exact chiral symmetry
(overlap, domain wall with $L_s \gg 1$)