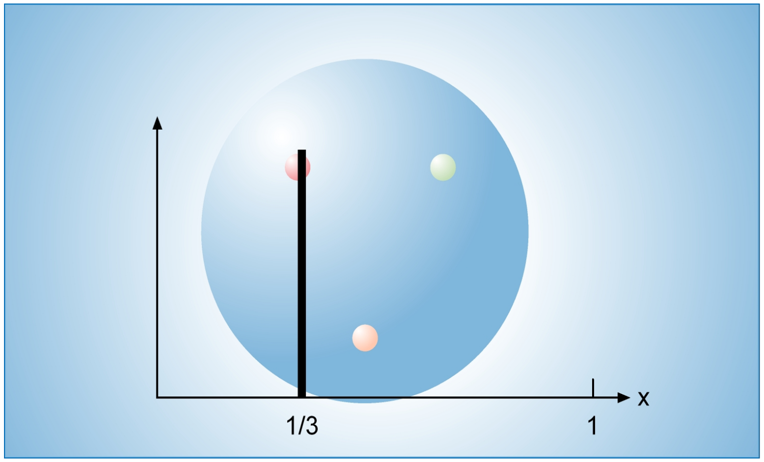
The Quest for Solving QCD: Light Quarks with Twisted Mass Fermions

Karl Jansen

- **Introduction**
- **New Formulations of Lattice Fermions: Overlap contra Twisted Mass Fermions**
- **Dynamical Quarks**
  - Understanding the Phase Structure of Lattice QCD
  - Breakthrough in Simulation Algorithm
- **Precision results from $N_f = 2$ dynamical twisted mass fermions**
- **Summary**

Quarks are the fundamental constituents of nuclear matter



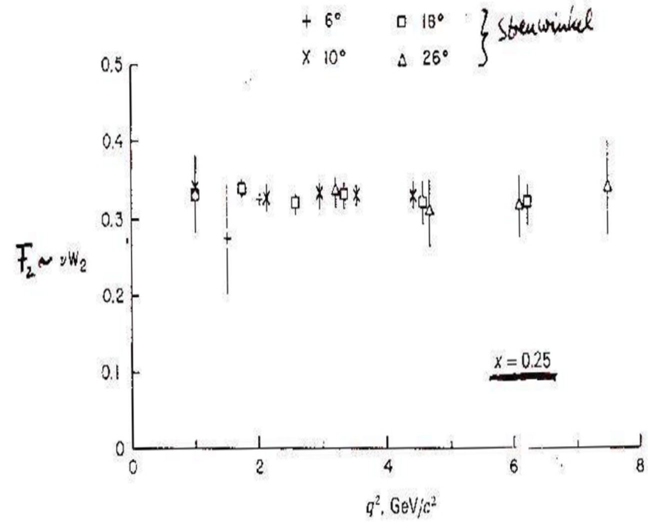


Fig. 7.17 νW_2 (or F_2) as a function of q^2 at $x = 0.25$. For this choice of x, there is practically no q^2-dependence, that is, exact "scaling". (After Friedman and Kendall 1972.)

Friedman and Kendall, 1972)

$f(x, Q^2)\big|_{x\approx 0.25, Q^2 > 10\mathrm{GeV}}$ independent of Q^2

(x momentum of quarks, Q^2 momentum transfer)

Interpretation (Feynman): scattering on single quarks in a hadron
$\longrightarrow$ (Bjorken) scaling

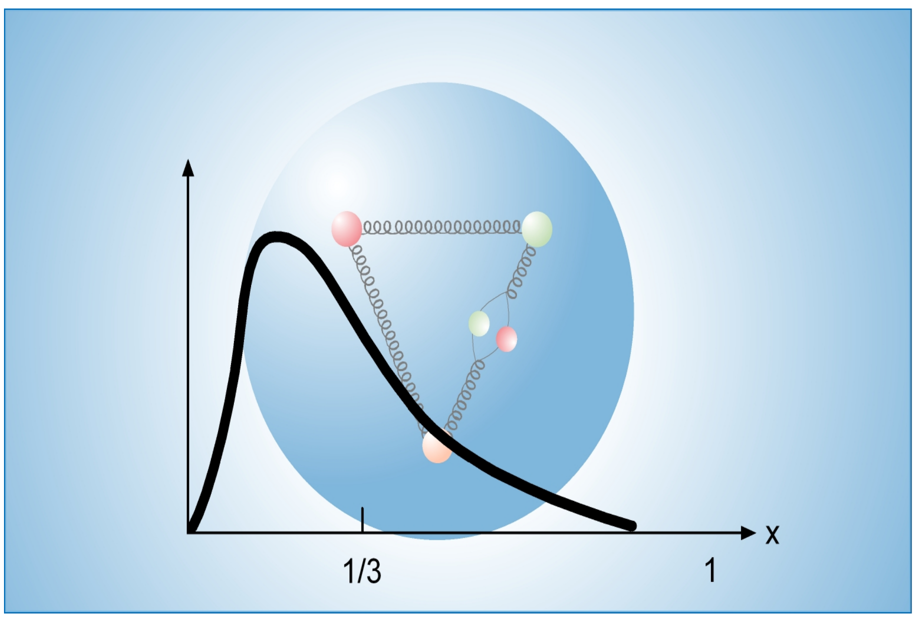
Quantum Fluctuations and the Quark Picture

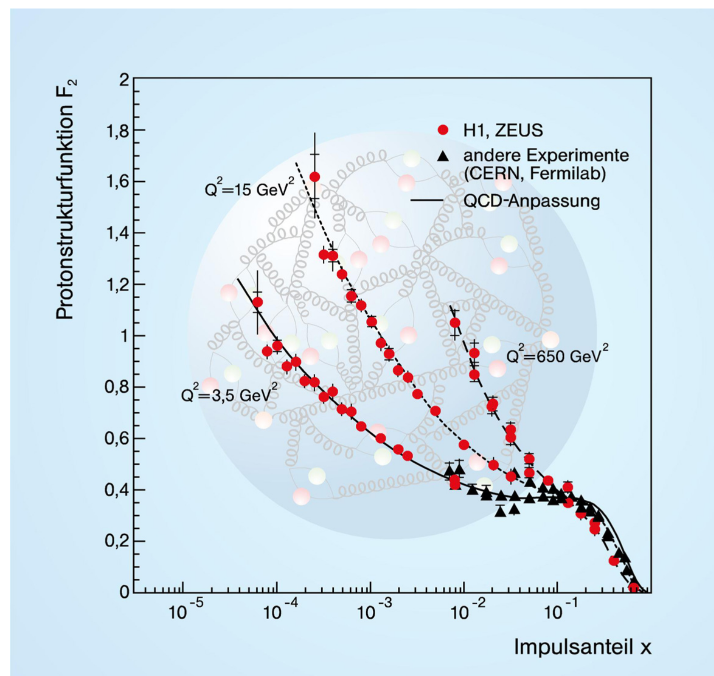
analysis in perturbation theory

$$\int_0^1 dx\, f(x,Q^2) = 3\left[1 - \frac{\alpha_s(Q^2)}{\pi} - a(n_f)\left(\frac{\alpha_s(Q^2)}{\pi}\right)^2 - b(n_f)\left(\frac{\alpha_s(Q^2)}{\pi}\right)^3\right]$$

– $a(n_f), b(n_f)$ calculable coefficients

deviations from scaling $\longrightarrow$ determination of strong coupling





Examples of quantities computable on the lattice

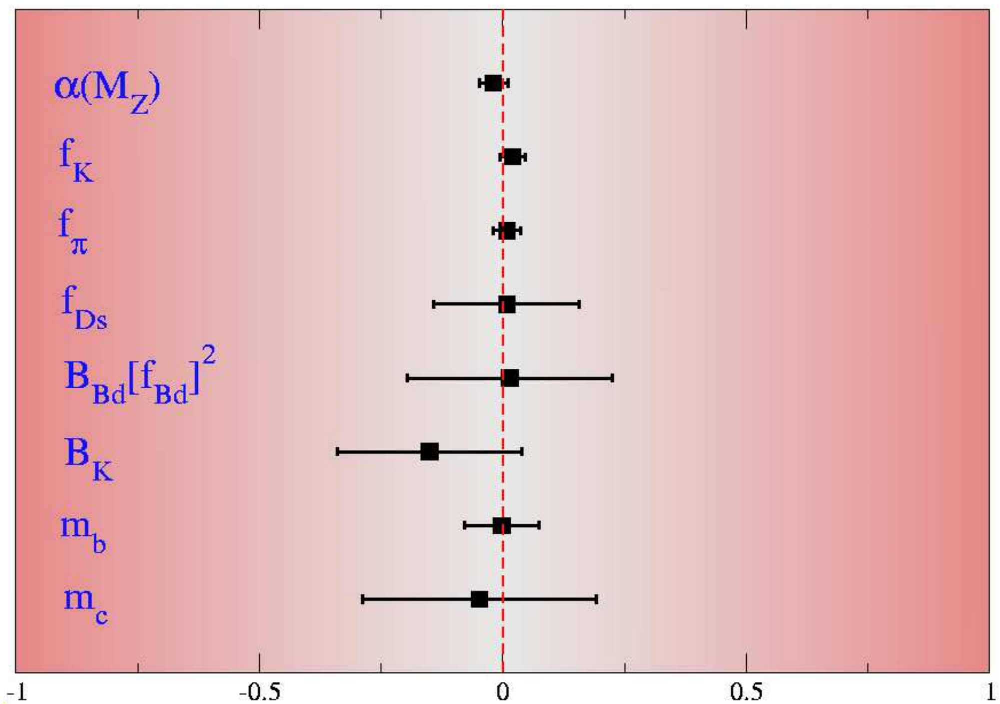
- Moments of structure functions: $\langle x^n \rangle = \int dx x^n f(x)$

  lowest moment, $\langle x \rangle$: corresponds to *average momentum of quark in hadron*

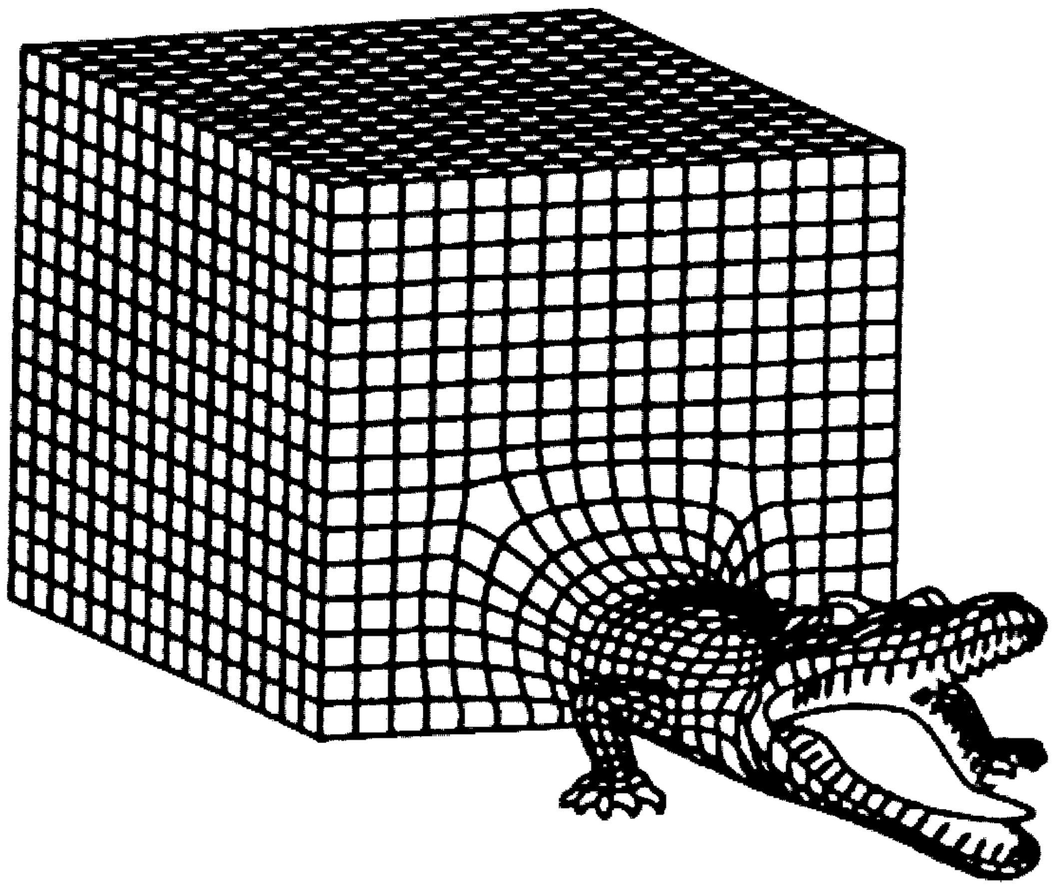
- Pion decay constant: $\langle 0|A_\mu|\pi(q)\rangle = f_\pi q_\mu$
  (A_μ Axial current, q momentum)

- Particle Masses, transition amplitudes, ...

$(O_{\rm Latt} - O_{\rm Exp})/O_{\rm Exp}$



There are dangerous lattice animals

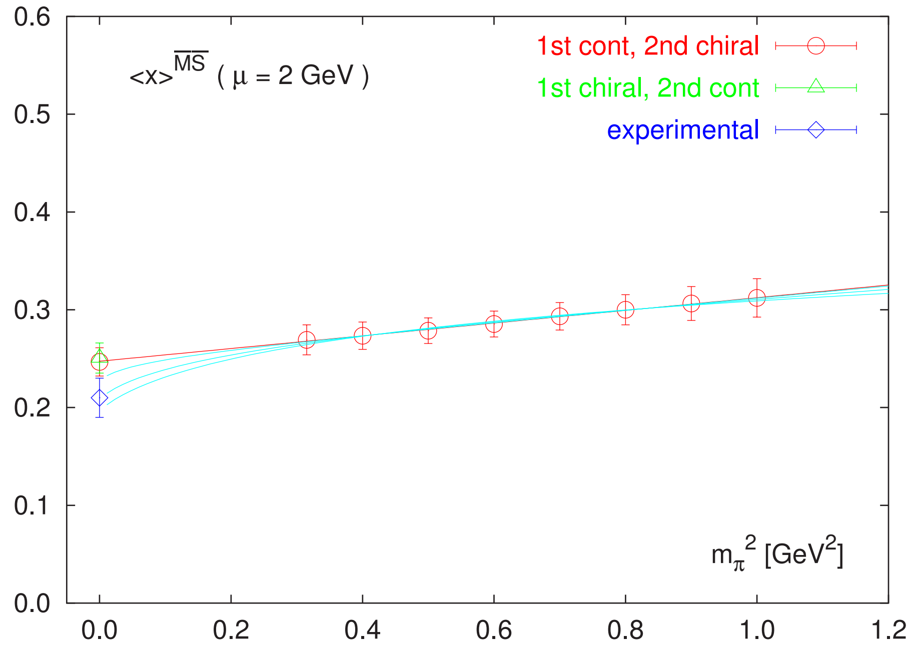


→ violation of chiral symmentry
(exchange of massless left- and right-handed quarks)

Problem to reach physical value of pion mass
quenched example: chiral extrapolation of $\langle x \rangle$

Guagnelli, K.J., Palombi, Petronzio, Shindler, Wetzorke

- Schrödinger Functional
- combined Wilson and $O(a)$-improved Wilson
- controlled
  - non-perturbative renormalization
  - continuum limit
  - finite volume effects
  - statisitical errors
- want to reach:
  $m_\pi^2 = 0.02$ [GeV^2]



solution, give up anti-commutation condition with γ_5: **Ginsparg-Wilson relation**

$$\boxed{\gamma_5 D + D\gamma_5 = 2aD\gamma_5 D} \qquad \Rightarrow D^{-1}\gamma_5 + \gamma_5 D^{-1} = 2a\gamma_5$$

Ginsparg-Wilson relation implies an *exact lattice chiral symmetry* (Lüscher):

for any operator D which satisfies the Ginsparg-Wilson relation, the action

$$S = \bar{\psi} D \psi$$

is invariant under the transformations

$$\boxed{\delta\psi = \gamma_5(1 - \tfrac{1}{2}aD)\psi \ , \qquad \delta\bar{\psi} = \bar{\psi}(1 - \tfrac{1}{2}aD)\gamma_5}$$

$\Rightarrow$ almost continuum like behaviour of fermions

one <u>local</u> (Hernández, Lüscher, K.J.) solution: overlap operator $D_{\rm ov}$ (Neuberger)

$$\boxed{D_{\rm ov} = \left[1 - A(A^\dagger A)^{-1/2}\right]}$$

with $A = 1 + s - D_{\rm w}(m_q = 0)$; s a tunable parameter, $0 < s < 1$

Wilson (Frezzotti, Rossi) twisted mass QCD (Frezzotti, Grassi, Sint, Weisz)

$$D_{\rm tm} = m_q + i\mu\tau_3\gamma_5 + \frac{1}{2}\gamma_\mu\left[\nabla_\mu + \nabla_\mu^*\right] - a\frac{1}{2}\nabla_\mu^*\nabla_\mu$$

quark mass parameter m_q , twisted mass parameter μ

- $m_q = m_{\rm crit} \rightarrow$ O(a) improvement for
  hadron masses, matrix elements, form factors, decay constants
- $\det[D_{\rm tm}] = \det[D_{\rm Wilson}^2 + \mu^2]$
  $\Rightarrow$ protection against small eigenvalues
- computational cost comparable to staggered
- simplifies mixing problems for renormalization
- serious competitor to Ginsparg-Wilson fermions

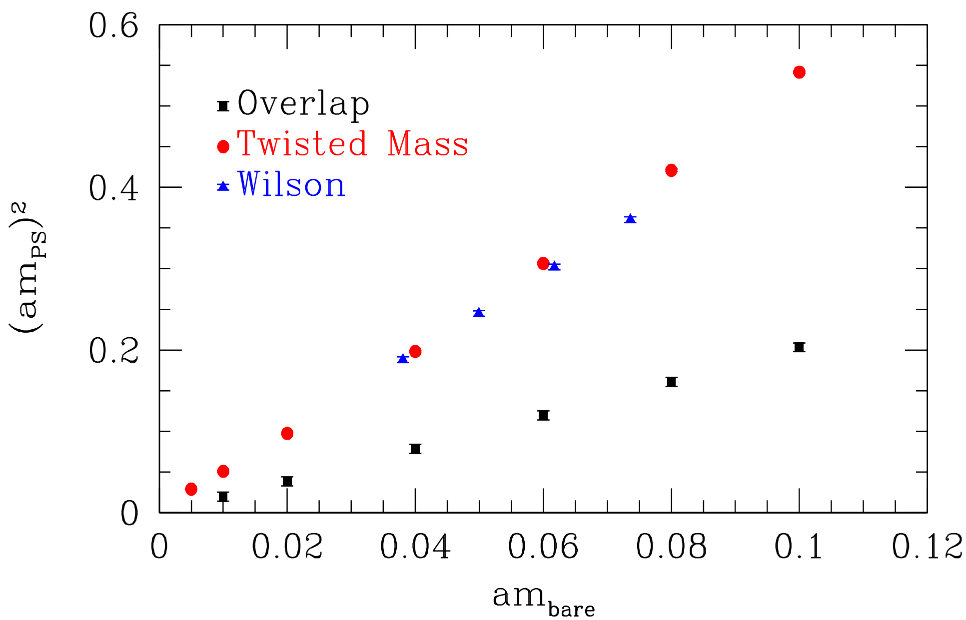
$\star$ **based on symmetry arguments $\Rightarrow$ check how it works in practise**

Drawback: *explicit breaking of isospin symmetry for any* $a > 0$

A first test
twisted mass against overlap fermions: how chiral can we go?

Bietenholz, Capitani, Chiarappa, Christian, Hasenbusch, K.J., Nagai, Papinutto,
Scorzato, Shcheredin, Shindler, Urbach, Wenger, Wetzorke

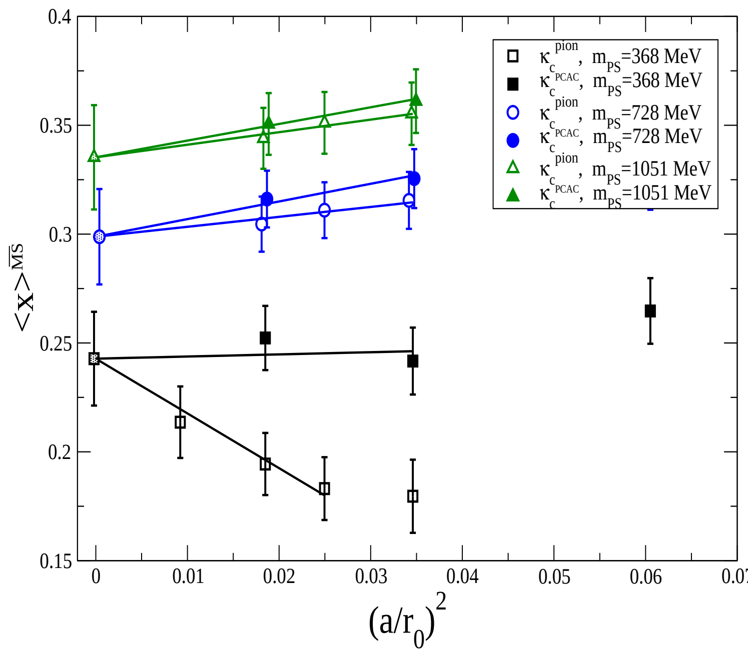
fixed lattice spacing of $a = 0.125$fm

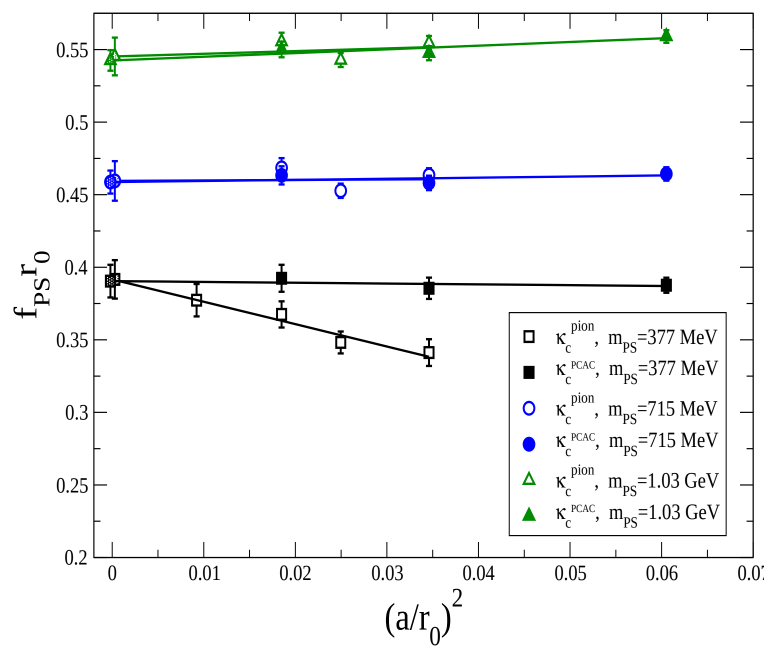


$\Rightarrow$ twisted mass simulations can reach quarks masses as small as overlap
substantially smaller than O(a)-improved Wilson fermions

Scaling of $\langle x \rangle$ and $F_{\rm PS}$ with twisted mass fermions

K.J., M. Papinutto, A. Shindler. C. Urbach. I. Wetzorke





→ O(a^2) scaling for two realizations of O(a)-improvement

→ $\kappa_c^{\rm PCAC}$ very small O(a^2) effects

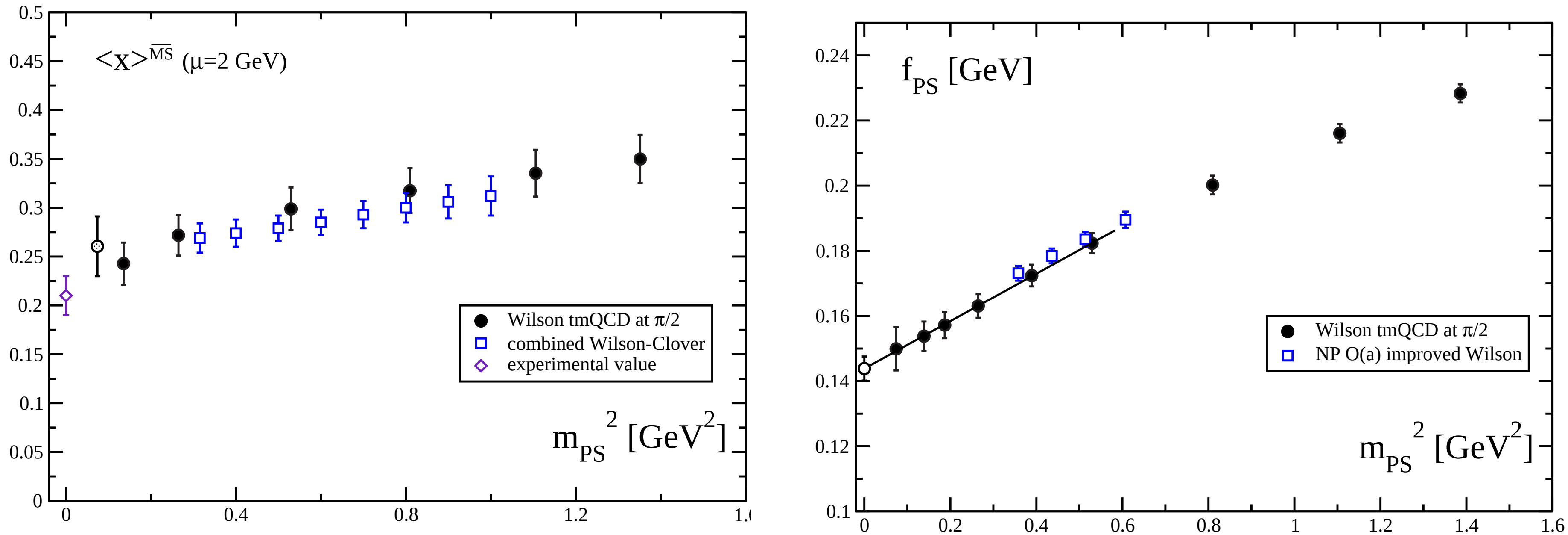
→ $\kappa_c^{\rm pion}$ larger O(a^2) effects, late scaling $\beta \geq 6$

→ consistent with theoretical considerations

(Frezzotti, Martinelli, Papinutto, Rossi; Sharpe, Wu; Aoki, Bär)

$F_{\rm PS}$ and $\langle x \rangle$ with twisted mass

(S. Capitani, K.J., M. Papinutto, A. Shindler, C. Urbach, I. Wetzorke)



Cost comparison

T. Chiarappa, K.J., K. Nagai, M. Papinutto, L. Scorzato,
A. Shindler, C. Urbach, U. Wenger, I. Wetzorke

V, m_π	Overlap	Wilson TM	rel. factor
12^4, 720Mev	48.8(6)	2.6(1)	18.8
12^4, 390Mev	142(2)	4.0(1)	35.4
16^4, 720Mev	225(2)	9.0(2)	25.0
16^4, 390Mev	653(6)	17.5(6)	37.3
16^4, 230Mev	1949(22)	22.1(8)	88.6

timings in seconds on Jump

Dynamical Quarks:
The phase structure of lattice QCD

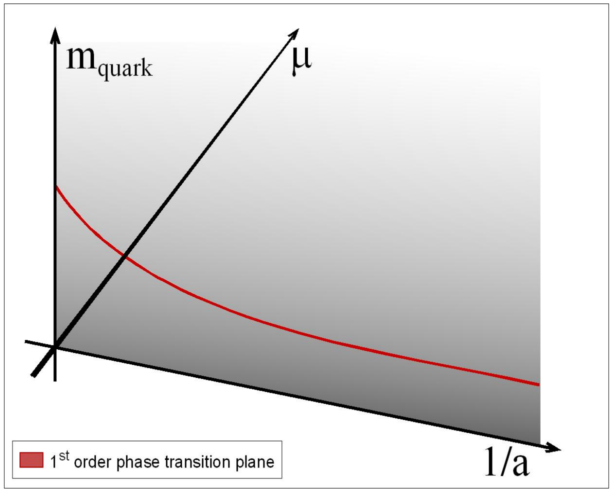
Farchioni, Frezzotti, Hofmann, K.J., Montvay, Münster,
Rossi, Scorzato,Scholz, Shindler, Ukita, Urbach, Wenger, Wetzorke

Let me describe a typical computer simulation:[...]
the first thing to do is to look for phase transitions (G. Parisi)

lattice simulations are done *under the assumption*
that the transition is continuum like

- first order, jump in $< \bar{\Psi}\Psi >$
  when quark mass m changes sign

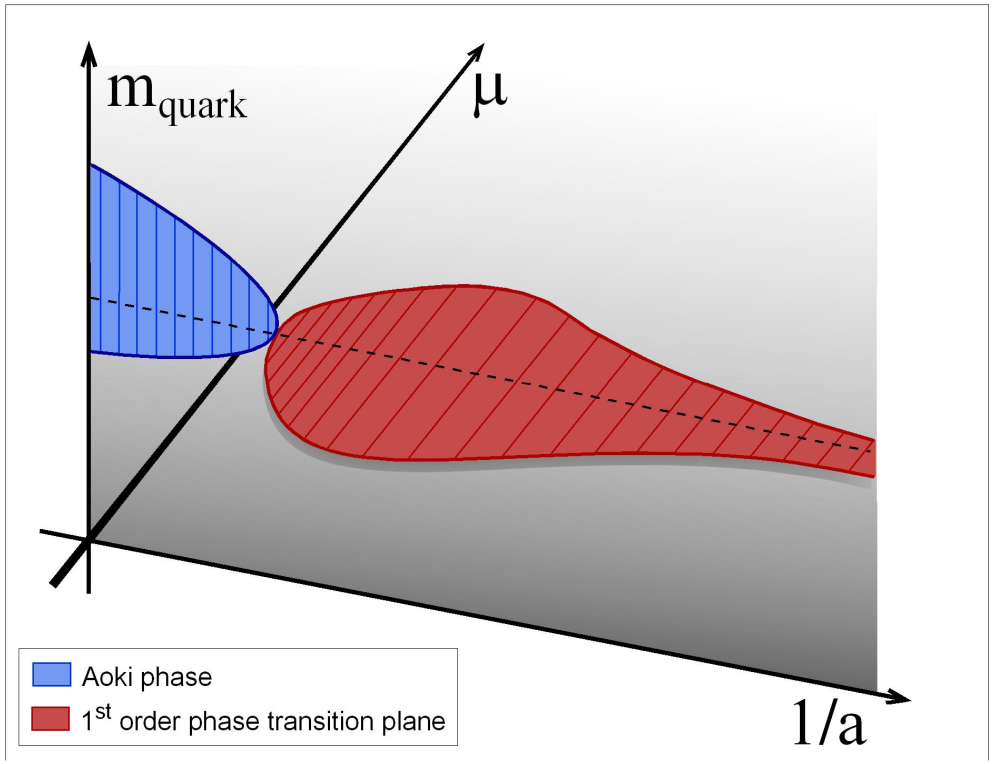
- pion mass vanishes at
  phase transition point



⇒ *single phase transition line*

→ twisted mass fermions offer a
tool to check this

Revealing the generic phase structure of lattice QCD



Aoki phase: Ilgenfritz, Müller-Preussker, Sternbeck, Stüben

→ Knowledge of phase structure for a particular formulation of lattice QCD: pre-requisite for numerical simulation

Chiral perturbation theory for the phase transition

Sharpe, Wu; Hofmann, Münster; Scorzato; Aoki, Bär

In the regime $m/\Lambda_{QCD} \gtrsim a\Lambda_{QCD}$

$$M = 2B_0/Z_P\sqrt{m_{PCAC,\chi}^2 + \mu^2} \qquad \Lambda_R = 4\pi F_0 \qquad \cos\omega = \frac{m_{PCAC,\chi}}{\sqrt{m_{PCAC,\chi}^2+\mu^2}}$$

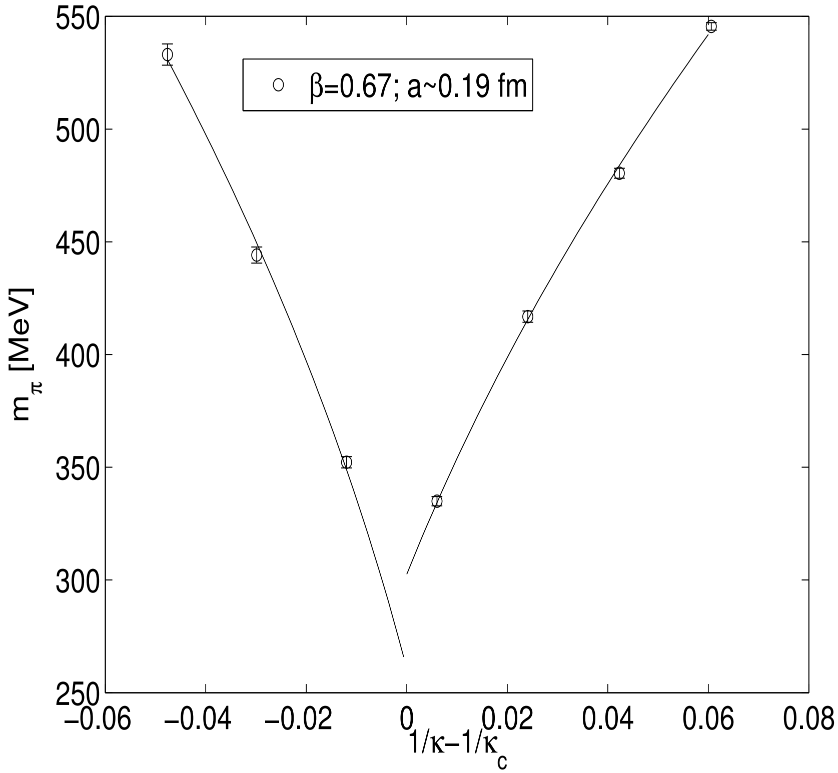
$$m_\pi^2 = M + \frac{8}{F_0{}^2}\left\{M^2(2L_{86} - L_{54}) + 4aM\cos\omega(w-\tilde{w})\right\} + \frac{M^2}{32F_0^2\pi^2}\log\left(\frac{M}{\Lambda_R^2}\right)$$

$$f_\pi = F_0 + \frac{4}{F_0}\left\{ML_{54} + 4a\cos\omega\tilde{w}\right\} - \frac{M}{16F_0\pi^2}\log\left(\frac{M}{\Lambda_R^2}\right)$$

$$g_\pi = B_0/Z_P\left[F_0 + \frac{4}{F_0}\left\{M(4L_{86} - L_{54}) + 4a\cos\omega(2w_s - \tilde{w})\right\} - \frac{M}{32F_0\pi^2}\log\left(\frac{M}{\Lambda_R^2}\right)\right]$$

parameters to fit: B_0/Z_P, F_0, L_{86}, L_{54}, w, $\tilde{w}$

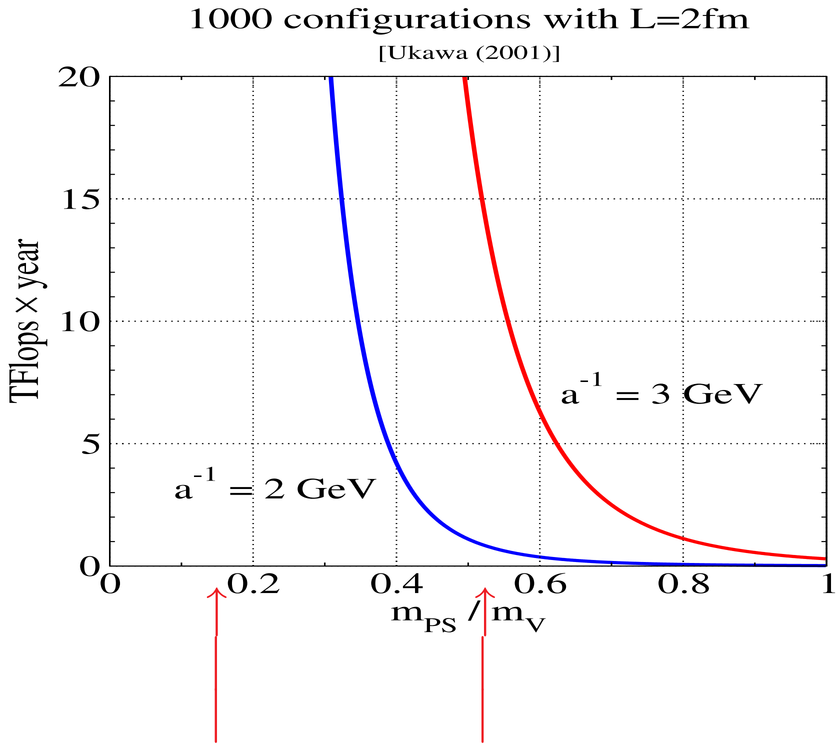
Serious Consequence: minimal pseudo scalar mass



- Continuum picture not realized
- pion does not vanish
  rather reaches a minimal value
- strength of phase transition depends
  on lattice spacing a
- minimal pion mass depends on
  strength of phase transition
  $m_{\rm PS}$ vanishes with rate $O(a)$

Costs of dynamical fermions simulations, the "Berlin Wall"

see panel discussion in Lattice2001, Berlin, 2001



physical point

contact to χPT (?)

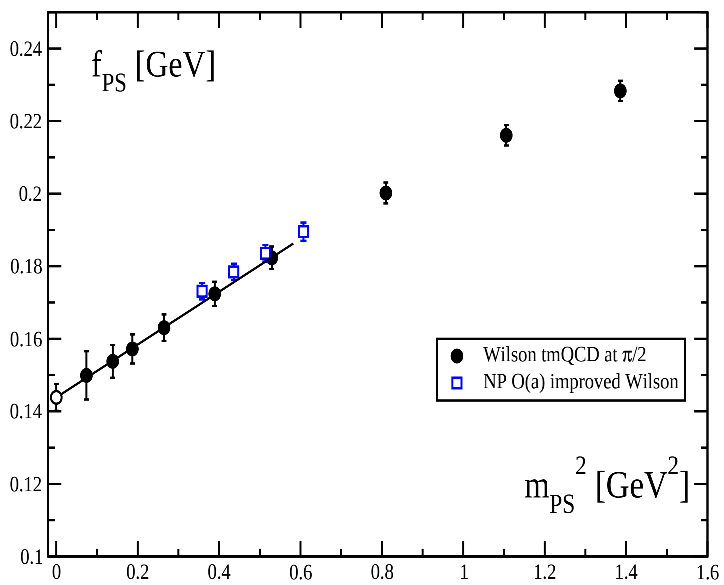
formula $C \propto \left(\frac{m_\pi}{m_\rho}\right)^{-z_\pi} (L)^{z_L} (a)^{-z_a}$

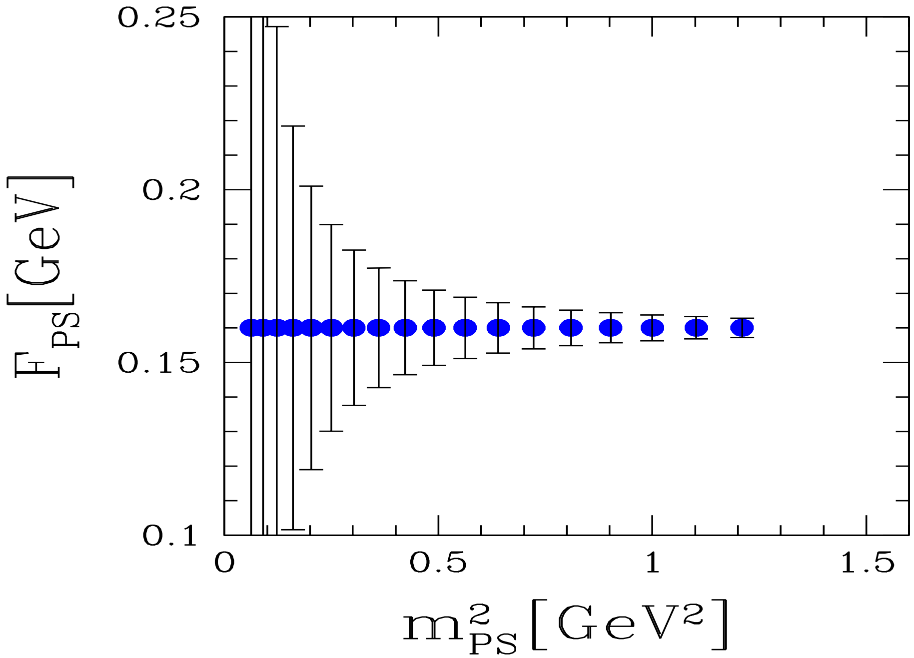
$$z_\pi = 6$$

$$z_L = 5$$

$$z_a = 7$$

A hypothetical dynamical computation of F_π in 2000
for up and down quarks ($N_f = 2$)





quenched ($N_f = 0$)

dynamical u and d quarks ($N_f = 2$)

European Twisted Mass Collaboration

The quest for solving QCD

B. Blossier, Ph. Boucaud, P. Dimopoulos,
F. Farchioni, R. Frezzotti, V. Gimenez,
G. Herdoiza, K. Jansen, V. Lubicz,
G. Martinelli, C. McNeile, C. Michael,
I. Montvay, M. Papinutto, O. Pène,
J. Pickavance, G.C. Rossi, L. Scorzato,
A. Shindler, S. Simula,
C. Urbach, U. Wenger

Target setup for $N_f = 2$ maximally twisted Dynamical Quarks

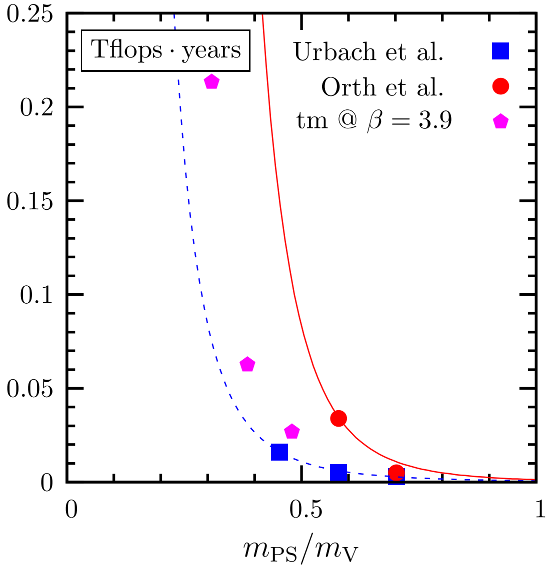
- $\beta = 3.9$, 5000 thermalized trajectories
- simulations at a smaller and a larger lattice spacing at matched pion masses and volumes are in progress
- test scaling and perform continuum limit

$L^3 \cdot T$	β	$\kappa_{\rm crit}$	$a\mu$	a[fm]	m_π[MeV]
$24^3 \cdot 48$	3.90	0.160856	0.0040	≈0.095	280
$24^3 \cdot 48$	3.90	0.160856	0.0064	≈0.095	350
$24^3 \cdot 48$	3.90	0.160856	0.0100	≈0.095	430
$24^3 \cdot 48$	3.90	0.160856	0.0150	≈0.095	510

Shift the Berlin Wall and Twist

New variant of HMC algorithm (Urbach, Shindler, Wenger, K.J.)
(see also SAP (Lüscher) and RHMC (Clark and Kennedy) algorithms)

- even/odd preconditioning
- (twisted) mass-shift (Hasenbusch trick)
- multiple time steps



– twisted mass at much smaller $m_{\mathrm{PS}}/m_{\mathrm{V}}$

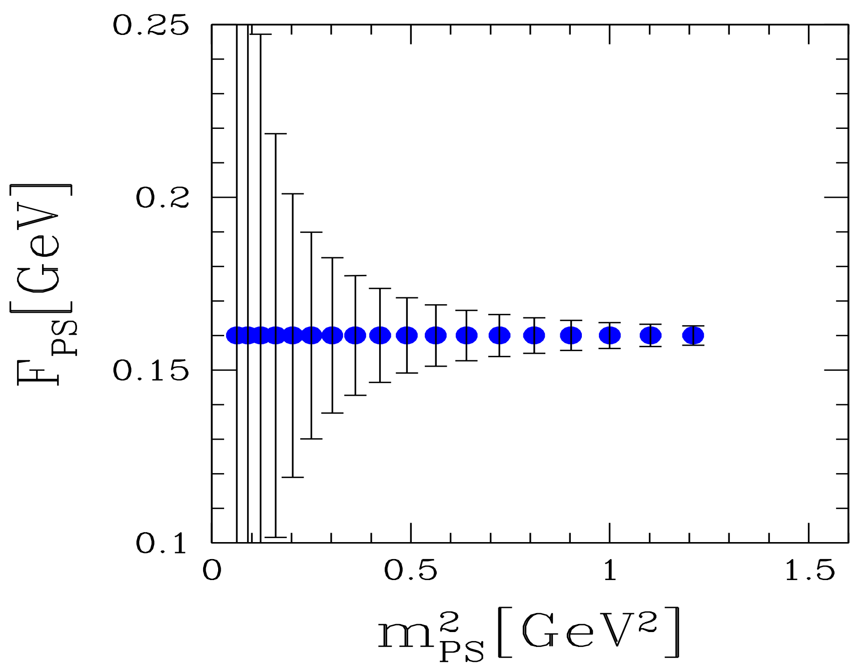
– compatible with (our own) Wilson
– compatible with staggered

– compatible with RHMC

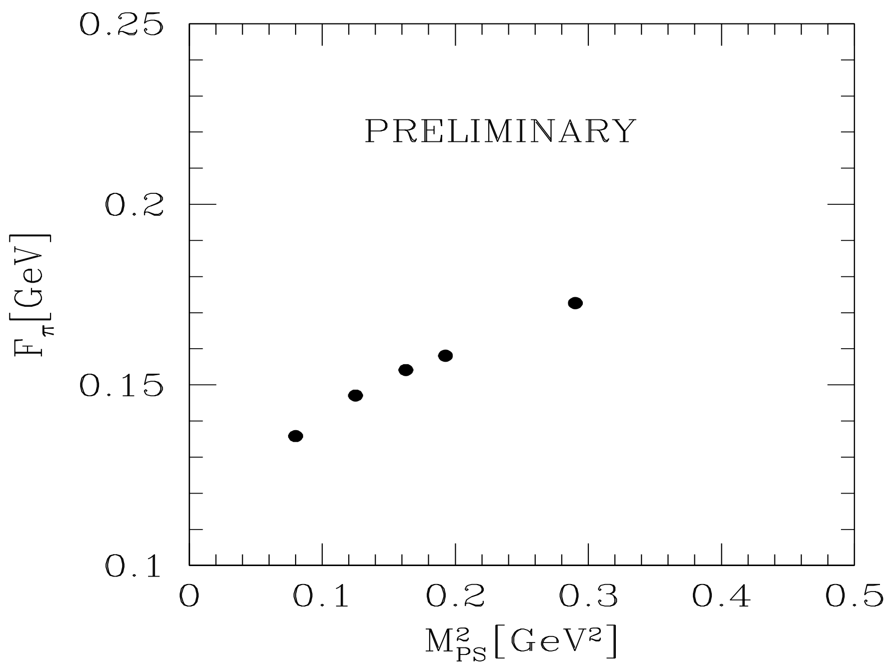
⇒ 3 algorithms to drive Wilson fermions towards the physical point

A computation of F_π in 2006

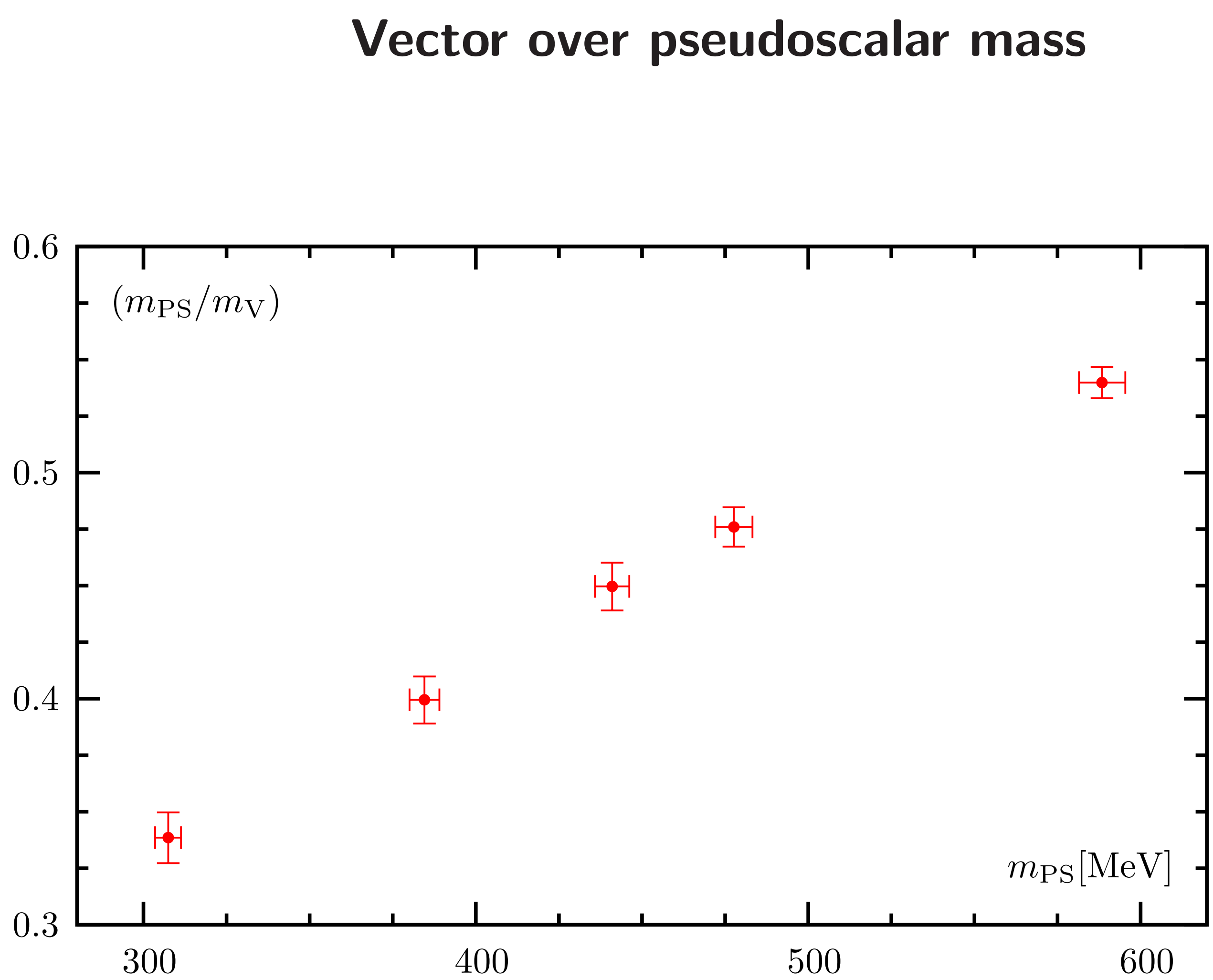
for up and down quarks ($N_f = 2$)



2000

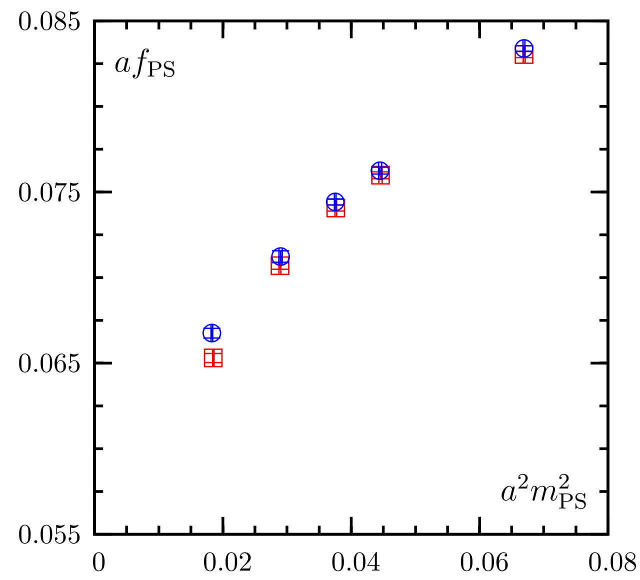


2006


Vector over pseudoscalar mass
0.6
0.5
0.4
0.3
300
400
500
600
$(m_{\rm PS}/m_{\rm V})$
$m_{\rm PS}$[MeV]

Pseudo scalar decay constant

- Results at one lattice spacing $a \approx 0.095\text{fm}$
- Finite Size corrections noticeable
- Curvature clearly visible



Comparison with Chrial Perturbation Theory

Precise numerical results for $m_{\rm PS}$ and $f_{\rm PS}$ calls for a comparison to chiral perturbation theory

$$m_{\rm PS}^2 = 2B_0\mu\,\left[1 + \xi\log(2B_0\mu/\Lambda_3^2)\right]\ ,\ \ \xi = 2B_0\mu/(4\pi F)^2$$

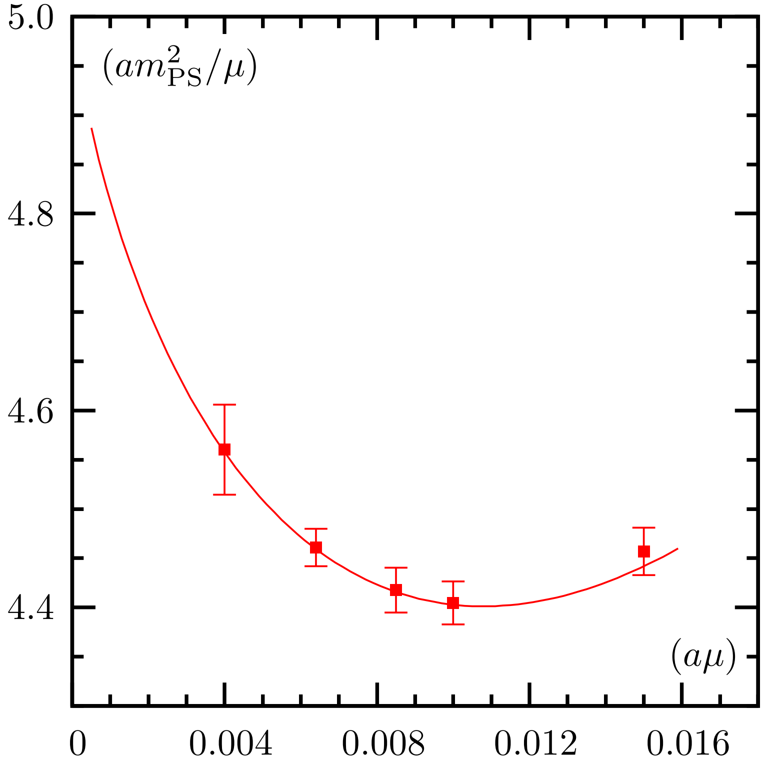
$$f_{\rm PS} = F\,\left[1 - 2\xi\log(2B_0\mu/\Lambda_4^2)\right]\ ,\ \ \xi = 2B_0\mu/(4\pi F)^2$$

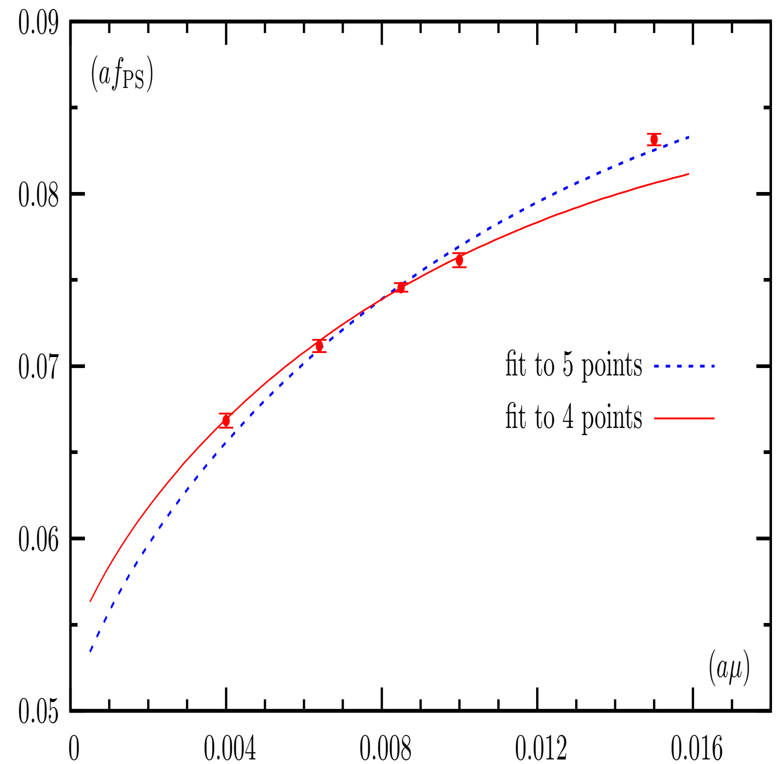
$\Rightarrow$ four unknown parameters: B_0, F, Λ_3, Λ_4

$\Rightarrow$ allow to determine physical observables, e.g.:

- scalar condensate $\Sigma_0 = \langle\bar{\Psi}\Psi\rangle$
- Pion decay constant F_π
- scalar pion radius $\langle r^2\rangle$
- s-wave scattering lengths a_{00}, a_{20}

Fits to chiral perturbation theory formulae





$\Rightarrow$ excellent description by chiral perturbation theory

$2aB_0 = 4.99(6), \quad aF = 0.0534(6)$

$a^2\bar{l}_3^{\,2} \equiv \log(a^2\Lambda_3^2) = -1.93(10), \quad a^2\bar{l}_4^{\,2} \equiv \log(a^2\Lambda_4^2) = -1.06(4)$

Comparison to other determinations

- ETMC:
  $\bar{l}_3 = 3.65 \pm 0.12$
  $\bar{l}_4 = 4.52 \pm 0.06$

- Other estimates Leutwyler, hep-ph/0612112

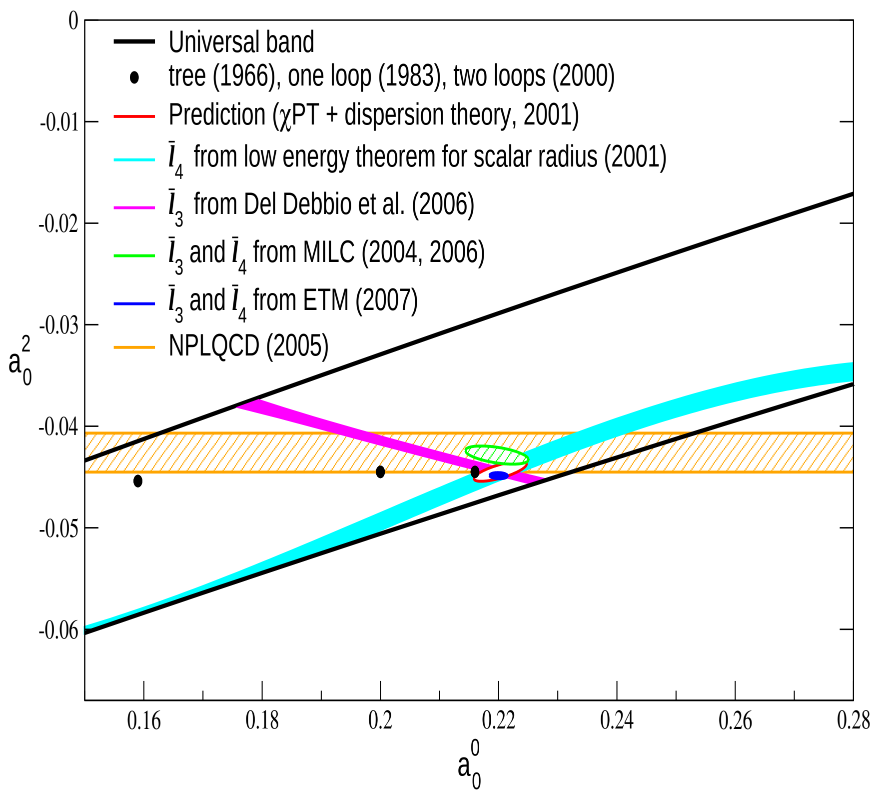
  phenomenological determinations

  $\bar{l}_3 = 2.9 \pm 2.4$ *from the mass spectrum of the pseudoscalar octet*
  $\bar{l}_4 = 4.4 \pm 0.2$ *from the radius of the scalar*

  other lattice determinations

  $\bar{l}_3 = 0.8 \pm 2.3$ from MILC (US-UK, staggered)
  $\bar{l}_3 = 3.0 \pm 0.6$ from lattice CERN group (Wilson)
  $\bar{l}_4 = 4.3 \pm 0.9$ from f_K/f_π *pion form factor*
  $\bar{l}_4 = 4.0 \pm 0.6$ *from MILC*

Narrowing scattering lengths (Leutwyler, private communication)



- Lattice calculations:
  only statistical errors
  → systematic effects under
  systematic inverstigation

- scalar pion radius (ETMC): $< r^2 >= 0.637(26)\mathrm{fm}^2$
  Colangelo, Gasser, Leutwyler: $< r^2 >= 0.61(4)\mathrm{fm}^2$
- swave scattering lengths:
  $a_{00} = 0.220 \pm 0.002, \;\; a_{20} = -0.0449 \pm 0.0003$

Quark Masses Preliminary!

$\longrightarrow$ prime example for lattice calculations

- up and down quarks:

  $m_{u,d}[\overline{\mathrm{MS}}, 2\ \mathrm{GeV}] = 3.8(3)\ \mathrm{MeV}$

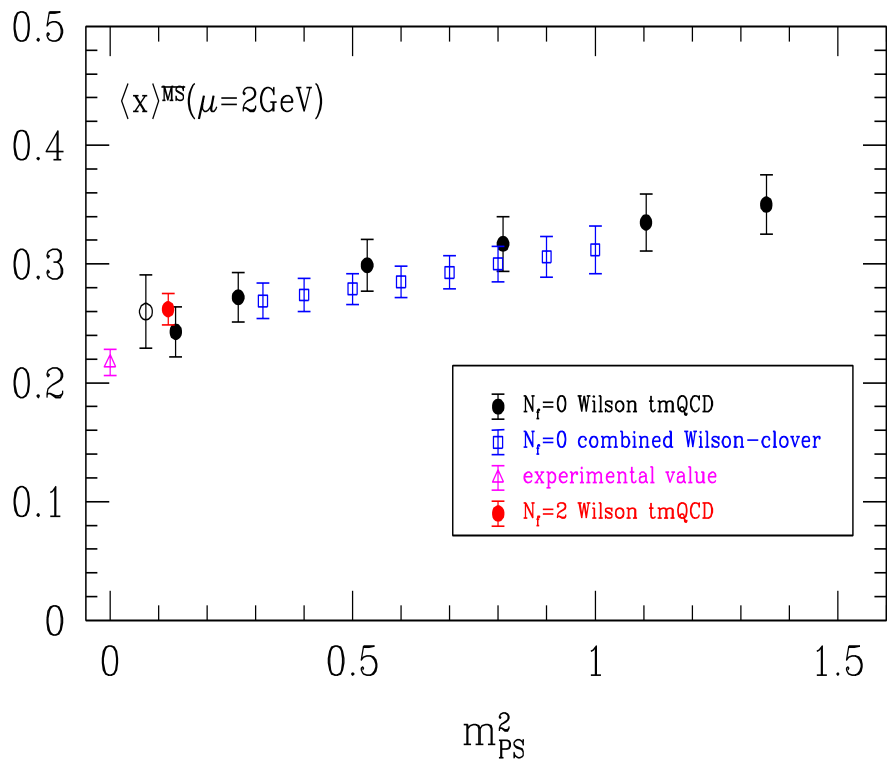
- strange quark:

  $m_s[\overline{\mathrm{MS}}, 2\ \mathrm{GeV}] = 115(2)\ \mathrm{MeV}$

- charm quark:

  $m_c[\overline{\mathrm{MS}}, 2\ \mathrm{GeV}] = 1.1(1)\ \mathrm{GeV}$

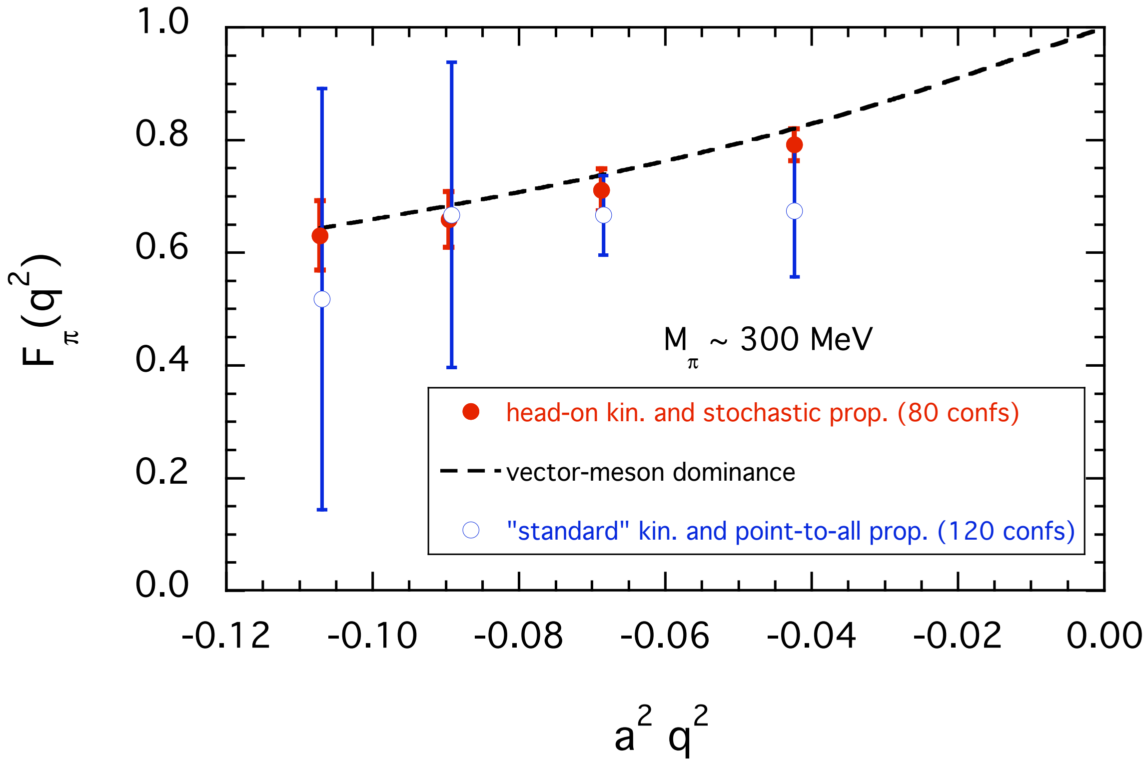
Example: Lowest Moment of Non-singlet, Pion Parton Distribution Function $\langle x \rangle$



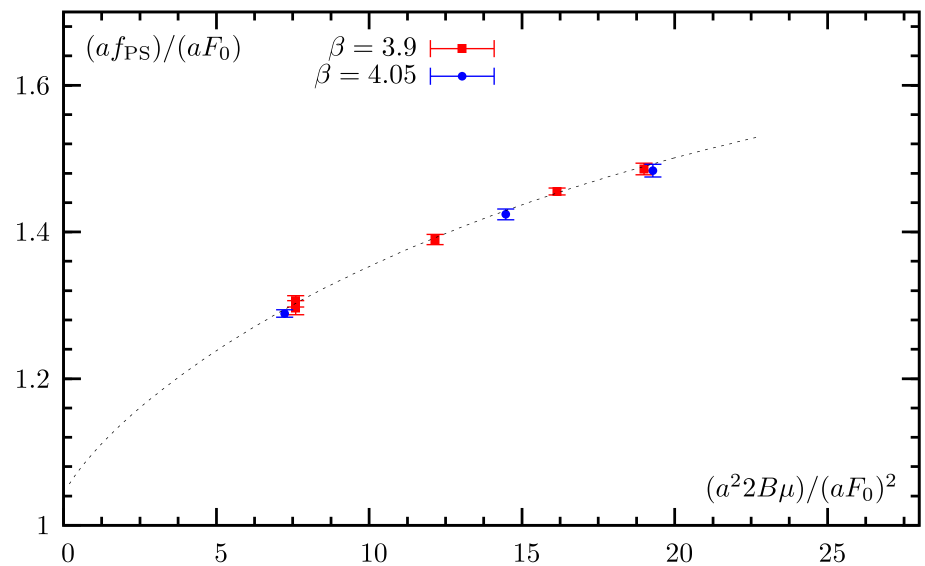
$\longrightarrow$ simulation at small pseudoscalar masses feasible

$\longrightarrow$ dynamical point consistent with quenched (?)

Pion Form Factor

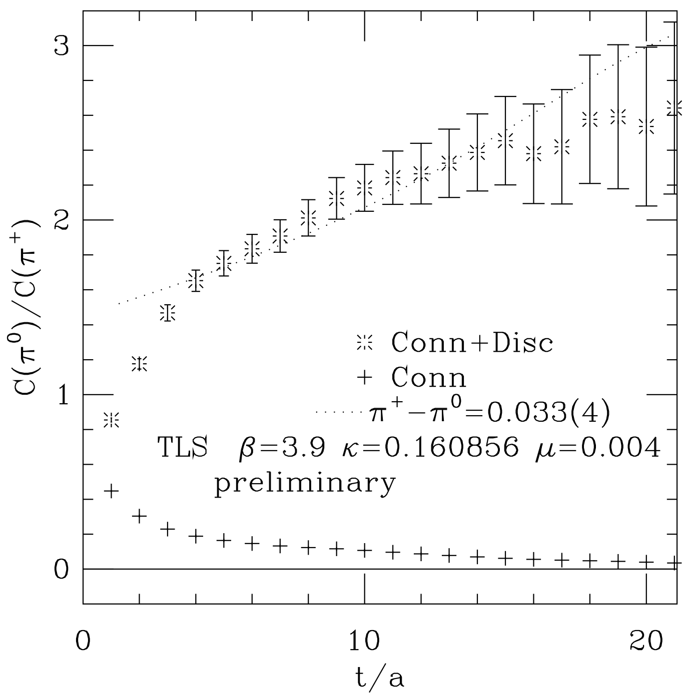


First Scaling result



Isospin breaking

- Isospin broken at $a > 0$
- strongest for $m_{\mathrm{PS}}^{+} - m_{\mathrm{PS}}^{0}$
- Effect vanishes as $m_{\mathrm{PS}}^{+} - m_{\mathrm{PS}}^{0} = c_2 a^2$
- Find at $a \approx 0.095\mathrm{fm}$
  and $250\mathrm{MeV}$ pion mass

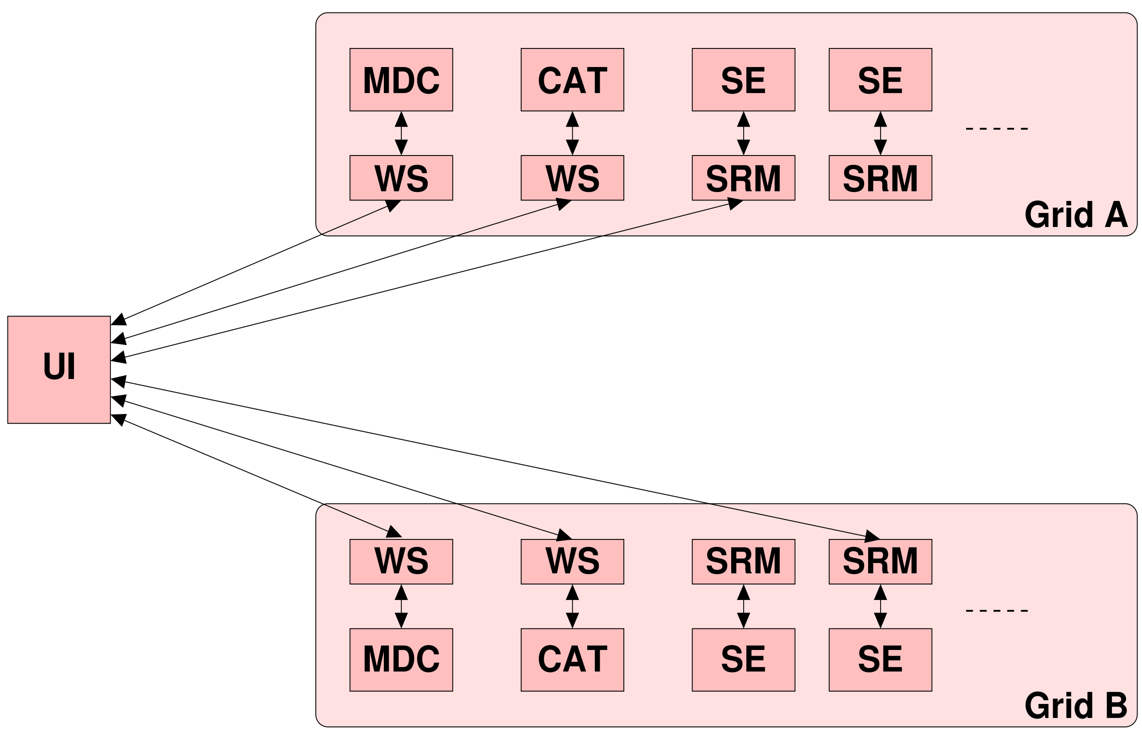


$$\Delta \equiv (m_{\mathrm{PS}}^{+} - m_{\mathrm{PS}}^{0})/m_{\mathrm{PS}}^{+} = (0.134 - 0.101)/0.134 \approx 25\%$$

- Preliminary: at $a \approx 0.075\mathrm{fm}$, $\Delta \approx 10\%$

International Lattice Data Grid

- Configurations stored within ILDG context
- storage elements:
  DESY Hamburg and Zeuthen, ZiB Berlin, FZ Jülich
- semantic based access to configuration data



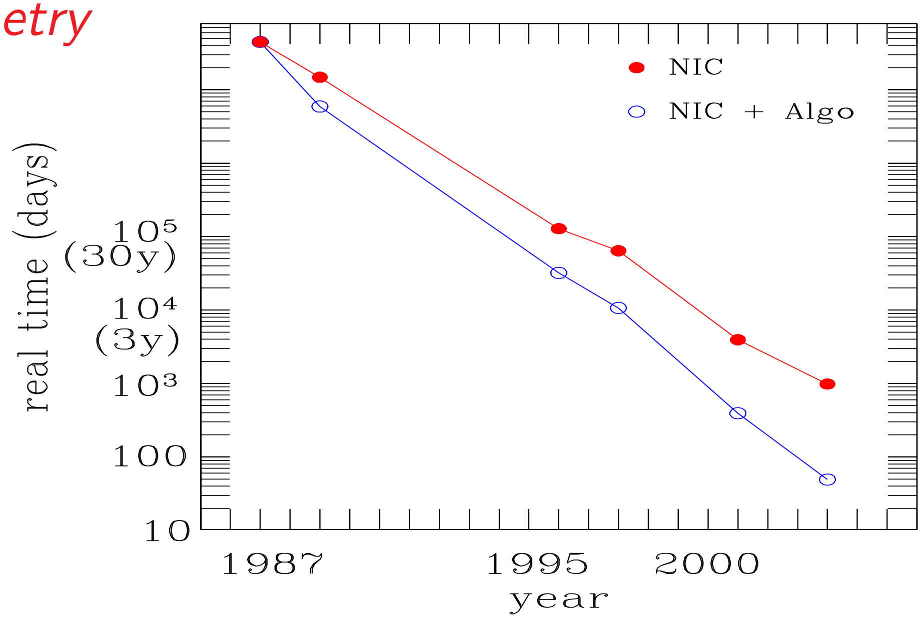
Summary

- Progress in solving outstanding problem in LGT
  $\longrightarrow$ reaching the chiral limit
  $\longrightarrow$ comparison to analytical approaches

  – Overlap fermions: *exact chiral symmetry*
  – Twisted mass fermions:
    $\longrightarrow$ *O(10-100) cheaper to simulate*
    $\longrightarrow$ *small quark masses reachable*
    $\longrightarrow$ *only chirally improved*

- Dramatic algorithm improvement

- New Computer Architectures
  $\Rightarrow$ **apeNEXT**
  $\Rightarrow$ enter area of precise dynamical results



Physics Plans and Machines in Germany

http://www-zeuthen.desy.de/latfor

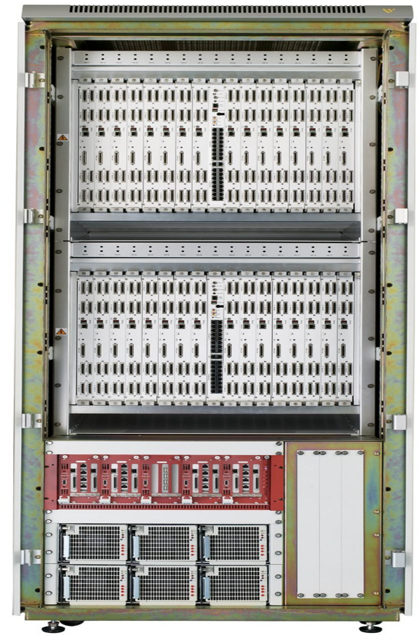
Physics Plans

SESAM	Action:	$N_\mathrm{f}=2$ Wilson, Wilson plaquette
GRAL	Links:	Germany, Italy, US
TXL	Policy:	open(*)
	Parameters:	m_π=0.4...1GeV, a=0.08...0.13fm, up to $V=24^3 40$
	Configurations:	19 ensembles (60K confs.), uploaded now 15K
QCDSF	Action:	$N_\mathrm{f}=2$ NP-Clover, Wilson plaquette
	Links:	Germany, UK, Japan, US
	Policy:	Open access to ensembles before 2006 (**)
		Immediate access to new data by agreement
	Parameters:	$m_\pi=$ 0.25...1GeV, a=0.05...0.11fm, up to $V=32^3 64$
	Configurations:	14 ensembles, O(14000) confs
ETMC	Action:	$N_\mathrm{f}=2$ maximally tmQCD, tlSym gauge
	Links:	Germany, France, Italy, UK
	Policy:	open (*)
	Parameters:	$a=0.075-0.12$fm, $L\approx 2.5$fm, $250<m_\pi<500$MeV
	Configurations:	3 ensembles O(3500) confs uploaded

(*) Acknowledgment in paper, draft paper in advance

(**) hep-ph/0502212 and hep-lat/0601004 should be cited

Supercomputer Infrastructure



- apeNEXT in Zeuthen 3Teraflops
  and Bielefeld 5Teraflops
  → dedicated to LGT

- NIC BlueGene/L System at FZ-Jülich
  45 Teraflops

- NIC IBM Regatta System at FZ-Jülich
  10 Teraflops

- Altix System at LRZ Munic
  26.2 Teraflops (since June 2006)
  upgrade to **60 Teraflops** mid 2007

The Future

Gauss Centre for Supercomputing (GCS)

The Gauss Centre for Supercomputing (GCS) provides the most powerful high-performance computing infrastructure in Europe.

- John von Neumann-Institut for Computing, Jülich
- Leibniz Rechenzentrum, München
- Höchstleistungsrechenzentrum, Stuttgart

– Multi-teraflops supercomputers

– Multi-petabyte storage

– Multi-gigabit communication links

$\longrightarrow$ compete for European Supercomputer Center

$\Rightarrow$ Super Computers with several 100 Teraflops in near future