Full QCD on fine lattices

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Lattice QCD

Goal

Computations in QCD of

- particle spectrum $\rightarrow$ **charmed meson and baryon masses**
- matrix elements (decay constants, pdfs, ...) $\rightarrow f_{\mathrm{D_s}}$
- running coupling
- quark masses $\rightarrow$ c **and** b **quark mass**
- ...

Method

Formulate theory on discrete Euclidean space-time

Numerical evaluation of path integral

Lattice QCD

Advantages

Non-perturbative method

QCD calculations also at low energies

Possiblity to vary parameters of QCD

Quark masses

$\rightarrow$ many simulations at non-physical masses

Flavor content

Simulations with N_f =2, 2+1,2+1+1, 8, 12 flavors
n.b. 2=two degenerate flavors (up and down have the same mass)

Gauge group

Use SU(2), SU(3), SU(4), etc $\rightarrow$ large N limit?

Disadvantages

Very expensive $\rightarrow$ need large computer resources & human effort

Statistical method, Euclidean time
$\rightarrow$ limited set of observables accessible.

Lattice computations

Formulate theory on lattice

Four dimensional lattice with finite lattice spacing a

Evaluate path integral

Markov Chain Monte Carlo: integration points $\rightarrow$ gauge fields

Necessily in finite volume $T \times L^3$

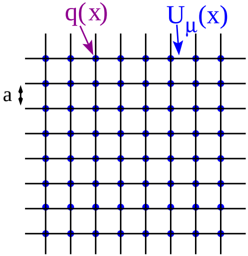
Continuum limit

Repeat calculation at several values of the lattice spacing a
extrapolate to $a = 0$

Finite volume

Control of finite volume effects
Requires simulation at larger-than-physical quark masses

Path integral



Computation of path integral

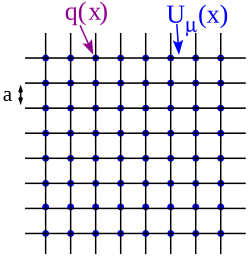
$$\langle A \rangle = \frac{1}{Z} \int \prod_{x,\mu} dU_{x,\mu} e^{-S[U]} \, A[U]$$

with

$$Z = \prod_{x,\mu} dU_{x,\mu} e^{-S[U]}$$

Fermions have been integrated out.
One SU(3) integration variable for each link.

Path integral



$$\langle A \rangle = \frac{1}{Z} \int \prod_{x,\mu} dU_{x,\mu} e^{-S[U]}\, A[U]$$

One SU(3) integration variable for each link.

128×64^3 lattice $\rightarrow 1.3 \cdot 10^8$ links

Classical numerical quadrature would need $N^{\#\text{variables}}$ function evaluations

Evaluation of the path integral

Monte Carlo
Replace integral by sum over measurements on field configurations

$$\langle A \rangle = \frac{1}{Z} \int \prod_{x,\mu} dU_{x,\mu} e^{-S[U]} \, A[U] = \frac{1}{N_{\text{conf}}} \sum_{i=1}^{N_{\text{conf}}} A[U_i] \times \, \{1 + \text{O}(1/\sqrt{N})\}$$

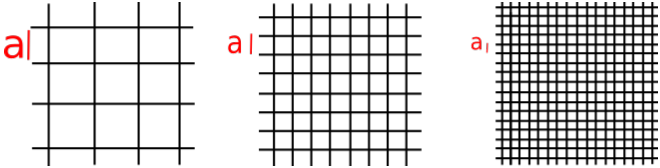
Markov Chain Monte Carlo
These gauge configurations are produced by a Markov process with propability $P[U] \propto e^{-S[U]}$

$$U_1 \to U_2 \to U_3 \to \cdots \to U_N$$

The generation of the gauge configurations takes a large fraction of the computer time, a full set several 100M core hours

Use configurations in many projects $\to$ joint effort

Continuum limit



Repeat calculation at several values of the lattice spacing a

Extrapolate to the continuum $a = 0\,\text{fm}$

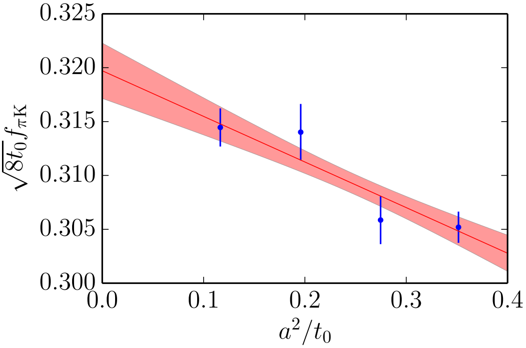
Expensive since in 4-dim box

$$\text{cost} \propto \text{number of points} \propto a^{-4}$$

Factor of 2 in lattice spacing $\Rightarrow$ $16\times$ cost

Systematic effects I

Discretization effects



Lattice spacing a

Pseudoscalar decay constant f_π in units of scale parameter $t_0 \approx 0.42$ fm.

$m_\pi \approx 420$ MeV

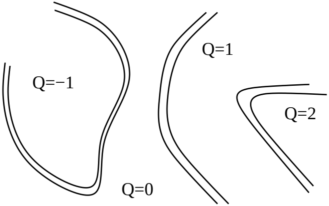
Major obstacle: Topological freezing

$$Q = -\frac{1}{32\pi^2} \int d\,x\,\epsilon_{\mu\nu\rho\sigma} \mathrm{tr}\, F_{\mu\nu} F_{\rho\sigma}$$

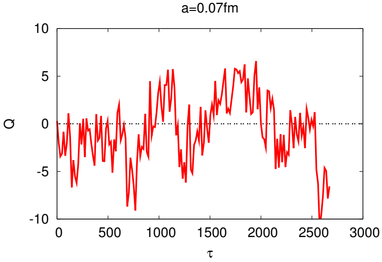
In continuum limit, disconnected **topological sectors** emerge.

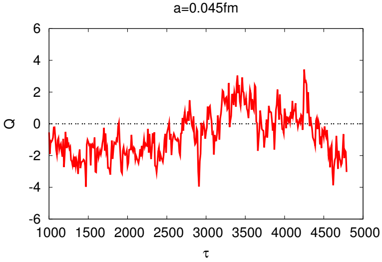
The probability of configurations "in between" sectors drops rapidly.
M. Lüscher, '10

Simulations get stuck in one sector.



Topological charge





$a \approx 0.08$fm

64×32^3

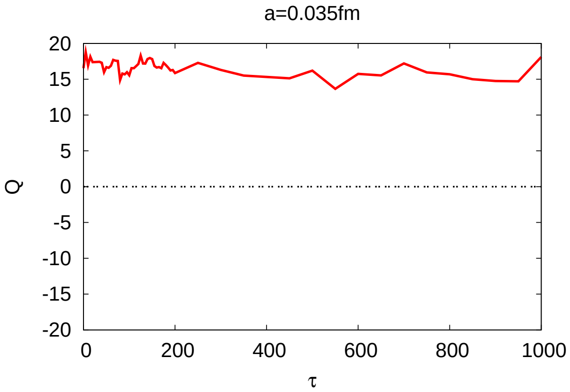
$m_\pi \approx 360$MeV

$a \approx 0.06$fm

64×32^3

$m_\pi \approx 460$MeV

A bad start



$a \approx 0.04$fm

128×64^3

$m_\pi \approx 480$MeV

Topological charge

Use open boundary conditions in time
→No freezing in the continuum, but still long autocorrelations

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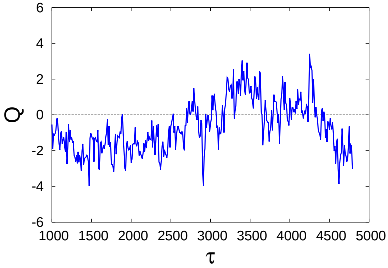
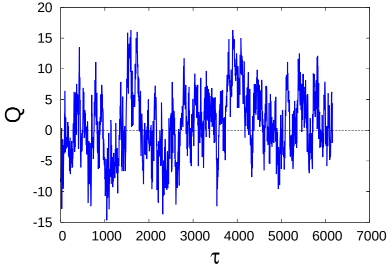
$N_\mathrm{f} = 2$, $a \approx 0.05\,$fm, periodic bc



DD-HMC algorithm

$N_\mathrm{f} = 2+1$, $a \approx 0.05\,$fm, open bc



Mass precond. HMC algorithm

Systematic effects II

Finite volume

Simulations necessarily in finite box

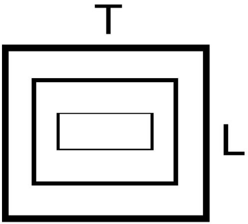
QCD has a mass gap (pions are lightest particle)

$$m_\pi(L) = m_\pi(\infty)(1 + \frac{c}{N_\mathrm{f}} \frac{(m_\pi/F_\pi)^2}{\sqrt{m_\pi L}} \exp(-m_\pi L) + \dots) \qquad \text{for} \qquad L \to \infty$$

To get sub-percent corrections, use

$$L > \frac{4}{m_\pi} \qquad \to \qquad \mathrm{cost} \propto m_\pi^{-4}$$

Verify size effects by simulating different volumes.



Systematic effects

Discretization effects

Need to simulate at several *fine* lattice spacings

$$a \ll \Lambda_{\mathrm{QCD}}^{-1} \qquad \text{and} \qquad a \ll m_q^{-1}$$

At physical light quark masses

$$\begin{aligned} m_\pi L > 4 \quad &\Rightarrow \quad L > 6\,\mathrm{fm} \\ a = 0.05\,\mathrm{fm} \quad &\Rightarrow \quad L/a > 120 \end{aligned}$$

Charm quarks

$$am_q \approx \frac{0.05\,\mathrm{fm} \cdot 1\,\mathrm{GeV}}{200\mathrm{MeV} \cdot \mathrm{fm}} = 0.25$$

Lattices of 0.05 fm and *finer* needed.

Need to make compromises

Simulate at larger pion masses

$\rightarrow$ control chiral extrapolation.

CLS 2+1

Berlin, Humboldt U
CERN
DESY
Dublin, Trinity College
Mainz
Madrid, U Autonoma
Milano, U Bicocca
Münster
Odense
Regensburg
Rome, La Sapienza
Rome, Tor Vergata
Valencia
Wuppertal

Based on blanc map ©Fobos92

Non-perturbatively improved Wilson fermions

$N_f = 2 + 1$ **dynamical flavors**

CLS 2+1

Unique features of the CLS simulations

Open boundary conditions Lüscher'10,Lüscher,S.S.'11

Solution of topological freezing problem

Twisted mass reweighting Lüscher, Palombi'08

Safe simulations with Wilson fermions at small quark masses

Deflated solver for Dirac equation Lüscher'07

Eliminates most of rising cost as $m_q \to 0$.

Monitoring of slow observables

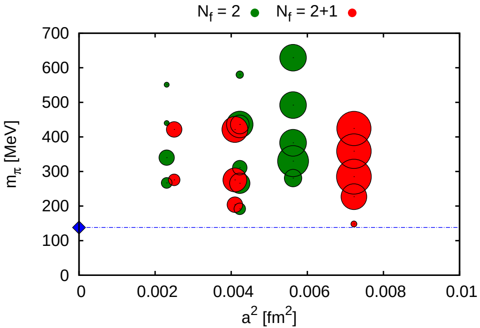
Tuning strategy and statistics based on flow observables

Use of publically available code Lüscher, S.S.'12

openQCD published before first large scale use by collaboration

CLS 2+1 configurations

Status 2014



Comparable statistics in $N_\mathrm{f} = 2$ and $N_\mathrm{f} = 2+1$ project.

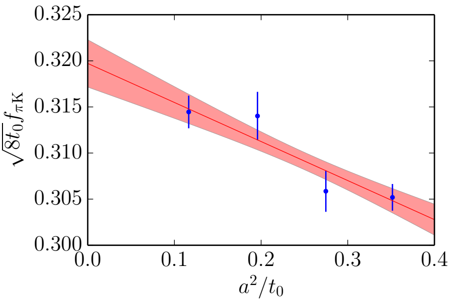
$N_\mathrm{f} = 2$ production 2007-2012

$N_\mathrm{f} = 2+1$ one year production $\rightarrow$ 100TB, 25′000 configs

...now we have 50′000 configs

M. Bruno *et al*, JHEP 1502 (2015) 043

Scale setting



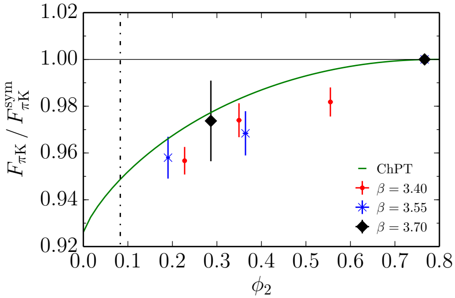
Use light pseudoscalar decay constants

$$f_{\pi K} = \frac{2}{3} \left[f_K + \frac{1}{2} f_\pi \right]$$

5% correction between coarsest lattice with $a \approx 0.086$ fm and continuum.

Chiral corrections

Decay constants



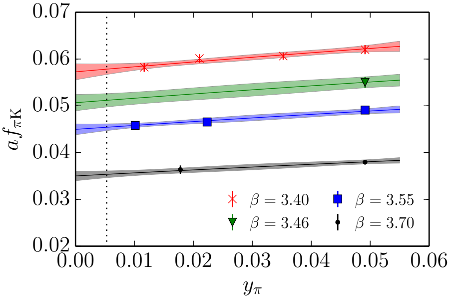
$$f_{\pi K} = f \left[1 + \frac{16\,B\,\mathrm{tr}(M)}{3f^2}(L_5 + 3L_4) + \mathrm{logs}\right]$$

In NLO ChPT combination const up to known log corrections.

$\phi_2 \propto m_{ud}$, $\mathrm{tr}(M)$ =const

NLO SU(3) ChPT prediction: no free parameters
works within 20% of the chiral effect

Lattice spacing



Measurements shifted to chiral trajectories which go through

$$y_\pi = \frac{m_\pi^2}{(4\pi f_{\pi K})^2} = y_\pi^{\mathrm{phys}} \qquad \text{and} \qquad y_K = \frac{m_K^2}{(4\pi f_{\pi K})^2} = y_K^{\mathrm{phys}}$$

Increased uncertainties with current data sets
→ lattice spacings at 2% level

Conclusions

Lattice QCD has made a lot of progress:

Reliable simulations at **small lattice spacing** and **small quark masses**.

CLS 2+1 has generated a standard set of gauge configurations
$\rightarrow$ still in course of being expanded

Finer lattices, smalle pion masses and different volumes will become available.

Scale setting in advanced stage.

Now ready for all kinds of physics projects

RTG comes just at the right time.