Introduction to Lattice QCD II

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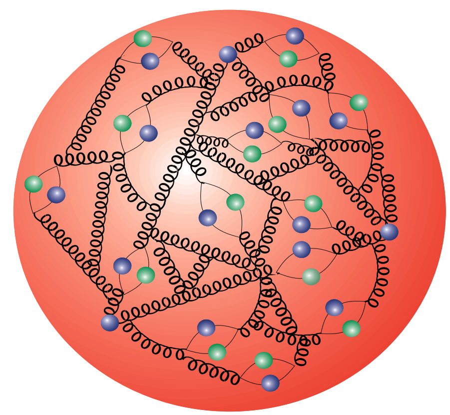
- **Task: compute the proton mass**



  - need an action
  - need an algorithm
  - need an observable
  - need a supercomputer

- **Anomalous magnetic moment of Muon**

Quantum Chromodynamics

Quantization via Feynman path integral

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

Fermion action

$$S_{\text{ferm}} = \int d^4x \bar{\Psi}(x) \left[\gamma_\mu D_\mu + m\right] \Psi(x)$$

gauge covriant derivative

$$D_\mu \Psi(x) \equiv (\partial_\mu - ig_0 A_\mu(x))\Psi(x)$$

with A_μ gauge potential, g_0 bare coupling, m bare quark mass

$$S_{\text{gauge}} = \int d^4x F_{\mu\nu} F_{\mu\nu}\ ,\ F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) + i\left[A_\mu(x), A_\nu(x)\right]$$

Lattice Gauge Theory had to be invented

$\rightarrow$ QuantumChromoDynamics

asymptotic freedom		confinement
distances $\ll 1\mathrm{fm}$		distances $\gtrsim 1\mathrm{fm}$
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

Reminder: Wilson fermions

introduce a 4-dimensional lattice with lattice spacing a

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

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

discretized fermion action

$$S \to a^4 \sum_x \bar{\Psi} \left[\gamma_\mu \partial_\mu - r \underbrace{\partial_\mu^2}_{\nabla_\mu^* \nabla_\mu} + m\right] \Psi(x) \quad , \qquad \partial_\mu = \frac{1}{2}\left[\nabla_\mu^* + \nabla_\mu\right]$$

discrete derivatives

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

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

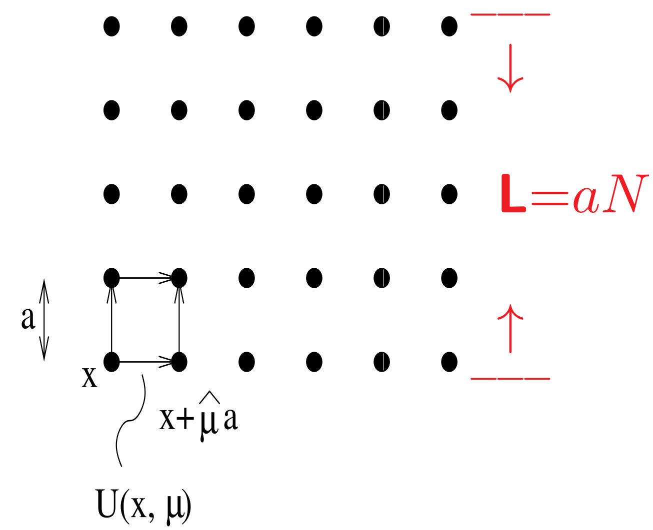
Nielsen-Ninimiya theorem: *The theorem simply states the fact that the Chern number is a cobordism invariant* (Friedan)

Reminder: Gauge fields

Introduce *group*-valued gauge field $U(x,\mu) \in \mathrm{SU}(3)$

Relation to gauge potential

$$U(x,\mu) = \exp(iaA_\mu^b(x)T^b) = 1 + iaA_\mu^b(x)T^b + \ldots$$



Discretization of the field strength tensor

$\Leftarrow$ principle of *local gauge invariance*

$$U(x,\mu)U(x+a\hat{\mu},\nu) - U(x,\nu)U(x+a\hat{\nu},\mu) = ia^2F_{\mu\nu}(x) + O(a^3)$$

$$F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) + i[A_\mu(x), A_\nu(x)]$$

Action for the gauge field, $(\beta = 6/g^2)$, plaquettes $\square$ (K.G. Wilson, 1974)

$$\boxed{S_{\mathrm{w}}(U) = \sum_\square \beta\left\{1 - \tfrac{1}{3}\mathrm{Re}\,\mathrm{tr}\,(U_\square)\right\} \xrightarrow{a\to 0} \tfrac{1}{2g^2}a^4\sum_x \mathrm{tr}\,(F_{\mu\nu}(x)^2) + O(a^6)}$$

Implementing gauge invariance

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

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

$\Rightarrow$ 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 Quantum Chromodynamics

Wilson Dirac operator

(K.G. Wilson, 1974)

$$D = m + \gamma_\mu D_\mu \rightarrow \quad \boxed{D_{\mathrm{w}} = m_q + \tfrac{1}{2}\{\underbrace{\gamma_\mu(\nabla_\mu + \nabla^\star_\mu)}_{\text{naive}} - \underbrace{a\nabla^\star_\mu \nabla_\mu}_{\text{Wilson}}\}}$$

bare quark mass m_q

gauge covariant lattice derivatives

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

$$\boxed{S_{\text{fermion}} = a^4 \textstyle\sum_x \bar{\Psi}(x) D_{\mathrm{w}} \Psi(x)}$$

Physical Observables

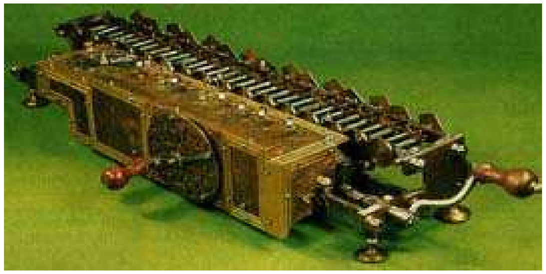
expectation value of physical observables $\mathcal{O}$

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

$\downarrow$ lattice discretization

$$0101110001110001110011$$

$$\downarrow$$



Monte Carlo Method

$$\langle f(x)\rangle = \int dx f(x) e^{-x^2}$$

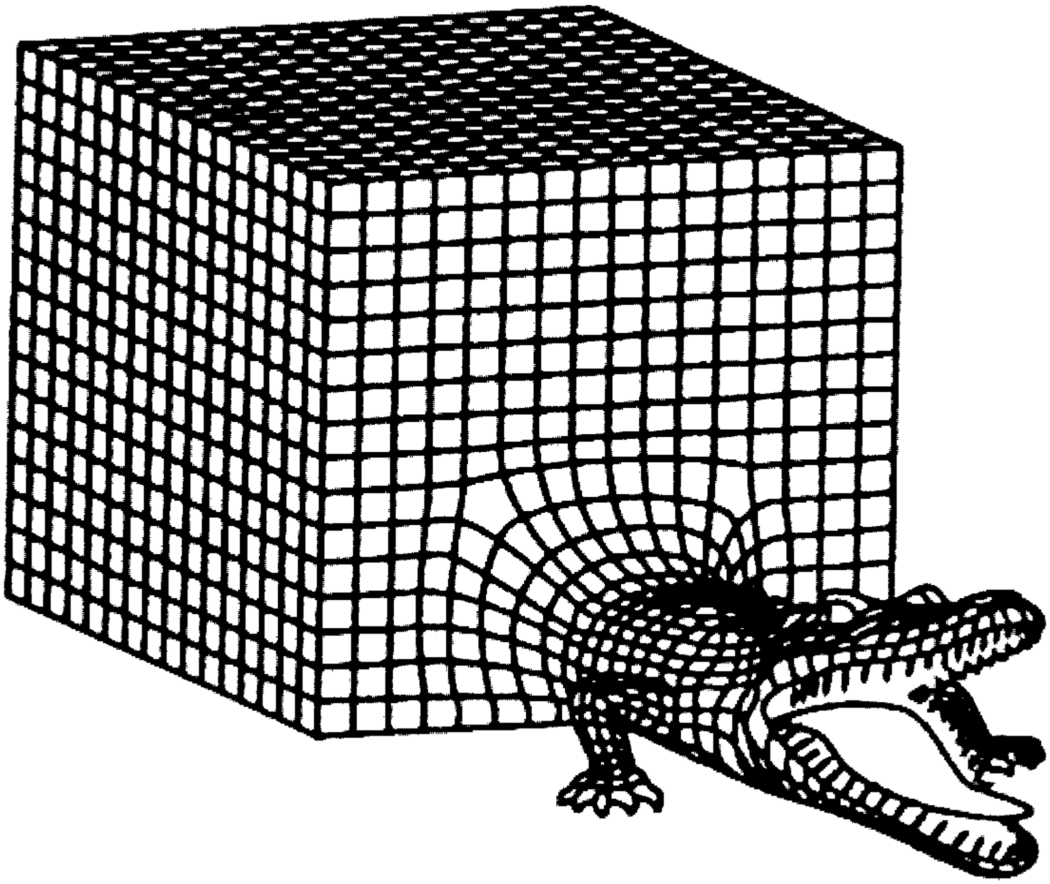
$\rightarrow$ importance sampling:
select points $x_i, i = 1, \cdots N$ with x_i Gaussian random number

$$\Rightarrow \langle f(x)\rangle \approx \frac{1}{N}\sum_i f(x_i)$$

Quantum Field Theory/Statistical Physics:

- sophisticated methods to generate the Boltzmann distribution e^{-S}
- x_i become *field configurations*
- $\langle . \rangle$ become physical observables

There are dangerous lattice animals



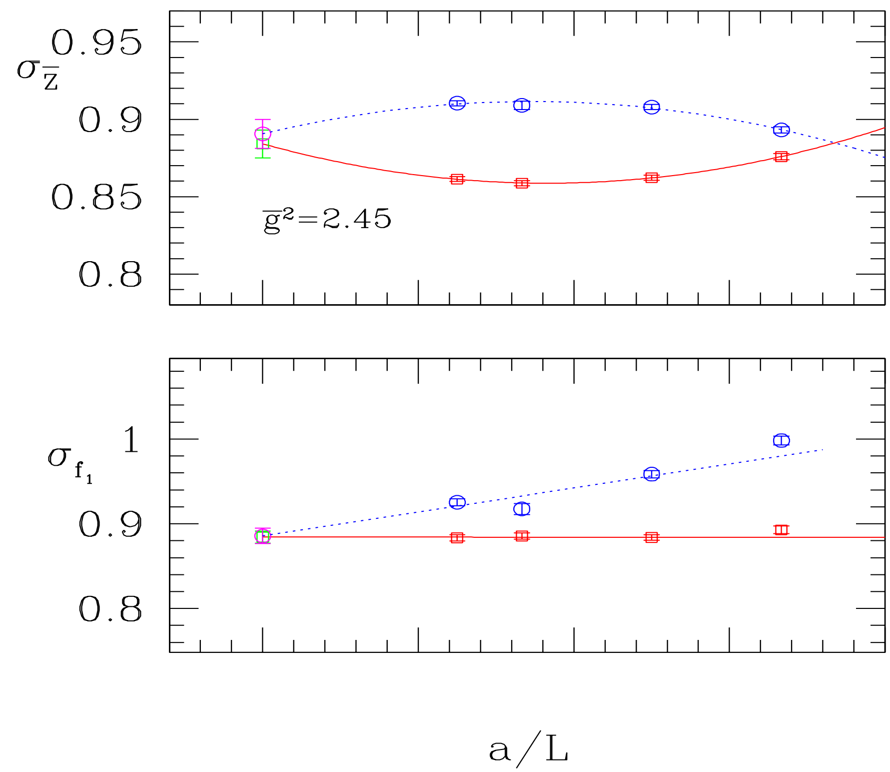
Wilson's Lattice Quantum Chromodynamics

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

lattice artefacts appear linear in a

→ possibly large lattice artefacts
$\Rightarrow$ need of fine lattice spacings
$\Rightarrow$ large lattices
(want $L = N \cdot a = 1\mathrm{fm}$ fixed)

→ simulation costs $\propto 1/a^{6-7}$



present (Wilson-type) solutions:

- clover-improved Wilson fermions
- maximally twisted mass Wilson fermions
- overlap/domainwall fermions ← 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:

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

$\rightarrow$ 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)

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

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

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

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

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

O(a) improvement

Symanzik expansion

$$\langle\mathcal{O}\rangle|_{(m_q,r)} = [\xi(r) + am_q\eta(r)]\,\langle\mathcal{O}\rangle|^{\rm cont}_{m_q} + a\chi(r)\,\langle\mathcal{O}_1\rangle|^{\rm cont}_{m_q}$$

$$\langle\mathcal{O}\rangle|_{(-m_q,-r)} = [\xi(-r) - am_q\eta(-r)]\,\langle\mathcal{O}\rangle|^{\rm cont}_{-m_q} + a\chi(-r)\,\langle\mathcal{O}_1\rangle|^{\rm cont}_{-m_q}$$

Using symmetry: $R_5 \times (r \to -r) \times (m_q \to -m_q)$, $R_5 = e^{i\omega\gamma_5\tau^3}$

- *mass average:* $\frac{1}{2}\left[\langle\mathcal{O}\rangle|_{m_q,r} + \langle\mathcal{O}\rangle|_{-m_q,r}\right] = \langle\mathcal{O}\rangle|^{\rm cont}_{m_q} + O(a^2)$
- *Wilson average:* $\frac{1}{2}\left[\langle\mathcal{O}\rangle|_{m_q,r} + \langle\mathcal{O}\rangle|_{m_q,-r}\right] = \langle\mathcal{O}\rangle|^{\rm cont}_{m_q} + O(a^2)$
- *automatic $O(a)$ improvement*
  $\rightarrow$ special case of mass average: $m_q = 0$

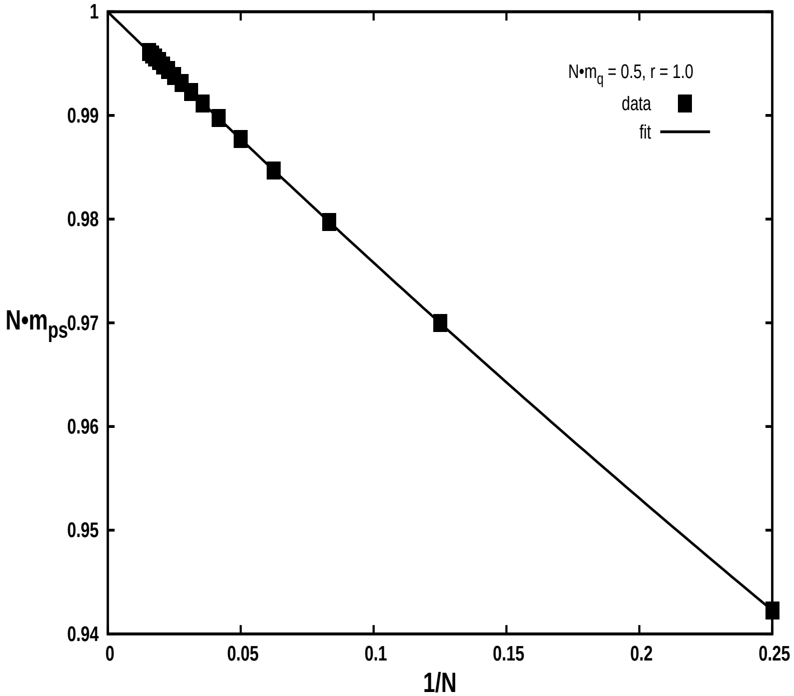
$$\Rightarrow \langle\mathcal{O}\rangle|_{m_q=0,r} = \langle\mathcal{O}\rangle|^{\rm cont}_{m_q} + O(a^2\ )$$

A first test: experiments in the free theory

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

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

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

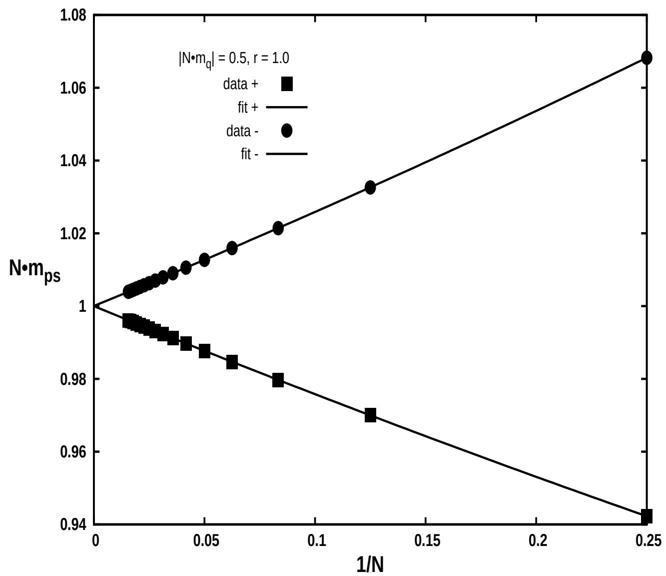


Scaling for pure Wilson fermions

at $Nm_q = 0.5$

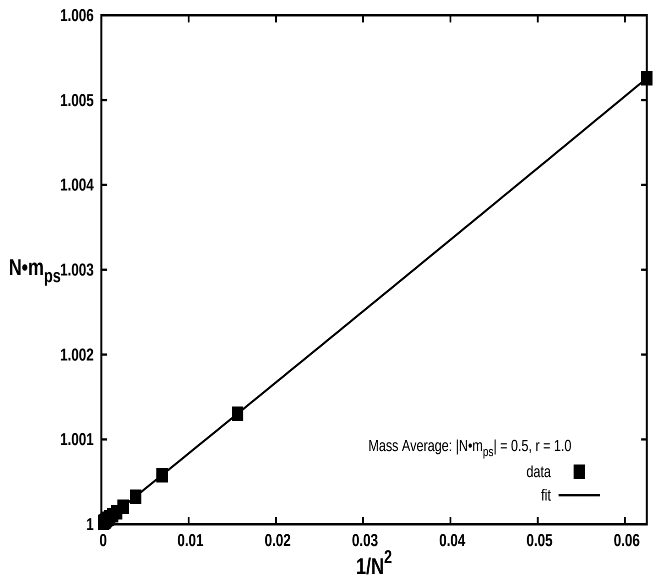
$N \cdot m_\pi$ versus $\mathbf{1/N} = a$

Averaging over the mass



Wilson fermions at $Nm_q = \pm 0.5$

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

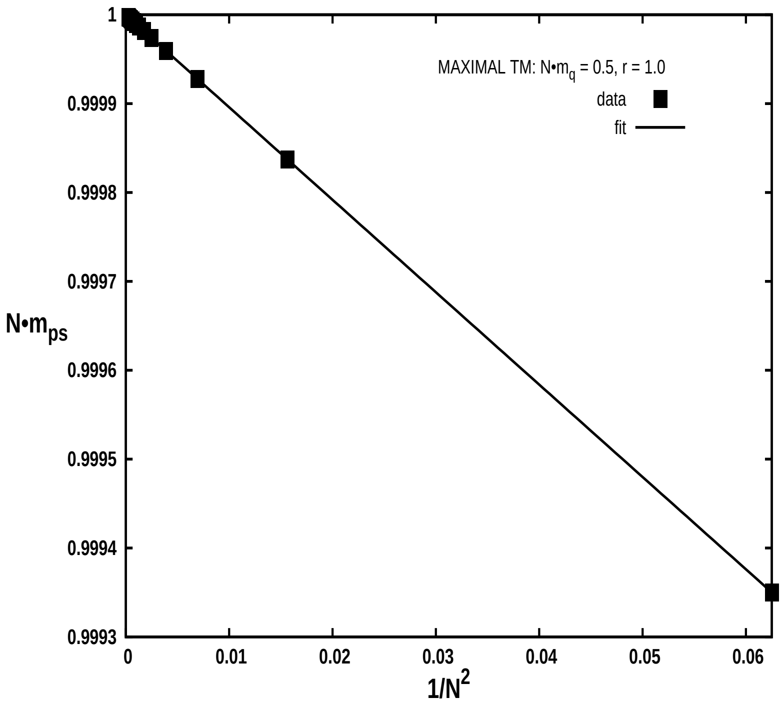


Averaging Wilson fermions at $Nm_q = \pm 0.5$

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

Twisted mass at maximal twist

choosing $m_q = 0 \quad \Rightarrow \quad \omega = \pi/2$



maximally twisted mass fermions

at $N\mu = 0.5$

$N \cdot m_\pi$ 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

Decide for an action

ACTION	ADVANTAGES	DISADVANTAGES
clover improved Wilson	computationally fast	breaks chiral symmetry needs operator improvement
twisted mass fermions	computationally fast automatic improvement	breaks chiral symmetry violation of isospin
staggered	computationally fast	fourth root problem complicated contraction
domain wall	improved chiral symmetry	computationally demanding needs tuning
overlap fermions	exact chiral symmetry	computationally expensive

For all actions: $O(a)$-improvement

$\Rightarrow \langle O^{\rm latt}_{\rm phys}\rangle = \langle O^{\rm latt}_{\rm cont}\rangle + O(a^2)$

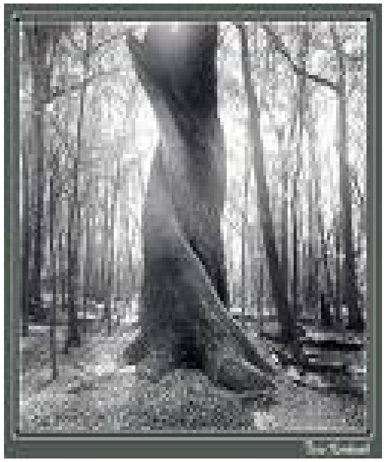
Here, example of twisted mass fermions

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

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

quark mass parameter m_q , twisted mass parameter μ

- $m_q = m_{\mathrm{crit}} \rightarrow$ O(a) improvement for
  hadron masses, matrix elements, form factors, decay constants
- $\det[D_{\mathrm{tm}}] = \det[D^2_{\mathrm{Wilson}} + \mu^2]$
  $\Rightarrow$ protection against small eigenvalues
- computational cost comparable to Wilson
- simplifies mixing problems for renormalization
- no operator specific improvement coefficients
- natural to twist



$\star$ **based on symmetry arguments**

Drawback: *explicit breaking of isospin symmetry for any* $a > 0$
$\Rightarrow$ possibly large cut-off effects in isospin zero sector

Need an algorithm

Molecular Dynamics

follow discussion of S. Chanddrasekar, Rev.Mod.Phys. 15 (1943) 1

Brownian motion [free particle in a fluid]

famous description

Langevin equation [stochastic differential equation]

$$\dot{\pi} = -\gamma\pi + \eta(t)$$

π particle momentum, γ friction coefficient

$\eta(t)$ Gaussian white noise: $< \eta(t) >= 0$
$< \eta(t)\eta(t') >= \delta(t - t')$

for a finite interval Δt we have

$$\pi(t + \Delta t) = \pi(t) - \gamma\pi(t)\Delta t + \int_t^{t+\Delta t} dt' \eta(t') \quad (1)$$

consider probability $P(\pi, t)$ to find a particle with momentum π at time t :

$$P(\pi + \Delta\pi, t + \Delta t) = \int d(\Delta\pi) P(\pi, t) W(\pi, \Delta\pi)$$

$W(\pi, \Delta\pi)$ *transition probability* that π
suffers an increment $\Delta\pi$ in the time interval Δt

transition probability determined from Gaussian noise:

$$W(\pi, \Delta\pi) = e^{-\int_0^{\Delta t} dt \eta(t)}$$

remember that $\Delta\pi = -\gamma\pi\Delta t + \int_0^{\Delta t} \eta(t)$

we can perform the integral and obtain

$$P(\pi + \Delta\pi, t + \Delta t) = e^{-(\gamma\pi + \int_0^{\Delta t} \eta(t))^2}$$

equation for the probabilities is equivalent to the Langevin equation

Taylor expansion $P(\pi + \Delta\pi, t + \Delta t)$, $W(\pi, \Delta\pi)$ in

$$P(\pi + \Delta\pi, t + \Delta t) = \int d(\Delta\pi) P(\pi, t) W(\pi, \Delta\pi)$$

find another equivalent description: Fokker-Planck equation

P probability to find a particle with momentum π at time t

$$\frac{\partial P(\pi,t)}{\partial t} = \gamma \frac{\partial}{\partial \pi}(\pi P) + \frac{1}{2}\frac{\partial^2 P}{\partial \pi^2}$$

this equation has a solution at infinite time:

$$\lim_{t\to\infty} P(\pi, t) \propto \exp\left\{-\frac{\gamma}{2}\pi^2\right\}$$

is a time independent stationary solution of the Fokker-Planck equation:
Maxwell distribution

Brownian motion in an external field

1.) External force $F = -\partial/\partial x V(x)$

2.) Consider stochastic differential equations for momenta π and the coordinates x, (η "white noise")

$$\begin{aligned} m\dot{x} &= \pi \\ \dot{\pi} &= -\gamma\pi + F + \eta(t) \end{aligned}$$

Equivalent generalized Fokker-Planck equation combined probability P of x and π

$$\frac{\partial P(x,\pi,t)}{\partial t} + \pi\frac{\partial P}{\partial x} + F(x)\frac{\partial P}{\partial \pi} = \gamma\frac{\partial}{\partial \pi}(\pi P) + \frac{1}{2}\frac{\partial^2 P}{\partial \pi^2}$$

Kramers equation

stochastic differential equation is called Kramers equation in Langevin form

stationary distribution $\lim_{t\to\infty} P(x,\pi,t) \propto e^{-\frac{\gamma}{2}\pi^2} e^{-V(x)}$

Monte Carlo Method

$$\langle f(x)\rangle = \int dx f(x) e^{-x^2} / \int dx e^{-x^2}$$

$\rightarrow$ solve numerically:

- at computer time τ_0 generate Gaussian random number x_0
- at computer time τ_i generate Gaussian random number x_i
- do this N-times

$$\Rightarrow \langle f(x)\rangle \approx \frac{1}{N}\sum_i f(x_i)$$

Monte Carlo Method

what if integral is more complicated?

$$\langle f(x)\rangle = \int dx f(x)e^{-V(x)} / \int dx e^{-V(x)}$$

write

$$\langle f(x)\rangle = \int dx \int d\pi f(x) \underbrace{e^{-\pi^2/2-V(x)}}_{e^H} / \int dx \int d\pi e^{-\pi^2/2-V(x)}$$

$\pi(t)$ Gaussian distributed: $\quad < \pi(t) >= 0$
$\qquad\qquad\qquad\qquad\qquad < \pi(t)\pi(t') >= \delta(t-t')$

$\rightarrow$ solve:

$$\begin{aligned}\dot{x} &= \pi \\ \dot{\pi} &= -\partial V(x)/\partial x\end{aligned}$$

Kramers equation: convergence to $e^{-\pi^2/2-V(x)}$ ($e^{-\pi^2/2}$ drops out)

Monte Carlo Method

$\rightarrow$ solve numerically:

- at τ_0 generate Gaussian distributed random π_0 and arbitrary x_0
- solve continuum equations

$$\begin{aligned} \dot{x} &= \pi \\ \dot{\pi} &= -\partial V(x)/\partial x \end{aligned}$$

by discrete time steps

$$\begin{aligned} x(\tau + \delta\tau) &= x(\tau) + \pi(\tau)\delta\tau \\ \pi(\tau + \delta\tau) &= \pi(\tau) - \partial V(x)/\partial x \delta\tau \end{aligned}$$

for N steps

Monte Carlo Method

non-vanishing integration step leads to discretization error

repaired by accept/reject step

$$P_{\mathrm{accept}} = \min\left(1, e^{H(x_i,\pi_i)-H(x_{i+1},\pi_{i+1})}\right)$$

$\Rightarrow \langle f(x)\rangle \approx \frac{1}{N}\sum_i f(x_i)$

find a transition probality $W(\phi, \phi')$ that brings us from a set of generic fields $\{\phi\} \to \{\phi'\}$ and which satisfies

- $W(\phi, \phi') > 0$ strong ergodicity ($W \geq 0$ is weak ergodicity)
- $\int d\phi' W(\phi, \phi') = 1$
- $W(\phi, \phi') = \int d\phi'' W(\phi, \phi'') W(\phi'', \phi')$ (Markov chain)
- $W(\phi, \phi')$ is measure preserving, $d\phi' = d\phi$

under these conditions, we are guaranteed

- to converge to a unique equilibrium distribution P^{eq} namely the Boltzmann distribution e^{-S}
- that this is independent from the initial conditions

Markov chain condition

$$W(\phi,\phi') = \int d\phi'' W(\phi,\phi'')W(\phi'',\phi')$$

can be rephrased when taking the equilibrium distribution itself

$$P(\phi') = \int d\phi W(\phi',\phi)P(\phi)$$

to fulfill (most of) our conditions it is *sufficient not neccessary* that W fulfills the detailled balance condition:

$$\frac{W(\phi,\phi')}{W(\phi',\phi)} = \frac{P(\phi')}{P(\phi)}$$

for example

$$\begin{aligned}\int d\phi P(\phi)W(\phi,\phi') &= \int d\phi P(\phi)\frac{P(\phi')}{P(\phi)}W(\phi',\phi) \\ &= \int d\phi P(\phi')W(\phi',\phi) = P(\phi')\end{aligned}$$

in the following discuss particular choices for W for problems of interest

Hybrid Monte Carlo Algorithm

expectation values in lattice field theory

$$\langle O \rangle = \frac{\int \mathcal{D}\Phi O e^{-S}}{\int \mathcal{D}\Phi e^{-S}}$$

do not change if field independent contributions are added to the action

$$\langle O \rangle = \frac{\int \mathcal{D}\Phi \int \mathcal{D}\pi O e^{-\frac{1}{2}\pi^2 - S}}{\int \mathcal{D}\Phi \int \mathcal{D}\pi e^{-\frac{1}{2}\pi^2 - S}}$$

field configurations are generated chronologically in a fictitious (computer) time τ

generation of equilibrium distribution: Langevin equation
take π's Gaussian distributed, satisfying

$$< \pi(t) >= 0, \;\; < \pi(t)\pi(t') >= \delta(t - t')$$

consider a 4-dimensional Hamiltonian

$$H = \tfrac{1}{2}\pi^2 + S$$

consider quantum mechanical action: $S = \sum_n (x(n+a) - x(n))^2 + m^2 x^2(n)$

in ficititious time τ the sytem develops according to
Hamilton's equations of motion

$$\frac{\partial}{\partial\tau}\pi(n) = -\frac{\partial}{\partial \mathbf{x(n)}} S \equiv \text{force}, \quad \frac{\partial}{\partial\tau}\mathbf{x(n)} = \pi(n)$$

$\Rightarrow$ conservation of energy

in practise, equations areeintegrated numerically up to time $T = 1$

divide T into N intervals of length $\delta\tau$ such that $T = N\delta\tau$: leap-frog scheme

$$\begin{aligned}
\pi(\delta\tau/2) &= \pi(0) - \frac{\delta\tau}{2}\frac{\partial}{\partial\mathbf{x}}S\Big|_{\mathbf{x}(0)} \\
\mathbf{x}(\delta\tau) &= \mathbf{x}(0) + \pi(\delta\tau/2)\delta\tau \\
\pi(3\delta\tau/2) &= \pi(\delta\tau/2) - \delta\tau\frac{\partial}{\partial\mathbf{x}}S\Big|_{\mathbf{x}(\delta\tau)} \\
&\vdots \\
\pi(T) &= \pi(N\delta\tau/2) - \frac{\delta\tau}{2}\frac{\partial}{\partial\mathbf{x}}S\Big|_{\mathbf{x}((N-1)\delta\tau)}
\end{aligned}$$

leap-frog scheme has a *finite* step-size $\delta\tau \Rightarrow$ energy is no longer conserved

$$H(\mathbf{x}_{\mathrm{in}}, \pi_{\mathrm{in}}) \neq H(\mathbf{x}_{\mathrm{end}}, \pi_{\mathrm{end}})$$

introduce a Metropolis like accept/reject step

accept new field configuration $\{\mathbf{x}_{\mathrm{end}}, \pi_{\mathrm{end}}\}$ with a probability

$$P_{\mathrm{accept}} = \min\left(1, e^{H(\mathbf{x}_{\mathrm{in}}, \pi_{\mathrm{in}}) - H(\mathbf{x}_{\mathrm{end}}, \pi_{\mathrm{end}})}\right)$$

Hybrid Monte Carlo algorithm

- fulfills detailled balance Exercise: proof this
  $\Leftarrow$ needs *reversibility* of the leap-frog integrator
- preserves measure
- Ergodicity?

The case of Lattice QCD

action for two flavors of fermions (up and down quark)

$$S = a^4 \sum_x \bar{\psi} M^\dagger M \psi$$

path integral

$$\mathcal{Z} = \prod_x d\bar{\psi}(x) d\Psi(x) e^{-S} = \prod_x d\Phi^\dagger(x) d\Phi(x) e^{-\Phi^\dagger \left[M^\dagger M\right]^{-1} \Phi}$$

interaction of the scalar fields is very complicated: inverse fermion matrix $\left[M^\dagger M\right]^{-1}$ couples all points on the lattice with each other

simulate with Hybrid Monte Carlo algorithm

$$\begin{aligned} \frac{d}{d\tau}\pi &= -\frac{dS}{d\Phi^\dagger} = \left[M^\dagger M\right]^{-1} \Phi \equiv \text{force} \\ \frac{d}{d\tau}\Phi &= \pi \end{aligned}$$

update of the momenta $\pi(x)$ is completely independent of update of Φ -field, non-locality of the action is not a problem to update the momenta, have to compute the vector

$$X = \left[M^\dagger M\right]^{-1} \Phi$$

$\Rightarrow$ solve an equation

$$\left[M^\dagger M\right] X = \Phi$$

Exercise:

estimate the number of flops to apply the twisted mass operator on a vector

assume you want to have 2000 thermalization and 5000 measurement steps on a $48^3 \cdot 96$ lattice

assume number of iterations to solve $\left[M^\dagger M\right] X = \Phi$ is 500

assume number of time steps in the HMC is 100

How long would the program run on your laptop?
(assume –unrealistic– efficiency of 50%)

If you save the 5000 configurations, would this fit on your laptop disk?

autocorrelation times

generating field configurations as a Markov process,
$\Rightarrow$ configurations are not independent from each other

free field theory again in Fourier space

$$S = \int d^4k \mathbf{x}(k)[k^2 + m_0^2]\mathbf{x}(k)$$

Langevin equation

$$\frac{d}{d\tau}\mathbf{x}(k,\tau) = -[k^2 + m_0^2]\mathbf{x}(k,\tau) + \eta(k,\tau)$$

then a solution may be written down

$$\mathbf{x}(k,\tau) = \int^{\tau} ds \exp\left\{-(\tau - s)[k^2 + m_0^2]\eta(k,s)\right\}$$

compute correlation of fields at $\tau = 0$ with fields at τ

consider the autocorrelation function

$$
\begin{aligned}
C(k,\tau) &= \mathbf{x}(k,0)\mathbf{x}(k,\tau) \\
&= \int ds_1 ds_2 \exp\left\{[k^2+m_0^2]s_1\left(-(\tau-s)[k^2+m_0^2]\right)\right. \\
&\qquad\qquad \left.\eta(k,s_1)\eta(k,s_2)\right\} \\
&\propto \frac{e^{-[k^2+m_0^2]\tau}}{k^2+m_0^2} \equiv \frac{e^{-\tau/\tau_0}}{k^2+m_0^2}
\end{aligned}
$$

- the autocorrelation function $C(k,\tau)$ decays exponentially autocorrelation time τ_0
- decay is lowest for the zero mode $k=0$
- $\tau \propto 1/m_0^2 \quad \Rightarrow$ the correlations become stronger closer to the critical point $m_0 = 0 \rightarrow$ *critical slowing down*
- scaling law $\tau_0 \propto 1/m^z$, $\quad z$ *the dynamical critical exponent*

A consequence from autocorrelations: Errors

measure average position of qunatum mechanical particle $\bar{x}$ from N measurements

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

This has a <u>variance</u>

$$\sigma = \frac{1}{N-1}\left(\bar{x^2} - \bar{x}^2\right)$$

and a standard deviation

$$\Delta_0 \equiv \sqrt{\sigma} \propto 1/\sqrt{N} \;\; \text{for} \;\; N \gg 1$$

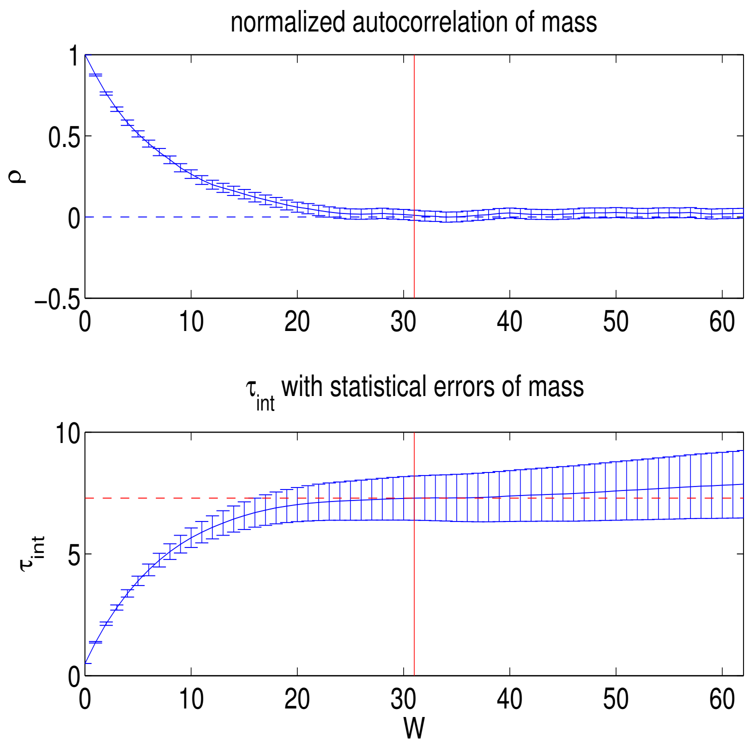
If we have an autocorrelation time $\tau \Rightarrow$ statistics reduces to $n = N/\tau$

$\Rightarrow \Delta_{\text{true}} \propto 1/\sqrt{n} = \sqrt{\tau}/\sqrt{N} = \sqrt{\tau}\Delta_0$

How to deal with the autocorrelation?

measure it:

$$\Gamma(\tau) = \langle x(\tau) \cdot x(0) \rangle / \langle x(0) \rangle^2 \propto e^{-\tau/\tau_{\rm int}}$$



Comment: *integrated auto correlation time* $\tau_{\rm int}$ observable dependent

The observable

QCD: the Mass Spectrum

goal: non-perturbative computation of bound state spectrum

$\rightarrow$ euclidean correlation functions
Reconstruction theorem relates this to Minkowski space

operator $O(\mathbf{x}, t)$ with quantum numbers of a given particle

correlation function decays exponentially: e^{-Et} , $E^2 = m^2 + \mathbf{p}^2$
$\Rightarrow$ mass obtained at zero momemtum

$$O(t) = \sum_{\mathbf{x}} O(\mathbf{x}, t)$$

correlation function

$$\begin{aligned} \langle O(0)O(t)\rangle &= \frac{1}{\mathcal{Z}} \sum_n \langle 0|O(0)e^{-\mathbf{H}t}|n\rangle\langle n|O(0)|0\rangle \\ &= \frac{1}{\mathcal{Z}} \sum_n |\langle 0|O(0)|n\rangle|^2 e^{-(E_n - E_0)t} \end{aligned}$$

connected correlation function

$$\lim_{t\to\infty}\left[\langle O(0)O(t)\rangle - |\langle O(0)\rangle|^2\right] \propto e^{-E_1 t}$$

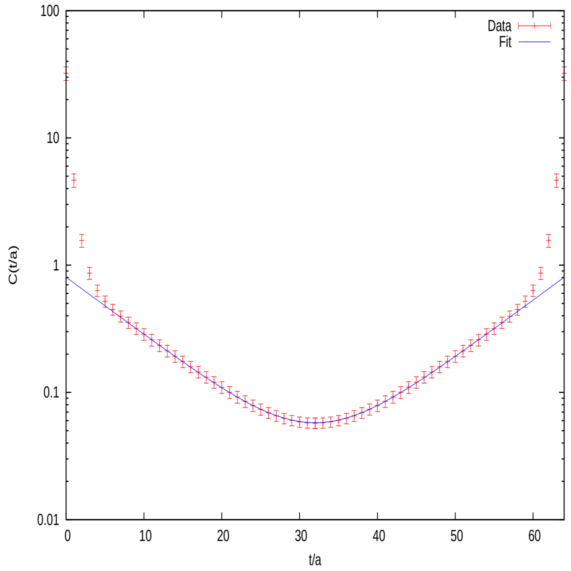
vanishing of connected correlation function at large times

$\rightarrow$ cluster property $\Rightarrow$ *locality of the theory*

periodic boundary conditions

$\langle O(0)O(t)\rangle_c = \sum_n c_n \left[e^{-E_n t} + e^{-E_n (T-t)}\right]$

$1 \ll t \ll T: \quad \langle O(0)O(t)\rangle_c \propto e^{-mt} + e^{-m(T-t)}$



Hadron Spectrum in QCD

hadrons are bound states in QCD

- mesons pion, kaon, eta, ...
- baryons neutron, proton, Delta, ..

for the computation of the hadon spectrum

- construct operators with the suitable quantum numbers
- compute the connected correlation function
- take the large time limit of the correlation function

Lorentz symmetry, parity and charge conjugation

rotational symmetry $\rightarrow$ hypercubic group: discrete rotations and reflections
classification of operators: irreducible representations R
(note hypercubic group is a subgroup of $SO(3)$)

parity	charge conjugation
$\Psi(\mathbf{x},t) \rightarrow \gamma_0 \Psi(-\mathbf{x},t)$	$\Psi(\mathbf{x},t) \rightarrow C\bar{\Psi}^T(\mathbf{x},t)$
$\bar{\Psi}(\mathbf{x},t) \rightarrow \bar{\Psi}(-\mathbf{x},t)\gamma_0$	$\bar{\Psi}(\mathbf{x},t) \rightarrow -\Psi^T(\mathbf{x},t)C^{-1}$

C charge conjugation matrix $C = \gamma_0\gamma_2$
C satisfies

$$C\gamma_\mu C^{-1} = -\gamma_\mu^T = -\gamma_\mu^*$$

Contraction

- 2-point-function calculation

$\mathcal{O}_\Gamma(x) = \bar{\psi}\Gamma\psi(0)$

$$
\begin{aligned}
&\langle \mathcal{O}_\Gamma(x)\mathcal{O}_\Gamma(0)\rangle = \\
&\bar{\psi}(x)\Gamma\bar{\psi}(0)\psi(x)\Gamma\psi(0) \\
&= tr[\Gamma S(x,0)\Gamma S(0,x)]
\end{aligned}
\tag{2}
$$

in terms of eigenvalues and eigenvectors:

$$
tr[\Gamma S(x,0)\Gamma S(0,x)] = \sum_{\lambda_i,\lambda_j} \frac{1}{\lambda_i\lambda_j} \sum_{\alpha\beta\gamma\delta} \left[(\phi_j^{\dagger\alpha}(x)\Gamma_{\alpha\beta}\phi_i^{\beta}(x))(\phi_i^{\dagger\gamma}(0)\Gamma_{\gamma\delta}\phi_j^{\delta}(0)) \right]
$$

Example: pion operator $\rightarrow$ need speudoscalar operator

$$O_{\mathrm{PS}}(\mathbf{x},t) = \bar{\Psi}(\mathbf{x},t)\gamma_0\gamma_5\Psi(\mathbf{x},t)$$

correlation function

$$\begin{aligned} f_{\mathrm{PS}}(t) \equiv \langle O_{\mathrm{PS}}(0) O_{\mathrm{PS}}(t)\rangle &= \sum_{\mathbf{x}} \left[\bar{\psi}(\mathbf{x},t)\gamma_0\gamma_5\Psi(\mathbf{x},t)\right]\left[\bar{\psi}(0,0)\gamma_0\gamma_5\Psi(0,0)\right] \\ &= \sum_{\mathbf{x}} \mathrm{Tr}\left[S_F(0,0;\mathbf{x},t)\gamma_0\gamma_5 S_F(\mathbf{x},t;0,0)\gamma_0\gamma_5\right] \end{aligned}$$

used Wick's theorem and $S_F = D^{-1}$ the fermion propagator

$\Rightarrow$ need to compute inverse of the fermion matrix

$$a \ll t \ll T: \quad f_{\mathrm{PS}}(t) = \underbrace{\frac{|\langle 0|P|\mathrm{PS}\rangle|^2}{2m_{\mathrm{PS}}}}_{\equiv F_{\mathrm{PS}}^2/2m_{\mathrm{PS}}} \cdot \left(e^{-m_{\mathrm{PS}}t} + e^{-m_{\mathrm{PS}}(T-t)}\right)$$

F_{PS} pion decay constant

Effective Masses

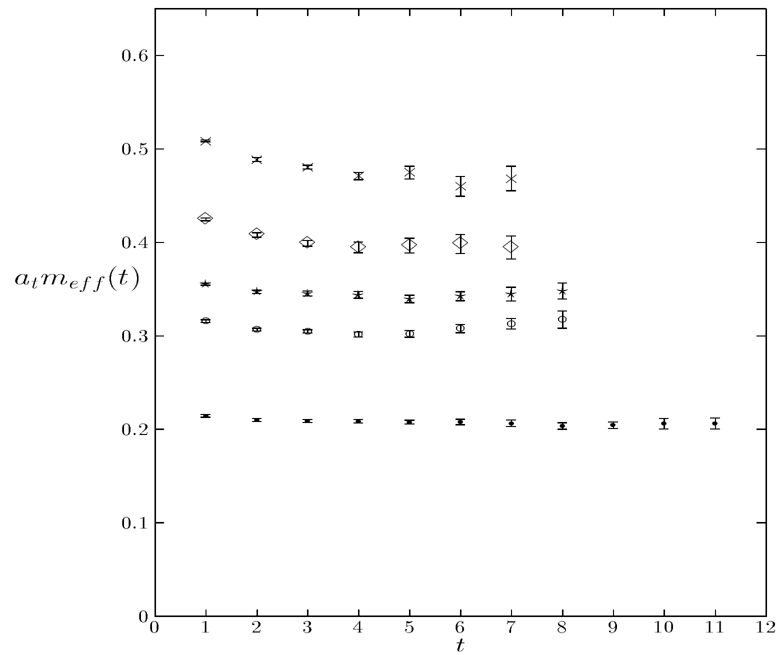
exponential deacy of correlator $\Gamma(t) = \langle O(0)O(t)\rangle_c$

define an effective mass $m_{\text{eff}}(t) = -\ln\frac{\Gamma(t+1)}{\Gamma(t)}$

periodic boundary conditions:

$f(t) = A\cosh(m_{\text{eff}}t)$

$\rightarrow$
solve $\frac{f(t+1)}{f(t)} = \frac{\Gamma(t+1)}{\Gamma(t}$)



The Proton

Nucleon: baryonic isospin-doublet, $I = \frac{1}{2}$:

proton (uud) $I_3 = +\frac{1}{2}$ and neutron (udd) $I_3 = -\frac{1}{2}$

local interpotating field of proton

$$P_\alpha(x) = -\epsilon_{abc} \left[\bar{d}_a(x)^C \gamma_5 u_b(x) \right] u_{c,\alpha}(x) \ , \quad [\ ]\,\text{spin trace}$$

u^C charged conjugate quark field

$$\psi^C(x) = C \bar{\psi}^T(x) \ , \quad \bar{\psi}^C = -\psi^T(x) C^{-1}$$

leading to

$$P_\alpha(x) = -\epsilon_{abc} \left[\bar{d}_a(x)^T C^{-1} \gamma_5 u_b(x) \right] u_{c,\alpha}(x)$$

$$\bar{P}_\beta(y) = -\epsilon_{def} u_{d,\beta}(y) \left[\bar{u}_e(y) \gamma_5 C \bar{d}_f^T(y) \right]$$

$$\Gamma_P(t) = \sum_{\vec{x}} \langle 0 | P(x) \bar{P}(0) | 0 \rangle$$

Exercise:

using the operator

$$P_\alpha(x) = -\epsilon_{abc}\left[\bar{d}_a(x)^T C^{-1}\gamma_5 u_b(x)\right] u_{c,\alpha}(x)$$

will we really get the proton?

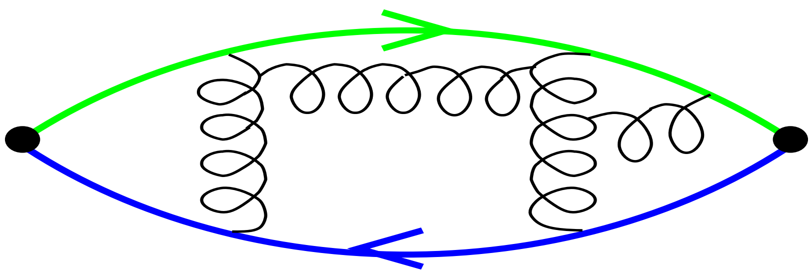
$\rightarrow$ check quantum numbers

Quenched approximation

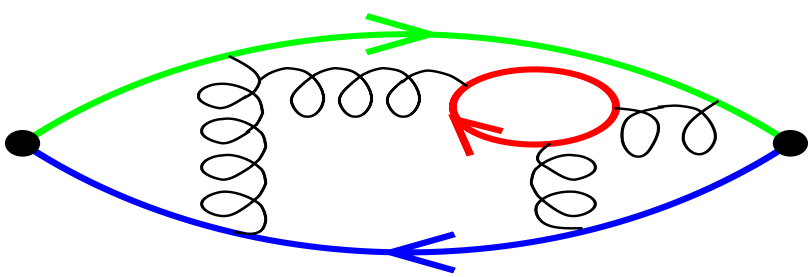
The Quenched Approximation

$\rightarrow$ neglect steady generation of quarks and antiquarks in physical quantum processes

$\Rightarrow$ *truncation*, works surprisingly well however



(A) Quenched QCD: no internal quark loops



(B) full QCD

A short history of proton mass computation

(take example of Japanese group)

1986 (Itoh, Iwasaki, Oyanagi and Yoshie)

quenched approximation, $12^3 \cdot 24$ lattice

$a \approx 0.15\mathrm{fm}$, 30 configurations

Machine: HITAC S810/20 $\rightarrow$ 630 Mflops

$\Rightarrow$ only meson masses, conclusion:
time extent of $T = 24$ too small to extract baryon ground state

1988 (plenary talk by Iwasaki at Lattice symposium at FermiLab)

quenched approximation, $16^3 \cdot 48$ lattice

$a \approx 0.11\mathrm{fm}$, 15 configurations

particle	lattice	experiment
Kaon	470(45)	494
Nucleon	866(108)	938
Ω	1697(89)	1672

The story goes on ...

1992 (Talk Yoshie at Lattice '92 in Amsterdam):

quenched approximation, $24^3 \cdot 54$ lattice

two lattice spacings: $a \approx 0.11\mathrm{fm}$, $a \approx 0.10\mathrm{fm}$, $O(200)$ configurations

Machine: QCDPAX 14 Gflops
$\Rightarrow$ worries about excited state effects
$\Rightarrow$ worries about finite size effects

1995 (paper by QCDPAX collaboration)

		stat.	sys.(fit-range)		sys.(fit-func.)		
$\beta = 6.00$	$m_N = 1.076$	± 0.060	$+0.047$	-0.020	$+0.0$	-0.017	GeV
$\beta = 6.00$	$m_\Delta = 1.407$	± 0.086	$+0.096$	-0.026	$+0.038$	-0.015	GeV

"Even when the systematic errors are included, the baryon masses at $\beta = 6.0$ do not agree with experiment. Our data are consistent with the GF11[1] data at finite lattice spacing, within statistical errors. In order to take the continuum limit of our results, we need data for a wider range of β with statistical and systematic errors much reduced."

[1] GF11 has been a 5.6Gflops machine developed by IBM research.

where the quenched story ends

2003 (Paper by CP-PACS collaboration):

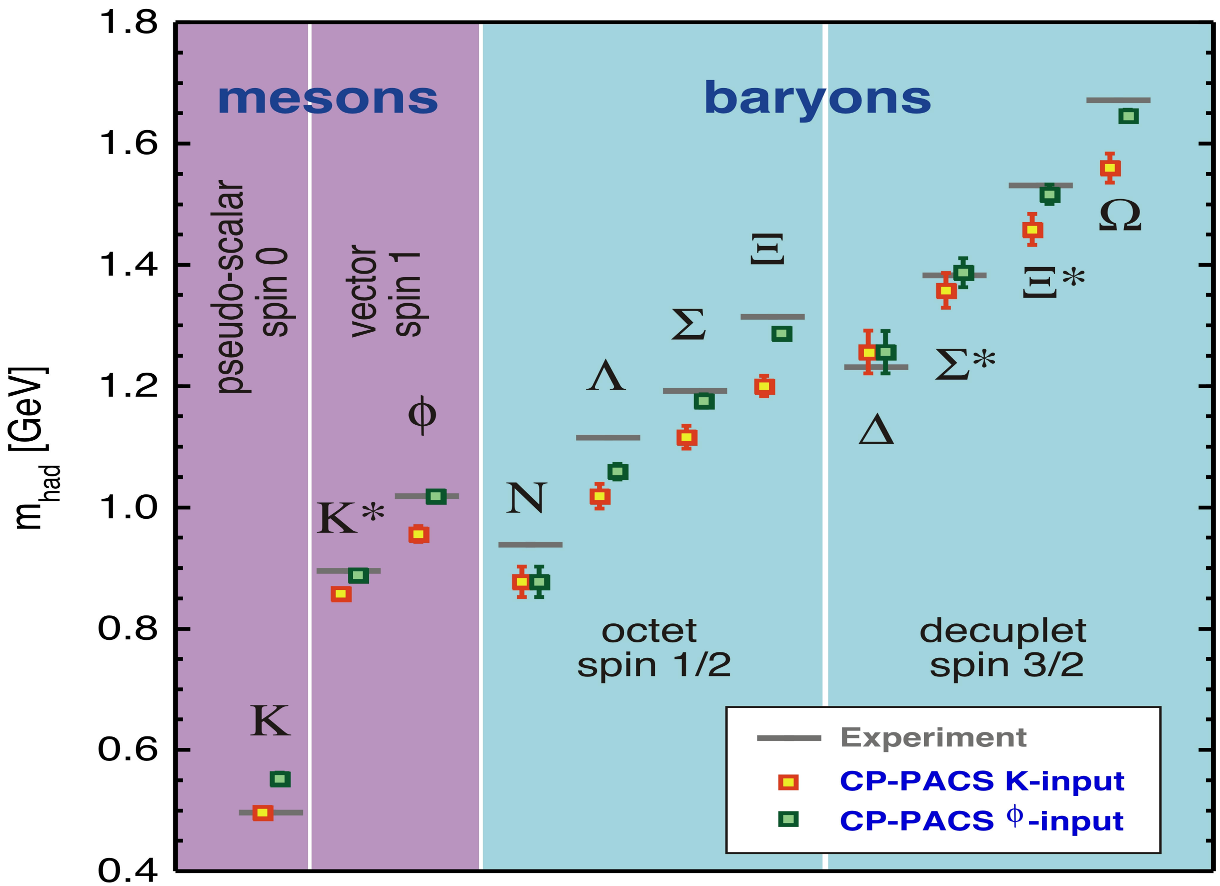
quenched approximation from $32^3 \cdot 56$ to $64^3 \cdot 112$ lattice

two lattice spacings: $a \approx 0.05\text{fm}\ - a \approx 0.10\text{fm}$, $O(150) - O(800)$configurations

Machine: CP-PACS, massively parallel, 2048 processing nodes,
completed september 1996

$\rightarrow$ reached 614Gflops

- control of systematic errors
  - finite size effects
  - lattice spacing
  - chiral extrapolation
  - excited states



quenched

quenched

CP-PACS collaboration

Solution of QCD?

$\rightarrow$ a number of systematic errors

Another example: glueballs

prediction of QCD: the existence of states made out of gluons alone, the glueballs

- hard to detect experimentally
- difficult to compute, of purely non-perturbative nature

$\Rightarrow$ challenge for lattice QCD

transformation laws for gauge links

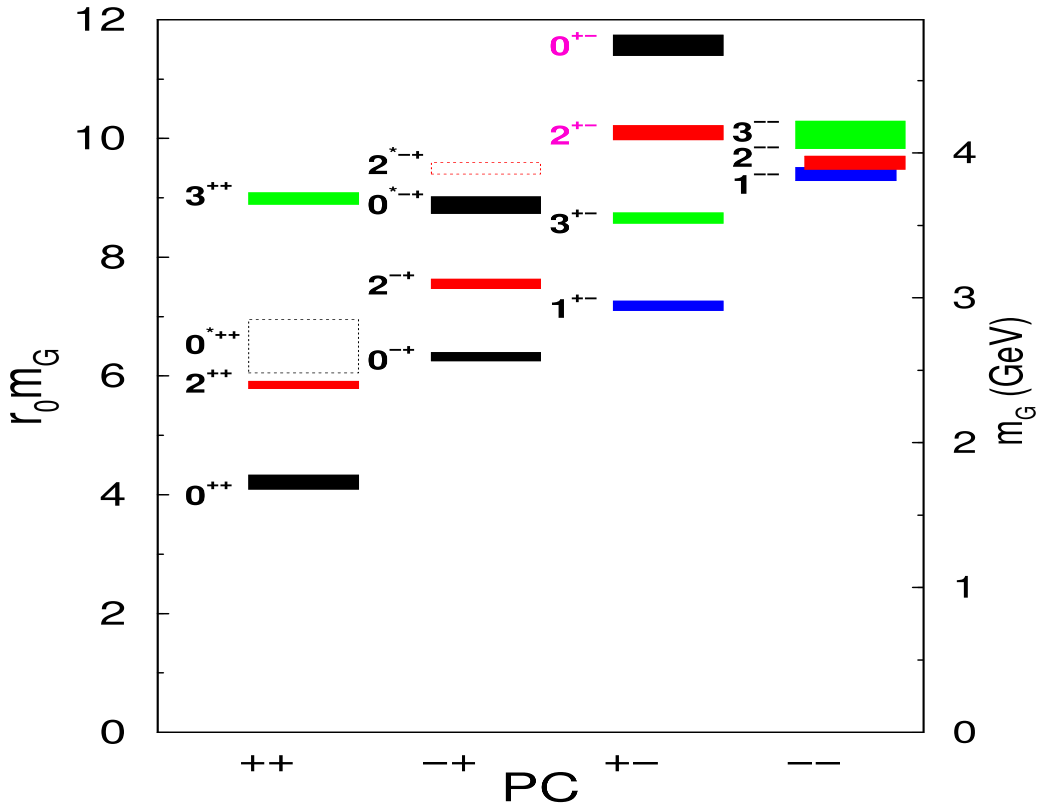
parity	charge conjugation
$U(\mathbf{x},t,4) \to U(-\mathbf{x},t,4)$	$U(\mathbf{x},t,4) \to U^*(\mathbf{x},t,4)$
$U(\mathbf{x},t,i) \to U(-\mathbf{x},t,-i)$	$U(\mathbf{x},t,i) \to U^*(\mathbf{x},t,i)$

example: combination of 1×1 Wilson loops $W(C)_{xy}$

$$O(\mathbf{x},t) = W_{(\mathbf{x},t),12} + W_{(\mathbf{x},t),13} + W_{(\mathbf{x},t),23}$$

invariant under hypercubic group, parity and charge conjugation $\to 0^{++}$

glueball spectrum → unique prediction from lattice QCD



quenched

quenched

‘

Morningstar and Peardon

start of dynamical (mass-degenrate up and down) quark simulations

1998 (Paper by UKQCD collaboration):

lattices: from $8^3 \cdot 24$ to $16^3 \cdot 24$

$a \approx 0.10\mathrm{fm}$, $m_\pi / m_\rho > 0.7$

Machine: CRAY T3E $\approx$ 1Tflop

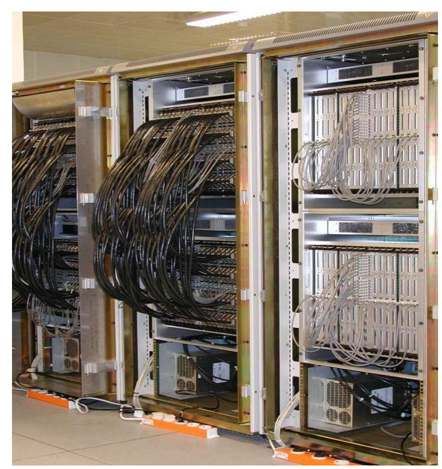
1999 (Paper by SESAM collaboration):

lattice: $16^3 \cdot 32$ lattice

$a \approx 0.10\mathrm{fm}$, $m_\pi / m_\rho > 0.7$

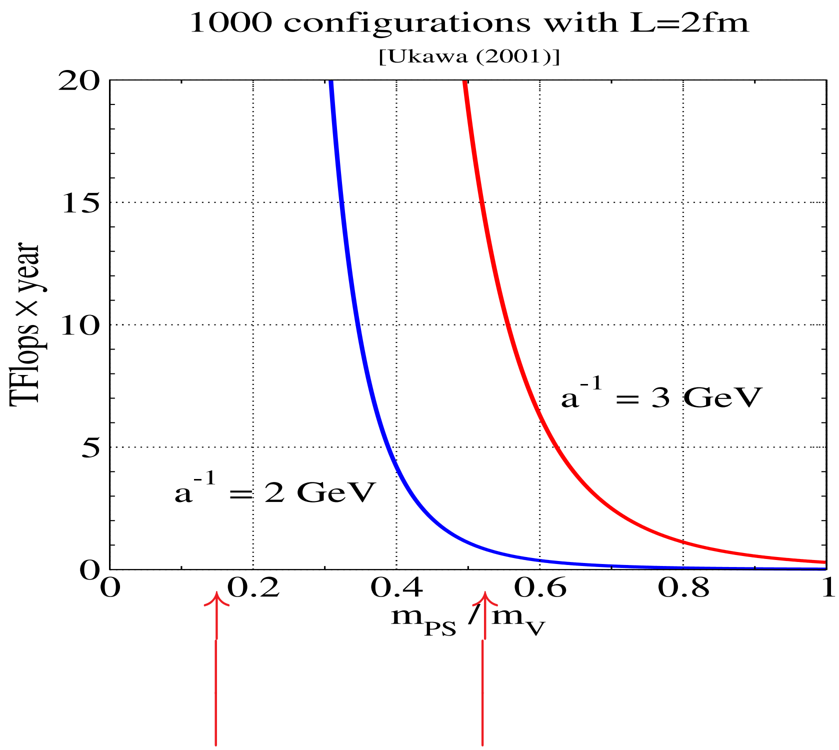
Machine: APE100 $\approx$ 100Gflop

- period of algorithm development
  - improved higher order integrators
  - multiboson algorithm
  - PHMC algorithm



Costs of dynamical fermions simulations, the “Berlin Wall”

see panel discussion in Lattice2001, Berlin, 2001



physical point

contact to χPT (?)

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

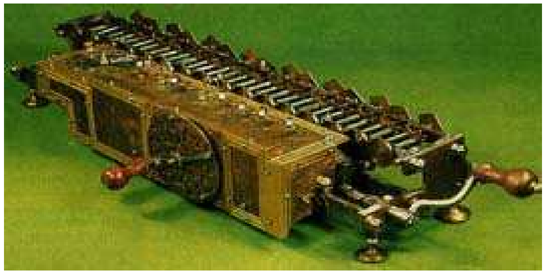
$$z_\pi = 6,\ \ z_L = 5,\ \ z_a = 7$$

“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**

Supercomputer

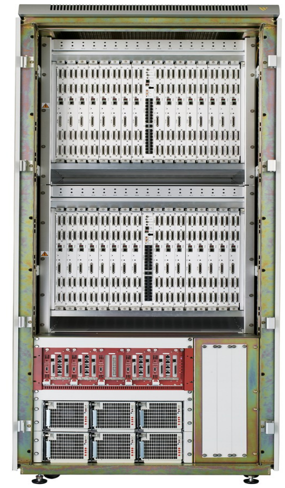
ca. 1700, Leibniz Rechenmaschine



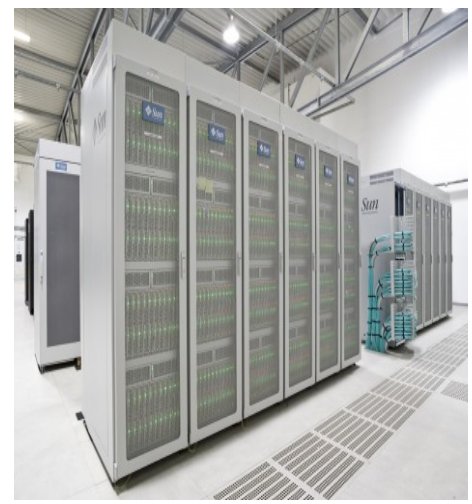
Denn es ist eines ausgezeichneten Mannes nicht würdig, wertvolle Stunden wie ein Sklave im Keller der einfachen Rechnungen zu verbringen. Diese Aufgaben könnten ohne Besorgnis abgegeben werden, wenn wir Maschinen hätten.

Because it is unworthy for an excellent man to spent valuable hours as a slave in the cellar of simple calculations. These tasks can be given away without any worry, if we would have machines.

German Supercomputer Infrastructure



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



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

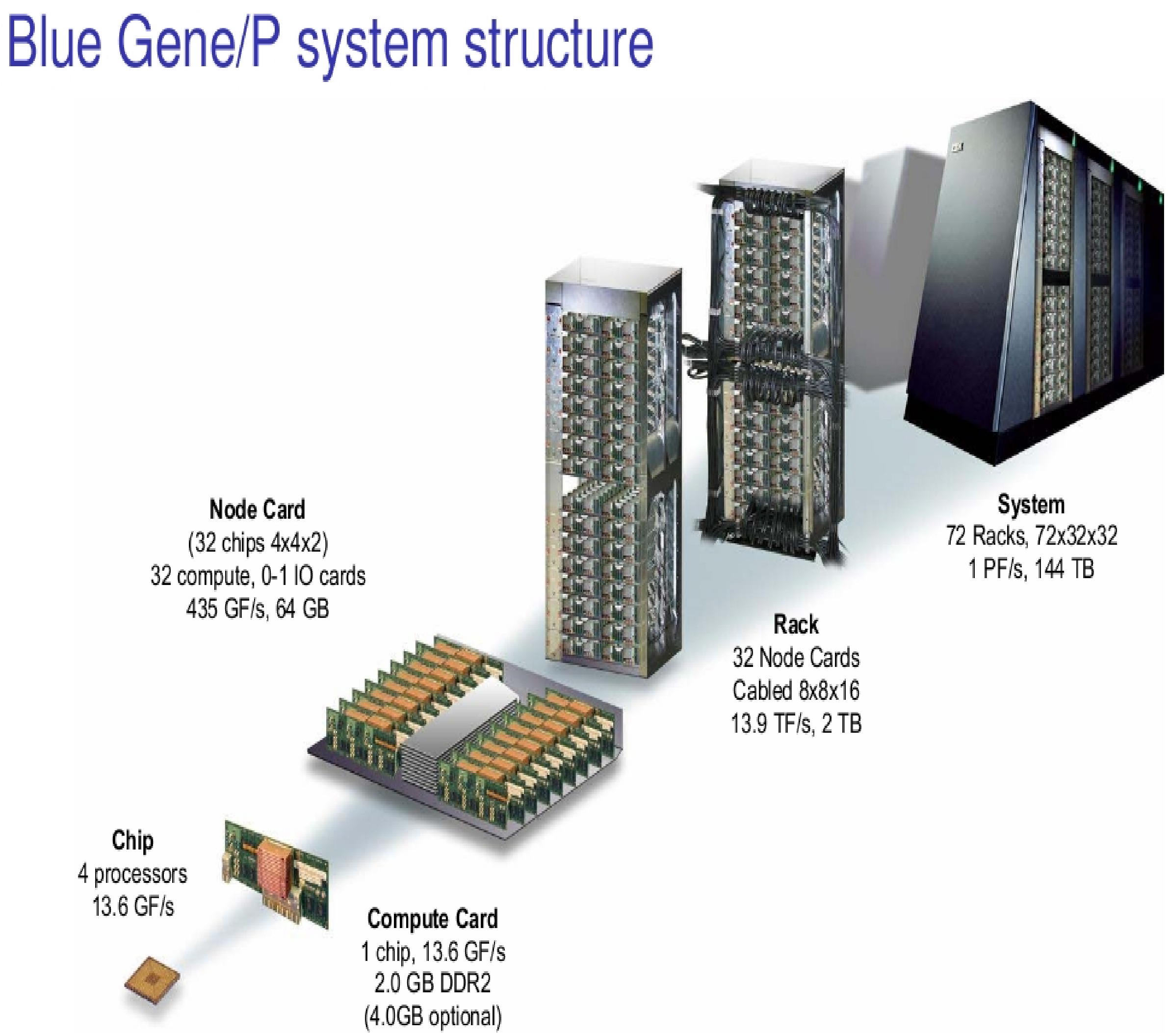
- 2208 Nehalem processor
  Cluster computer:
  208 Teraflops

- Altix System at LRZ Munic

- SGI Altix ICE 8200 at HLRN (Berlin, Hannover)
  31 Teraflops
  → will be upgraded to a **3 Petaflops system**

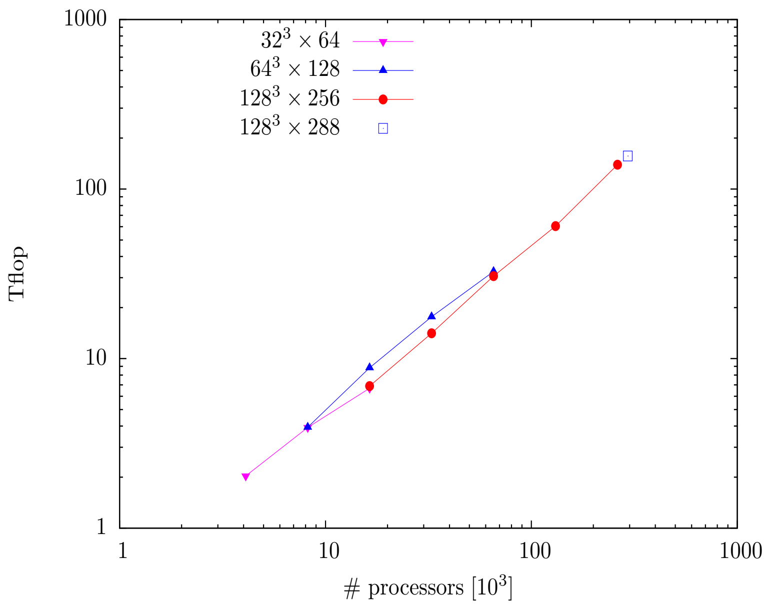
State of the art

- **BG/P**

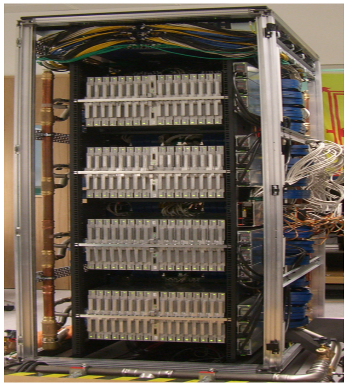


Strong Scaling

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



Low budget machines



- QPACE 4+4 Racks in Jülich und Wuppertal
  1900 PowerXCell 8i nodes **190 TFlops (peak)**
  based on cell processor
  3-d torus network
  low power consumption 1.5W/Gflop

- **Videocards (NVIDIA Tesla)**
  CUDA programming language (C extension)

enlarged to a cluster

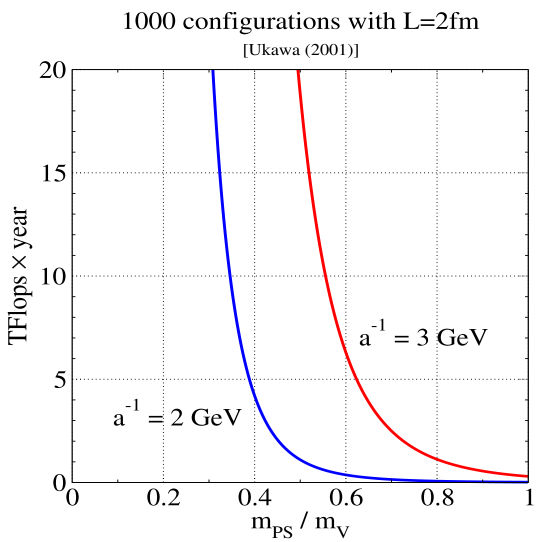
- challenge for 2020: **Exaflop Computing**

- already 2006: workshop on **Zetaflop computing**

A generic improvement for Wilson type fermions

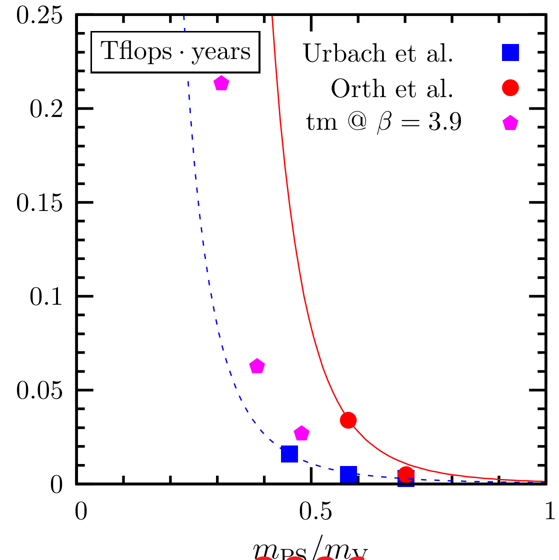
New variant of HMC algorithm (Urbach, Shindler, Wenger, K.J.)
(see also SAP (Lüscher) and RHMC (Clark and Kennedy) algorithms)

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



2001

$\longrightarrow$



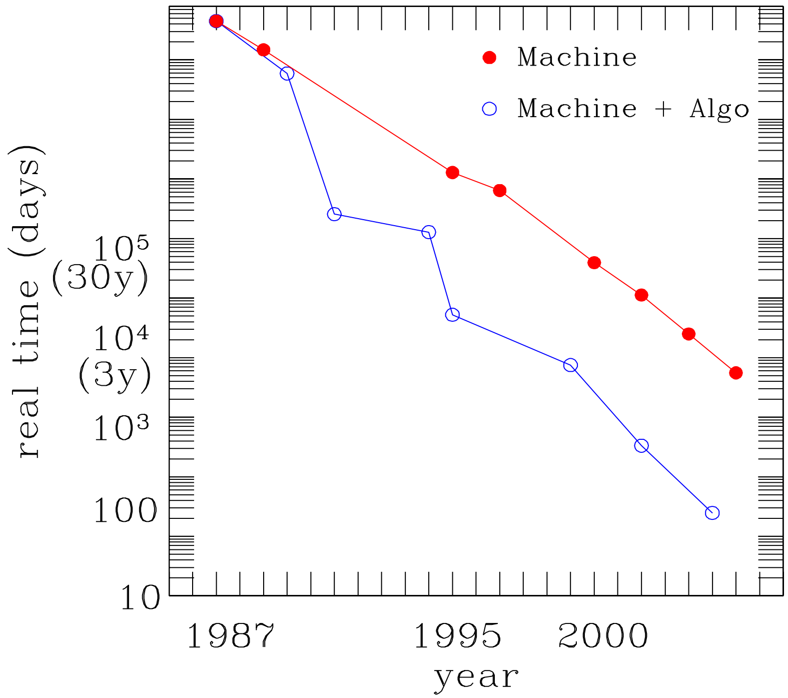
2006

– comparable to staggered

– reach small pseudo scalar masses $\approx 300\text{MeV}$

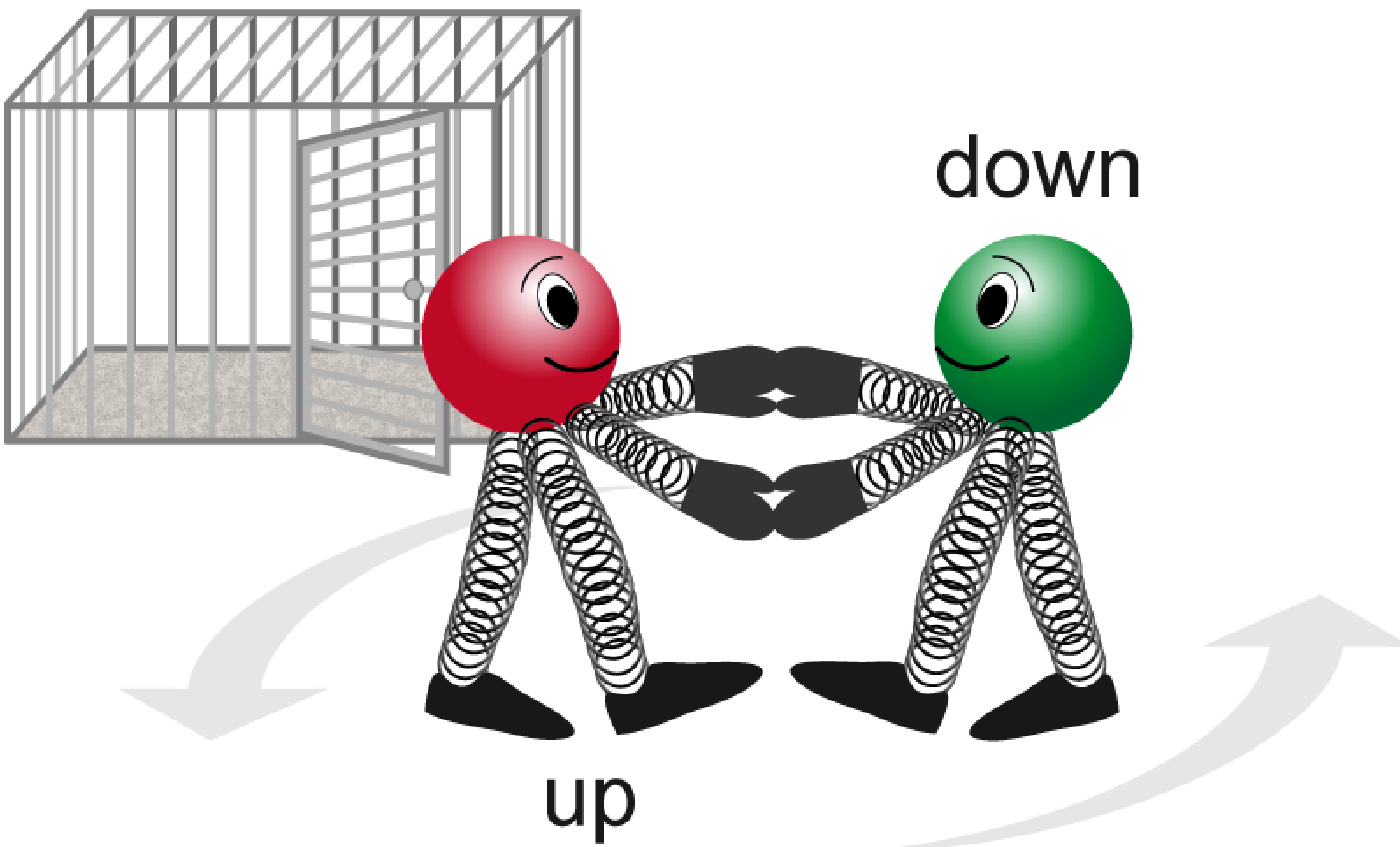
Computer and algorithm development over the years

time estimates for simulating $32^3 \cdot 64$ lattice, 5000 configurations



$\rightarrow$ O(few months) nowadays with a typical collaboration supercomputer contingent

$N_f = 2$ **dynamical flavours**



Examples of present Collaborations (using Wilson fermions)

- CERN-Rome collaboration
  Wilson gauge and clover improved Wilson fermions

- ALPHA
  Wilson gauge and clover improved Wilson fermions
  Schrödinger functional

- QCDSF
  tadpole improved Symanzik gauge and clover improved Wilson fermions

- ETMC
  tree-level Symanzik improved gauge and
  maximally twisted mass Wilson fermions

- RBC
  domain wall fermions

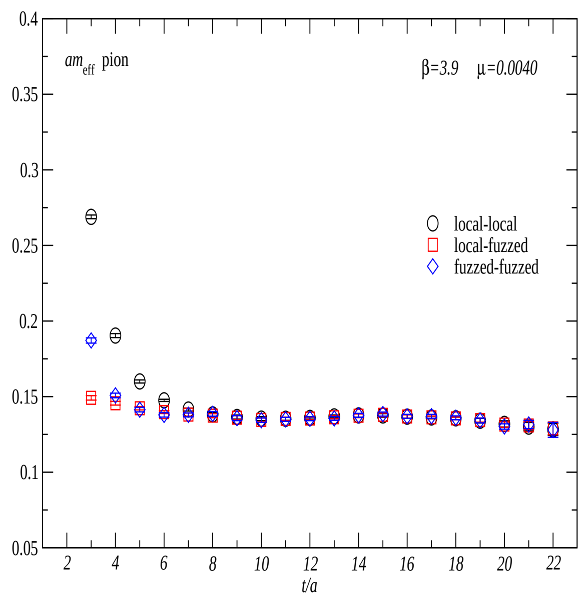
- BMW
  improved gauge and
  non-perturbatively imporved, 6 stout smeared Wilson fermions

- **Cyprus (Nicosia)**
  C. Alexandrou, T. Korzec, G. Koutsou
- **France (Orsay, Grenoble)**
  R. Baron, 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)**
  B. Bloissier, F. Farchioni, X. Feng, J. González López, G. Herdoiza, M. Marinkovic, I. Montvay, G. Münster, D. Renner, T. Sudmann, C. Urbach, M. Wagner, K.J.

European Twisted Mass Collaboration

Extraction of Masses

- Quark propagator: stochastic, fuzzed sources
- Change the location of the time-slice source: reduce autocorrelations



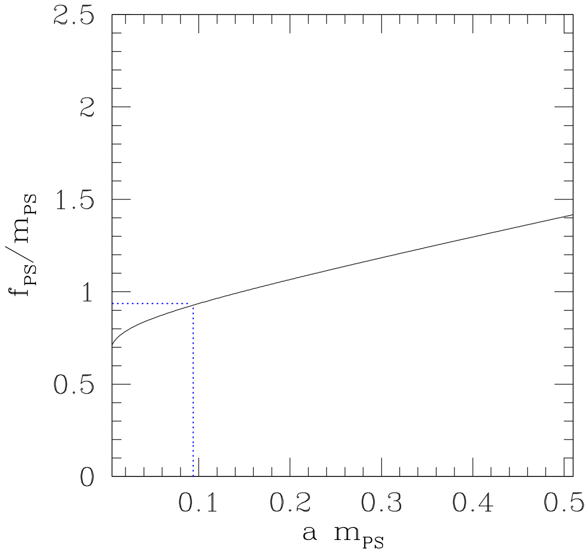
- effective mass of $\pi^{\pm}$
- isolate ground state : small statistical errors

$\Rightarrow$ get a number, but what does it mean? How to get physical units?

Setting the scale

$$m_{\rm PS}^{\rm latt} = a m_{\rm PS}^{\rm phys}\ , \quad f_{\rm PS}^{\rm latt} = a f_{\rm PS}^{\rm phys}$$

$$\frac{f_{\rm PS}^{\rm phys}}{m_{\rm PS}^{\rm phys}} = \frac{f_{\rm PS}^{\rm latt}}{m_{\rm PS}^{\rm latt}} + {\rm O}(a^2)$$



$\longrightarrow$ setting $\frac{f_{\rm PS}^{\rm latt}}{m_{\rm PS}^{\rm latt}} = 130.7/139.6$

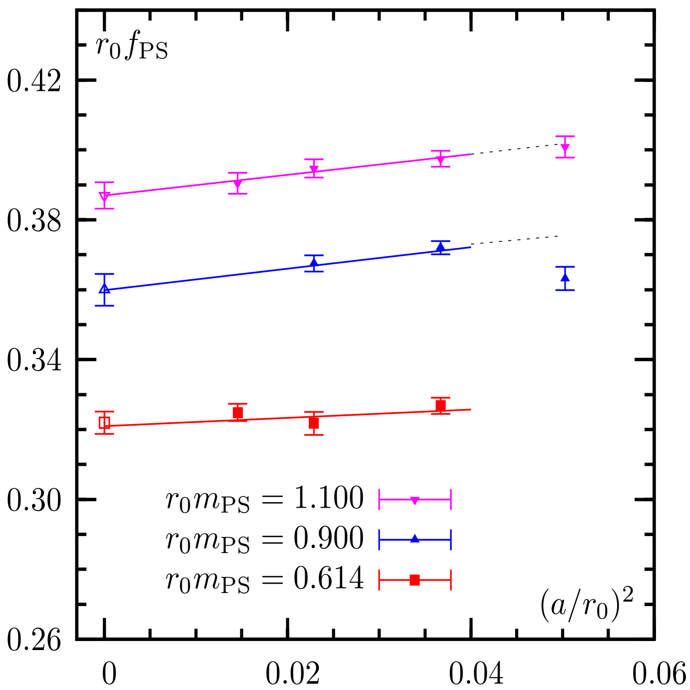
$\longrightarrow$ obtain $m_{\rm PS}^{\rm latt} = a139.6$[Mev]

$\longrightarrow$ value for lattice spacing a

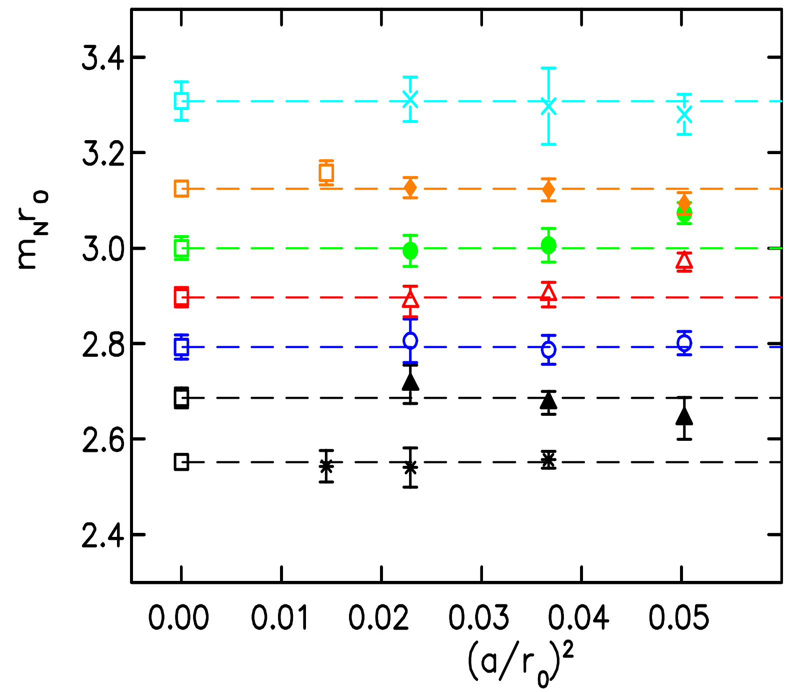
available configurations (free on ILDG)

β	a [fm]	$L^3 \cdot T$	L [fm]	$a\mu$	N_{traj} $(\tau = 0.5)$	m_{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

Continuum limit scaling



$f_{\rm PS}$



$M_{\rm N}$

observe small $O(a^2)$ effects

Chiral perturbation theory

$$r_0 f_{\mathrm{PS}} = r_0 f_0 \left[1 - 2\xi \log\left(\frac{\chi_\mu}{\Lambda_4^2}\right) + \ldots \right.$$

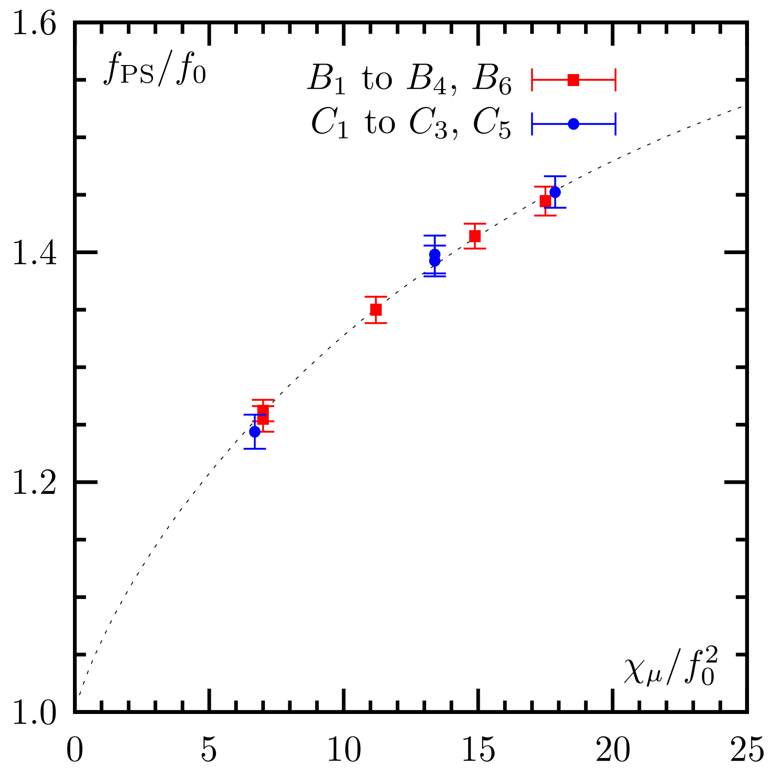
$$(r_0 m_{\mathrm{PS}})^2 = \chi_\mu r_0^2 \left[1 + \xi \log\left(\frac{\chi_\mu}{\Lambda_3^2}\right) + \ldots \right.$$

where

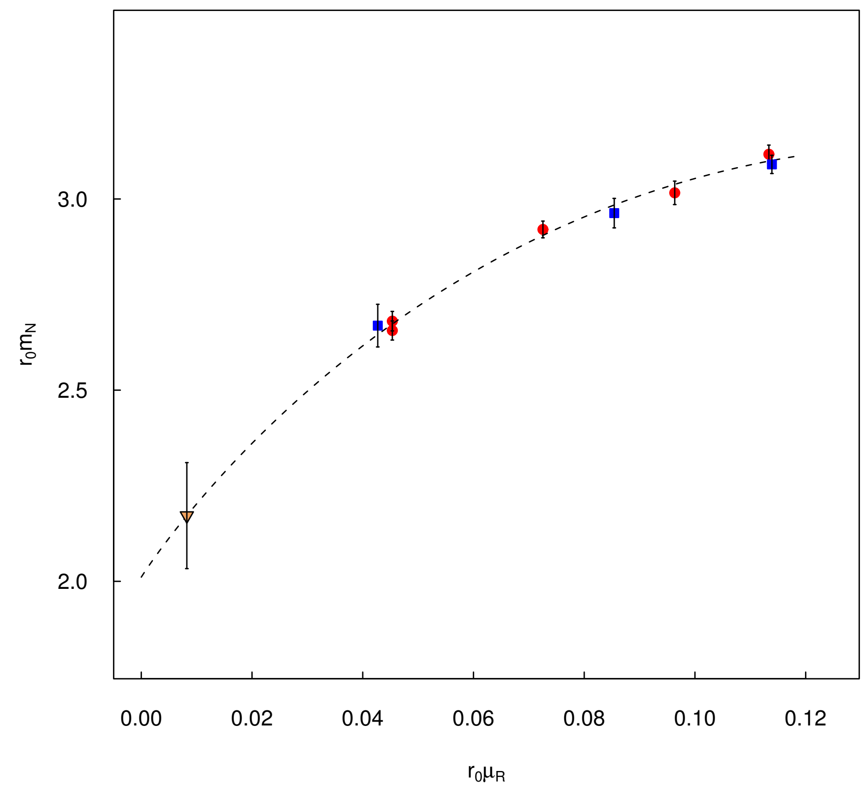
$$\xi \equiv 2B_0\mu_q/(4\pi f_0)^2, \quad \chi_\mu \equiv 2B_0\mu_R, \quad \mu_R \equiv \mu_q/Z_{\mathrm{P}}$$

Chiral fits

Pion decay constant



nucleon mass



Chiral perturbation theory

$\rightarrow$ add finite volume and lattice spacing dependence:

$$r_0 f_{\mathrm{PS}} = r_0 f_0 \left[1 - 2\xi \log\left(\frac{\chi_\mu}{\Lambda_4^2}\right) + D_{f_{\mathrm{PS}}} a^2/r_0^2 + T_f^{\mathrm{NNLO}} \right] K_f^{\mathrm{CDH}}(L)$$

$$(r_0 m_{\mathrm{PS}})^2 = \chi_\mu r_0^2 \left[1 + \xi \log\left(\frac{\chi_\mu}{\Lambda_3^2}\right) + D_{m_{\mathrm{PS}}} a^2/r_0^2 + T_m^{\mathrm{NNLO}} \right] K_m^{\mathrm{CDH}}(L)^2$$

$$r_0/a(a\mu_q) = r_0/a + D_{r_0}(a\mu_q)^2$$

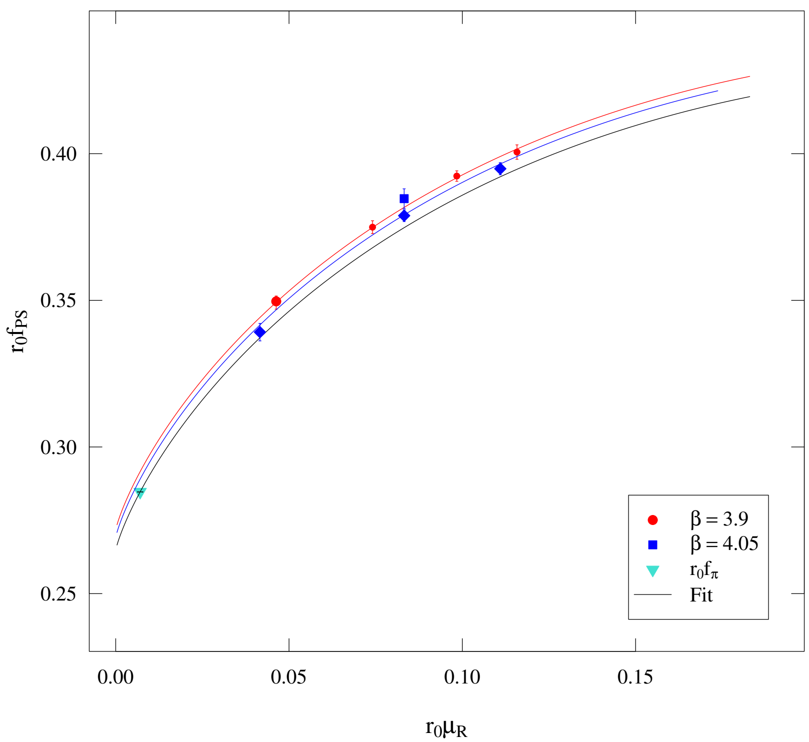
where

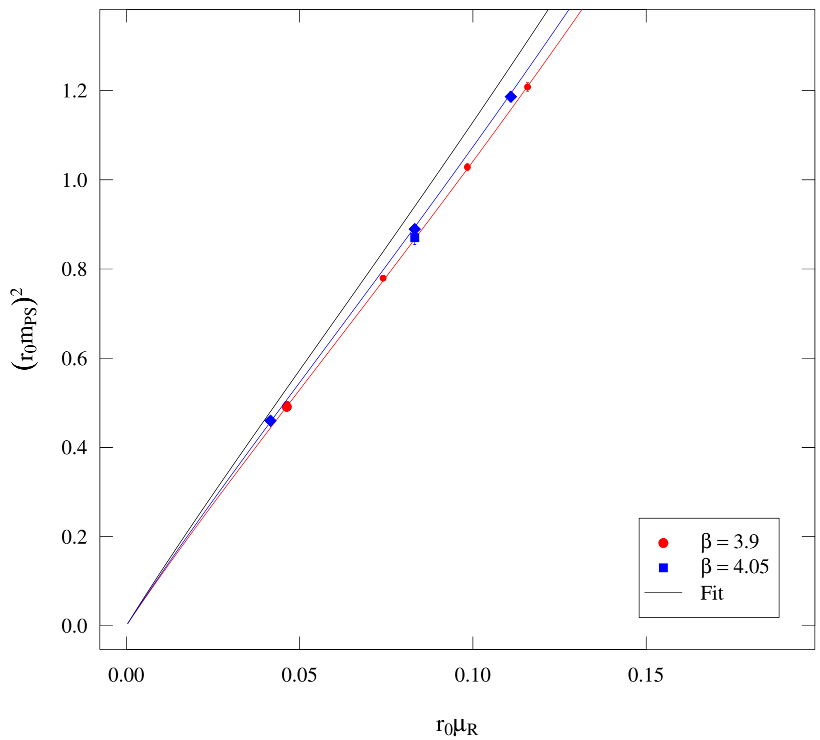
$$\xi \equiv 2B_0\mu_q/(4\pi f_0)^2, \quad \chi_\mu \equiv 2B_0\mu_R, \quad \mu_R \equiv \mu_q/Z_{\mathrm{P}}$$

- $D_{f,m}$ parametrize lattice artefacts
- $K_{f,m}^{\mathrm{CDH}}(L)$ Finite size corrections Colangelo *et al.*, 2005
- $T_{f,m}^{\mathrm{NNLO}}$ NNLO correction

Chiral perturbation theory

- Fit B: NLO continuum χPT, $T_{m,f}^{\mathrm{NNLO}} \equiv 0$, $D_{m_{\mathrm{PS}},f_{\mathrm{PS}}}$ fitted





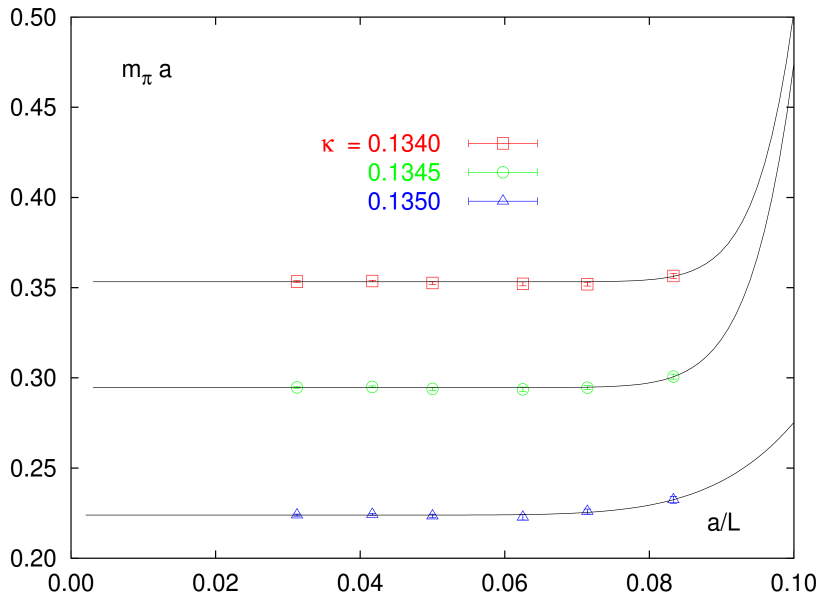
two values of the lattice spacing $\rightarrow$ $D_m = -1.07(97)$, $D_f = 0.71(57)$

Chiral perturbation theory

$\rightarrow$ fit variety:

- Fit A: NLO continuum χPT, $T_{m,f}^{\mathrm{NNLO}} \equiv 0$, $D_{m_{\mathrm{PS}},f_{\mathrm{PS}}} \equiv 0$
- Fit B: NLO continuum χPT, $T_{m,f}^{\mathrm{NNLO}} \equiv 0$, $D_{m_{\mathrm{PS}},f_{\mathrm{PS}}}$ fitted
- Fit C: NNLO continuum χPT, $D_{m_{\mathrm{PS}},f_{\mathrm{PS}}} \equiv 0$
- Fit D: NNLO continuum χPT, $D_{m_{\mathrm{PS}},f_{\mathrm{PS}}}$ fitted

Finite Size Effects



General *analytical* description:

$$m_\pi(L) = m_\pi^{L=\infty} + c_1/L^{3/2}\exp(-m_\pi^\infty L)$$

M. Lüscher

different κ correspond to different m_π

$\longrightarrow$ Analytical finite size corrections known for many quantities, and to high precision

e.g. higher order correction terms from χPT Colangelo, Dürr

$$\begin{aligned} R_{m_\pi}(L) &\simeq \frac{3}{8\pi^2}\left(\frac{m_\pi}{F_\pi}\right)^2\left[\frac{K_1(m_\pi L)}{m_\pi L} + \frac{2\ K_1(\sqrt{2}\ m_\pi L)}{\sqrt{2}\ m_\pi L}\right] \\ &\simeq \frac{3}{4(2\pi)^{3/2}}\left(\frac{m_\pi}{F_\pi}\right)^2\left[\frac{e^{-m_\pi L}}{(m_\pi L)^{3/2}} + \frac{2\ e^{-\sqrt{2}\ m_\pi L}}{(\sqrt{2}\ m_\pi L)^{3/2}}\right] \end{aligned}$$

Finite size effects

Comparison of data at several volumes to :

- NLO χPT : GL [Gasser, Leutwyler, 1987, 1988]
- resummed Lüscher formula : CDH [Colangelo, Dürr, Haefeli, 2005]
- relative deviation : $R_O = (O_L - O_\infty)/O_\infty$

obs. O	β	$m_{\mathrm{PS}}L$	meas. [%]	GL [%]	CDH [%]
m_{PS}	3.90	3.3	+1.8	+0.6	+1.1
f_{PS}	3.90	3.3	−2.5	−2.5	−2.4
m_{PS}	4.05	3.0	+6.2	+2.2	+6.1
f_{PS}	4.05	3.0	−10.7	−8.8	−10.3
m_{PS}	4.05	3.5	+1.1	+0.8	+1.5
f_{PS}	4.05	3.5	−1.8	−3.4	−2.9

- for R_{CDH} : parameters estimates from [CDH, 2005] were used as input
- CDH describes data in general better than GL but needs more parameters

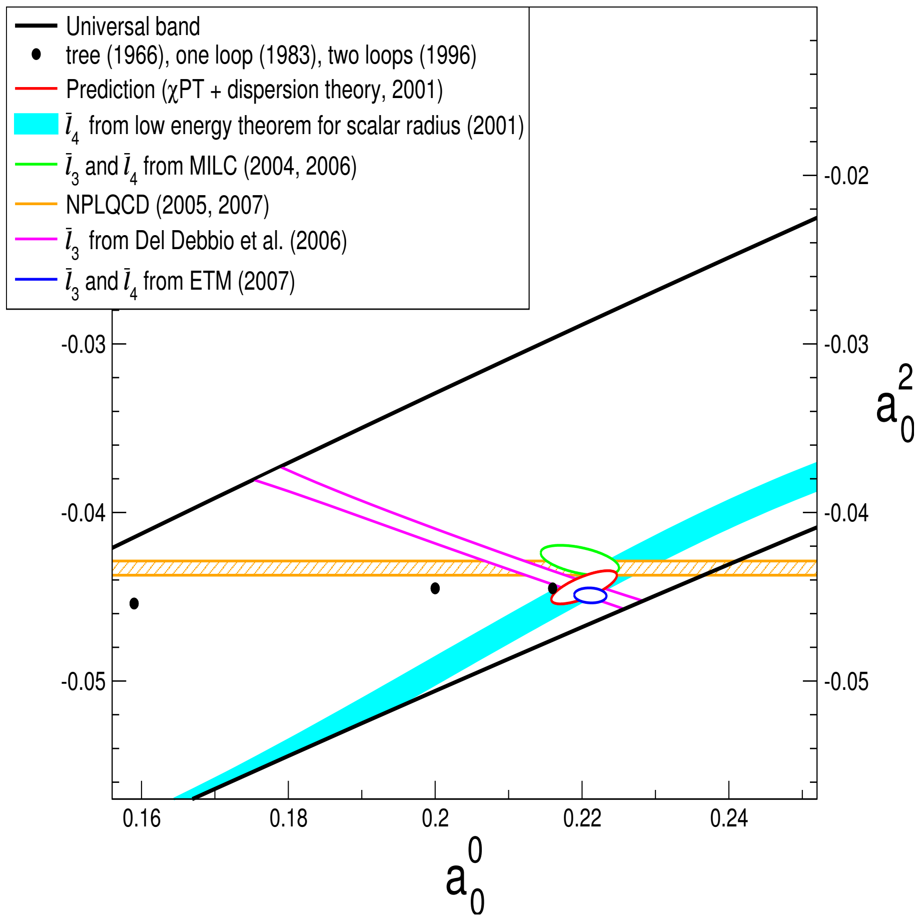
Chiral perturbation theory: results

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	$1.0734(40)$

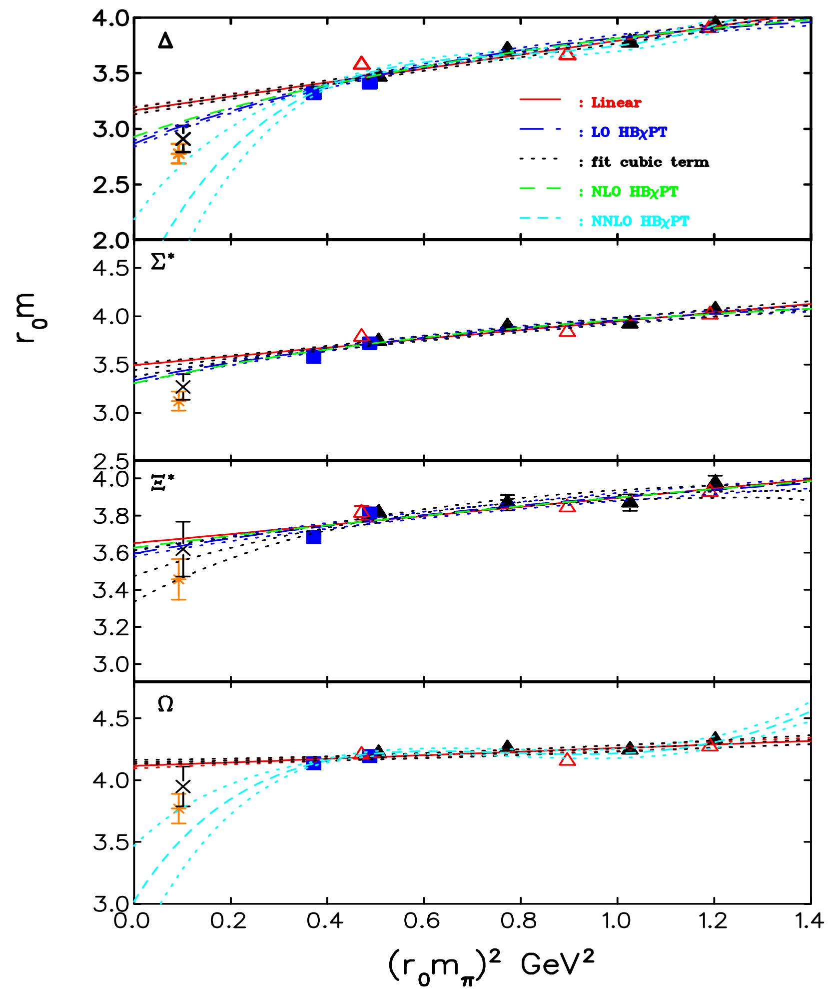
- averaged over many fit results, weighted with confidence levels
- B_0, Σ, $m_{u,d}$ renormalised in $\overline{\mathrm{MS}}$ scheme at scale $\mu = 2$ GeV
- LECs can be used to compute further quantities: scattering lengths

Chiral perturbation theory

S-wave scattering lengths a_0^0 and a_0^2 Leutwyler

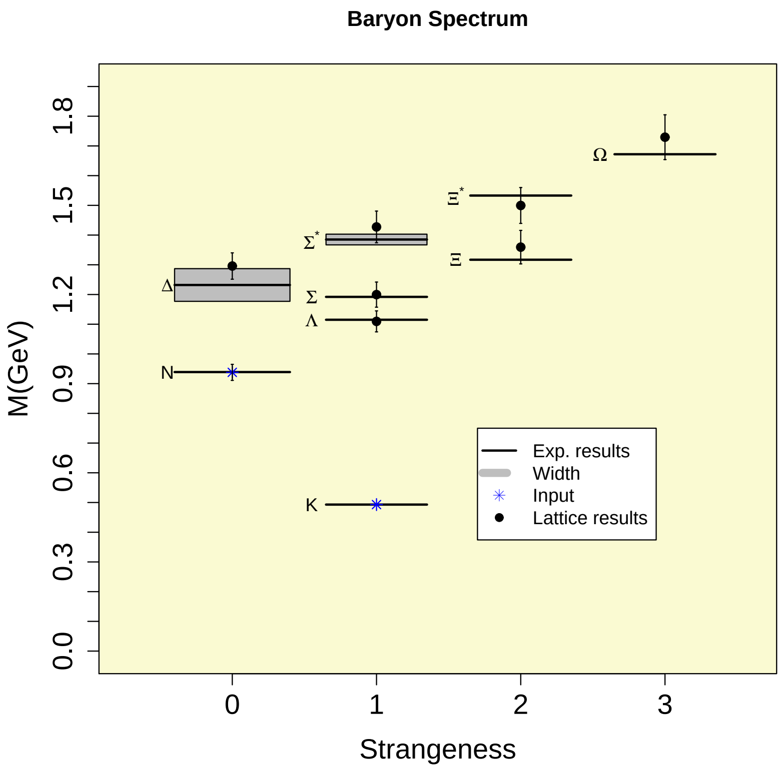


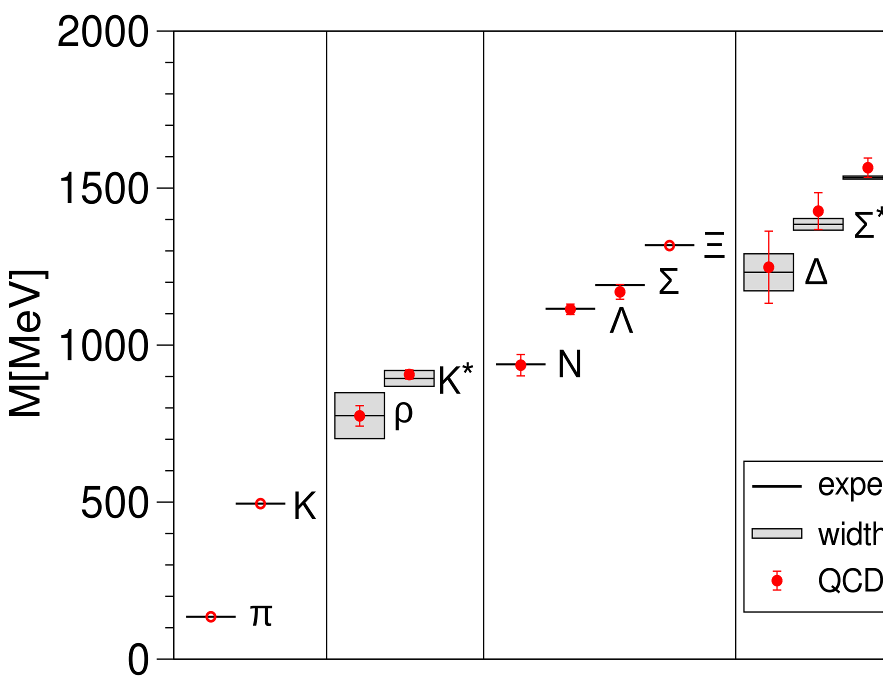
Chiral extrapolation of strange Baryons



The lattice QCD benchmark calculation: the spectrum

ETMC ($N_f = 2$), BMW ($N_f = 2 + 1$)

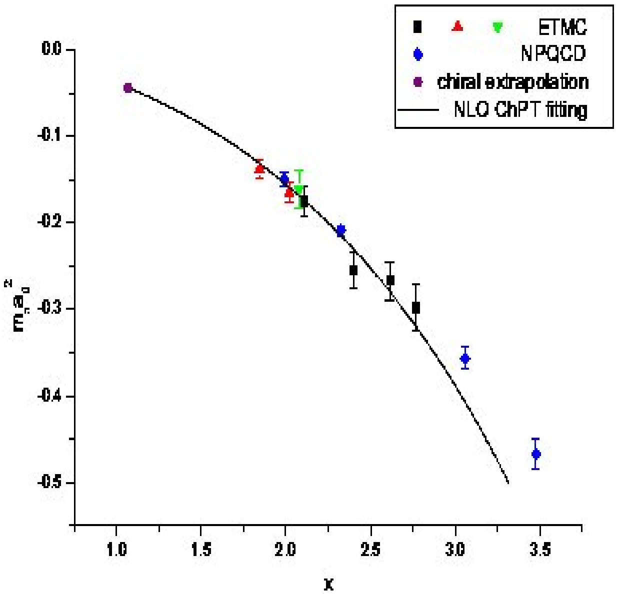


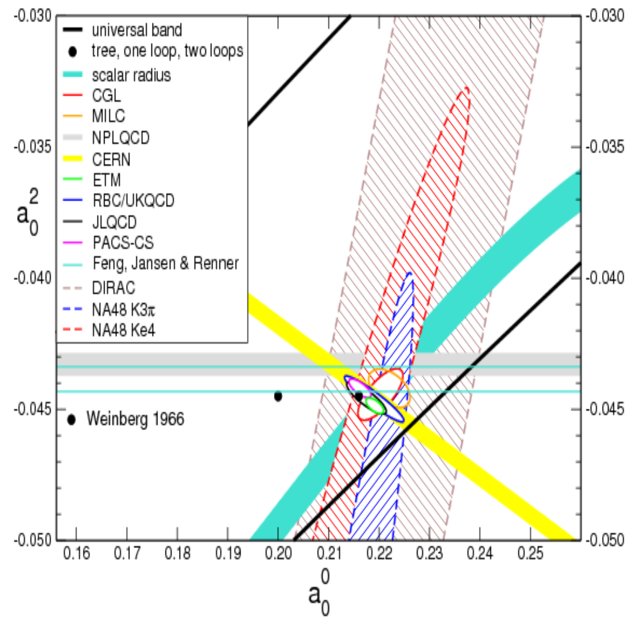


$N_f = 2$ $\qquad$ $N_f = 2 + 1$

I=2 Pion scattering length

(X. Feng, D. Renner, K.J.)





energy determined from

$R(t) = \langle(\pi^+\pi^+)^\dagger(t+t_s)(\pi^+\pi^+)(t_s)\rangle / \langle(\pi^+)^\dagger(t+t_s)\pi^+(t_s)\rangle^2$

$\rightarrow \quad \Delta E = c/L^3 \cdot a_{\pi\pi}^{I=2}(1+O(1/L))$

E865 (BNL) $m_\pi a_{\pi\pi}^{I=0} = 0.203\,(33)$ and $m_\pi a_{\pi\pi}^{I=2} = -0.055\,(23)$.

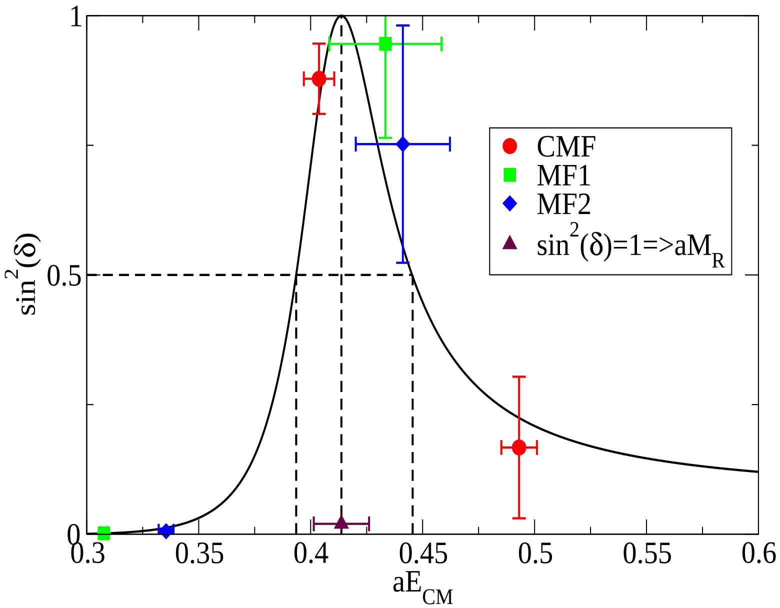
NA48/2 (CERN) $m_\pi a_{\pi\pi}^{I=0} = 0.221\,(5)$ and $m_\pi a_{\pi\pi}^{I=2} = -0.0429\,(47)$.

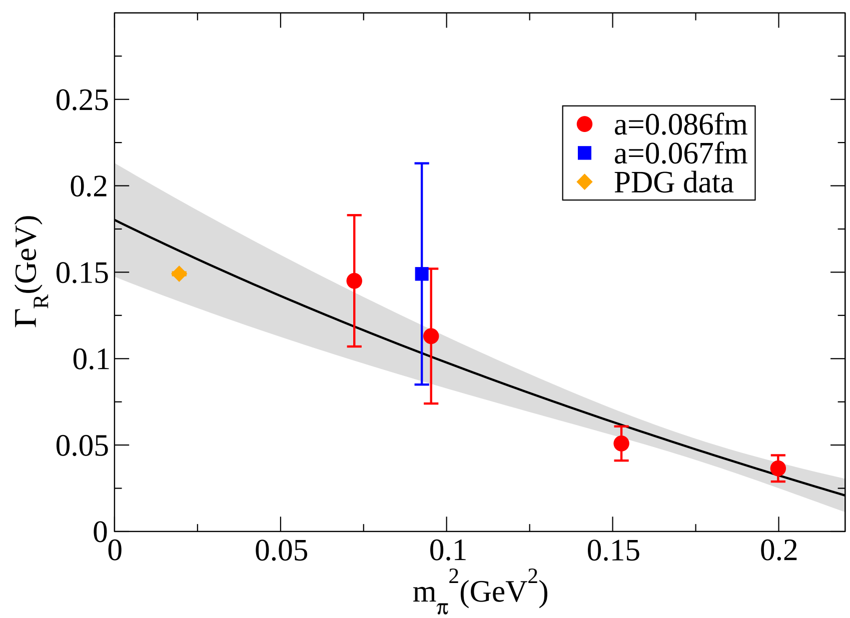
our work $m_\pi a_{\pi\pi}^{I=2} = -0.04385\,(28)(38)$

The ρ-meson resonance: dynamical quarks at work

(X. Feng, D. Renner, K.J.)

- usage of three Lorentz frames





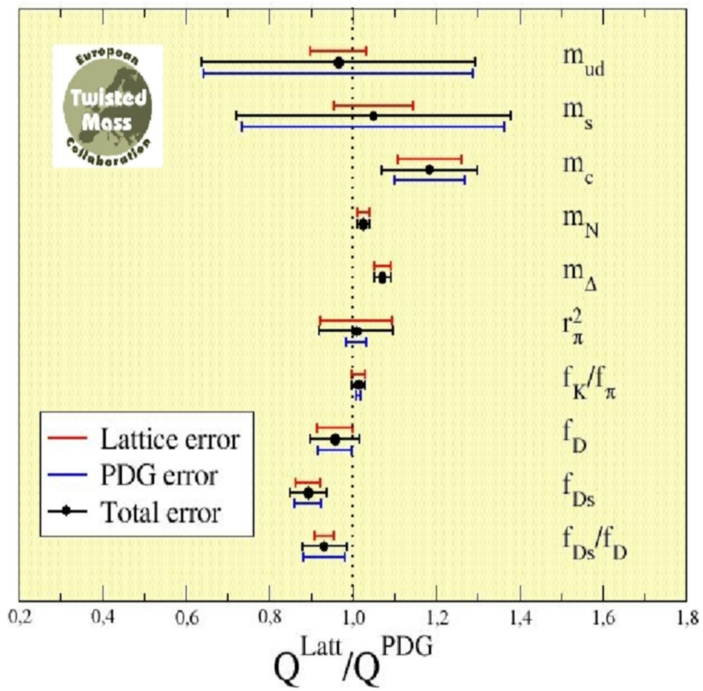
$m_{\pi^+} = 330$ MeV, $a = 0.079$ fm, $L/a = 32$

fitting $z = (M_\rho + i\frac{1}{2}\Gamma_\rho)^2$

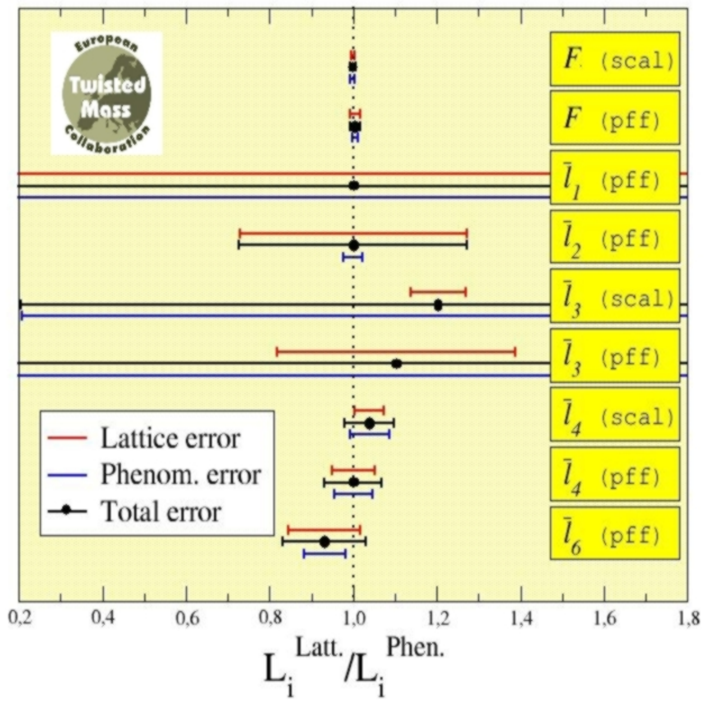
$m_\rho = 1033(31)$ MeV, $\Gamma_\rho = 123(43)$ MeV

Selected results for $N_f = 2$

Simulation results versus PDG



Low energy constants



Summary

- wanted to show basic step for proton mass computation
- 25 years effort
  - conceptual developments: $O(a)$-improved actions
  - algorithm developments (see also Buividovic and Urbach)
  - machine developments
- mission of hadron spectrum benchmark calculation completed
- read for more complicated observables
  $\longrightarrow$ (lectures by M. Göckeler and R. Sommer)

General articles

Lectures, review articles

- R. Gupta
  Introduction to Lattice QCD, hep-lat/9807028
- C. Davies
  Lattice QCD, hep-ph/0205181
- M. Lüscher
  Advanced Lattice QCD, hep-lat/9802029
  Chiral gauge theories revisited, hep-th/0102028
- A.D. Kennedy
  Algorithms for Dynamical Fermions, hep-lat/0607038

Books about Lattice Field Theory

- **C. Gattringer and C. Lang**
  Quantum Chromodynamics on the Lattice
  Lecture Notes in Physics 788, Springer, 2010
- **T. DeGrand and C. DeTar**
  Lattice methods for Quantum Chromodynamics
  World Scientific, 2006
- **H.J. Rothe**
  Lattice gauge theories: An Introduction
  World Sci.Lect.Notes Phys.74, 2005
- **J. Smit** *Introduction to quantum fields on a lattice: A robust mate*
  Cambridge Lect.Notes Phys.15, 2002
- **I. Montvay and G. Münster**
  Quantum fields on a lattice
  Cambridge, UK: Univ. Pr., 1994
- **Yussuf Saad**
  Iterative Methods for sparse linear systems
  Siam Press, 2003