The Quest of Solving QCD

Recent Progress in Lattice QCD

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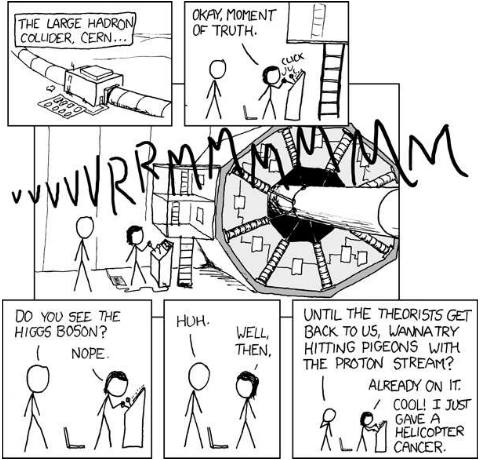
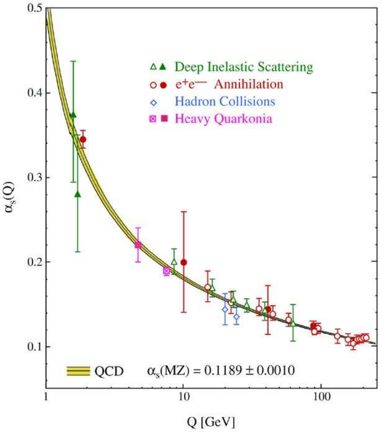
Motivation



xkcd.com

- LHC collides protons
- LHC is a QCD machine
- accurate predictions for both background and signal
  need understanding of QCD

Motivation



[Bethke, 2006]

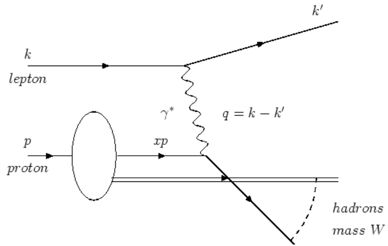
Quantum Chromo-dynamics
the theory of strong interactions

describes both

- asymptotic freedom
  at large energies
  $\alpha_s \ll 1$
  $\rightarrow$ perturbation theory
- confinement
  at low energies
  $\alpha_s \approx 1$
  $\rightarrow$ non-perturbative

$\Rightarrow$ Lattice QCD is a non-perturbative, ab-initio method

Motivation



- large momentum transfer
- deep inelastic scattering of an electron and a proton
- interested in cross-section

- to leading order in α_s

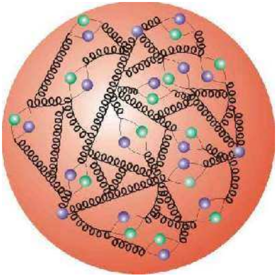
$$\sigma(l(k)p(p) \to l(k') + X) = \int_0^1 dx \sum_f f_f(x) \sigma(l(k) q_f(xp) \to l(k') + q_f(p'))$$

- parton distribution functions f_f: probability density of finding constituent with momentum fraction x
- PDF's are non-perturbative

Motivation: Hydrogen Atom versus Proton (QED vs. QCD)

- Hydrogen Atom:
  - electron mass: 0.5 MeV
  - proton mass: 938 MeV
  - binding energy: 13.5 eV
- Proton:
  - u-quark mass: $\sim$ 3 MeV
  - d-quark mass: $\sim$ 6 MeV
  - proton mass: 938 MeV

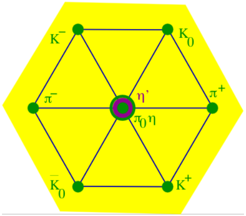
  $\longrightarrow$ QCD origin of mass
- moreover: quarks cannot be observed, confinement



- accuracy of strong coupling $\alpha_s(m_Z) = 0.119(1)$
- fine structure constant $\alpha^{-1} = 137.035\,999\,697(94)$

Flavour Singlet Pseudo-Scalar Mesons

- nine lightest pseudo-scalar mesons show a peculiar spectrum:
  - 3 very light pions (140 MeV)
  - Kaons and the η around 600 MeV
  - the η' has mass around 1 GeV



- The large mass of the η' meson is thought to be caused by the QCD vacuum structure and the $U(1)_A$ anomaly
- η' meson is not a (would be) Goldstone Boson
- η' is massive even in the chiral limit
- Lattice QCD allows to study this

Chiral Symmetry

- in QCD with massless quarks
  chiral symmetry is spontaneously broken
- consequences:
  - 8 massless Goldstone bosons
    in the limit of 3 massless quarks: 3 pions, 4 Kaons, η
- quark masses break chiral symmetry explicitly
  e.g. pions acquire mass

$$m_\pi^2 \propto (m_u + m_d)$$

- Chiral Perturbation Theory (χPT) provides effective description
  however, Low Energy Constants (LECs) are unknown
- lattice QCD offers the unique possibility
  to investigate the quark mass dependence

Outline

1. Lattice Methods
   - Regularisation
   - Monte Carlo for Lattice QCD
   - Theoretical Developments: $\mathcal{O}(a)$ Improvement

2. Physics Results
   - Meson Sector
   - Baryon Sector

3. Conclusion and Outlook

QCD in Euclidean Space-Time

- expectation values in path-integral quantisation

$$\langle \mathcal{O} \rangle \propto \int \mathcal{D}A_\mu \, \mathcal{D}\bar{\psi} \, \mathcal{D}\psi \; \mathcal{O} \; e^{-S[A_\mu,\bar{\psi},\psi]}$$

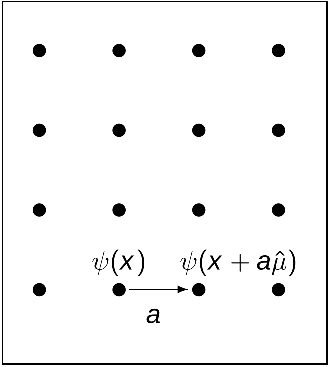
- with action (N_f mass degenerate quark flavours, $c = \hbar = 1$)

$$S[A_\mu, \bar{\psi}, \psi] = \int d^4x \; \left\{ \frac{1}{4} F_{\mu\nu}^2 + \bar{\psi} \, (\gamma_\mu D_\mu + m_q) \, \psi \right\} = S_{\mathrm{G}} + S_f$$

- analogy: e^{-S} can be interpreted as Boltzmann factor
- stochastic integration with Monte-Carlo methods importance sampling
- still need to regularise the theory $\longrightarrow$ Lattice

Lattice Quantum Chromo-dynamics

Introduce finite space-time lattice $L^3 \times T$



[Wilson, 1974, 1975]

- lattice spacing a
- momentum cut-off: $k_{\max} \propto 1/a$.
- fermionic fields on space-time points
- functional integral:

$$\int \mathcal{D}\psi \mapsto \int \prod_x d\psi(x)$$

- what about the gauge potential A_μ?

Lattice Quantum Chromo-dynamics

The principle of local gauge invariance

- gauge covariant derivative D_μ

$$D_\mu \psi(x) \; = \lim_{a\to 0} \frac{1}{a}[U(x, x + a\hat{\mu})\psi(x + a\hat{\mu}) - \psi(x)]$$

- transformation laws

$$\psi(x) \; \to \; V(x)\psi(x) \, , \qquad U(x,y) \; \to \; V(x)U(x,y)V^\dagger(y)$$

with $U, V \in \mathrm{SU}(3)$

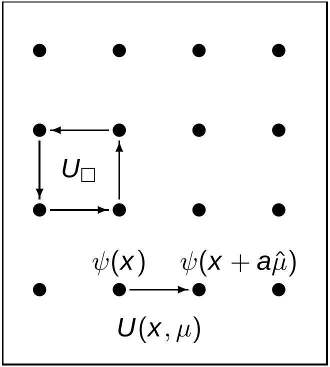
- for infinitesimal a

$$U(x, x + a\hat{\mu}) = \exp\left[-igA^i_\mu(x + \frac{a}{2}\hat{\mu})\lambda^i + \mathcal{O}(a^3)\right]$$

Lattice Quantum Chromo-dynamics

The principle of local gauge invariance

space-time lattice $L^3 \times T$:



- discretised gauge action

$$S_{\mathrm{G}}[U] = \sum_{\Box} \beta \left\{ 1 - \frac{1}{3} \mathrm{Re}\,\mathrm{Tr}(U_\Box) \right\}$$

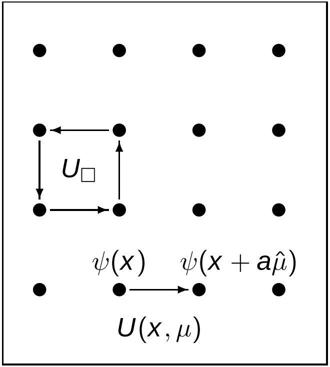
$(\beta = 6/g_0^2)$

[Wilson, 1974, 1975]

Lattice Quantum Chromo-dynamics

The principle of local gauge invariance

space-time lattice $L^3 \times T$:



- discretised gauge action

$$S_G[U] = \sum_\square \beta \left\{ 1 - \frac{1}{3} \mathrm{Re}\,\mathrm{Tr}(U_\square) \right\}$$

$(\beta = 6/g_0^2)$

- covariant difference operators

$$\nabla_\mu \psi(x) = \frac{1}{a}\Big[U(x,\mu)\psi(x + a\hat{\mu}) - \psi(x)\Big]$$

$$\nabla^*_\mu \psi(x) = \frac{1}{a}\Big[\psi(x) - U(x,-\mu)\psi(x - a\hat{\mu})\Big]$$

[Wilson, 1974, 1975]

Wilson Formulation

Wilson Dirac Operator

$$D_{\mathrm{W}}[U] + m_0 = \frac{1}{2}\sum_{\mu}\left[\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - a\nabla^*_\mu\nabla_\mu\right] + m_0$$

- Wilson Term $-a\nabla^*_\mu\nabla_\mu$
  - solves the fermion doubling problem,
- but:
  - chiral symmetry is explicitly broken, $\{D_{\mathrm{W}}, \gamma_5\} \neq 0$,
  - therefore m_0 renormalises additively (and multiplicatively)

$$m_q = m_0 - m_{\mathrm{crit}} \ ,$$

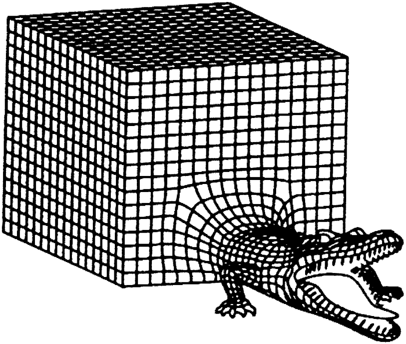
  - leading lattice artifacts are $\mathcal{O}(a)$

QCD on the Lattice

- For given parameters lattice calculations are exact (up to statistical errors). . .

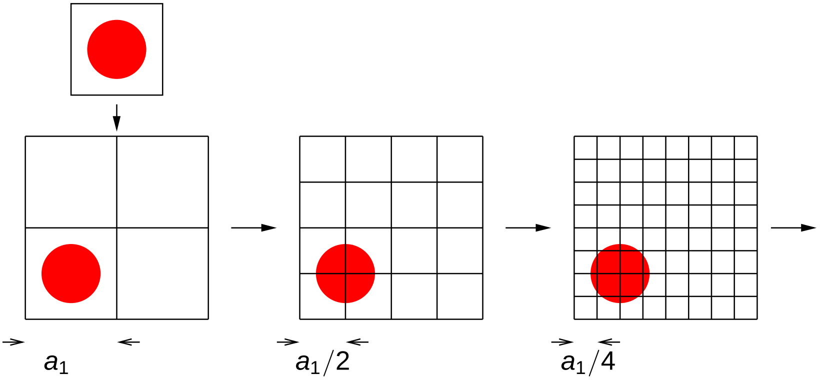
QCD on the Lattice

- For given parameters lattice calculations are exact (up to statistical errors). . .
- but, there are dangerous animals on the lattice



A Glimpse at the Extrapolations

1. go to infinite volume
2. remove cut-off at fixed volume and physics



The Goal: Precision Lattice QCD Results

- . . . we need to control systematic errors:
  - lattice spacing effects $\Rightarrow$ continuum limit, lattice spacing $a \to 0$,
    $\Rightarrow$ remove leading order lattice artifacts
  - finite size effects $\Rightarrow$ thermodynamic limit, physical volume $L^3 \to \infty$,
    $\Rightarrow$ use chiral effective field theories.
  - chiral effects $\Rightarrow$ chiral limit, $m_{\mathrm{PS}} \to m_\pi$,
    $\Rightarrow$ use chiral effective field theories.

$\Rightarrow$ be aware: subtle interplay of limits

- from experience: we need

$$\begin{aligned} a &< 0.1\,\mathrm{fm}, \\ L &> 2\,\mathrm{fm}, \\ m_{\mathrm{PS}} &< 300\,\mathrm{MeV}. \end{aligned}$$

Outline

Why are Fermions expensive to simulate?

- we need to evaluate (ψ Grassman valued):

$$\int \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, e^{-\bar{\psi}(\gamma_\mu D_\mu + m_0)\psi} \propto \det(\gamma_\mu D_\mu + m_0)$$

- determinant can be represented by bosonic fields:

$$\det(\gamma_\mu D_\mu + m_0) \propto \int \mathcal{D}\phi^\dagger\, \mathcal{D}\phi\, e^{-\phi^\dagger(\gamma_\mu D_\mu + m_0)^{-1}\phi}$$

- solving linear equations

$$\xi = (\gamma_\mu D_\mu + m_0)^{-1}\phi$$

for ξ given ϕ using iterative solver (e.g. CG)
requires $\mathcal{O}(1000)$ applications of $D^{\mathrm{lat}} \equiv \gamma_\mu D_\mu + m_0$

Why are Fermions expensive to simulate?

- original Hybrid Monte Carlo (HMC) algorithm
  [Duane, Kennedy, Pendleton, Rowet, 1987]
  typical parameter values: $a = 0.1$ fm, $m_{\mathrm{PS}} = 350$ MeV
  - one application of D^{lat} per lattice site: 1400 flops
  - 16^4 lattice: $\sim$ 90 Mflops
  - solve $\xi = (D^{\mathrm{lat}})^{-1}\phi$ 200 times: $\sim 200 \times 260$ Gflops $=$ 50 Tflops
  - 5000 configurations: $\sim$ 250 Pflops

- Scaling of the 4-dimensional problem:
  - keep fixed box size: $L \cdot a \approx 2$ fm
  - continuum limit $a \to 0$:
    halfing $a \quad \Rightarrow \quad$ no. of points increase by 2^4
  - in addition: factor 4 to 8 from algorithm

- wait for bigger computers ...

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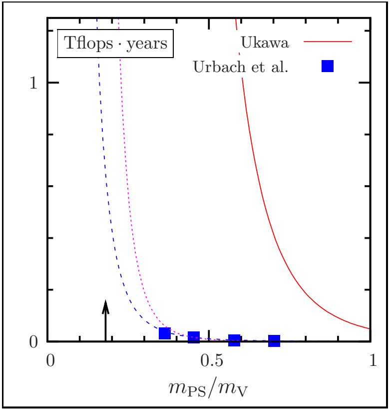
    halfing $a \Rightarrow$ no. of points increase by 2^4
  - in addition: factor 4 to 8 from algorithm

- wait for bigger computers ... or invent better algorithms!

Algorithmic Improvements

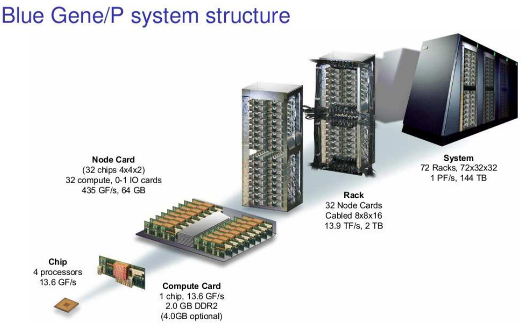
Cost for 1000 configurations, $a = 0.08\ \mathrm{fm}$, Wilson fermions



- trick:
  separate slowly varying expensive modes from rapidly varying cheap modes
- integrate on multiple time-scales
- much faster than standard HMC
- similar developments [Lüscher; QCDSF; Peardon et al.; Clark, Kennedy]

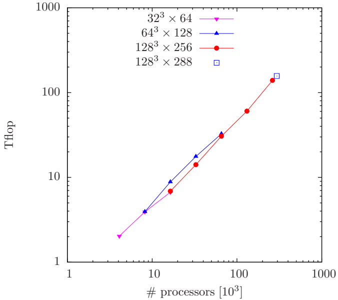
Computer Resources

Lattice QCD still needs Peta Flop machines

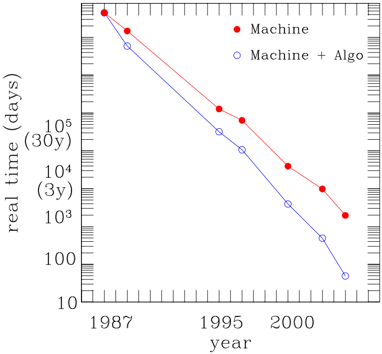


- e.g. Jugene at FZ Jülich
- 72 racks with 1 Peta Flop (peak)

- special programming needed
- code [Jansen, C.U., 2009] speedup:



Resources vs. Algorithm



- real time needed for a standard problem
- machine only reflects Moore's law
- algorithmic improvements contribute almost two orders of magnitude

Outline

Lattice Artifacts

- any quantity affected by lattice artifacts

$$\langle O\rangle^{\mathrm{lat}} = \langle O\rangle^{\mathrm{c}} + a\,\langle O'\rangle^{\mathrm{c}} + a^2\,\langle O''\rangle^{\mathrm{c}}$$

  operators O', O'', ... depend on O and on the symmetries of your action

- discretisation offers large freedom
  not unique

- add (irrelevant) counter terms to the action
  $\Rightarrow$ Symanzik improvement programme

- or try to find a particular discretisation
  where all terms linear in a vanish by symmetries

Twisted Mass Fermions

- Consider the continuum 2-flavour fermionic action

  [Frezzotti, Grassi, Sint, Weisz, '99]

$$S_F = \int d^4x \; \bar{\psi} \; [D + m_q + i\mu\gamma_5\tau_3] \; \psi$$

  with
  - twisted mass parameter μ
  - τ_3 third Pauli matrix acting in flavour space

- S_F is form invariant under a change of variables with angle ω:

$$\psi \to e^{i\omega\gamma_5\tau_3/2}\psi, \qquad \bar{\psi} \to \bar{\psi}e^{i\omega\gamma_5\tau_3/2}.$$

$\longrightarrow$ more general form of the action

Wilson Twisted Mass Fermions

Wilson Twisted Mass Dirac operator [Frezzotti, Grassi, Sint, Weisz, '99]

$$D_{\rm tm} = \frac{1}{2}\sum_\mu \left[\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - a\nabla^*_\mu\nabla_\mu\right] + m_0 + i\mu\gamma_5\tau_3$$

- when $m_0 = m_{\rm crit}$ (maximal twist)
  physical observables are $\mathcal{O}(a)$ improved

  [Frezzotti, Rossi, 2003]

  (proof basically by Parity symmetry of continuum action in Symanzik expansion)

Drawback:

- flavour symmetry explicitly broken

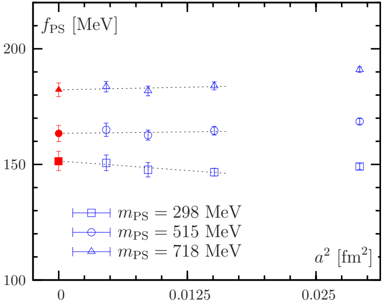
$\mathcal{O}(a)$ Improvement at Maximal Twist

- shown to work in practise
  in the quenched approximation

  [Jansen et al., 2004, 2005]

  [Abdel-Rehim et al., 2004, 2005]

- twisted mass μ relates directly
  to physical quark mass
  only multiplicative renormalisation



- only one parameter $m_0 \to m_{\mathrm{crit}}$ must be tuned
  no additional operator improvement!

- many mixings under renormalisation are simplified

- flavour symmetry breaking appears at $\mathcal{O}(a^2)$
  in practise only important for neutral pion mass

Outline

Choice of Ensembles

- collaborative effort:
  European Twisted Mass Collaboration (ETMC)
- $N_f = 2$ mass-degenerate Wilson quarks at maximal twist
- four values of the lattice spacings:
  $a \sim 0.10$ fm, $a \sim 0.09$ fm, $a \sim 0.07$ fm, $a \sim 0.055$ fm
  in terms of inverse gauge coupling:
  $\beta = 3.80$, $\beta = 3.9$, $\beta = 4.05$, $\beta = 4.2$
- values for m_{PS} range from 260 to 600 MeV
- $L^3 \times 2L$ lattices with $L > 2$ fm
- ≥ 5000 equilibrated trajectories per ensemble

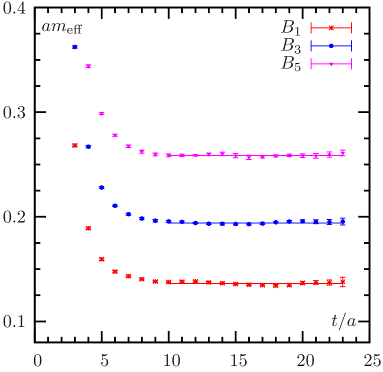
Pion Sector: m_{PS} and f_{PS}

- m_{PS} from exponential decay
  of appropriate correlation functions
- f_{PS} can be extracted at maximal twist from

$$f_{\mathrm{PS}} = \frac{2\mu_q}{m_{\mathrm{PS}}^2} |\langle 0|P^1(0)|\pi\rangle|$$

  [Frezzotti, Grassi, Sint, Weisz]
  due to an exact lattice Ward identity
- no renormalisation factor needed!
  - since $Z_\mu = 1/Z_P$
  - similar to overlap fermions (exact chiral symmetry)
  - unlike pure Wilson

Pion Sector: Mass Determination



- correlator (zero momentum):

$$\langle O(0)O(t)\rangle$$
$$\propto \sum_n \langle 0|O(0)|n\rangle e^{-Ht}\langle n|O(0)|0\rangle$$
$$\propto \sum_n e^{-(E_n-E_0)t}$$

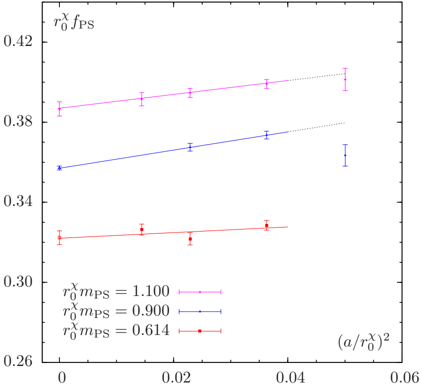
- pseudo-scalar correlator

$$C_\pi(t/a) \propto e^{-am_{\mathrm{PS}}t/a}$$

- effective mass:

$$am_{\mathrm{eff}} = \log \frac{C_\pi(t/a)}{C_\pi(t/a+1)}$$

Continuum Extrapolation f_{PS} in Finite Volume



- finite volume $L/r_0 \sim 5.0$
- linear interpolation to reference points
  $r_0 m_{\mathrm{PS}} = \mathrm{const}$
- linear extrapolation $a^2 \to 0$
  largest a-value not included

$\Rightarrow$ Only small lattice artifacts!

Can we use continuum chiral perturbation theory to describe the data?

[ETMC, C.U., 2009]

Quark Mass Dependence and Chiral Perturbation Theory

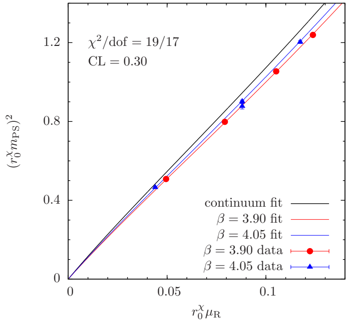
- chiral perturbation theory χPT: low energy effective theory
- describe mass dependence with $n_f = 2$ NLO χPT plus leading lattice artifacts

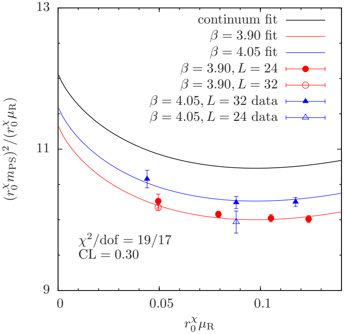
$$m^2_{\mathrm{PS}} = \chi_\mu \left[1 + \xi \log(\chi_\mu/\Lambda_3^2 + D_m a^2)\right] \quad K_m^2(L)$$
$$f_{\mathrm{PS}} = f_0 \left[1 - 2\xi \log(\chi_\mu/\Lambda_4^2) + D_f a^2\right] K_f(L)$$

with $\chi_\mu = 2\hat{B}_0 Z_\mu \mu_q$ and $\xi = \chi_\mu/(2\pi f_0)^2$

- finite size corrections $K_m(L), K_f(L)$ from continuum χPT
  [Gasser, Leutwyler, 1987, 1988; Colangelo, Dürr, Haefeli, 2005]
- fit simultaneously to our data at $a = 0.085$ fm and $a = 0.066$ fm
- 16 data points $300\ \mathrm{MeV} \leq m_{\mathrm{PS}} \leq 500\ \mathrm{MeV}$

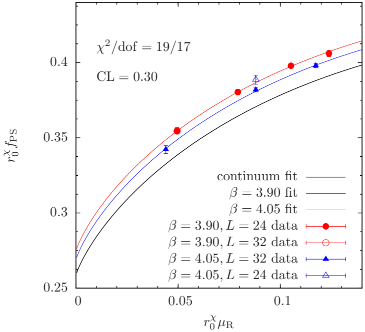
Pion Sector: $(m_{\mathrm{PS}})^2$ as Function of the Quark Mass





- at first glance completely linear
- sensitivity to Λ_3 clearly visible

Pion-Sector: f_{PS} as Function of the Quark Mass



some results:

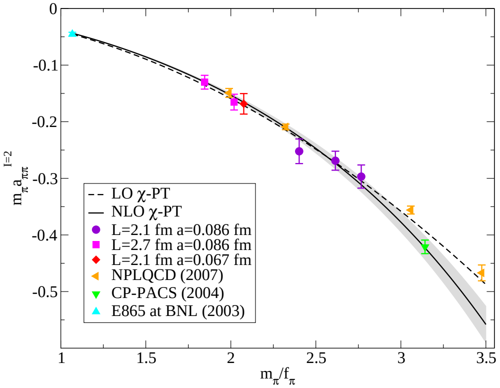
$m_{u,d}$ [MeV]†	$3.54(19)(^{+16}_{-17})$
$\bar{\ell}_3$	$3.50(9)(^{+9}_{-30})$
$\bar{\ell}_4$	$4.66(4)(^{+4}_{-33})$
$\lvert\Sigma\rvert^{1/3}$ [MeV]†	$270(5)(^{+3}_{-4})$
f_0 [MeV]	$121.5(0.1)(^{+1.1}_{-0.1})$
f_π/f_0	$1.0755(6)(^{+8}_{-94})$

†: at 2 GeV in $\overline{\mathrm{MS}}$

- $\bar{\ell}_{3,4} \equiv 2\log(\Lambda_{3,4}/m_\pi)$
- control systematics by averaging over $\mathcal{O}(80)$ different fits

[ETMC, 2009]

$\pi\pi$ Scattering: S-wave Scattering Length $a_{\pi\pi}^{I=2}$



[ETMC, Feng, Jansen, Renner, 2009]

- Lüscher formula:
  don't fear
  but use finite volume!
- $a_{\pi\pi}^{I=2}$ from
  energy shift
  in finite volume
- extrapolated using χPT

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

Flavour Singlet Pseudo-Scalar Mesons

- η' acquires mass through QCD vacuum structure and anomaly
- $2+1$ flavours of quarks:
  mixing between light and strange interpolating operators

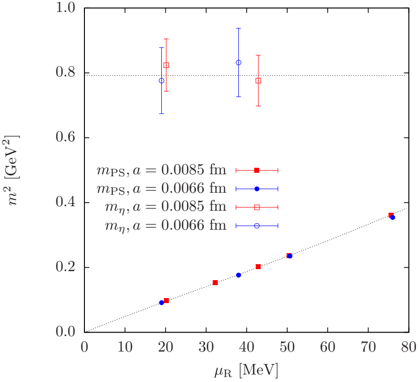
$$\eta \approx 0.58(\bar{u}\gamma_5 u + \bar{d}\gamma_5 d) - 0.57\bar{s}\gamma_5 s$$

$$\eta' \approx 0.40(\bar{u}\gamma_5 u + \bar{d}\gamma_5 d) + 0.82\bar{s}\gamma_5 s$$

- 2 flavours of quarks:
  only one singlet state (η_2) which is related to the "real world" $\eta'(958)$
- η_2 should have mass around 800 MeV [McNeile, Michael, 2000]

Flavour Singlet Pseudo-Scalar Meson η_2

Comparison of quark mass dependence of $m_{\rm PS}$ and m_{η_2}



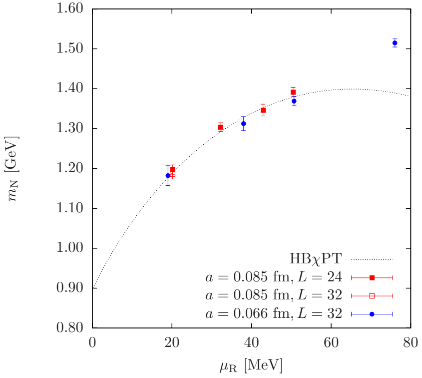
- η_2 mass results down to $m_{\rm PS} \sim 300$ MeV
- small lattice artifacts
- η_2 data consistent with non-zero value in the chiral limit
- $m_{\eta_2} \approx 880$ MeV

[ETMC: K. Jansen, C. Michael, C.U., 2008]

Chiral Extrapolation of the Nucleon Mass

using HBχPT [Jenkins, Manohar, 1991; Becher, Leutwyler, 1999]

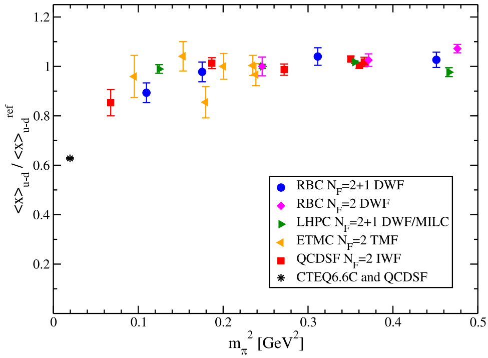
$$m_N = M_N - 4c_1\chi_\mu - \frac{6g_A^2}{32\pi f_0^2}(\chi_\mu)^{3/2}$$



- finite volume effects for smallest mass value at $\beta = 3.9$ negligible
- $m_{\rm N} = 962(45)(10)(3)$
- $c_1 = -1.13(27)(5)(20)$
  $g_A = 1.13(21)(5)(10)$
- still large uncertainty
  can we do better?
- does the extrapolation work?

Moments of Parton Distribution Functions of the Nucleon

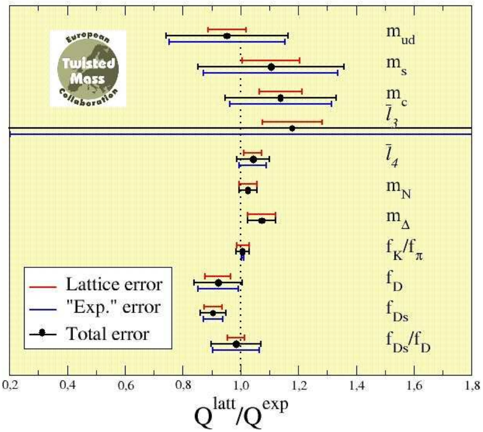
Lattice can compute only moments of PDF's



- curvature hardly visible
- finite size effects?
- need even smaller quark masses!

[Renner, 2009]

A Collection of Results



[ETMC, 2009]

Conclusion

Lattice QCD has made significant progress towards solving QCD

- improved algorithms
- largely reduced systematic errors
- starting to obtain phenomenologically intersting physical results
  - masses and decay constants
  - scattering properties
  - hadron structure
  - ...

Lattice QCD offers the opportunity to work on

- algorithm and computer oriented questions
- quantum field theoretical questions
- interesting physics

Outlook

In lattice QCD

- $2 + 1 + 1$ quark flavours (in progress),
- higher precision,
- more observables, ...

What, if the Higgs mechanism is not realised in nature?

- there are other ways to address electroweak symmetry breaking
- for instance extended technicolour
  - strongly coupled gauge theories
  - must have other properties than QCD: walking and conformal theories
- one possible future challenge for lattice gauge theory