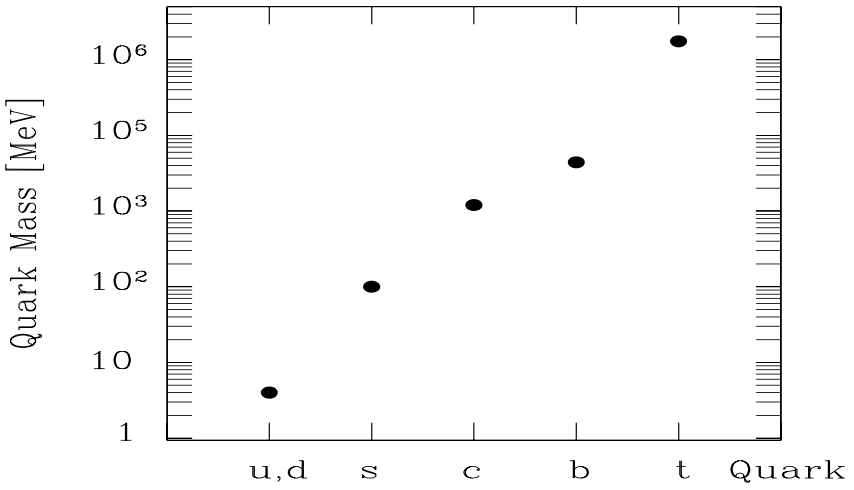
The Quest for Solving QCD: Simulations with Light Quarks

Karl Jansen

- **Introduction**
- **Studying strong interaction by a 4-dimensional lattice**
  - Breakthrough in Simulation Algorithm
  - Selected Results
- **Short remark about Higgs boson mass**
- **Summary**

Comparing QED and QCD

- binding energy
  - hydrogen atom: O(eV)
  - Proton: O(GeV)
    (while quark mass O(MeV))
  - accurcay of strong coupling:
    $\alpha_s(M_Z) = 0.118(3)$
  - comparison to anomalous
    magnetic momenent of electron:

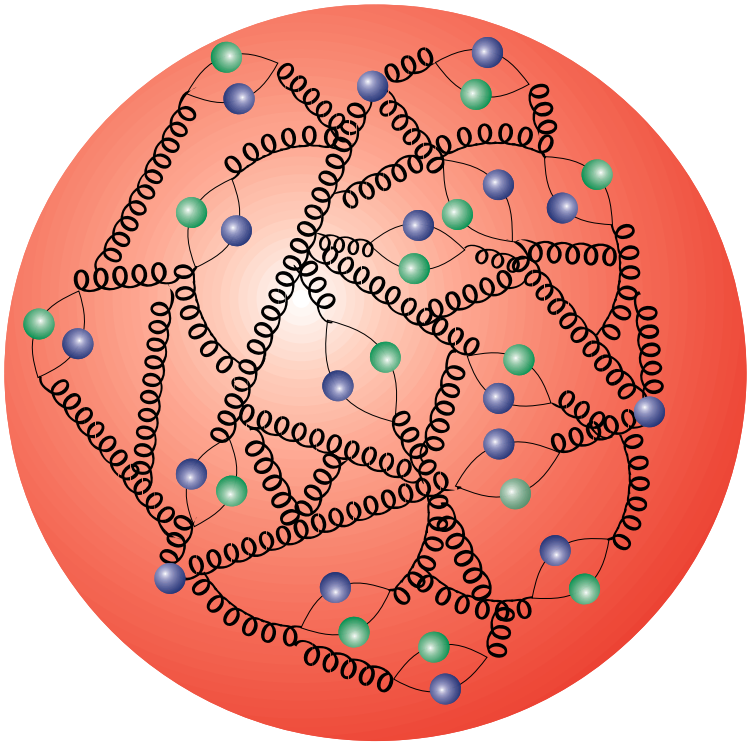


$$a_e(\text{theory}) = 1159652201.1(2.1)(27.1) \cdot 10^{-12}$$
$$a_e(\text{experiment}) = 1159652188.4(4.3) \cdot 10^{-12}$$

- completely novel situation in QCD:
  constituent particles cannot
  be observed themselves!
  $\rightarrow$ confinement phenomenon

Why Perturbation Theory fails for the Strong Interaction

- situation becomes incredibly complicated



- value of the coupling (expansion parameter) $\alpha_{\text{strong}}(1\text{fm}) \approx 1$

$\Rightarrow$ need different ("exact") method

$\Rightarrow$ has to be non-perturbative

- Wilson's Proposal: Lattice Quantum Chromodynamics

Lattice Gauge Theory had to be invented

→ QuantumChromoDynamics

asymptotic freedom		confinement
distances $\ll 1\text{fm}$		distances $\gtrsim 1\text{fm}$
world of quarks and gluons		world of hadrons and glue balls
perturbative description		non-perturbative methods

Unfortunately, it is not known yet whether the quarks in quantum chromodynamics actually form the required bound states. To establish whether these bound states exist one must solve a strong coupling problem and present methods for solving field theories don't work for strong coupling.

Wilson, Cargese Lecture notes 1976

Schwinger model: 2-dimensional Quantum Electrodynamics

Schwinger 1962

(typical system explored in DESY summerstudent programme; www.desy.de/summerstudents/)

Quantization via Feynman path integral

$$\mathcal{Z} = \int \mathcal{D}A_\mu \mathcal{D}\Psi \mathcal{D}\bar{\Psi} e^{-S_{\rm gauge} - S_{\rm ferm}}$$

Fermion action

$$S_{\rm ferm} = \int d^2x \bar{\Psi}(x) \left[D_\mu + m \right] \Psi(x)$$

gauge covriant derivative

$$D_\mu \Psi(x) \equiv (\partial_\mu - i g_0 A_\mu(x)) \Psi(x)$$

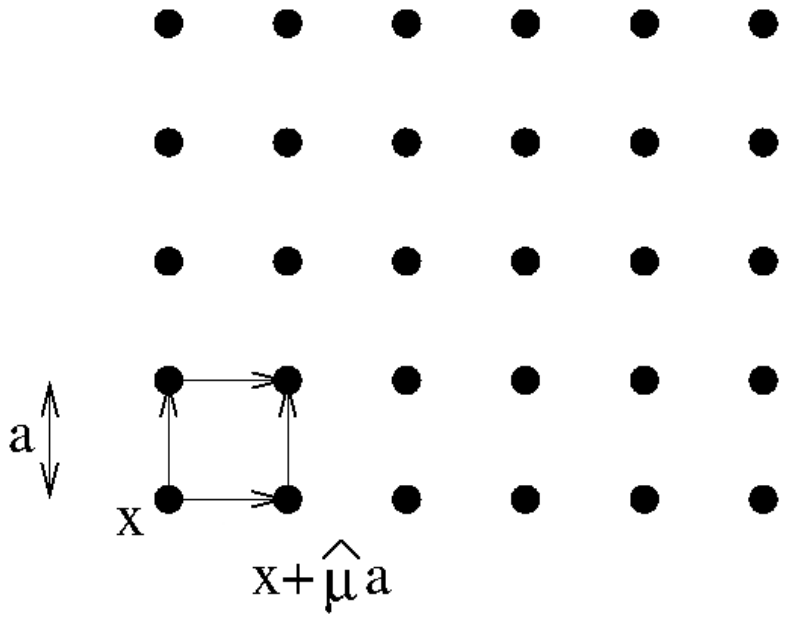
with A_μ gauge potential, g_0 bare coupling

$$S_{\rm gauge} = \int d^2x F_{\mu\nu} F_{\mu\nu} \ , \ F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)$$

equations of motion: obtain classical Maxwell equations

Lattice Schwinger model

introduce a 2-dimensional lattice with
lattice spacing a



fields $\Psi(x)$, $\bar{\Psi}(x)$ on the lattice sites

$x = (t, \mathbf{x})$ integers

discretized fermion action

$$S \to a^2 \sum_x \bar{\Psi} \left[\gamma_\mu \partial_\mu - r \underbrace{\partial_\mu^2}_{\nabla_\mu^* \nabla_\mu} + m\right] \Psi(x)$$

$$\partial_\mu = \tfrac{1}{2}\left[\nabla_\mu^* + \nabla_\mu\right]$$

discrete derivatives

$$\nabla_\mu \Psi(x) = \tfrac{1}{a}\left[\Psi(x + a\hat{\mu}) - \Psi(x)\right] \ , \quad \nabla_\mu^* \Psi(x) = \tfrac{1}{a}\left[\Psi(x) - \Psi(x - a\hat{\mu})\right]$$

second order derivative $\to$ remove doubler $\leftarrow$ break chiral symmetry

Implementing gauge invariance

Wilson's fundamental observation: introduce Paralleltransporter connecting the points x and $y = x + a\hat{\mu}$:

$$U(x,\mu) = e^{iaA_\mu(x)} \in U(1)$$

$\Rightarrow$ lattice derivatives

$$\begin{aligned} \nabla_\mu \Psi(x) &= \frac{1}{a}\left[U(x,\mu)\Psi(x+\mu) - \Psi(x)\right] \\ \nabla^*_\mu \Psi(x) &= \frac{1}{a}\left[\Psi(x) - U^{-1}(x-\mu,\mu)\Psi(x-\mu)\right] \end{aligned}$$

action gauge invariant under

$$\Psi(x) \to g(x)\Psi(x), \;\; \bar{\Psi}(x) \to \bar{\Psi}(x)g^*(x),$$

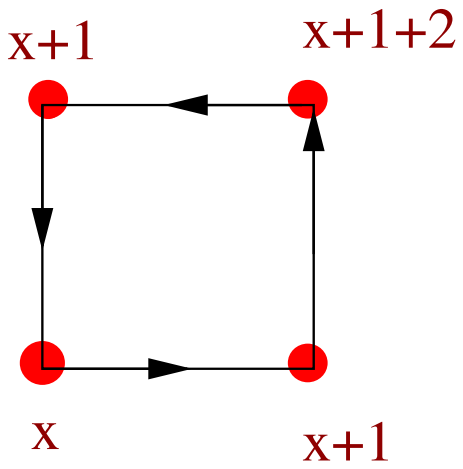
$$U(x,\mu) \to g(x)U(x,\mu)g^*(x+\mu)$$

Lattice Action

$$\mathcal{Z} = \int_{\text{fields}} e^{-S}$$

Partition functions (pathintegral) with Boltzmann weight (action) S

$$S = a^2 \sum_x \left\{ \beta \left[1 - \mathrm{Re}(U_{(x,p)}) \right] + \bar{\psi} \left[m_0 + \tfrac{1}{2} \{ \gamma_\mu (\partial_\mu + \partial_\mu^\star) - a \partial_\mu^\star \partial_\mu \} \right] \psi \right\}$$



lattice derivatives

$$\partial_\mu \Psi(x) = \tfrac{1}{a} \left[U(x,\mu) \Psi(x+\mu) - \Psi(x) \right]$$

$$U(x,\mu) = e^{iaA_\mu(x)}$$

$$U_p = U(x,\mu) U(x+\mu,\nu) U^{-1}(x+\nu,\mu) U^{-1}(x,\nu) \rightarrow F_{\mu\nu} F^{\mu\nu}(x) \quad \text{for} \quad a \rightarrow 0$$

Physical Observables

expectation value of physical observables $\mathcal{O}$

$$\underbrace{\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int_{\text{fields}} \mathcal{O} e^{-S}}$$

$\downarrow$ lattice discretization

$$0101110001110001111001 1$$

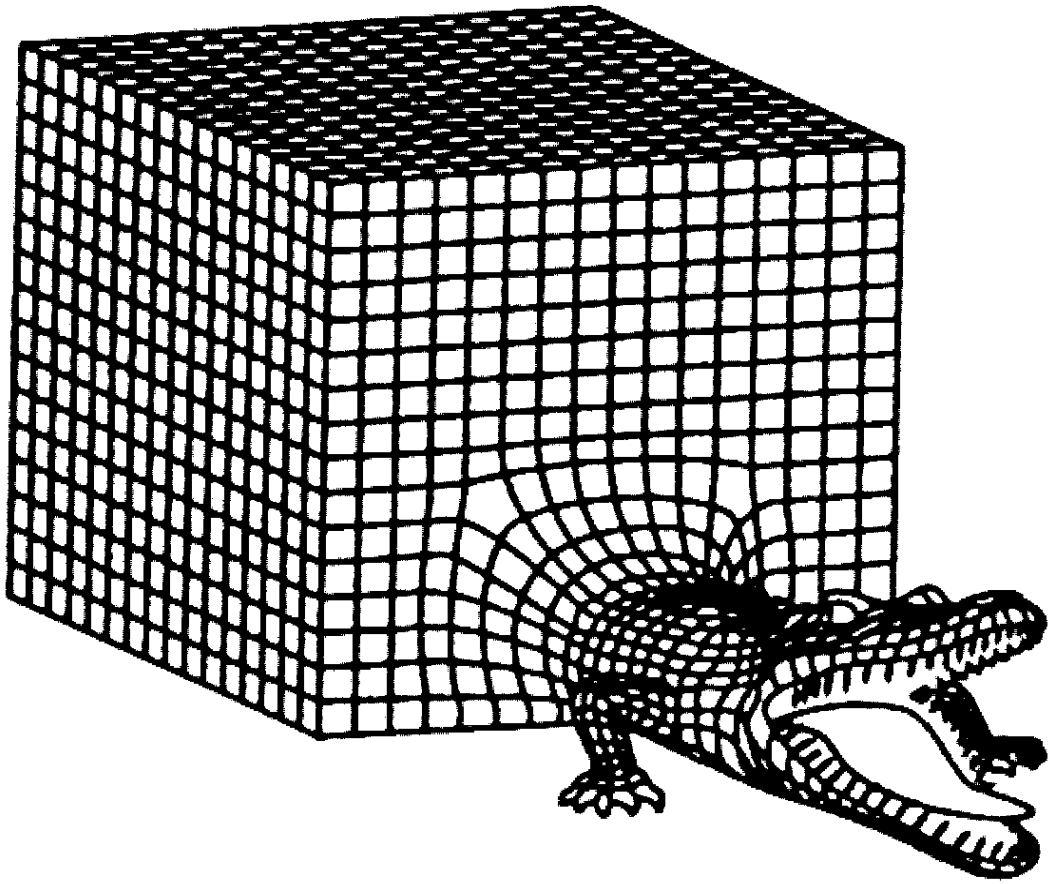
$\downarrow$

Lattice QCD

change:

- 2-d $\longrightarrow$ 4-d
- gauge field $U(x,\mu) \in U(1) \longrightarrow U(x,\mu) \in SU(3)$
- Pauli matrices $\sigma_\mu \longrightarrow$ Dirac-matrices γ_μ
- spinors become 12-component complex vectors
- theory needs renormalization

There are dangerous lattice animals

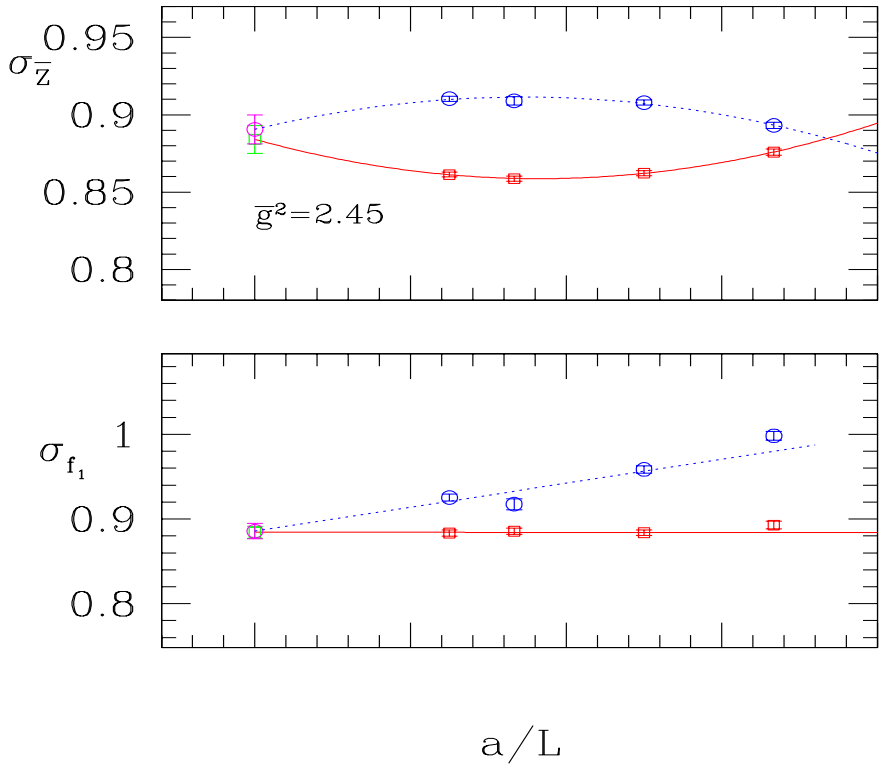


Wilson's Lattice Quantum Chromodynamics

$$S = \underbrace{S_{\mathrm{G}}}_{\mathrm{O}(a^2)} + \underbrace{S_{\mathrm{naive}}}_{\mathrm{O}(a^2)} + \underbrace{S_{\mathrm{wilson}}}_{\mathrm{O}(a)}$$

lattice artefacts appear linear in a

$\rightarrow$ possibly large lattice artefacts
$\Rightarrow$ need of fine lattice spacings
$\Rightarrow$ large lattices
(want $L = N \cdot a = 1\mathrm{fm}$ fixed)
$\rightarrow$ simulation costs $\propto 1/a^{6-7}$



present (Wilson-type) solutions:

- clover-improved Wilson fermions
- maximally twisted Wilson fermions
- overlap/domainwall fermions $\leftarrow$ exact (lattice) chiral symmetry

Realizing $\mathrm{O}(a)$-improvement

Continuum lattice QCD action $S = \bar{\Psi}\left[m + \gamma_\mu D_\mu\right]\Psi$

an *axial transformation*: $\Psi \to e^{i\omega\gamma_5\tau_3/2}\Psi\ , \quad \bar{\Psi} \to \bar{\Psi}e^{i\omega\gamma_5\tau_3/2}$

changes only the mass term:

$m \to me^{i\omega\gamma_5\tau_3} \equiv m' + i\mu\gamma_5\tau_3\ , \quad m = \sqrt{m'^2 + \mu^2}\ , \quad \tan\omega = \mu/m$

$\to$ generalized form of continuum action

- $\omega = 0$: standard QCD action
- $\omega = \pi/2 : S = \bar{\Psi}\left[i\mu\gamma_5\tau_3 + \gamma_\mu D_\mu\right]\Psi$
- general ω : smooth change between both actions

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

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

quark mass parameter m_q , twisted mass parameter μ

difference to continuum situation:
Wilson term not invariant under axial transformations

$\Psi \to e^{i\omega\gamma_5\tau_3/2}\Psi\ , \quad \bar\Psi \to \bar\Psi e^{i\omega\gamma_5\tau_3/2}$

2-point function: $\left[m_q + i\gamma_\mu \sin p_\mu a + \frac{r}{a}\sum_\mu(1-\cos p_\mu a) + i\mu\tau_3\gamma_5\right]^{-1}$

$\propto (\sin p_\mu a)^2 + \left[m_q + \frac{r}{a}\sum_\mu(1-\cos p_\mu a)\right]^2 + \mu^2$

$\lim_{a\to 0}: \quad p_\mu^2 + m_q^2 + \mu^2 + \underbrace{am_q\sum_\mu p_\mu}_{O(a)}$

- setting $m_q = 0 \ \ (\omega = \pi/2):$ no $O(a)$ lattice artefacts
- quark mass is realized by twisted mass term alone

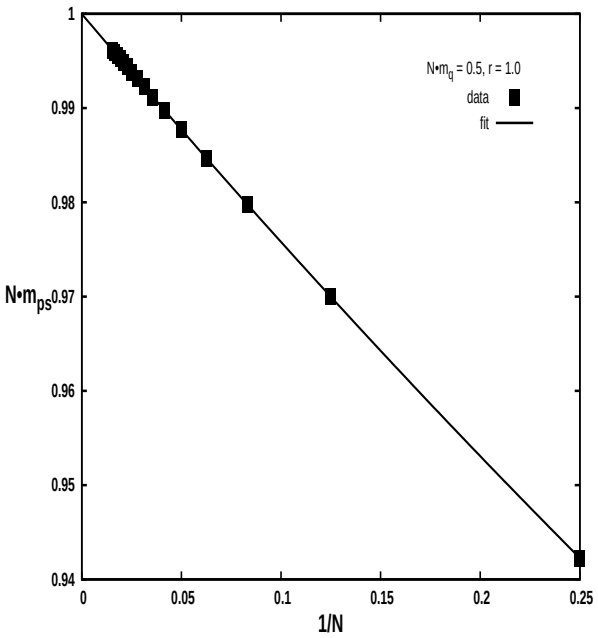
A demonstration in the free theory

(K. Cichy, J. Gonzales Lopez, A. Kujawa, A. Shindler, K.J.)

free fields: imagine study system for $L[\mathrm{fm}] < \infty$

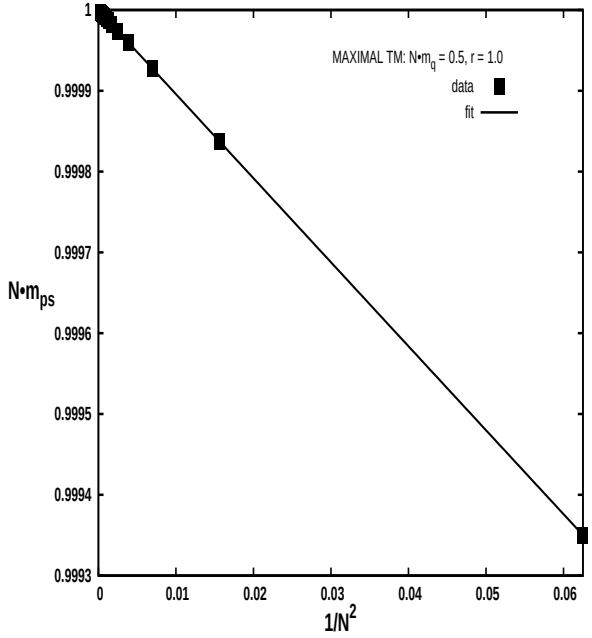
$\Rightarrow \quad L = N \cdot a \quad \rightarrow a \rightarrow 0 \leftrightarrow N \rightarrow \infty$

Wilson fermions at $m_q = 0.5$



$N \cdot m_\pi$ versus $\mathbf{1/N = a}$

twisted mass at $m_q = 0.0$, $\mu_q = 0.5$



$N \cdot m_\pi$ versus $\mathbf{1/N^2 = a^2}$

Overlap fermions: exact lattice chiral symmetry

starting point: **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 local (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, $0 < s < 1$

The "No free lunch theorem"

A 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
$12^4, 720$Mev	48.8(6)	2.6(1)	18.8
$12^4, 390$Mev	142(2)	4.0(1)	35.4
$16^4, 720$Mev	225(2)	9.0(2)	25.0
$16^4, 390$Mev	653(6)	17.5(6)	37.3
$16^4, 230$Mev	1949(22)	22.1(8)	88.6

timings in seconds on Jump

- nevertheless chiral symmetric lattice fermions can be advantageous
  - e.g., Kaon Physics, B_K, $K \to \pi\pi$
  - ϵ-regime of chiral perturbation theory
  - topology
  - use in valence sector

Why are fermions so expensive?

- need to evaluate

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\bar{\psi}\{D^{\text{Dirac}}_{\text{lattice}}\}\psi} \propto \det[D^{\text{Dirac}}_{\text{lattice}}]$$

- bosonic representation of determinant

$$\det[D^{\text{Dirac}}_{\text{lattice}}] \propto \int \mathcal{D}\Phi^\dagger\mathcal{D}\Phi e^{-\Phi^\dagger\{D^{-1}_{\text{lattice}}\}\Phi}$$

- need vector $X = D^{-1}_{\text{lattice}}\Phi$

- solve linear equation $D_{\text{lattice}}X = \Phi$

  D_{lattice} matrix of dimension $1\text{million} \otimes 1\text{million}$ (however, sparse)

- number of such "inversions": $O(100)$ for one field configuration

- want: $O(1000 - 10000)$ such field configurations

The need for parallelization

lattice size: $24^3 \cdot 48$

computer: one rack of a BG/P system with 4096 processors

harvest: about 200 gauge field configurations per day

Need: $\langle \mathcal{O} \rangle$ requires about 5000 of such configurations

$\Rightarrow$ clear need of parallelization

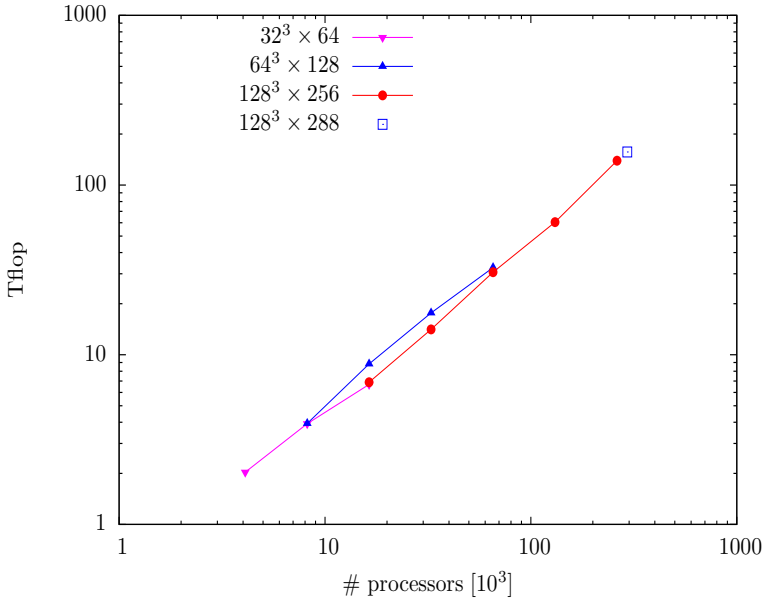
general form interaction $\bar{\Psi}^{(i,\alpha)}(x) U^{(i,j)}(x,\mu) \Gamma^{\alpha,\beta} \Psi^{(j,\beta)}(x + a\hat{\mu})$.

- indices $i = 1, 2, 3$ representing colour
- $\alpha = 1, 2, 3, 4$ representing Dirac structure
- gauge field $U^{(i,j)}(x,\mu)$ is SU(3)-matrix describing gluon degrees of freedom

$\Rightarrow$ clear possibility for parallelization

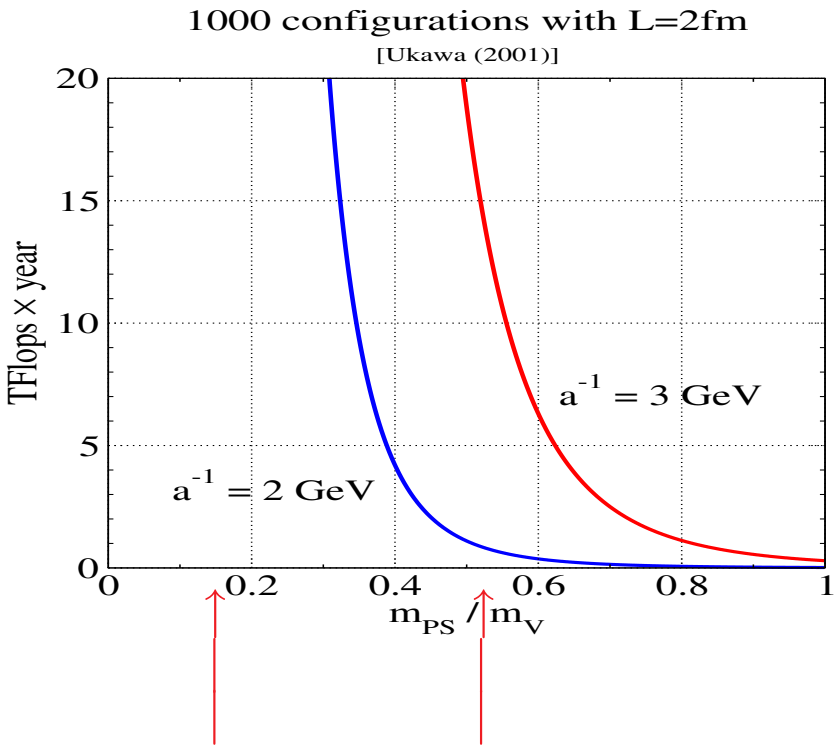
Strong Scaling

- Test on 72 racks BG/P installation at supercomputer center Jülich (Gerhold, Herdioza, Urbach, K.J.)
- using tmHMC code (Urbach, K.J.)



Costs of dynamical fermions simulations, the "Berlin Wall"

see panel discussion in Lattice2001, Berlin, 2001



physical point

contact to χPT (?)

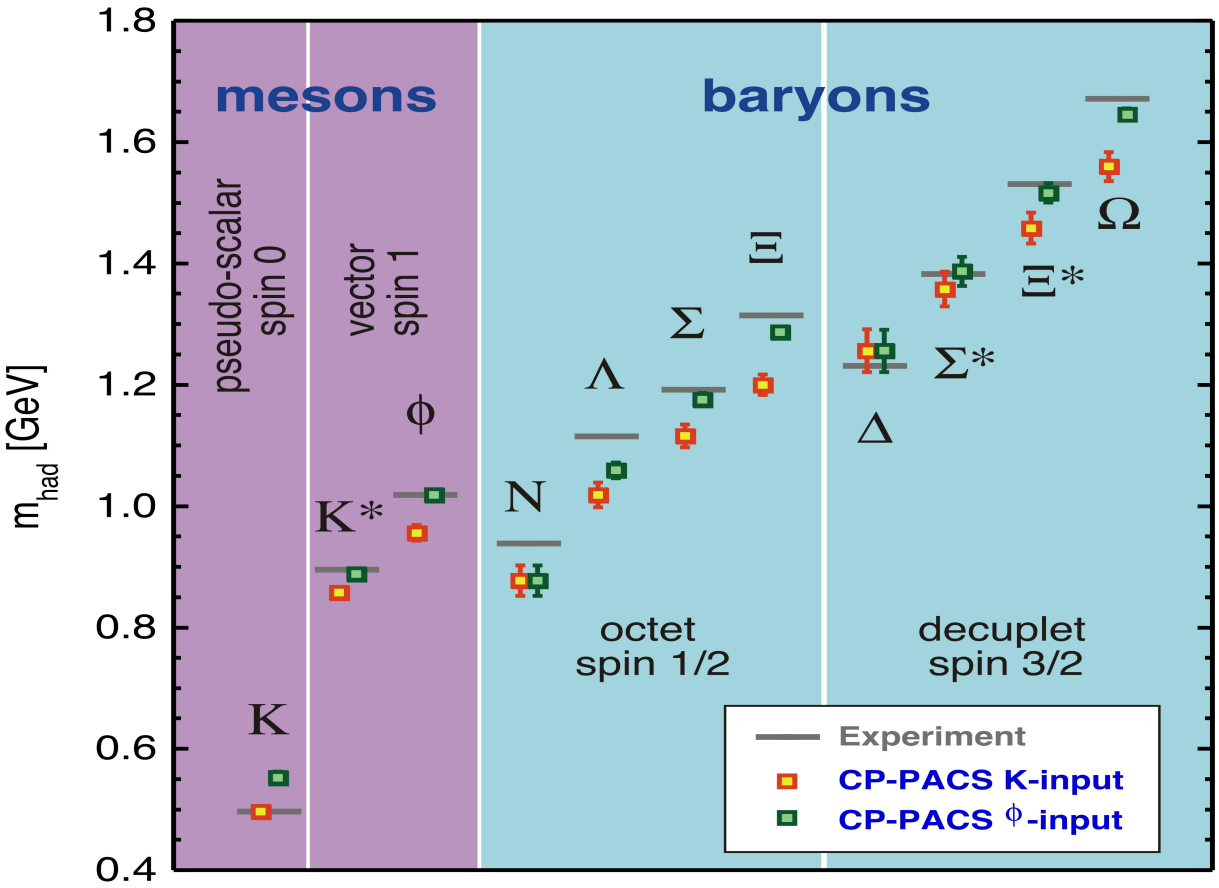
formula $C \propto \left(\frac{m_\pi}{m_\rho}\right)^{-z_\pi} (L)^{z_L} (a)^{-z_a}$

$$z_\pi = 6, \;\; z_L = 5, \;\; z_a = 7$$

"both a 10^8 increase in computing power AND spectacular algorithmic advances before a useful interaction with experiments starts taking place."
(Wilson, 1989)

$\Rightarrow$ need of **Exaflops Computers**

Quenched approximation



CP-PACS collaboration, 2000

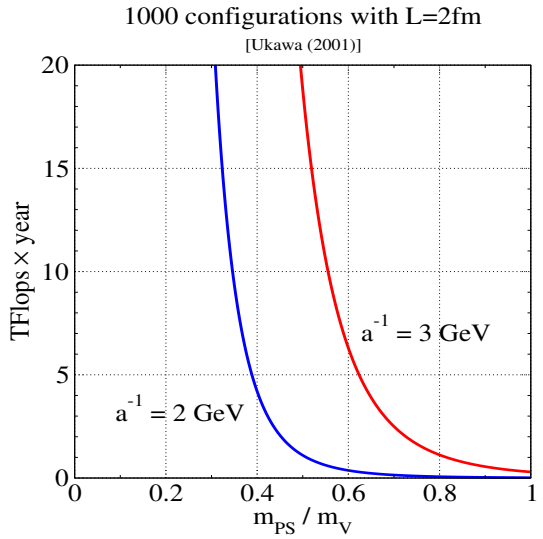
Solution of QCD?

→ a number of systematic errors

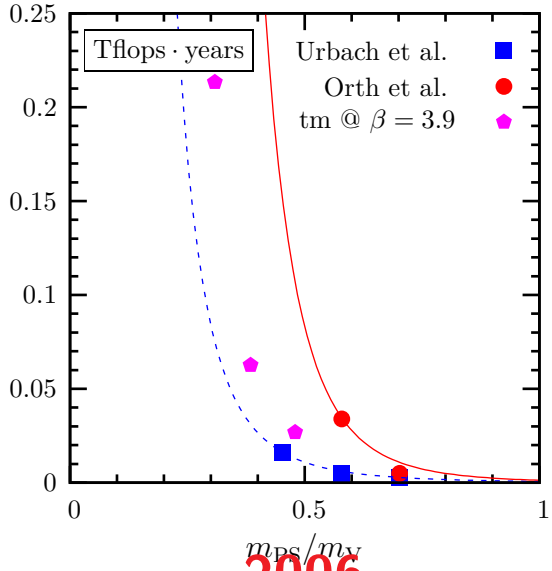
A generic improvement for Wilson type fermions

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



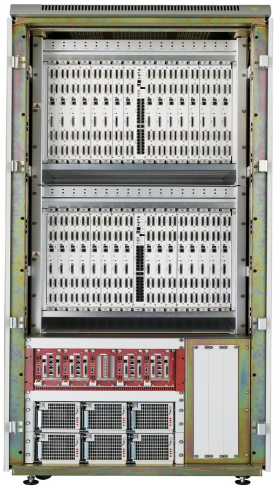
2001



2006

- comparable to staggered
- reach small pseudo scalar masses ≈ 300MeV

German Supercomputer Infrastructure

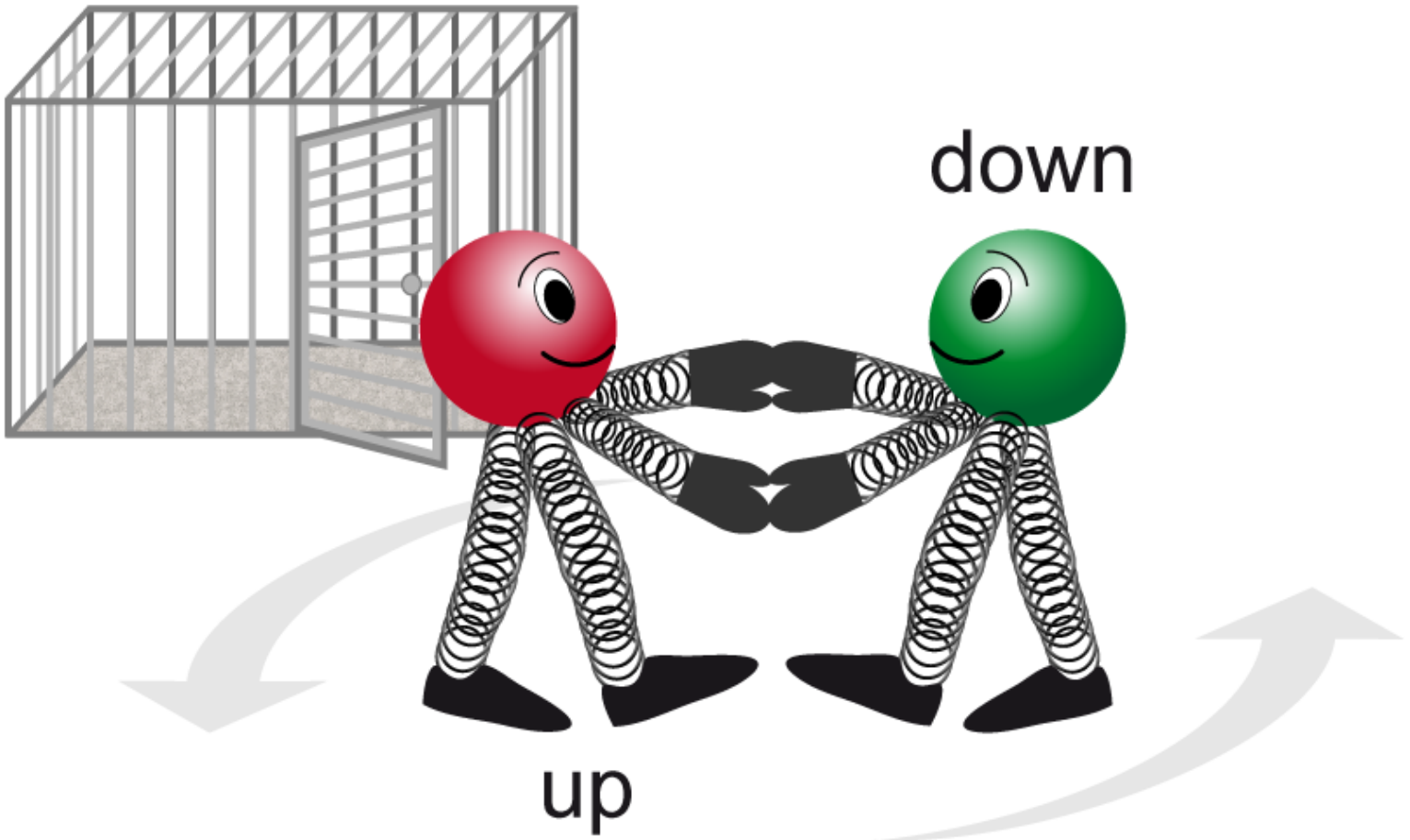


- apeNEXT in Zeuthen 3Teraflops
  and Bielefeld 5Teraflops
  $\longrightarrow$ dedicated to LGT

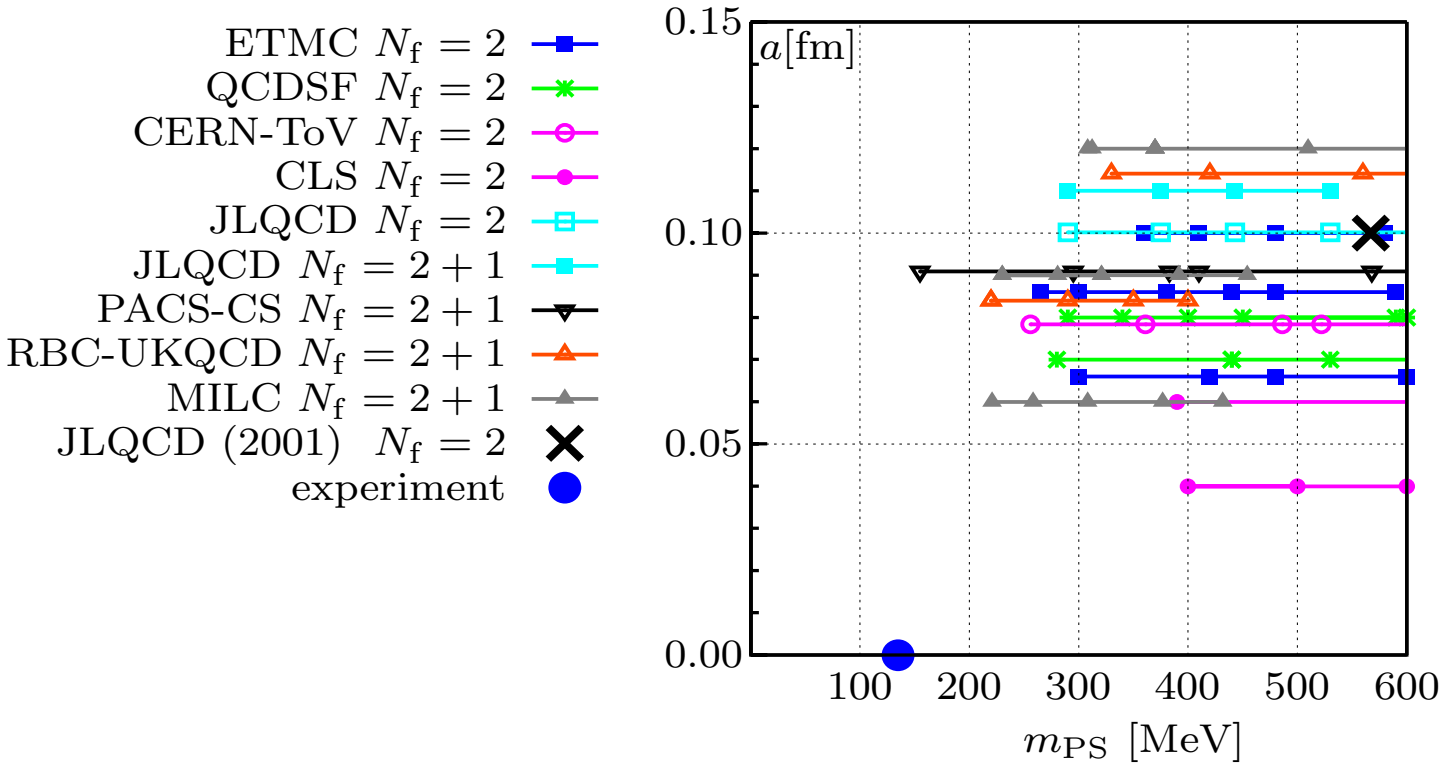
- NIC 72 racks of BG/P System
  at FZ-Jülich **1 Petaflops**

- 2208 Nehalem processor
  Cluster computer:
  208 Teraflops
- Altix System at LRZ Munic
- SGI Altix ICE 8200 at HLRN (Berlin, Hannover)
  31 Teraflops
- QPACE 4+4 Racks in Jülich und Wuppertal
  1900 PowerXCell 8i nodes **190 TFlops (peak)**
- University machines, e.g. University of Mainz:
  280 nodes Dual Quadcore AMD Barcelona + Infiniband

$N_f = 2$ dynamical flavours



Simulation landscape



- **Cyprus (Nicosia)**
  C. Alexandrou, M. Constantinou, T. Korzec, G. Koutsou
- **France (Orsay, Grenoble)**
  R. Baron, B. Bloissier, Ph. Boucaud, M. Brinet, J. Carbonell, V. Drach, P. Guichon, P.A. Harraud, Z. Liu, O. Pène
- **Italy (Rome I,II,III, Trento)**
  P. Dimopoulos, R. Frezzotti, V. Lubicz, G. Martinelli, G.C. Rossi, L. Scorzato, S. Simula, C. Tarantino
- **Netherlands (Groningen)**
  A. Deuzeman, E. Pallante, S. Reker
- **Poland (Poznan)**
  K. Cichy, A. Kujawa
- **Spain (Valencia)**
  V. Gimenez, D. Palao
- **Switzerland (Bern)**
  U. Wenger
- **United Kingdom (Glasgow, Liverpool)**
  G. McNeile, C. Michael, A. Shindler
- **Germany (Berlin/Zeuthen, Hamburg, Münster)**
  F. Farchioni, X. Feng, J. González López, G. Herdoiza, K. Jansen, I. Montvay, G. Münster, M. Petschlies, D. Renner, T. Sudmann, C. Urbach, M. Wagner

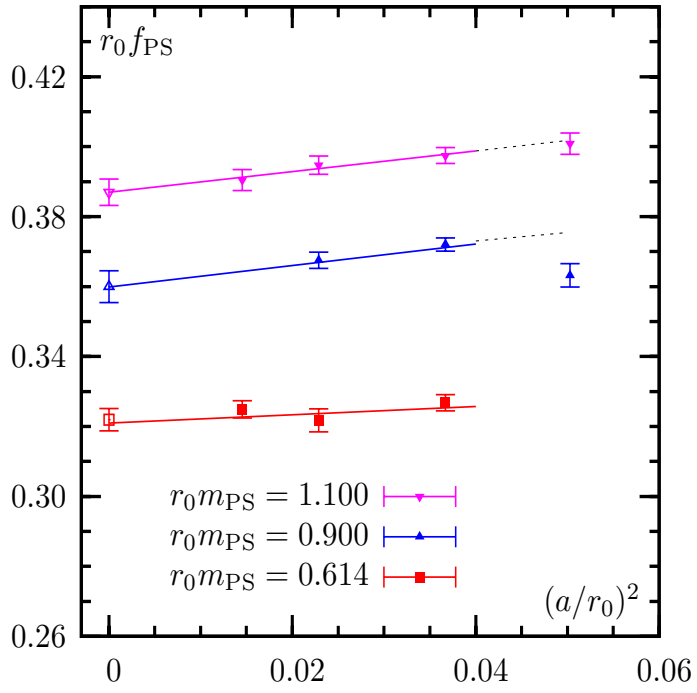
European Twisted Mass Collaboration

available configurations (free on ILDG)

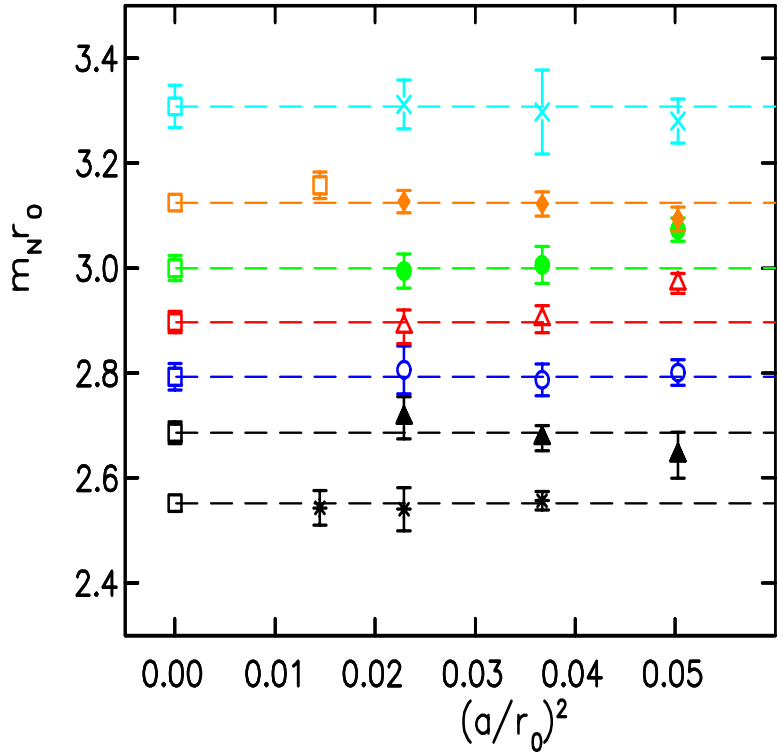
β	a [fm]	$L^3 \cdot T$	L [fm]	$a\mu$	$N_{\rm traj}$ $(\tau = 0.5)$	$m_{\rm PS}$ [MeV]
4.20	~ 0.050	$48^3 \cdot 96$	2.4	0.0020	5200	~ 300
		$32^3 \cdot 64$	2.1	0.0060	5600	~ 420
4.05	~ 0.066	$32^3 \cdot 64$	2.2	0.0030	5200	~ 300
				0.0060	5600	~ 420
				0.0080	5300	~ 480
				0.0120	5000	~ 600
3.9	~ 0.086	$32^3 \cdot 64$	2.8	0.0030	4500	~ 270
				0.0040	5000	~ 300
		$24^3 \cdot 48$	2.1	0.0064	5600	~ 380
				0.0085	5000	~ 440
				0.0100	5000	~ 480
				0.0150	5400	~ 590
3.8	~ 0.100	$24^3 \cdot 48$	2.4	0.0060	4700×2	~ 360
				0.0080	3000×2	~ 410
				0.0110	2800×2	~ 480
				0.0165	2600×2	~ 580

Lattice spacing scaling

Pion decay constant



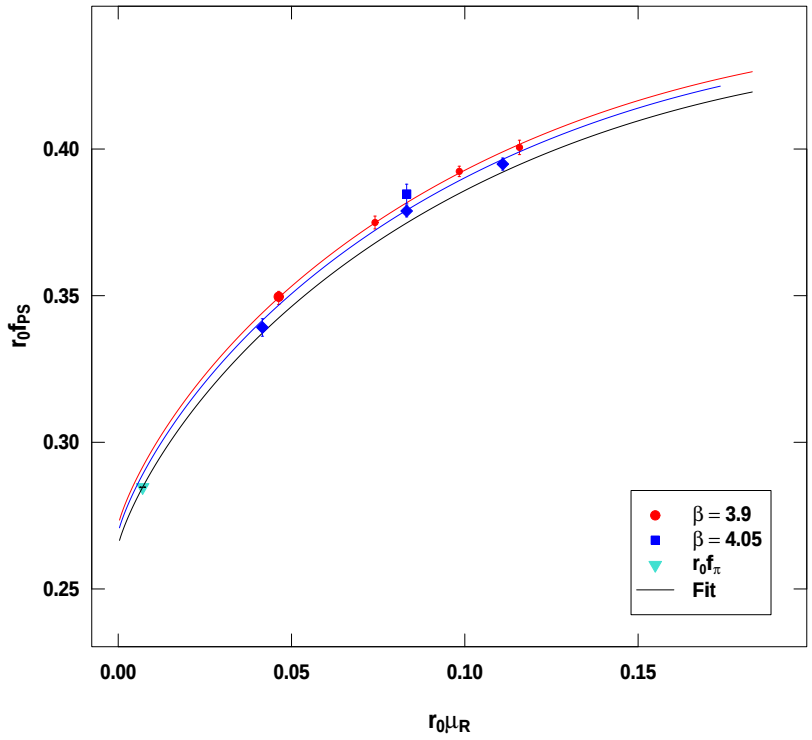
Nucleon mass

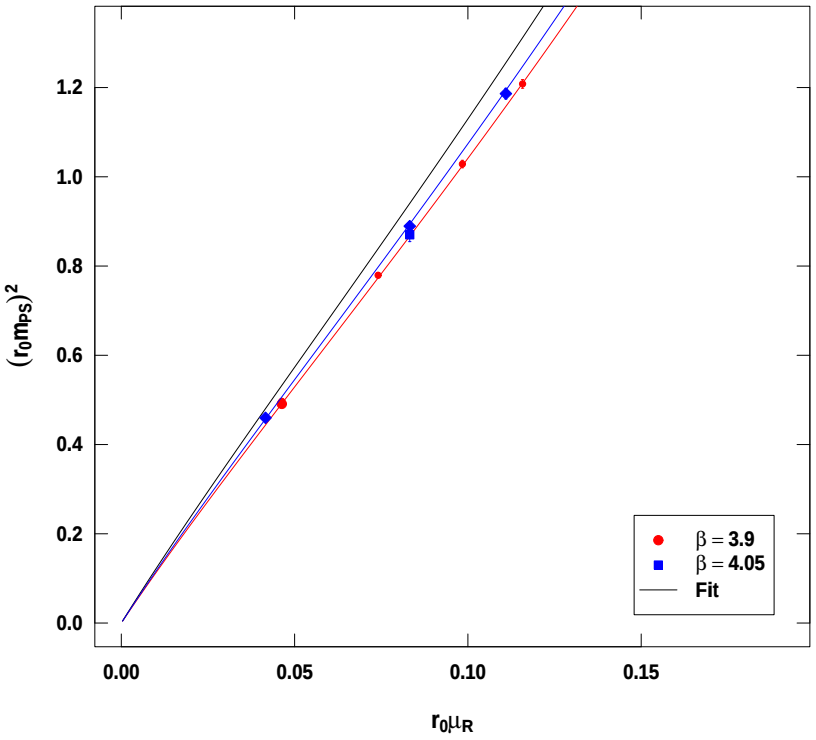


$\rightarrow$ observe (flat) $O(a^2)$ scaling

Chiral perturbation theory

- Fit: Next Leading Order continuum χPT fitted





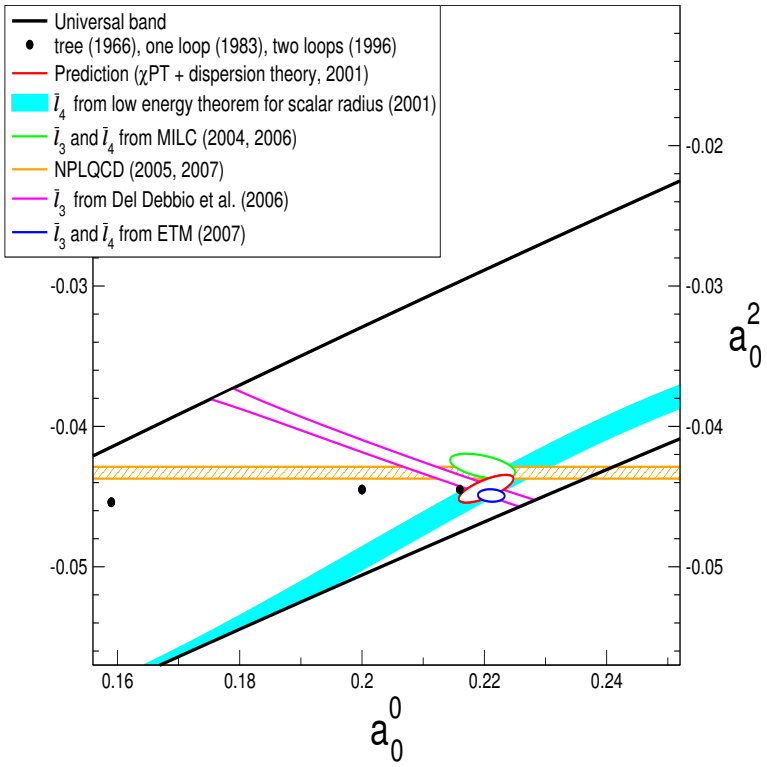
Chiral perturbation theory: results (preliminary)

quantity	value
$m_{u,d}$ [MeV]	3.37(23)
$\bar{\ell}_3$	3.49(19)
$\bar{\ell}_4$	4.57(15)
f_0 [MeV]	121.75(46)
B_0 [GeV]	2774(190)
r_0 [fm]	0.433(14)
$\langle r^2 \rangle_s$	0.729(35)
$\Sigma^{1/3}$ [MeV]	273.9(6.0)
f_π / f_0	1.0734(40)

- averaged fit results, weighted with confidence levels
- B_0, Σ, $m_{u,d}$ renormalised in $\overline{\mathrm{MS}}$ scheme at scale $\mu = 2$ GeV

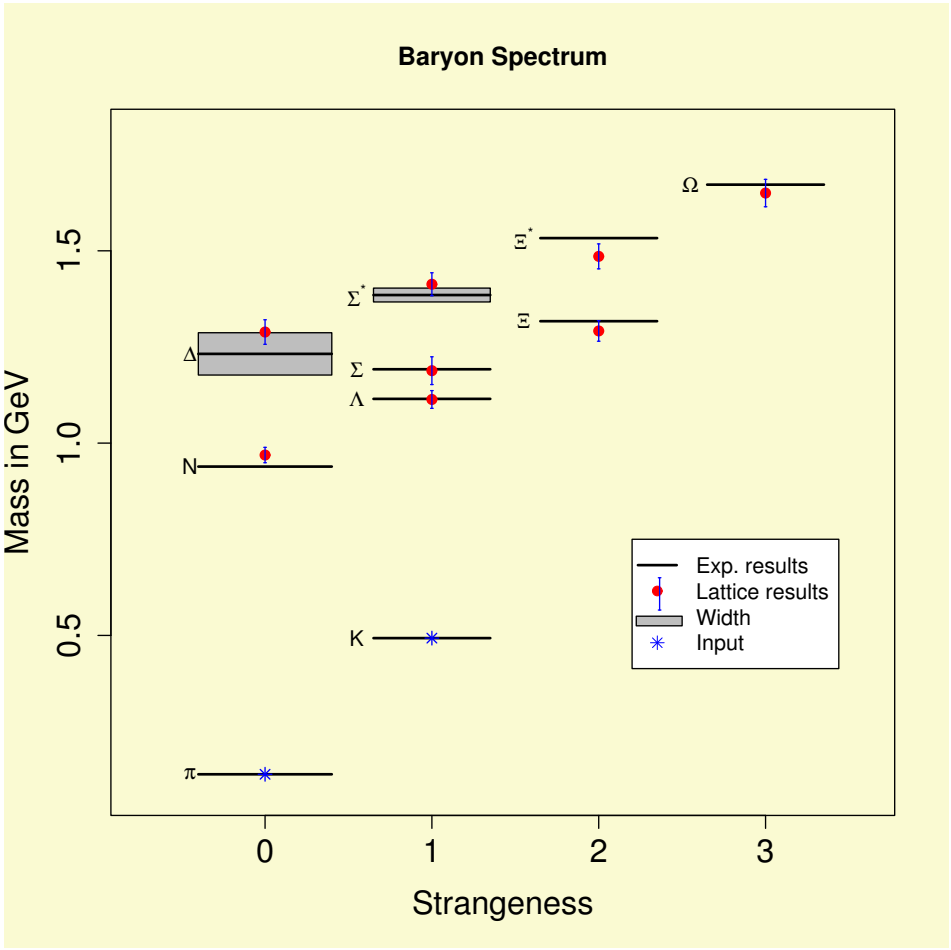
Chiral perturbation theory

using low energy constants:
S-wave scattering lengths a_0^0 and a_0^2 (Leutwyler, 2007)

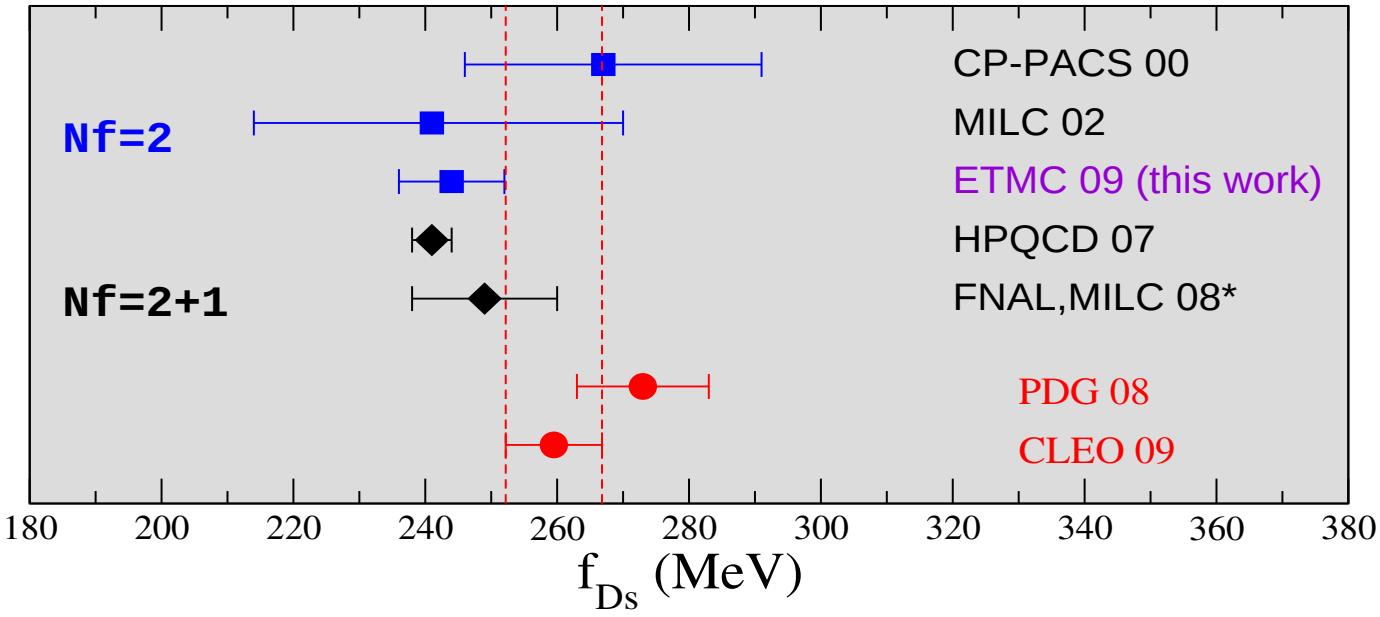


→ consistent with direct lattice calculation (X. Feng, D. Renner, K.J.)

(Strange) Baryon spectrum



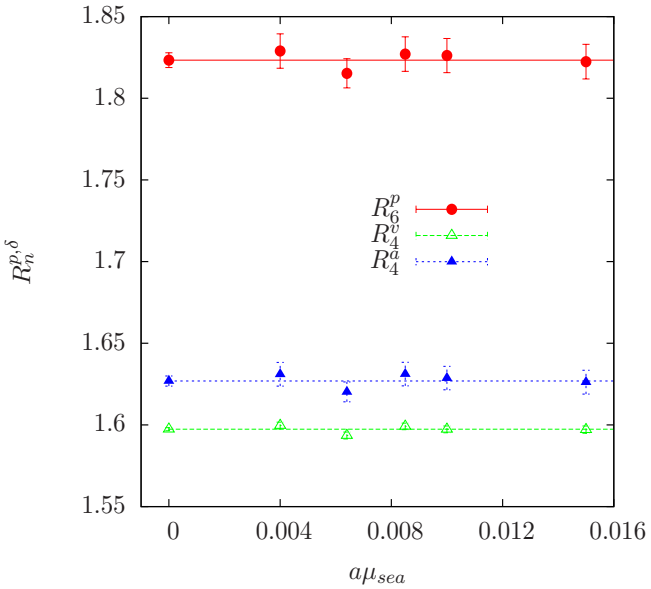
f_{D_s} a compilation (ETMC)

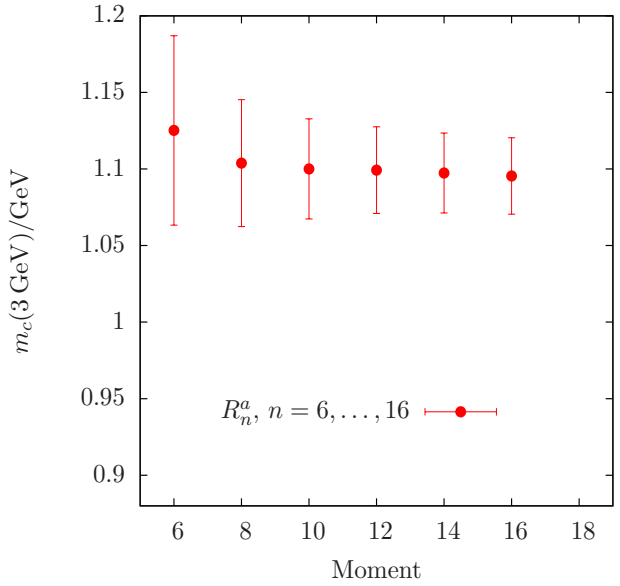


- tension with experiment very much weakened

Connection to Perturbation Theory

- **Charm quark mass from moments of correlators**
  (Petschlies, Urbach, K.J.)





$\Leftarrow$ needs input from high order loop perturbation theory

- large momentum behaviour of gluon and quark propagators,
  $\longrightarrow$ check existence of non-perturbative condensates
- lattice pertubation theory (talk by Roman Rogalyov)

Lattice in India

Chiral Anomaly in Lattice QCD with Twisted Mass Wilson Fermion

A. K. De, A. Harindranath, S. Mondal, Saha Institue of Nuclear Physics, Kolkata

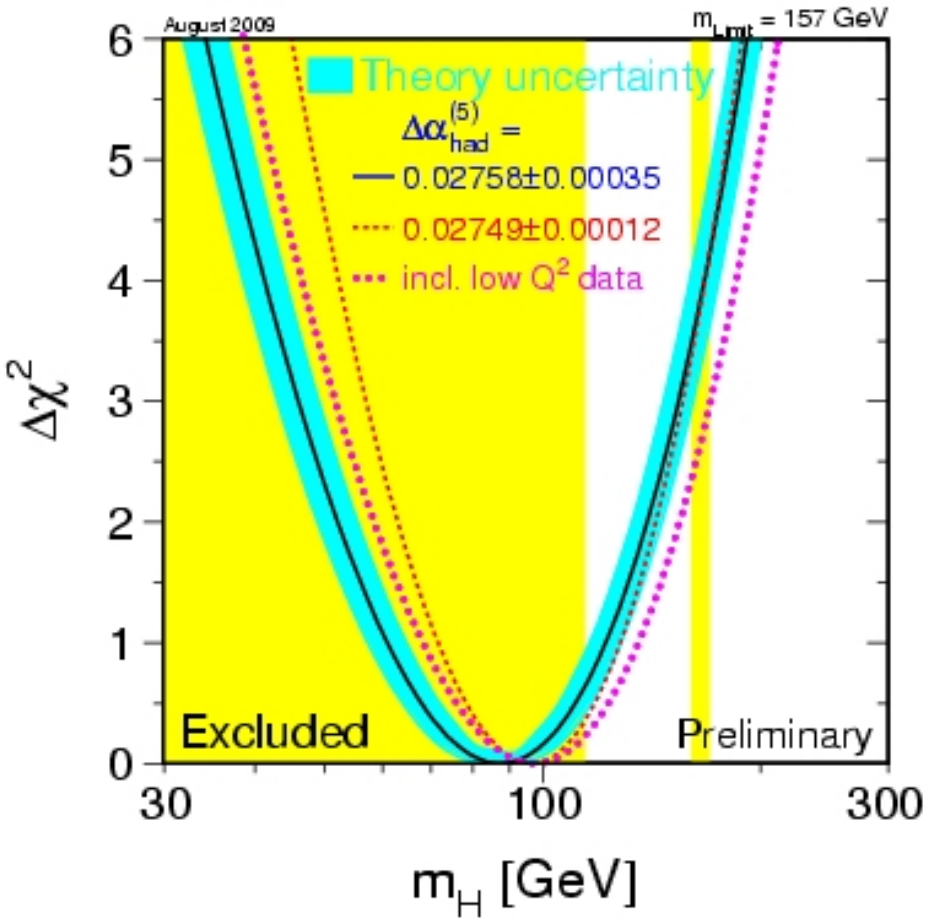
Thermodynamics of the ideal overlap quarks on the lattice

D. Banerjee, R.V. Gavai, S. Sharma, Tata Inst. of Fundamental Research, Mumbai

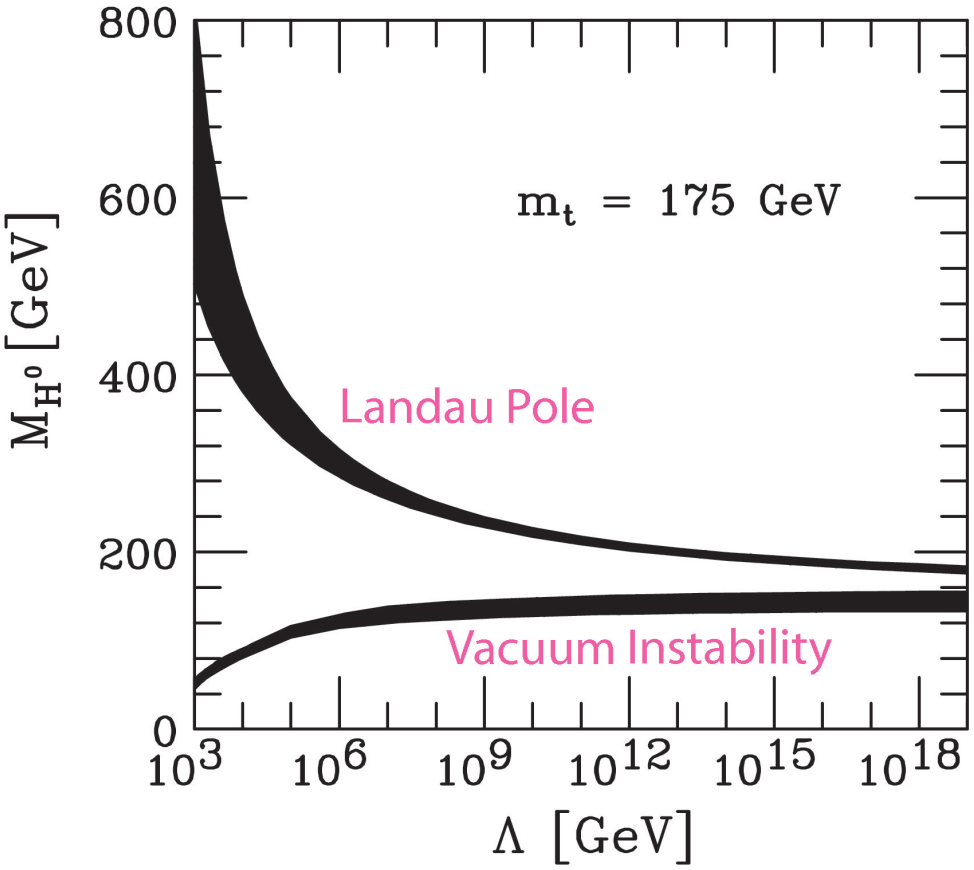
Properties of the SU(N(c)) Gluon Plasma

S. Datta, S. Gupta, Tata Inst. of Fundamental Research, Mumbai

Experimental bounds on the Higgs boson mass



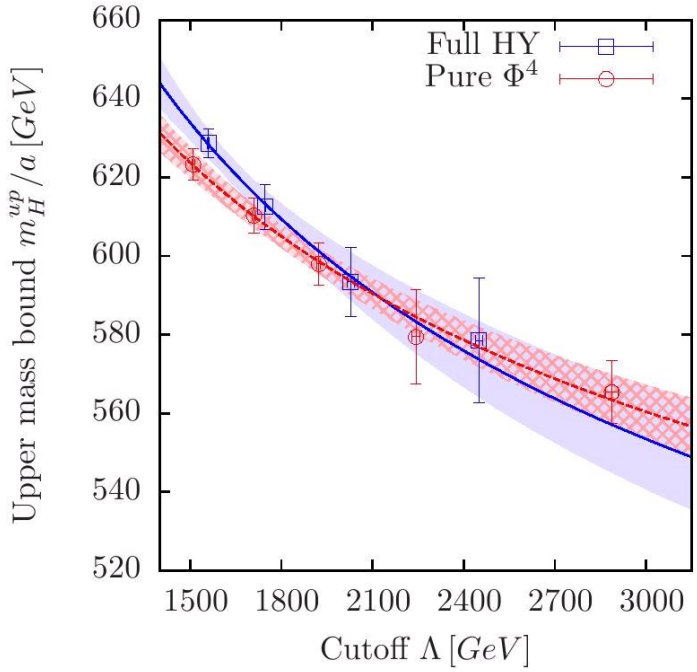
Theoretical bounds on the Higgs boson mass

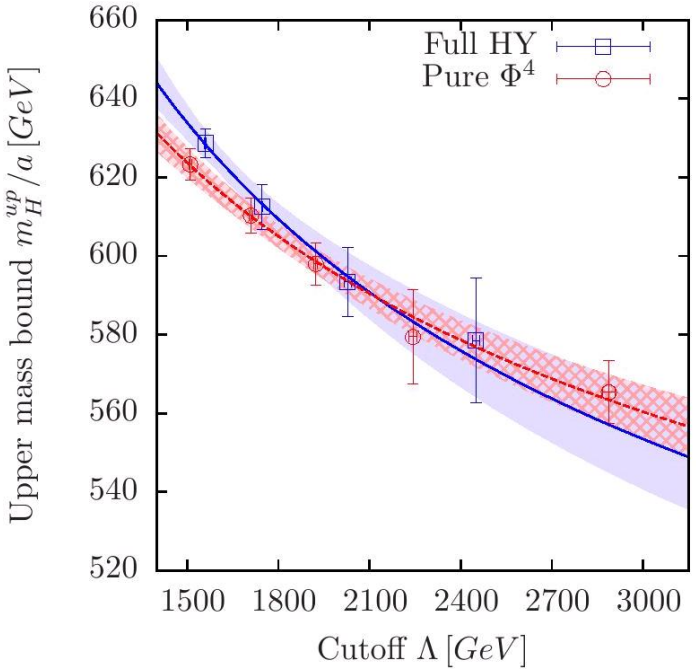


- upper bound from triviality
- lower bound from vacuum instability

Non-perturbative lattice bounds on the Higgs boson mass

P. Gerhold, K.J.



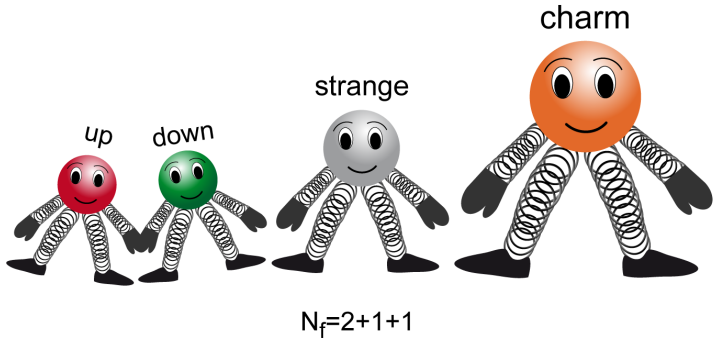
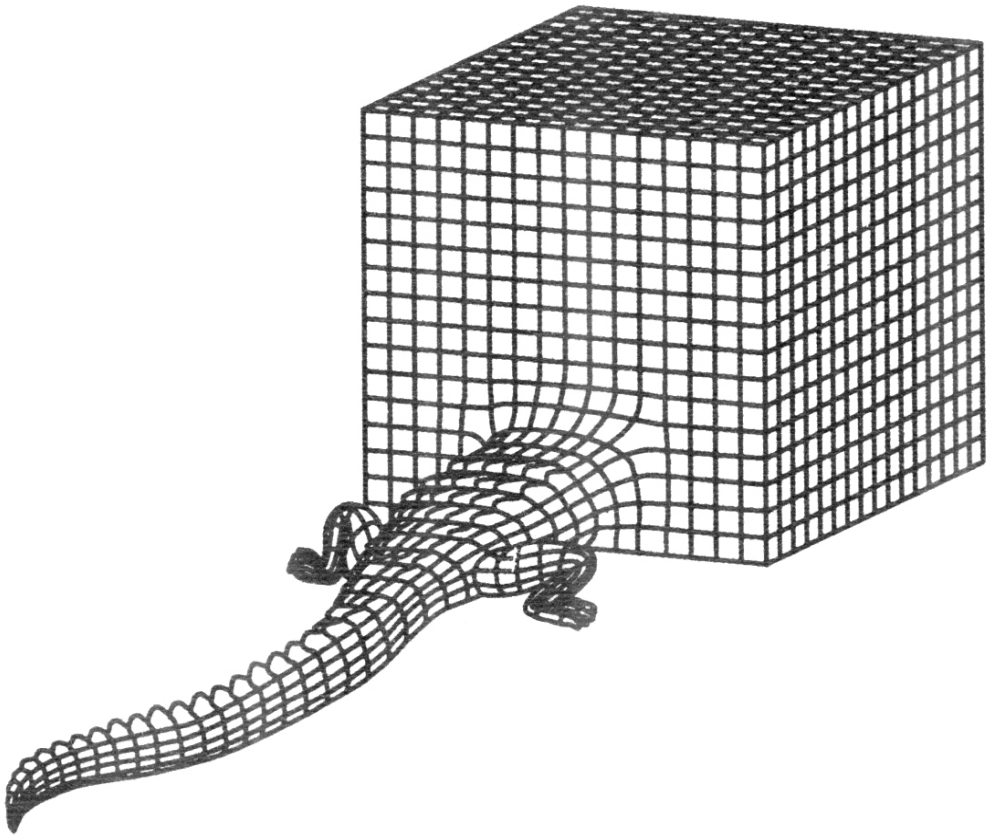


$\Rightarrow$ knowing Higgs boson mass

$\rightarrow$ determine energy scale when standard model becomes invalid

Summary

- Progress in solving QCD with lattice techniques
  - O(a)-improved fermion actions
  - dramatic algorithm improvements
  - new supercomputer architectures
- offers possibility to
  - compute bound states of the strong interactions
  - decay constants, matrix elements, form factors, ...
  - determine non-perturbative bounds of Higgs boson mass
- many challenges
  - glueball spectrum, resonances, scattering processes
  - include strange and charm degrees of freedom
  - simulations at physical point



Goodbye from the lattice and to the alligator