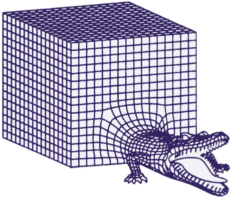
Lattice QCD Basics

Christian B. Lang

Inst. f. Physik, FB Theoretische Physik

Universität Graz

June 2017



Warning!

This is a lettuce field:

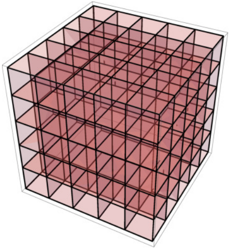
(Go to an agriculture lecture!)

Warning!

This is a lettuce field:

(Go to an agriculture lecture!)

This is a lattice field:



(Stay here!)

Outline

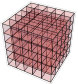
Further reading

I do not quote the standard texts on Quantum Field Theory (like Peskin/Schroeder or Ramond). For this please ask your favorite QFT lecturer.

- Lattice QCD specific web sites:
  http://www.scholarpedia.org/article/Lattice_gauge_theories
  https://arxiv.org/archive/hep-lat
- Lattice QCD specific monographs:
  - E. Seiler: Gauge Theories as a Problem of Constructive QFT and Statistical Mechanics, Vol. 159 of Springer Lecture Notes in Physics (Springer, 1982)
  - M. Creutz: Quarks, Gluons and Lattices (Cambridge Univ. Press, 1983)
  - H. J. Rothe: Lattice Gauge Theories - An Introduction (World Scientific, 1992)
  - I. Montvay and G. Münster: Quantum Fields on a Lattice (Cambridge University Press: 1997)
  - J. Smit: Introduction to Quantum Fields on a Lattice (Cambridge University Press: 2002)
  - J. Zinn-Justin: Quantum Field Theory and Critical Phenomena (Clarendon Press, Oxford, UK: 2002)
  - Thomas Degrand und Carleton Detar: Lattice Methods for Quantum Chromodynamics (World Scientific: 2006)
  - Christof Gattringer and Christian B. Lang: Quantum Chromodynamics on the Lattice - an Introductory Presentation (Springer: 2010)
  - Francesco Knechtli, Michael Günther, and Michael: Lattice Quantum Chromodynamics, Practical Essentials (Springer: 2017)

Texts and software on the Web

- Introductory lectures
  - Martin Lüscher, Computational Strategies in Lattice QCD, arXiv 1002.4232
  - Sinéad Ryan, INT Lectures on Hadron Spectroscopy, http://www.maths.tcd.ie/ryan/INT2012/
  - William Detmold, Hadron Interactions and Many-Body Physics, INT Summer School on Lattice QCD for Nuclear Physics, http://www.int.washington.edu/PROGRAMS/12-2c/Lectures.html
  - Anna Hasenfratz, Introduction to Lattice QCD, Summer School on Lattice QCD for Nuclear Physics, http://www.int.washington.edu/PROGRAMS/12-2c/Lectures.html
  - Christian Hoelbling, Lattice QCD: Concepts, techniques and some results, Acta Physica Polon. B45 no.12, 2143, 2014.
  - Daniel Mohler, Bound states on the lattice, lectures at IUTP 2017, http://physik.uni-graz.at/iutp2017/lecturenotes.php
- Other sources
  - Annual lattice proceedings, many of them at Proceedings of Science: https://pos.sissa.it/
  - HEP-LAT Preprint Server: https://arxiv.org/archive/hep-lat
- Software
  - openQCD: http://luscher.web.cern.ch/luscher/openQCD/
  - LQCD Software (SciDAC): https://www.usqcd.org/software.html



1. Lattice Gauge Theory

"Declaration of QCD"

- We assume that QCD is *the* quantum field theory of quarks and gluons, defined by a Lagrangian and action of the form

$$
\begin{aligned}
L &= \frac{1}{2\,g^2}\,\mathrm{Tr}\,F_{\mu\nu}F_{\mu\nu} + \sum_f \overline{\psi}_f\,(\not{D} + m_f)\,\psi_f \\
S &= \int d^4x\;L
\end{aligned}
$$

- This theory can be solved from first principles, with minimal number of input parameters (bare quark masses and a scale fixing parameter).
- Hadron properties should be computable from QCD.

Euclidean space-time: x_μ real, $x_4 = \mathrm{i}\, t$.

Quarks $\psi_{f,i,\alpha}$:
- flavor f= u, d, s, c, t, b;
- color i= 1, 2, 3;
- Dirac α=1,2,3,4

Gluons $A_\mu \in \mathbf{su}(3)$: $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + \mathrm{i}\,[A_\mu, A_\nu]$

Parameters (couplings): g, m_u, m_d, m_s, m_c, m_t, m_b (note: bare parameters, scale dependence!)

Homework (1.1)

Discuss: what changes for $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + \mathrm{i}\,[A_\mu, A_\nu]$, $A_\mu \in \mathbf{s}u(3)$, if $SU(3) \to U(1)$.

A local transformation with an SU(3) matrix $\Omega(x)$:

$$\begin{aligned}
\psi(x) &\rightarrow \psi'(x) = \Omega(x)\psi(x) \\
\overline{\psi}(x) &\rightarrow \overline{\psi}'(x) = \overline{\psi}(x)\Omega(x)^\dagger \\
A_\mu(x) &\rightarrow A'_\mu(x) = \Omega(x)A_\mu(x)\Omega(x)^\dagger + \mathrm{i}\big(\partial_\mu\Omega(x)\big)\Omega(x)^\dagger
\end{aligned}$$

leaves the action invariant

$$S[\psi', \overline{\psi}', A'] = S[\psi, \overline{\psi}, A]$$

- $\Omega \in \mathrm{SU}(3) \rightarrow \Omega(x)^\dagger\Omega(x) = \mathbb{1}$
- Cf. rotation invariance, e.g., $\overline{\psi}(x)\Omega(x)^\dagger\Omega(x)\psi(x) = \overline{\psi}(x)\psi(x)$
- Action and observable (asymptotic) states have to be color singlets!
- This is the **SU(3)$_{color}$ gauge invariance!**

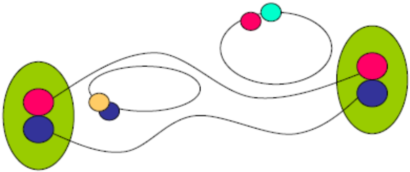
Quantization via Feynman path integral:

$$C_N(t) = \langle \overline{N}(t) N(0) \rangle \quad \propto \quad \int [\mathcal{D}A\, \mathcal{D}\overline{\psi}\, \mathcal{D}\psi]\, \mathrm{e}^{-S(A,\overline{\psi},\psi)}\, \overline{N}(t)\, N(0)$$
$$\sim \quad \exp(-E_N\, t)$$

Observables (like N) are built from A, ψ and $\overline{\psi}$

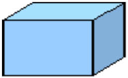
Gluons: bosonic variables are commuting: $A(x)A(y) = A(y)A(x)$

Quarks: Grassmann variables are anti-commuting: $\psi(x)\psi(y) = -\psi(y)\psi(x)$



Quantization by path integral

Path integral =
integral over all field configurations =
integral over all field values at all space-time points!



How to sum over all ∞^∞ field configurations?

We need

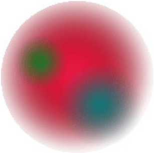
- *Regularization and renormalization:*
  Momentum cut-off, dimensional regularization, lattice
- *Approximation:*
  Perturbation theory or non-perturbative methods

Problems using perturbation theory

Problems that cannot be attacked with perturbation theory:

- Chiral symmetry breaking
  - Explicit: Non-zero quark masses
  - Spontaneous: The pion is a Goldstone boson

- Confinement and the low energy properties of hadrons
  - Hadron masses
  - Low energy parameters (decay constants, current quark masses, LEC and parameters of Chiral Perturbation Theory)
  - Form factors, matrix elements, structure functions
  - Temperature and chemical potential



We need non-perturbative methods!

Why the lattice?

- Continuum QFT is singular:

regular formulation needed

Why the lattice?

- Continuum QFT is singular:

  regular formulation needed ✔

- Hadrons are non-perturbative compounds:

  non-pert. method needed

Why the lattice?

- Continuum QFT is singular:

  regular formulation needed ✓

- Hadrons are non-perturbative compounds:

  non-pert. method needed ✓

- Gauge invariance is important:

  gauge inv. formulation preferred

Why lattice?

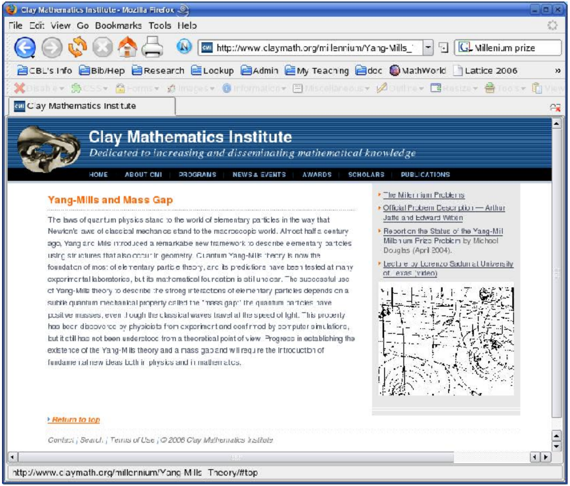
Why the lattice?

- Continuum QFT is singular:
  regular formulation needed ✓
- Hadrons are non-perturbative compounds:
  non-pert. method needed ✓
- Gauge invariance is important:
  gauge inv. formulation preferred ✓
- Limit to “continuum QCD”:
  should be controllable

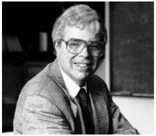
Why the lattice?

- Continuum QFT is singular:
  regular formulation needed ✓
- Hadrons are non-perturbative compounds:
  non-pert. method needed ✓
- Gauge invariance is important:
  gauge inv. formulation preferred ✓
- Limit to "continuum QCD":
  should be controllable ✓

Non-perturbative results are hard to get. A rigorous proof of confinement brings a 1,000.000 $ prize from the Clay Mathematics institute



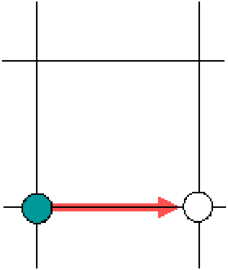
Lattice QCD



Kenneth Wilson suggested 1974 to regularize QCD by introducing a 4-d (Euclidean) space-time lattice.
Phys.Rev. D10 (1974) 2445-2459. (cited 4500!)

Gauge field variables $U_\mu(x) \in SU(3)$
(3x3 complex, unitary matrices on each link)

Quark field variables $\psi(x)$, $\overline{\psi}(x)$
($\psi^{(f)}_{\alpha,c}(x)$ are color 3-vectors, Dirac 4-spinors, n_f vectors and Grassmann variables, on each lattice site)



Continuum: Free fermion action (Dirac operator):

$$S_F^0[\psi,\overline{\psi}] = \int d^4x\, \overline{\psi}(x)\Big(\gamma_\mu \partial_\mu + m\Big)\psi(x)$$

Derivative:

$$\partial_\mu \psi(x) \;\rightarrow\; \frac{1}{2a}\Big(\psi(n+\hat{\mu}) - \psi(n-\hat{\mu})\Big)$$

Lattice action:

$$S_F^0[\psi,\overline{\psi}] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n)\left(\sum_{\mu=1}^{4} \gamma_\mu\, \frac{\psi(n+\hat{\mu}) - \psi(n-\hat{\mu})}{2a} \;+\; m\,\psi(n)\right)$$

Gauge invariance = invariance under gauge transformations:

$$\begin{aligned} \psi(n) \to \psi'(n) &= \Omega(n)\,\psi(n) \\ \overline{\psi}(n) \to \overline{\psi}'(n) &= \overline{\psi}(n)\,\Omega(n)^\dagger \end{aligned}$$

Note: each $\Omega(n) \in SU(3)$ is a unitary 3x3 matrix: $\Omega(n)^\dagger\,\Omega(n) = \mathbf{1}$.
It may be different for each site (gauge symmetry = local symmetry)!

Gauge invariance of lattice action?

$$\begin{aligned} \overline{\psi}(n)\psi(n) &\to \overline{\psi}'(n)\,\psi'(n) = \overline{\psi}(n)\,\Omega(n)^\dagger\,\Omega(n)\,\psi(n) = \overline{\psi}(n)\psi(n) \quad ✓ \\ \overline{\psi}(n)\psi(n+\hat{\mu}) &\to \overline{\psi}'(n)\,\psi'(n+\hat{\mu}) = \overline{\psi}(n)\,\Omega(n)^\dagger\,\Omega(n+\hat{\mu})\,\psi(n+\hat{\mu}) \quad ✗ \end{aligned}$$

Gauge transporter

We replace the term by a new form with a new field variable:

$$\overline{\psi}(n)\, U_\mu(n)\, \psi(n+\hat{\mu})$$

The new field is the gauge (transporter) field $U_\mu(n) \in SU(3)$ with the transformation

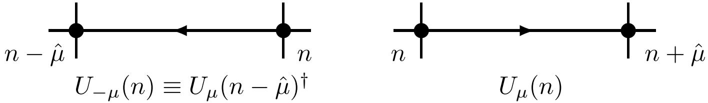
$$U_\mu(n) \;\to\; U'_\mu(n) = \Omega(n)\, U_\mu(n)\, \Omega(n+\hat{\mu})^\dagger$$

Then

$$\begin{aligned}
&\overline{\psi}'(n)\, U'_\mu(n)\, \psi'(n+\hat{\mu}) \\
&\qquad = \overline{\psi}(n)\, \Omega(n)^\dagger\, U'_\mu(n)\, \Omega(n+\hat{\mu})\, \psi(n+\hat{\mu}) \\
&\qquad = \overline{\psi}(n)\, \Omega(n)^\dagger\, \Omega(n)\, U_\mu(n)\, \Omega(n+\hat{\mu})^\dagger\, \Omega(n+\hat{\mu})\, \psi(n+\hat{\mu}) \\
&\qquad = \overline{\psi}(n)\, U_\mu(n)\, \psi(n+\hat{\mu}) \;\checkmark
\end{aligned}$$

Lattice gauge field: oriented link variable

$$U_{-\mu}(n) \equiv U_\mu(n-\hat{\mu})^\dagger$$



Compare with the continuum *gauge transporter*

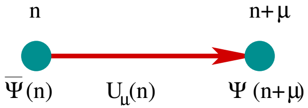
$$G(x,y) = P \exp\left(\mathrm{i}\int_{\mathcal{C}_{xy}} A\cdot \mathrm{d}s\right)$$

along a link from $x = n$ to $y = n+\hat{\mu}$:

$$\begin{aligned} G(n, n+\hat{\mu}) &= \exp\left(\mathrm{i}\, a\, A_\mu(n)\right) \\ &= U_\mu(n) = \mathbb{1} + \mathrm{i}\, a\, A_\mu(n) + \mathcal{O}(a^2) \end{aligned}$$

$$S_F[\psi, \overline{\psi}, U] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n) \left[\sum_{\mu=1}^{4} \gamma_\mu \frac{U_\mu(n)\psi(n+\hat{\mu}) - U_{-\mu}(n)\psi(n-\hat{\mu})}{2a} + m\psi(n) \right]$$

"Link term":



Homework (1.2)

Prove that up to $\mathcal{O}(a)$ the "naive" fermion action

$$S_F[\psi, \overline{\psi}, U] = a^4 \sum_{n\in\Lambda} \overline{\psi}(n) \left[\sum_{\mu=1}^{4} \gamma_\mu \frac{U_\mu(n)\psi(n+\hat{\mu}) - U_{-\mu}(n)\psi(n-\hat{\mu})}{2a} + m\psi(n) \right]$$

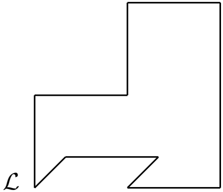
gives the continuum action.

Discuss the difference between this version of continuum limit and the true continuum limit.

Can we build action terms just with gauge field variables?
Any term like that will do:

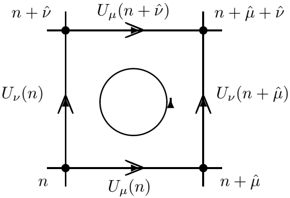
$$L[U] = \mathrm{Tr}\left[\prod_{(n,\mu)\in\mathcal{L}} U_\mu(n)\right]$$

($\mathcal{L}$ is a closed loop of links.)



Why? Consider the smallest (non-trivial) loop: a plaquette!

$$\begin{aligned} U_{\mu\nu}(n) &= U_\mu(n)\,U_\nu(n+\hat\mu) \\ &\quad \times U_{-\mu}(n+\hat\mu+\hat\nu)\,U_{-\nu}(n+\hat\nu) \\ &= U_\mu(n)\,U_\nu(n+\hat\mu)\,U_\mu(n+\hat\nu)^\dagger\,U_\nu(n)^\dagger \end{aligned}$$



Is $\mathrm{Tr}U_{\mu\nu}(n)$ gauge invariant?

Gauge transformation $\{\Omega(n)\}$ of the plaquette term:

$$\mathrm{Tr}\left[U'_\mu(n)\,U'_\nu(n+\hat\mu)\,U'_\mu(n+\hat\nu)^\dagger\,U'_\nu(n)^\dagger\right] =$$

$$\mathrm{Tr}\Big[\Omega(n)U_\mu(n)\,\Omega(n+\hat\mu)^\dagger\Omega(n+\hat\mu)\,U_\nu(n+\hat\mu)\,\Omega(n+\hat\nu+\hat\mu)^\dagger$$
$$\times\Omega(n+\hat\nu+\hat\mu)\,U_\mu(n+\hat\nu)^\dagger\,\Omega(n+\hat\nu)^\dagger\Omega(n+\hat\nu)U_\nu(n)^\dagger\Omega(n)^\dagger\Big] =$$
$$\mathrm{Tr}\left[U_\mu(n)\,U_\nu(n+\hat\mu)\,U_\mu(n+\hat\nu)^\dagger\,U_\nu(n)^\dagger\right]$$

(note: $(A\,B\,C)^\dagger = C^\dagger\,B^\dagger\,A^\dagger$)

Gauge transformation $\{\Omega(n)\}$ of the plaquette term:

$$
\begin{aligned}
&\mathrm{Tr}\left[U'_\mu(n)\, U'_\nu(n+\hat\mu)\, U'_\mu(n+\hat\nu)^\dagger\, U'_\nu(n)^\dagger\right] = \\
&\mathrm{Tr}\Big[\Omega(n)U_\mu(n)\,\Omega(n+\hat\mu)^\dagger\Omega(n+\hat\mu)\,U_\nu(n+\hat\mu)\,\Omega(n+\hat\nu+\hat\mu)^\dagger \\
&\quad\times\Omega(n+\hat\nu+\hat\mu)\,U_\mu(n+\hat\nu)^\dagger\,\Omega(n+\hat\nu)^\dagger\Omega(n+\hat\nu)U_\nu(n)^\dagger\Omega(n)^\dagger\Big] = \\
&\mathrm{Tr}\left[U_\mu(n)\,U_\nu(n+\hat\mu)\,U_\mu(n+\hat\nu)^\dagger\,U_\nu(n)^\dagger\right]
\end{aligned}
$$

(note: $(A\,B\,C)^\dagger = C^\dagger\,B^\dagger\,A^\dagger$)

Gauge transformation $\{\Omega(n)\}$ of the plaquette term:

$$
\begin{aligned}
&\mathrm{Tr}\left[U'_\mu(n)\, U'_\nu(n+\hat\mu)\, U'_\mu(n+\hat\nu)^\dagger\, U'_\nu(n)^\dagger\right] = \\
&\mathrm{Tr}\Big[\Omega(n) U_\mu(n)\, \Omega(n+\hat\mu)^\dagger \Omega(n+\hat\mu)\, U_\nu(n+\hat\mu)\, \Omega(n+\hat\nu+\hat\mu)^\dagger \\
&\quad \times \Omega(n+\hat\nu+\hat\mu)\, U_\mu(n+\hat\nu)^\dagger\, \Omega(n+\hat\nu)^\dagger \Omega(n+\hat\nu) U_\nu(n)^\dagger \Omega(n)^\dagger\Big] = \\
&\mathrm{Tr}\left[U_\mu(n)\, U_\nu(n+\hat\mu)\, U_\mu(n+\hat\nu)^\dagger\, U_\nu(n)^\dagger\right]
\end{aligned}
$$

(note: $(A\,B\,C)^\dagger = C^\dagger\, B^\dagger\, A^\dagger$)

Wilson gauge action:

$$S_G[U] = \frac{2}{g^2} \sum_{n\in\Lambda} \sum_{\mu<\nu} \mathrm{Re}\,\mathrm{Tr}\left[\mathbb{1} - U_{\mu\nu}(n)\right]$$

- ...is a sum over all plaquettes
- For small lattice spacing a and $U_\mu(n) = \exp\left(\mathrm{i}\, a\, A_\mu(n)\right)$ the leading term of the expansion gives

$$S_G[U] = \frac{2}{g^2} \sum_{n\in\Lambda} \sum_{\mu<\nu} \mathrm{Re}\,\mathrm{Tr}\left[1 - U_{\mu\nu}(n)\right] = \frac{a^4}{2\,g^2} \sum_{n\in\Lambda} \sum_{\mu,\nu} \mathrm{Tr}\left[F_{\mu\nu}(n)^2\right] + \mathcal{O}(a^2)$$

  This is called the “naive” continuum limit...
- More complicated gauge actions involve longer closed loops (but should give the same continuum limit!).

Homework problems

Homework (1.3)

Prove that up to $\mathcal{O}(a^2)$ the Wilson gauge action reproduces the continuum action. Do not forget, that the gauge field variables for non-abelian groups do not commute! For this proof you need the Baker-Campbell-Hausdorff formula:

$$\exp(A)\,\exp(B) = \exp\left(A + B + \frac{1}{2}[A, B] + \ldots\right) .$$

Homework (1.4)

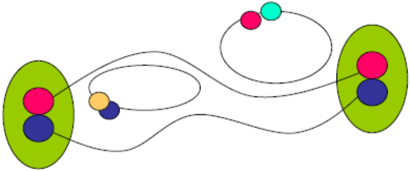
Write first parts of a program for $U(1)$ gauge theory, As a first step implement (a) initialization (ordered or disordered), and (b) plaquette measurement) the updating steps will be discussed later). Make it modular such that you can later easily extend it to include further tasks. Can you do this for $SU(2)$ as well?

Lattice path integral for expectation values (n-point functions):

$$\langle O_2(t)\, O_1(0)\rangle = \frac{1}{Z}\int \mathcal{D}[\psi,\overline{\psi}]\,\mathcal{D}[U]\; \mathrm{e}^{-S_F[\psi,\overline{\psi},U]-S_G[U]}\, O_2[\psi,\overline{\psi},U]\, O_1[\psi,\overline{\psi},U]$$

Partition function:

$$Z = \int \mathcal{D}[\psi,\overline{\psi}]\,\mathcal{D}[U]\; \mathrm{e}^{-S_F[\psi,\overline{\psi},U]-S_G[U]}\ .$$



Key points

- The Euclidean lattice formulation has site variables (quarks) and link variables (gaugefields). The gaugefield variables are in the group (not in the algebra).
- The Wilson gauge field action is a sum over plaquettes.
- Quantization amounts to summing over all gauge- and fermion-configurations.
- The naive continuum limit ($a \to 0$ in the action) reproduces the continuum expressions. (Does this hold for the quantized theory?)
- The formulation is explicitly gauge invariant.

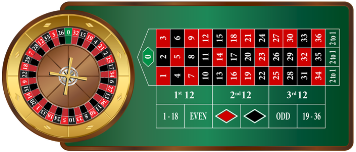
2. Monte Carlo Integration

We want to compute expectation values like

$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}[U]\, \mathrm{e}^{-S_G[U]}\, O[U] \quad \text{with} \quad Z = \int \mathcal{D}[U]\, \mathrm{e}^{-S_G[U]} \, .$$

Monte Carlo simulation = approximation

$$\langle O \rangle \approx \frac{1}{N} \sum_{n=1}^{N} \mathrm{e}^{-S[U_n]}\, O[U_n] \approx \frac{1}{N} \sum_{\substack{U_n \text{ with} \\ \text{probability} \\ \propto\, \mathrm{e}^{-S[U_n]}}} O[U_n] \, ,$$

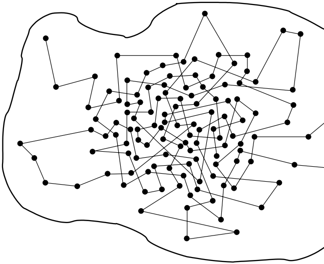


Markov chain of configurations:

$$U_0 \longrightarrow U_1 \longrightarrow U_2 \longrightarrow \dots$$

$$P(U_n = U'|U_{n-1} = U) = T(U' \leftarrow U) \equiv T(U'|U)$$

$$0 \leq T(U'|U) \leq 1 \;, \quad \sum_{U'} T(U'|U) = 1$$



configuration space

Balance condition $P(\text{hop into } U') = P(\text{hop out of } U')$:

$$\sum_U T(U'|U)\, P(U) \stackrel{!}{=} \sum_U T(U|U')\, P(U') = P(U')$$

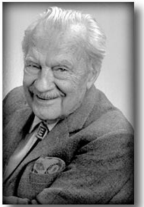
ensures:

$$P^{(0)} \stackrel{T}{\to} P^{(1)} \stackrel{T}{\to} P^{(2)} \stackrel{T}{\to} \dots \stackrel{T}{\to} P \qquad (= \text{equilibrium distribution})$$

Detailed balance :

$$T(U'|U)\,P(U) = T(U|U')\,P(U')$$

is a sufficient condition.



Nick Metropolis

Metropolis algorithm

Step 1: Choose some candidate configuration U' according to some *a priori selection probability* $T_0(U'|U)$, where $U = U_{n-1}$.

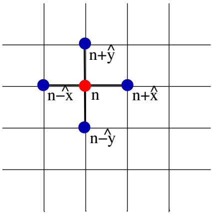
Step 2: Accept the candidate configuration U' as the new configuration U_n with the acceptance probability

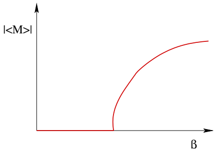
$$T_A(U'|U) = \min\left(1,\ \frac{T_0(U|U')\exp\left(-S[U']\right)}{T_0(U'|U)\exp\left(-S[U]\right)}\right) .$$

Step 3: Repeat these steps from the beginning.

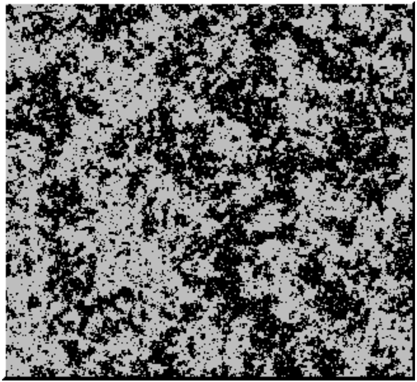
Example: Ising model

- Spin configuration: spins $s_n \in \{-1, 1\}$
- $S[s] = \kappa \sum_{n,\mu} \; s_n s_{n+\hat{\mu}}$
- $s'_n = -s_{n,old}$
- $T_A(s'|s) = \min\left(1, \exp\left[-(S[s'] - S[s])\right]\right)$
  i.e. accept if
  $\exp\left(-(S[s'] - S[s])\right) > \text{random number} \in (0, 1)$
  Note: ΔS is local due to
  $S[s'] - S[s] = [\kappa(s_{n+\hat{1}} + s_{n-\hat{1}} + s_{n+\hat{2}} + s_{n-\hat{2}})](s'_n - s_n)$
- Test/update each spin once for all spins = one sweep
- Measure observables after each sweep

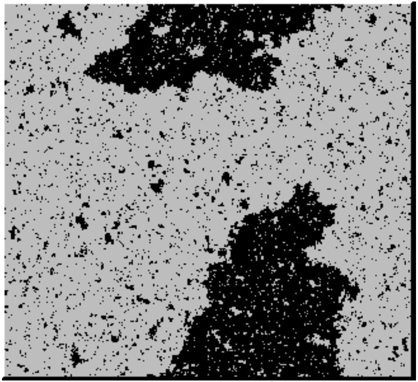




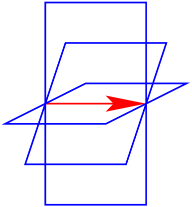
Examples for Ising spin configurations
(cf.http://latticeguy.net/mypubs/xtoys/xtoys.html run:/executables/xising)



hot (disordered)



cold (ordered)



(3 orthogonal directions!)

The gauge action has locally the form

$$S[U_\mu(n)']_{\mathrm{loc}} = \frac{\beta}{N} \mathrm{Re\,Tr}\left[6\,\mathbb{1} - U_\mu(n)'\,A\right]$$
$$\text{with } A = \sum_{i=1}^{6} P_i$$

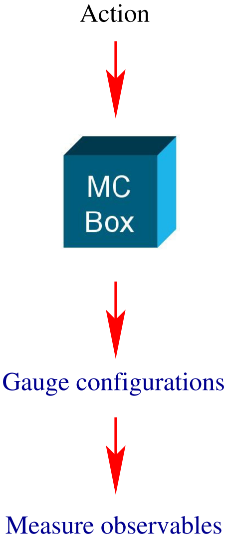
i.e., sum over "staples" P_i

We need the change of the action:

$$\Delta S = S[U_\mu(n)']_{\mathrm{loc}} - S[U_\mu(n)]_{\mathrm{loc}} = -\frac{\beta}{N} \mathrm{Re\,Tr}\left[\left(U_\mu(n)' - U_\mu(n)\right) A\right]$$

Note: A is not affected by the change of $U_\mu(n)$! Updating one link requires only information from the bordering plaquettes (staples)

Mike Creutz



Let's compute:

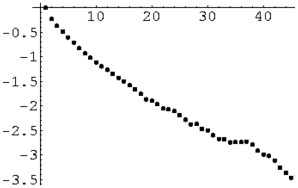
- Start with some (e.g. hot or cold) configuration.
- Update each link of the configuration = one sweep.
- Run for many equilibrating sweeps.
- Continue sweeping and measure observables every k sweeps (k depends on the autocorrelation time).

Autocorrelation time τ_X for an observable X (t=MC time):

$$C_X(t) = \langle (X_0 - \langle X \rangle)(X_t - \langle X \rangle) \rangle$$

$$\Gamma_X(t) = \frac{C_X(t)}{C_X(0)} \propto e^{-t/\tau_X}$$

$$\tau_{exp} = \sup_X \tau_X$$



Approximated by

$$\tau_{X,int} = \frac{1}{2} + \sum_{t=1}^{\infty} \Gamma_X(t)$$

Estimate:

$$n_{indep} = \frac{n}{2\tau_{A,int}}$$

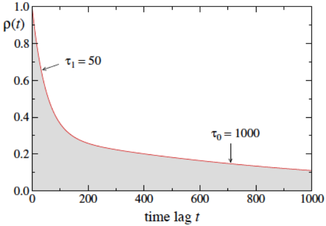


Fig. from M. Lüscher, arXiv/1009.5877

MC simulation $\rightarrow$ raw data $\{C\}$ $\rightarrow$ analysis $\rightarrow$ the golden number $\theta \equiv \theta(\{C\})$
Errors propagate over several stepa - how to estimate the variance of θ?

Jackknife method:

Assume that $\{C\}$ is a set of N configurations, then

- choose subset $\{C\}_i$ by removing configuration i
- compute $\theta_i \equiv \theta(\{C\}_i)$
- repeat for all i, then an estimate for variance is

$$\sigma_\theta^2 = \frac{N-1}{N} \sum_{i=1}^{N} (\theta_i - \theta)^2$$

Unbiased estimate: $\theta - (N-1)(\tilde{\theta} - \theta)$ with $\tilde{\theta} \equiv \frac{1}{N} \sum_{i=1}^{N} \theta_i$

(Caveat: Jackknife does not know about autocorrelation!)

Homework problems

Homework (2.1)

For the $U(1)$ program (earlier homework) write a subroutine that applies a random gauge transformation. Measure the mean plaquette before and after applying the gauge transformation. It should not change!

Homework (2.2)

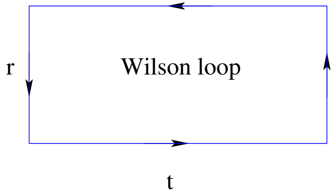
Extend your $U(1)$ gauge theory program with a Monte-Carlo updating routine (Metropolis algorithm). Perform some equilibration and measuring (mean plaquette!) runs. Make it modular such that you can later easily extend it to Wilson-loop and Polyakov loop measurements.

More on MC algorithms: Lectures by Alexei Bazavov

Consider the observable "Wilson loop":

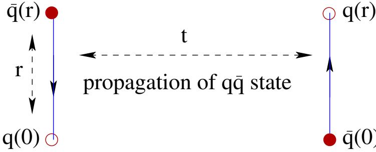
$$W[U] = \mathrm{Tr}\left[\prod_{(n,\mu)\in\mathcal{C}_{r\times t}} U_\mu(n)\right]$$

where $\mathcal{C}_{r\times t}$ is a closed loop around a $r \times t$ rectangle.



Its expectation value defines a "static potential" $V(r)$ at spatial separation r between a quark and an anti-quark:

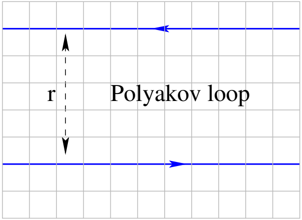
$$\begin{aligned}\langle W_{\mathcal{L}}\rangle &\propto e^{-t\,V(r)}\left(1+\mathcal{O}(e^{-t\,\Delta E})\right)\\ &= e^{-n_t\,a\,V(r)}\left(1+\mathcal{O}(e^{-n_t\,a\,\Delta E})\right)\end{aligned}$$



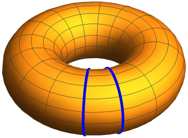
Strong coupling expansion: $\rightarrow V(r = a\,n_r) = \sigma\,r$ with $\sigma = -\frac{1}{a^2}\log(\beta/18) \neq 0$
(Wilson confinement criterion)

Alternative observable: Polyakov loop

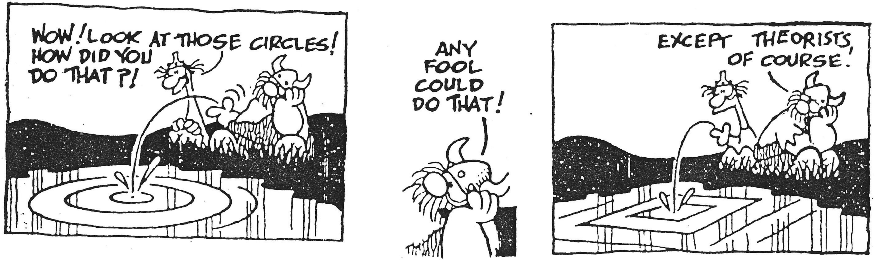
$$P(\vec{m}) = \mathrm{Tr}\left[\prod_{j=0}^{N_T-1} U_4(\vec{m}, j)\right]$$

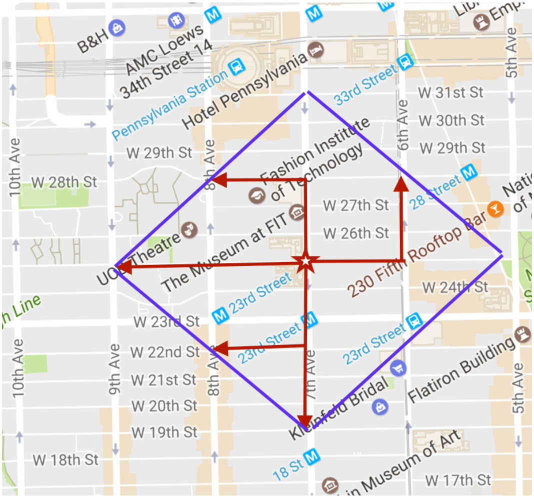


$$\langle P(\vec{m})P(\vec{n})^\dagger \rangle \propto \mathrm{e}^{-N_T a\, V(r)} \left(1 + \mathcal{O}(\mathrm{e}^{-N_T a \Delta E})\right)$$



"Static" potential: potential between "static" charges (not well-defined for dynamical sea quarks → string breaking)


WOW! LOOK AT THOSE CIRCLES! HOW DID YOU DO THAT?!
ANY FOOL COULD DO THAT!
EXCEPT THEORISTS, OF COURSE!



Taxi geometry

Rotational ($O(4)$) symmetry returns for $a \to 0$:

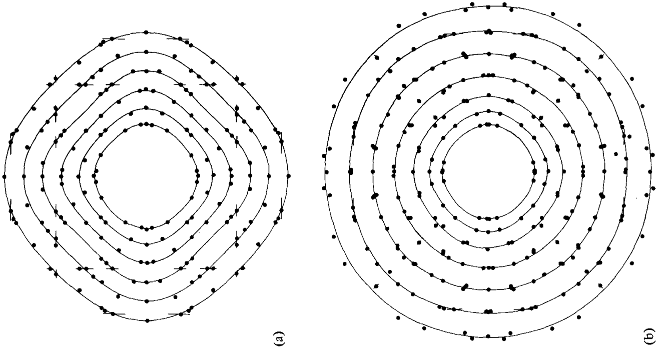
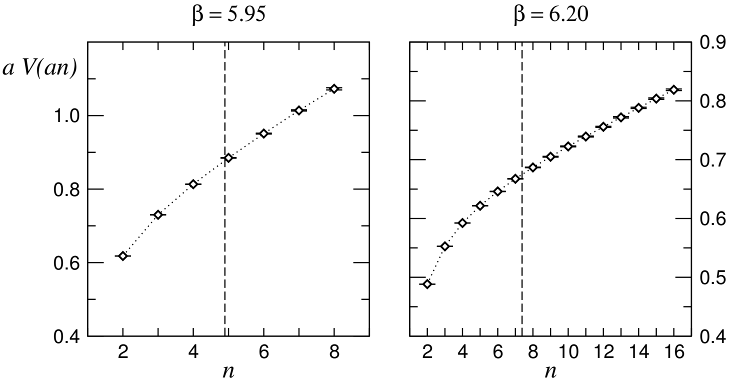


Fig. 1. Restoration of rotational invariance from (a) $\beta = 2$, $n_s = 8$, $n_t = 4$ to (b) $\beta = 2.25$, $n_s = 16$, $n_t = 6$; the equipotential curves are obtained through fits as described in the text.

CBL & C. Rebbi, PLB 115B(1982)137



Example for evaluation of the static potential: linearly rising!

The lattice spacing is not yet fixed. We need a physical scale parameter to fix it and thus set the scale.

(R. Sommer radius)

1. Experiment (analysed with non-rel. Schrödinger equation) gives for the force the dimensionless combination $r_0^2\, F(r_0) = 1.65$ at $r_0 = 0.5$ fm.
2. We then find the position x in the lattice potential, where that value is observed; thus $x = r_0/a$ or $a = r_0/x$
3. Compare with lattice potential:

$$F(r) = \frac{dV(r)}{dr} = \frac{d}{dr}\left(A + \frac{B}{r} + \sigma\, r\right) = -\frac{B}{r^2} + \sigma$$

4. B and $\sigma\, a^2$ determined from a fit to the lattice potential.

This has to be done at each value of the gauge coupling $\beta = 6/g^2$ and gives $a(\beta)$.

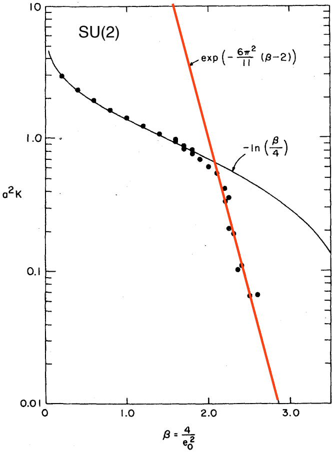
M. Creutz, PRD 21 (1980) 2308.

Scaling according to renormalization group (running coupling constant)

$$a(g) = \frac{1}{\Lambda_L} \left(\beta_0 g^2\right)^{-\frac{\beta_1}{2\beta_0^2}} \exp\left(-\frac{1}{2\beta_0 g^2}\right) \left(1 + \mathcal{O}(g^2)\right)$$

is confirmed by the lattice results.

Monte Carlo study of quantized $SU(2)$ gauge theory.

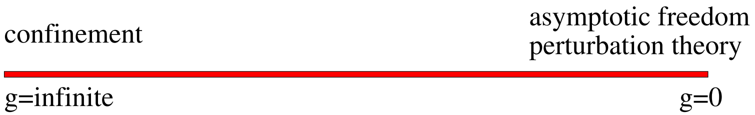


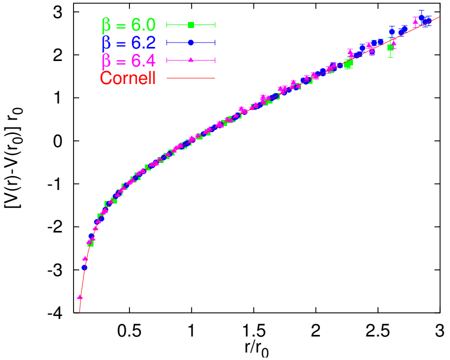
The cutoff squared times the string tension as a function of β. The solid lines are the strong- and weak-coupling limits.

QCD phase diagram

One finds $a(g \to 0) \to 0$!

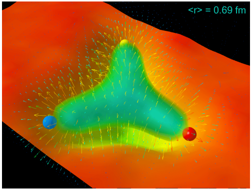
In full LGT (including the quark sea) one can take measured hadron masses to set the scale.





The static potential derived from Wilson loops shows correct scaling (Bali, Phys. Rep. 343 (2001) 1)

Supports the string picture:



© Leinweber et al.,
www.physics.adelaide.edu.au/cssm/research

- One needs $N_f + 1$ parameters: $\alpha(g), m_u(g), m_d(g), m_s(g), m_c(g), m_b(g), m_t(g)$ (all scale-variant!).
  Thus one needs N_f masses $(m_\pi, m_K, m_D, \ldots)$ and one scale parameter.
  The scale should be measurable in experiment and in LQCD, statistically reliable, and weakly dependent on the quark masses.
  (cf. review of Rainer Sommer, PoS LATTICE2013 (2014) 015, arXiv:1401.3270)
- Use some hadron mass parameter (e.g., m_Ω or f_π or f_K); needs extrapolation to or work at the physical point.
- Static force (see above): r_0 or r_1 (similar definition; not optimal on coarse lattices).
- Gradient flow: t_0 or w_0

Gradient flow: behaviour of plaquette expectation value under differential (infinitesimal staut smearing) equation in 'time' τ for the gauge links:

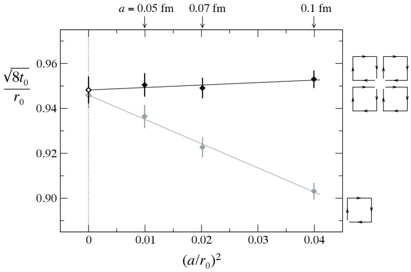
$$\frac{dV(\tau)}{d\tau} = -\frac{\partial S_P(V)}{dV} V(\tau) \quad \text{with } V(0) = U \,.$$

Then find the dimensionless values of t_0 (Lüscher,) or w_0 (BMW) such that

$$\tau^2 \langle E(\tau)\rangle|_{\tau=t_0} = 0.3 \quad \text{or} \quad \tau \frac{d}{d\tau} \langle \tau^2 E(\tau)\rangle|_{\tau=w_0^2} = 0.3$$

where $E = \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu}$ (field strength $G^a_{\mu\nu}$)

Fig. from M. Lüscher, JHEP 1008, 071 (2010)



- M. Lüscher, JHEP 1008, 071 (2010); see also PoS(LATTICE 2013)016
- BMW, JHEP 1209, 010 (2012) :
  $w_0\, a = w_{0,phys} = 0.1755(18)(04) fm.$

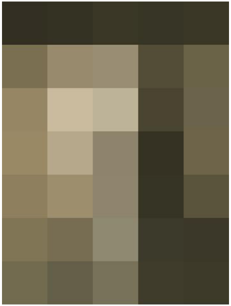
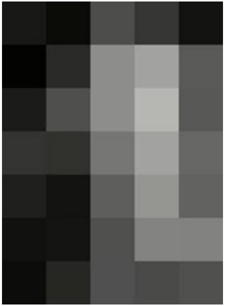
The three limits of LQCD

- Continuum limit: $a(g,m) \to 0 \qquad (g \to 0)$
  Lattice artifacts should become small
  $\to$ Improvement programme

- Thermodynamic limit: $L \to \infty \quad (L \cdot a = const.)$
  Hadron physics in a box of a few fm
  $\to$ Finite volume effects can be utilized

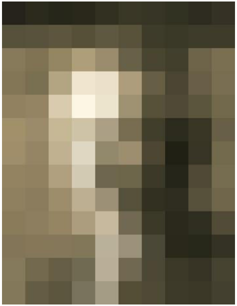
- Chiral limit: $m \to m_0 \quad (M_\pi \to M_{\pi,\mathrm{exp}})$
  Physical u, d quark masses are small
  $\to$ We want to understand chiral symmetry breaking

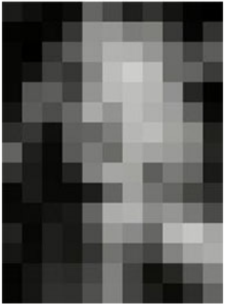
Continuum limit

The same physical image represented on lattices of linear extent 5, 10, 15, 20, 30 (in units of *a*) corresponding to lattice spacings *a* of 30 mm, 15 mm, 7.5 mm, and 5mm.

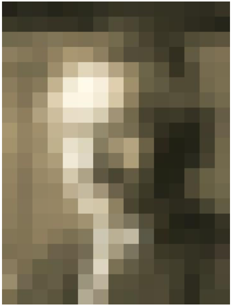
Continuum limit

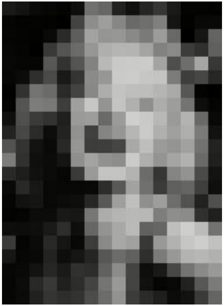




The same physical image represented on lattices of linear extent 5, 10, 15, 20, 30 (in units of *a*) corresponding to lattice spacings *a* of 30 mm, 15 mm, 7.5 mm, and 5mm.

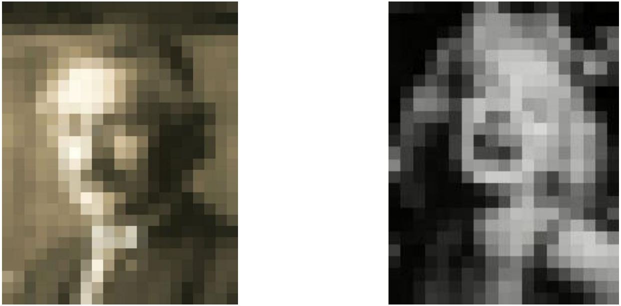
Continuum limit





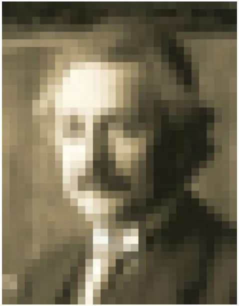
The same physical image represented on lattices of linear extent 5, 10, 15, 20, 30 (in units of a) corresponding to lattice spacings a of 30 mm, 15 mm, 7.5 mm, and 5mm.

Continuum limit



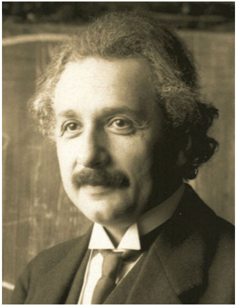
The same physical image represented on lattices of linear extent 5, 10, 15, 20, 30 (in units of *a*) corresponding to lattice spacings *a* of 30 mm, 15 mm, 7.5 mm, and 5mm.

Continuum limit



The same physical image represented on lattices of linear extent 5, 10, 15, 20, 30 (in units of a) corresponding to lattice spacings a of 30 mm, 15 mm, 7.5 mm, and 5mm.

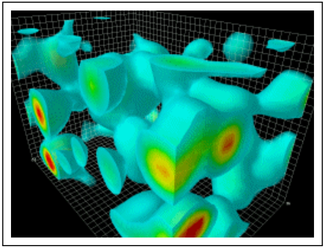
Continuum limit



The same physical image represented on lattices of linear extent 5, 10, 15, 20, 30 (in units of a) corresponding to lattice spacings a of 30 mm, 15 mm, 7.5 mm, and 5mm.

Key points

- QCD can be formulated on a Euclidean space-time lattice
- Quantization amounts to summing over all gauge configuration; this can be approximated by Monte Carlo sums
- Strong coupling confinement can be proven, towards weaker coupling MC calculations show non-vanishing string tension and asymptotic freedom
- The lattice spacing “runs”: $a(\beta)$
- The three limits of LQCD: continuum, thermodynamic, chiral.



Gluonic vacuum fluctuations
movie © Leinweber et al.,
www.physics.adelaide.edu.au/cssm/research

Homework (2.3)

Are the operators $\overline{\psi}_n \psi_n$, $\overline{\psi}_n U_{n,\mu} \psi_{n+\hat{\mu}}$, and $\overline{\psi}_n \psi_{n+\hat{\mu}}$ gauge invariant?
Which gauge invariant operators can you construct out of site-fermions and link-gaugefields?
What particle states could they couple to?
What would be a glueball operator?

3. Quarks

Fermions

QFT path integral:

$$\langle A \rangle = \frac{1}{Z} \int \mathcal{D}[U]\, \mathcal{D}[\psi, \overline{\psi}]\, e^{-S_G[U] - S_F[\psi, \overline{\psi}, U]}\, A[\psi, \overline{\psi}, U]$$

$$= \frac{1}{Z} \int \mathcal{D}[U]\, e^{-S_G[U]} \left\{ \mathcal{D}[\psi, \overline{\psi}]\, e^{-S_F[\psi, \overline{\psi}, U]}\, A[\psi, \overline{\psi}, U] \right\}$$

Bosons: usual integration (a group integral for each link)

Fermions: Grassmann variables (“anti-commuting c-numbers”)

Fermions

QFT path integral:

$$\langle A \rangle = \frac{1}{Z} \int \mathcal{D}[U]\, \mathcal{D}[\psi, \overline{\psi}]\, e^{-S_G[U] - S_F[\psi, \overline{\psi}, U]}\, A[\psi, \overline{\psi}, U]$$

$$= \frac{1}{Z} \int \mathcal{D}[U]\, e^{-S_G[U]} \left\{ \mathcal{D}[\psi, \overline{\psi}]\, e^{-S_F[\psi, \overline{\psi}, U]}\, A[\psi, \overline{\psi}, U] \right\}$$

Bosons: usual integration (a group integral for each link)

Fermions: Grassmann variables (“anti-commuting c-numbers”)

Grassmann variables

- ...are anti-commuting numbers:

$$\eta_i \, \eta_j \;=\; -\,\eta_j \, \eta_i$$

  for all i, j, thus $\eta_i \, \eta_i = 0$

- ...have the integration rules:

$$d^N\eta = d\eta_N \, d\eta_{N-1} \, \ldots \, d\eta_1 \;, \quad d\eta_i \, d\eta_j = -\, d\eta_j \, d\eta_i \;, \quad d\eta_i \, \eta_j = -\eta_j \, d\eta_i$$

$$\int d\eta_i \, 1 = 0 \;, \quad \int d\eta_i \, \eta_i = 1 \;,$$

  e.g.

$$\int d\eta_2 \, d\eta_1 \, (1 + 2\,\eta_1 - 42\,\eta_1\eta_2) = -42$$

cf. http://en.wikipedia.org/wiki/42_(number)

- These rules lead to, e.g., the Matthews-Salam formula:

$$Z_F = \int d\eta_N d\overline{\eta}_N \; \ldots \; d\eta_1 d\overline{\eta}_1 \; \exp\left(\sum_{i,j=1}^{N} \overline{\eta}_i M_{ij} \eta_j\right) \; = \; \det[M],$$

where M is a complex $N \times N$ matrix.

Note: This looks almost like Gaussian integration for bosons, except that there the result is $\det[M]^{-1}$*!*

The **generating functional for fermions** is then given by

$$W[\theta,\overline{\theta}] = \int \prod_{i=1}^{N} \mathrm{d}\eta_i \mathrm{d}\overline{\eta}_i \exp\left(\sum_{k,l=1}^{N} \overline{\eta}_k M_{kl} \eta_l + \sum_{k=1}^{N} \overline{\theta}_k \eta_k + \sum_{k=1}^{N} \overline{\eta}_k \theta_k\right)$$

$$= \det[M] \exp\left(-\sum_{n,m=1}^{N} \overline{\theta}_n \left(M^{-1}\right)_{nm} \theta_m\right)$$

and, e.g.,

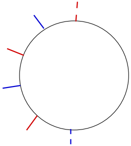
$$\frac{\partial}{\partial\theta_m}\frac{\partial}{\partial\overline{\theta}_n} W[\theta,\overline{\theta}]\Big|_{\theta,\overline{\theta}=0} = \int \prod_{i=1}^{N} \mathrm{d}\eta_i \mathrm{d}\overline{\eta}_i \; \eta_n \overline{\eta}_m \exp\left(\sum_{k,l=1}^{N} \overline{\eta}_k M_{kl} \eta_l\right)$$

$$= -\det[M] \left(M^{-1}\right)_{nm}$$

N-point functions can be computed by (Wick's theorem):

$$\langle \eta_{i_1}\overline{\eta}_{j_1} \ldots \eta_{i_n}\overline{\eta}_{j_n}\rangle_F = \frac{1}{Z_F}\int \prod_{k=1}^{N} \mathrm{d}\eta_k \mathrm{d}\overline{\eta}_k \; \eta_{i_1}\overline{\eta}_{j_1} \ldots \eta_{i_n}\overline{\eta}_{j_n} \exp\left(\sum_{l,m=1}^{N} \overline{\eta}_l M_{lm} \eta_m\right)$$
$$= \frac{1}{Z_F} \frac{\partial}{\partial\theta_{j_1}} \frac{\partial}{\partial\overline{\theta}_{i_1}} \cdots \frac{\partial}{\partial\theta_{j_n}} \frac{\partial}{\partial\overline{\theta}_{i_n}} W\left[\theta,\overline{\theta}\right]\Big|_{\theta,\overline{\theta}=0}$$

with $Z_F = \det[M]$.



Quarks and anti-quarks:

$$\eta_i \to \psi^{(f)}(x,\alpha,a) \quad \text{or, e.g.} \quad u(x,\alpha,a)$$
$$\overline{\eta}_i \to \overline{\psi}^{(f)}(x,\alpha,a) \quad \text{or, e.g.} \quad \overline{u}(x,\alpha,a)$$
$$M \to D \quad \text{lattice Dirac operator = matrix}$$

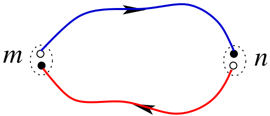
Important: ψ and $\overline{\psi}$ are independent variables!

Meson propagators

Some examples for meson propagators:

Quark:

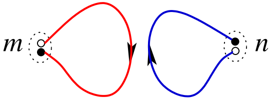
$$\langle u(n)\,\overline{u}(m)\rangle_F = D_u^{-1}(n|m)$$



Connected piece of a meson correlator

(Isovector) meson operator $O_T = \overline{d}\,\Gamma\,u$ (e.g. π^+):

$$\begin{aligned}\left\langle O_T(n)\,\overline{O}_T(m)\right\rangle_F &= \left\langle \overline{d}(n)\Gamma u(n)\,\overline{u}(m)\Gamma d(m)\right\rangle_F \\ &= -\mathrm{Tr}\left[\Gamma D_u^{-1}(n|m)\,\Gamma D_d^{-1}(m|n)\right]\end{aligned}$$



Disconnected piece of a meson correlator

(Isoscalar) meson operator $O_S = \overline{d}\,\Gamma\,d$ (e.g. f_0):

$$\begin{aligned}\left\langle O_S(n)\,\overline{O}_S(m)\right\rangle_F &= \mathrm{Tr}\left[\Gamma D_u^{-1}(n|n)\right]\mathrm{Tr}\left[\Gamma D_u^{-1}(m|m)\right] \\ &\quad -\mathrm{Tr}\left[\Gamma D_u^{-1}(n|m)\Gamma D_u^{-1}(m|n)\right]\end{aligned}$$

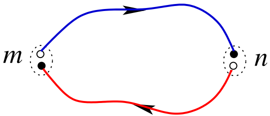
Some examples for meson propagators:

Quark:

$$\langle u(n)\,\overline{u}(m)\rangle_F = D_u^{-1}(n|m)$$

(Isovector) meson operator $O_T = \overline{d}\,\Gamma\,u$ (e.g. π^+):

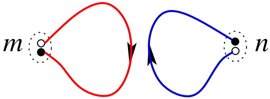
$$\left\langle O_T(n)\,\overline{O}_T(m)\right\rangle_F = \left\langle \overline{d}(n)\Gamma u(n)\,\overline{u}(m)\Gamma d(m)\right\rangle_F = -\mathrm{Tr}\left[\Gamma D_u^{-1}(n|m)\,\Gamma D_d^{-1}(m|n)\right]$$



Connected piece of a meson correlator

(Isoscalar) meson operator $O_S = \overline{d}\,\Gamma\,d$ (e.g. f_0):

$$\left\langle O_S(n)\,\overline{O}_S(m)\right\rangle_F = \mathrm{Tr}\left[\Gamma D_u^{-1}(n|n)\right]\mathrm{Tr}\left[\Gamma D_u^{-1}(m|m)\right] - \mathrm{Tr}\left[\Gamma D_u^{-1}(n|m)\Gamma D_u^{-1}(m|n)\right]$$



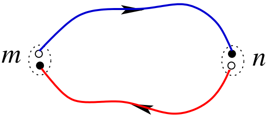
Disconnected piece of a meson correlator

Meson propagators

Some examples for meson propagators:

Quark:

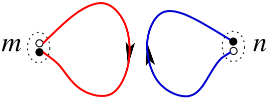
$$\langle u(n)\,\overline{u}(m)\rangle_F = D_u^{-1}(n|m)$$



Connected piece of a meson correlator

(Isovector) meson operator $O_T = \overline{d}\,\Gamma\,u$ (e.g. π^+):

$$\begin{aligned}\left\langle O_T(n)\,\overline{O}_T(m)\right\rangle_F &= \left\langle \overline{d}(n)\Gamma u(n)\,\overline{u}(m)\Gamma d(m)\right\rangle_F \\ &= -\mathrm{Tr}\left[\Gamma D_u^{-1}(n|m)\,\Gamma D_d^{-1}(m|n)\right]\end{aligned}$$



Disconnected piece of a meson correlator

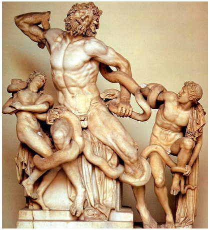
(Isoscalar) meson operator $O_S = \overline{d}\,\Gamma\,d$ (e.g. f_0):

$$\begin{aligned}\left\langle O_S(n)\,\overline{O}_S(m)\right\rangle_F &= \mathrm{Tr}\left[\Gamma D_u^{-1}(n|n)\right]\,\mathrm{Tr}\left[\Gamma D_u^{-1}(m|m)\right] \\ &\quad -\mathrm{Tr}\left[\Gamma D_u^{-1}(n|m)\Gamma D_u^{-1}(m|n)\right]\end{aligned}$$

Homework (3.1)

Compute the Grassmann integral(s):

1. $\int d\eta_1 d\eta_2 \exp\left(\eta_1 + \eta_2 + a\,\eta_1\,\eta_2\right)$.
2. $\int dx_1 dx_2 dy_1 dy_2 \exp\left(\vec{x}^T \cdot A \cdot \vec{y}\right)$, where $A = (a_{ij})$ is a 2×2 matrix.
3. $\left\langle \overline{d}(n)\Gamma u(n)\,\overline{u}(m)\Gamma d(m) \right\rangle_F$.



Naive fermion action:

$$\begin{aligned} S_F[\psi,\overline{\psi},U] &= a^4 \sum_{n\in\Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{U_\mu(n)\psi(n+\hat{\mu}) - U_{-\mu}(n)\psi(n-\hat{\mu})}{2a} + m\,\psi(n) \right) \\ &= a^4\, \overline{\psi}(n)\, D(n|m)\, \psi(m) \end{aligned}$$

(omitting Dirac and color indices)

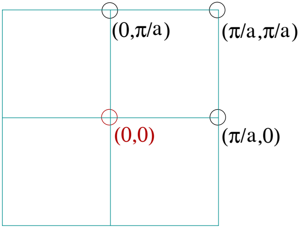
Free fermions ($U = 1$):

$$D(n|m) = \sum_{\mu=1}^{4} \gamma_\mu \frac{\delta_{n+\hat{\mu},m} - \delta_{n-\hat{\mu},m}}{2a} + m\,\delta_{n,m}$$

The lattice Dirac operator D is a matrix with $n_{sites} \times n_{color} \times n_{Dirac} = 12\, N_s^3 \times n_t$ *rows and columns!*

Let us Fourier-transform the free fermion matrix:

$$\begin{aligned}
\widetilde{D}(p|q) &= \frac{1}{|\Lambda|}\sum_{n,m\in\Lambda} e^{-ip\cdot na}\, D(n|m)\, e^{iq\cdot ma} \\
&= \frac{1}{|\Lambda|}\sum_{n\in\Lambda} e^{-i(p-q)\cdot na}\left(\sum_{\mu=1}^{4}\gamma_\mu \frac{e^{+iq_\mu a}-e^{-iq_\mu a}}{2a} + m\mathbb{1}\right) \\
&= \delta(p-q)\,\widetilde{D}(p)\ , \\
\widetilde{D}(p) &= m\mathbb{1} + \frac{i}{a}\sum_{\mu=1}^{4}\gamma_\mu \sin(p_\mu a) \\
\widetilde{D}(p)^{-1} &= \frac{m\mathbb{1} - ia^{-1}\sum_\mu \gamma_\mu \sin(p_\mu a)}{m^2 + a^{-2}\sum_\mu \sin(p_\mu a)^2}\ .
\end{aligned}$$



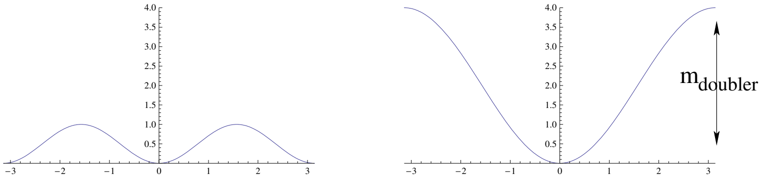
→ the massless propagator D^{-1} has 16 poles in the Brillouin-zone → “doubler fermions”!

Wilson suggested to add another term:

$$\widetilde{D}(p) = m\mathbb{1} + \frac{i}{a}\sum_{\mu=1}^{4}\gamma_\mu \sin(p_\mu a) + \mathbb{1}\frac{1}{a}\sum_{\mu=1}^{4}\left(1-\cos(p_\mu a)\right)$$

$\rightarrow$ changes the denominator of D^{-1}:

$$\sum_\mu \sin(p_\mu a)^2 \quad\rightarrow\quad \sum_\mu \sin(p_\mu a)^2 + \left(\sum_{\mu=1}^{4}(1-\cos(p_\mu a))\right)^2$$



... gives extra mass $2\,k/a$ to the doublers!

Summing up the Wilson fermion action (N_f flavors):

$$S_F[\psi,\overline{\psi},U] = \sum_{f=1}^{N_f} a^4 \sum_{n,m\in\Lambda} \overline{\psi}^{(f)}(n)\, D^{(f)}(n|m)\, \psi^{(f)}(m)\ ,$$

$$D^{(f)}(n|m) = \left(m^{(f)} + \frac{4}{a}\right)\delta_{\alpha\beta}\,\delta_{ab}\,\delta_{n,m} - \frac{1}{2a}\sum_{\mu=\pm 1}^{\pm 4}(\mathbb{1}-\gamma_\mu)_{\alpha\beta}\, U_\mu(n)_{ab}\,\delta_{n+\hat{\mu},m},$$

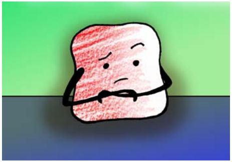
$$\text{with}\quad \gamma_{-\mu} = -\gamma_\mu\ ,\quad \mu = 1,2,3,4\ .$$

Homework problems

Homework (3.2)

Compute the naive continuum limit (fixed p) of the lattice Dirac operator in momentum space $\widetilde{D}(p)$ for free (naive) fermions. What are the eigenvalues of D? How can you find the quark propagator in real space?

Be naive and curious.
That's all you need to become a scientist.
(Abhijit Naskar)



Homework (3.3)

Consider a 2-dimensional lattice system of free bosons $\phi(n) \in \Re$ (where n denotes the site vector $n = (x_1, x_2)$. .A possible action is

$$S = \sum_{nm} \phi(n) D(n|m) \phi(m)$$

where

$$D(n|m) = \delta_{nm} - \kappa \sum_{\mu=1}^{2} (\delta_{n+\hat{\mu},m} + \delta_{n-\hat{\mu},m}).$$

Find the boson propagator (in momentum space and in real space) by the method of Fourier transformation. What is the mass $m(\kappa)$?

Homework (3.4)

Write a Monte Carlo simulation program (Metropolis algorithm) for a free 2D boson system (given by the action in the earlier problem) and determine the boson propagator for a boson with some mass and vanishing momentum.
(Attention: In the action each link enters twice; this gives a factor 2 in the updating!)

Homework (3.5)

Write a Monte Carlo simulation program (Metropolis algorithm) for a free 2D boson system (given by the action in the earlier problem) and determine the boson propagator for a boson with some mass and vanishing momentum.
(Attention: In the action each link enters twice; this gives a factor 2 in the updating!)

It's trivial. Believe me!

Charge conjugation

$$
\begin{aligned}
\psi(n) &\xrightarrow{\mathcal{C}} \psi(n)^{\mathcal{C}} = C^{-1}\,\overline{\psi}(n)^T , \\
\overline{\psi}(n) &\xrightarrow{\mathcal{C}} \overline{\psi}(n)^{\mathcal{C}} = -\psi(n)^T\, C . \\
U_\mu(n) &\xrightarrow{\mathcal{C}} U_\mu(n)^{\mathcal{C}} = U_\mu(n)^* = \left(U_\mu(n)^\dagger\right)^T .
\end{aligned}
$$

Parity and Euclidean reflections

$$
\begin{aligned}
\psi(\vec{n},n_4) &\xrightarrow{\mathcal{P}} \psi(\vec{n},n_4)^{\mathcal{P}} = \gamma_4\,\psi(-\vec{n},n_4) , \\
\overline{\psi}(\vec{n},n_4) &\xrightarrow{\mathcal{P}} \overline{\psi}(\vec{n},n_4)^{\mathcal{P}} = \overline{\psi}(-\vec{n},n_4)\,\gamma_4 , \\
U_i(\vec{n},n_4) &\xrightarrow{\mathcal{P}} U_i(\vec{n},n_4)^{\mathcal{P}} = U_i(-\vec{n}-\hat{\imath},n_4)^\dagger , \quad i = 1,2,3 , \\
U_4(\vec{n},n_4) &\xrightarrow{\mathcal{P}} U_4(\vec{n},n_4)^{\mathcal{P}} = U_4(-\vec{n},n_4) .
\end{aligned}
$$

γ_5-hermiticity

$$(\gamma_5\, D)^\dagger = \gamma_5\, D \quad \text{or, equivalently,} \quad D^\dagger = \gamma_5\, D\, \gamma_5 .$$

Consequences of γ_5-hermiticity

Example: general local iso-triplet meson operator: $O_T = \overline{d}\,\Gamma\,u$

Propagator:

$$\begin{aligned} C_T(n,m) &= \left\langle O_T(n)\,\overline{O}_T(m)\right\rangle_F &&= \left\langle \overline{d}(n)\Gamma u(n)\,\overline{u}(m)\Gamma d(m)\right\rangle_F \\ &= -\left\langle \Gamma u(n)\,\overline{u}(m)\Gamma d(m)\overline{d}(n)\right\rangle_F &&= -\mathrm{Tr}\left[\Gamma\,\langle u(n)\,\overline{u}(m)\rangle_F\,\Gamma\left\langle d(m)\overline{d}(n)\right\rangle_F\right] \\ &= -\mathrm{Tr}\left[\Gamma D_u^{-1}(n|m)\,\Gamma D_d^{-1}(m|n)\right] \end{aligned}$$

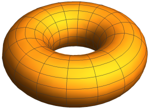
Using γ_5-hermiticity: $D^{-1} = (\gamma_5\,D^{-1\dagger}\,\gamma_5)$ gives $D^{-1}(m,n) = \gamma_5\,D^{-1*}(n,m)\,\gamma_5$, therefore

$$C_T(n,m) = -\mathrm{Tr}\left[\gamma_5\Gamma D_u^{-1}(n|m)\,\Gamma\,\gamma_5 D_d^{-1*}(n|m)\right]$$

For the pion $\Gamma = \gamma_5$ and one gets the simple form

$$C_\pi(n,m) = -\mathrm{Tr}\left[D_u^{-1}(n|m)\,D_d^{-1*}(n|m)\right]$$

A word on boundary conditions



Gaugefields: Usually periodic, $U_\mu(x) = U_\mu(x + N_\nu k_\nu)$ for lattice size $N_1 \times N_2 \times N_3 \times_4$.

Fermions: For Osterwalder-Schrader positivity (existence of a Minkowski theory) at least one direction should be anti-periodic $\psi(x) = -\psi(x + L)$, usually in the temporal direction $L = (0, 0, 0, N_t)$.

In general we can write

$$f(x + \hat{\mu} N_\mu) \;=\; \mathrm{e}^{\mathrm{i}2\pi\theta_\mu} f(x) \;,$$

Periodic | Anti-periodic | Twisted b.c.: $\theta_\mu = 0 \mid \frac{1}{2} \mid \frac{1}{3}$.
Momentum space

$$\widetilde{\Lambda} \;=\; \{p = (p_1, p_2, p_3, p_4) \mid p_\mu = \frac{2\pi}{a N_\mu}(k_\mu + \theta_\mu), k_\mu = -\frac{N_\mu}{2} + 1, \ldots, \frac{N_\mu}{2}\} \;.$$

Furthermore: Fixed b.c., open b.c.,...

Actually: Boundary conditions should not matter in the infinite volume limit...:

Why is the fermion vacuum full of loops?

Hopping expansion

Let us write (removing an overall factor and for just one flavor)

$$D = (1 - \kappa H) \quad \text{with the “Hopping term”} \quad H_{nm} = \sum_{\mu=\pm 1}^{\pm 4} (\mathbb{1} - \gamma_\mu)\, U_\mu(n)\, \delta_{n+\hat{\mu},m} \ .$$

with $\kappa = 1/(m + 4/a)$.

A propagator then can be expanded:

$$D^{-1}_{nm} = (1 - \kappa H)^{-1} = 1_{nm} + \kappa\, H_{nm} + \kappa^2\, (H^2)_{nm} + \kappa^3\, (H^3)_{nm} \ldots$$

i.e., H^K_{nm} is sum of paths of length K from site n to site m.

This is called the “Hopping expansion”.

Theoretically intriguing.

Practically unfeasible due to convergence problems for smaller quark masses! Sorry!

Why is the fermion vacuum full of loops?

Hopping expansion

Let us write (removing an overall factor and for just one flavor)

$$D = (1 - \kappa H) \quad \text{with the “Hopping term”} \quad H_{nm} = \sum_{\mu=\pm 1}^{\pm 4} (\mathbb{1} - \gamma_\mu)\, U_\mu(n)\, \delta_{n+\hat{\mu},m} \; .$$

with $\kappa = 1/(m + 4/a)$.

A propagator then can be expanded:

$$D^{-1}_{nm} = (1 - \kappa H)^{-1} = 1_{nm} + \kappa\, H_{nm} + \kappa^2\, (H^2)_{nm} + \kappa^3\, (H^3)_{nm} \ldots$$

i.e., H^K_{nm} is sum of paths of length K from site n to site m.

This is called the “Hopping expansion”.

Theoretically intriguing.

Practically unfeasible due to convergence problems for smaller quark masses! Sorry!

Hopping expansion

Let us write (removing an overall factor and for just one flavor)

$$D = (1 - \kappa H) \quad \text{with the “Hopping term”} \quad H_{nm} = \sum_{\mu=\pm1}^{\pm4} (\mathbb{1} - \gamma_\mu)\, U_\mu(n)\, \delta_{n+\hat{\mu},m} \ .$$

with $\kappa = 1/(m + 4/a)$.

A propagator then can be expanded:

$$D^{-1}_{nm} = (1 - \kappa H)^{-1} = 1_{nm} + \kappa\, H_{nm} + \kappa^2\, (H^2)_{nm} + \kappa^3\, (H^3)_{nm} \ldots$$

i.e., H^K_{nm} is sum of paths of length K from site n to site m.

This is called the “Hopping expansion”.

☺ Theoretically intriguing.

☹ Practically unfeasible due to convergence problems for smaller quark masses! Sorry!

Hopping expansion

Let us write (removing an overall factor and for just one flavor)

$$D = (1 - \kappa H) \quad \text{with the “Hopping term”} \quad H_{nm} = \sum_{\mu=\pm 1}^{\pm 4} (\mathbb{1} - \gamma_\mu)\, U_\mu(n)\, \delta_{n+\hat{\mu},m} \; .$$

with $\kappa = 1/(m + 4/a)$.

A propagator then can be expanded:

$$D^{-1}_{nm} = (1 - \kappa H)^{-1} = 1_{nm} + \kappa\, H_{nm} + \kappa^2\, (H^2)_{nm} + \kappa^3\, (H^3)_{nm} \ldots$$

i.e., H^K_{nm} is sum of paths of length K from site n to site m.

This is called the “Hopping expansion”.

☺ Theoretically intriguing.

☹ Practically unfeasible due to convergence problems for smaller quark masses! Sorry!

Hopping expansion

The determinant

$$\det[D] = \det[\mathbb{1} - \kappa H] = \exp\left(\mathrm{Tr}\ln\left(\mathbb{1} - \kappa H\right)\right) = \exp\left(-\sum_{j=1}^{\infty} \frac{1}{j}\,\kappa^j \mathrm{Tr}\left[H^j\right]\right)$$

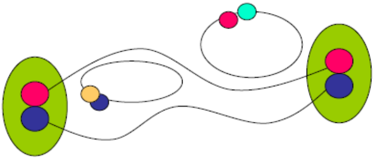
is a sum of closed loops (due to the trace).

"When fermions, the most antisocial type of quantum particle, do get together, they pair up in a wondrous dance..." from: ScienceDaily (Dec. 23, 2005)

"Full QCD":

$$C(t) \propto \int \mathcal{D}[U]\, \mathcal{D}[\psi, \overline{\psi}]\, e^{-S_G[U] - \overline{\psi}\, D[U]\, \psi}\, N(t)\bar{N}(0)$$
$$= \int \mathcal{D}[U]\, e^{-S_G[U]}\, (\det D_u \det D_d \ldots)$$
$$\times \left[D_u^{-1} D_d^{-1} \ldots + \ldots \right]$$

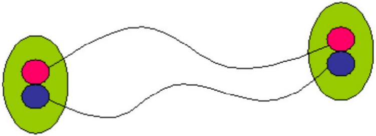
- Set $\det D \equiv 1$ (no dynamical fermion vacuum, i.e. no sea quarks)
- Gauge field vacuum is fully dynamical (Monte Carlo)
- Consider only the valence quarks
- Hadron correlation functions are built from the quark propagators



Quenched approximation:

$$\begin{aligned} C(t) &\propto \int \mathcal{D}[U]\, \mathcal{D}[\psi,\overline{\psi}]\, \mathrm{e}^{-S_G[U]-\overline{\psi}\, D[U]\, \psi}\, N(t)\bar{N}(0) \\ &= \int \mathcal{D}[U]\, \mathrm{e}^{-S_G[U]}\, (\det D_u \det D_d \ldots) \\ &\quad \times \left[D_u^{-1} D_d^{-1} \ldots + \ldots\right] \end{aligned}$$

- Set $\det D \equiv 1$ (no dynamical fermion vacuum, i.e. no sea quarks)
- Gauge field vacuum is fully dynamical (Monte Carlo)
- Consider only the valence quarks
- Hadron correlation functions are built from the quark propagators



Dynamical fermions:

$$\text{Bosons:} \quad \det[A]^{-1} = \pi^{-N} \int \mathcal{D}[\phi]\mathcal{D}[\phi_I]\, \mathrm{e}^{-\phi^\dagger A \phi}$$

$$\text{Fermions:} \quad \det[A] = \int \mathcal{D}[\psi]\mathcal{D}[\overline{\psi}]\, \mathrm{e}^{-\overline{\psi} A \psi}$$

Replace fermions by pseudofermions:

$$\int \mathcal{D}[\psi]\mathcal{D}[\overline{\psi}]\, \mathrm{e}^{-\overline{\psi}_u D \psi_u - \overline{\psi}_d D \psi_d} = \pi^{-N} \int \mathcal{D}[\phi_R]\mathcal{D}[\phi_I]\, \mathrm{e}^{-\phi^\dagger (D D^\dagger)^{-1} \phi} \, .$$

Doubling is (for this kind of Dirac operator) necessary in order to ensure positivity:

$$\det[D]\, \det[D] = \det[D]\, \det[D^\dagger] = \det[D\, D^\dagger] \geq 0$$

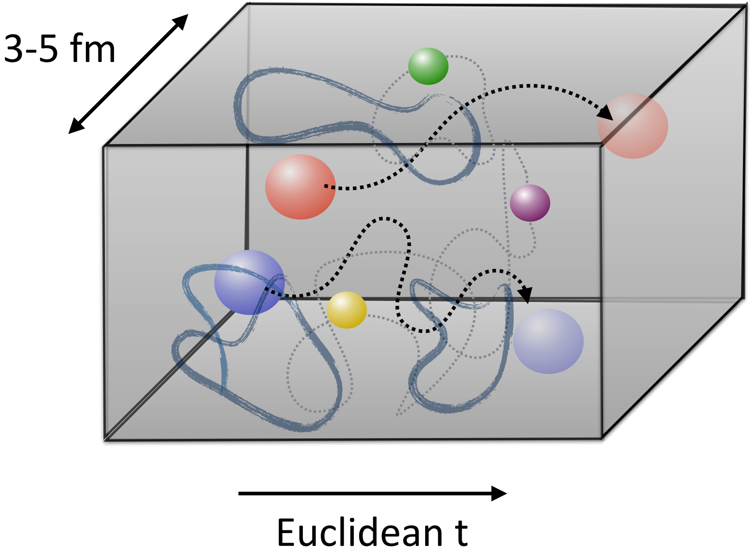
Simulation with Hybrid Monte Carlo (HMC) algorithm:

$$\begin{aligned}\langle O\rangle_Q &= \frac{\int \mathcal{D}[U]\ \exp(-S[U])\ O[U]}{\int \mathcal{D}[U]\ \exp(-S[U])}\\ &= \frac{\int \mathcal{D}[U]\,\mathcal{D}[P]\ \exp(-\frac{1}{2}P^2 - S[U])\ O[U]}{\int \mathcal{D}[U]\,\mathcal{D}[P]\ \exp(-\frac{1}{2}P^2 - S[U])} = \langle O\rangle_{P,U}\ .\end{aligned}$$

For the dynamical fermion simulation $S[U]$ and $\mathcal{D}[U]$ include the pseudofermion terms.

Microcanonical ensemble $\to$ canonical ensemble

More on HMC: Lecture by Alexei Bazavov


3-5 fm
Euclidean t

Key points

- In the path integral fermions are Grassmann variables.
- The lattice Dirac operator is a huge matrix. Quark propagators are entry of the inverse matrix, hadron propagators are built from quark propagators.
- In the naive action there are 16-fold too many fermions. Wilson's action moves these doublers to higher masses.
- The hopping expansion visualizes the quark paths.
- Dynamical fermions are "simulated" by pseudofermions (=bosons) in the Hybrid Monte Carlo algorithm.

4. Exploring the femtoverse

"There's Plenty of Room at the Bottom"
(Richard Feynman)

What do we want?

- ...determine hadron masses
- ...determine decay properties (e.g., phases shifts and resonance properties)
- ...measure low energy constants, e.g. quark masses, condensate, decay constants
- ...matrix elements, e.g. electromagnetic form factors, transition form factors, etc.
- ...study extreme environments (temperature, matter density)
- ...understand other quantum field theories (e.g., other gauge groups and fermions)

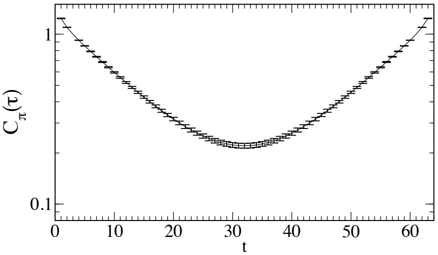
...and many more (see other lectures and the topics in the annual lattice proceedings...

Lattice2017

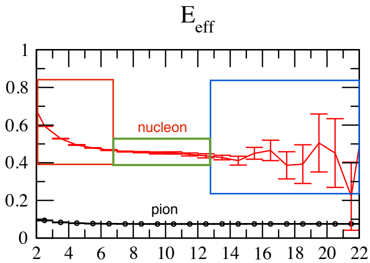
Algorithms and Machines
Applications Beyond QCD
Chiral Symmetry
Hadron Spectroscopy and Interactions
Hadron Structure
Nonzero Temperature and Density
Physics Beyond the Standard Model
Software Development
Standard Model Parameters and Renormalization
Theoretical Developments
Vacuum Structure and Confinement
Weak Decays and Matrix Elements

Measure correlation functions like

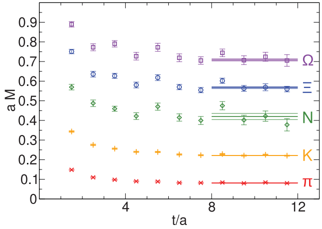
$$C_\pi(t) \propto \langle \pi_t \bar{\pi}_0 \rangle \sim \exp(-a\, m_\pi\, t) + \exp(-a\, m_\pi\, (T - t))$$



Result of a Monte Carlo simulation on a $32^3 \times 64$ lattice at lattice spacing $a \approx 0.09$ fm; log-plot for the pion correlation function.



$a = 0.0907$ fm, $m_\pi \approx 157$ MeV, $m_N \approx 970$ MeV, PACS-CS data, analysis CBL et al.. PRD 95, 014510 (2017).arXiv:1610.01422



$a = 0.085 - 0.125$ fm, $m_\pi \approx 190$ MeV, Dürr et al..(BMW collab.) Science 322, 1224-1227 (2008). arXiv:0906.3599.

Effective energy $E(t)$ from

$$\frac{C(t)}{C(t+1)} = \frac{\cosh(E(t - N_t/2))}{\cosh(E(t+1-N_t/2))}$$

Simpler version:

$$\frac{C(t)}{C(t+1)} = \frac{\exp(-Et)}{\exp(-E(t+1))}$$

Signal:

$$C_A(t) = \langle A(t)A^\dagger(0)\rangle = \sum_n \langle A(0)|n\rangle e^{-E_A t}\langle n|A^\dagger(0)\rangle \propto e^{-E_{A_0} t}$$

Noise:

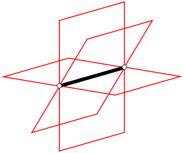
$$N\sigma^2 \approx \langle |C_A|^2\rangle = \langle C_A C_A^\dagger\rangle = \langle A(t)A(t)^\dagger A(0)A^\dagger(0)\rangle \propto e^{-E_{A\bar{A}} t}$$

The ratio depends on lowest energy in A- and $A\bar{A}$- channels.

A = pion $\quad\rightarrow\quad N\sigma^2 \propto e^{-2m_\pi t}$, $C_A \propto e^{-m_\pi t} \quad\rightarrow\quad \frac{C_A}{\sigma} \propto \frac{1}{\sqrt{N}}$

A = nucleon $\quad\rightarrow\quad N\sigma^2 \propto e^{-3m_\pi t}$, $C_A \propto e^{-m_N t} \quad\rightarrow\quad \frac{C_A}{\sigma} \propto \frac{1}{\sqrt{N}} e^{-(m_N - 3/2 m_\pi) t}$

Improving the signal: gauge field smoothing, source/sink smearing, more operators, ...



- APE smearing

$$V_\mu(x) = (1-\alpha)U_\mu + \alpha \sum_{\text{staples}} C_{\mu\nu}$$

New link $U' \in SU(3)$ maximises $\mathrm{ReTr}(VU')$.
M. Albanese et al.: Phys. Lett. B 192, 163 (1987)

- Hyp smearing
Average over paths in the hypercube containing U
A. Hasenfratz and F. Knechtli: Phys. Rev. D 64, 034504 (2001)

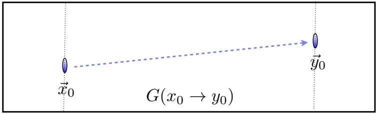
- Stout smearing
Projection to $SU(3)$ by a detour to the algebra.
C. Morningstar and M. Peardon: Phys. Rev. D 69, 054501 (2004)

Dirac op. M, source vector S, quark propagator

$$G_S(y) = M^{-1}(y,x)S(y) \qquad \rightarrow \textit{solve} \quad M(yx,y)G_S(y) = S(x)$$

Point sources: "point-to-all"

$$G(y,x_0) = M^{-1}(y,x)\delta_{x,x_0}$$



Smeared: "smeared-to-all"

$$G(y,S_i) = M^{-1}(y,x)S_i(x)$$

E.g. Jacobi smearing $S_i(x) = \sum_n \kappa^n H^n \delta_{x,0}$ with H the spatial covariant Laplacian

- Fewer quark propagators
- Derivative sources are possible
- Combination allows nodes in the interpolating operators

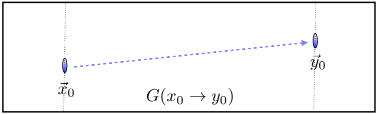
Quark propagators: source smearing

Dirac op. M, source vector S, quark propagator

$$G_S(y) = M^{-1}(y,x)S(y) \qquad \rightarrow \textit{solve} \quad M(yx,y)G_S(y) = S(x)$$

Point sources: "point-to-all"

$$G(y,x_0) = M^{-1}(y,x)\delta_{x,x_0}$$



Smeared: "smeared-to-all"

$$G(y,S_i) = M^{-1}(y,x)S_i(x)$$

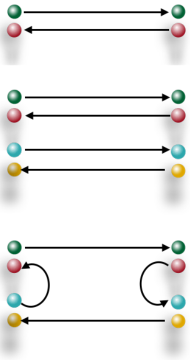
E.g. Jacobi smearing $S_i(x) = \sum_n \kappa^n H^n \delta_{x,0}$ with H the spatial covariant Laplacian

- Fewer quark propagators
- Derivative sources are possible
- Combination allows nodes in the interpolating operators

All-to-all propagators

For some processes (with annihilations) we need all-to-all propagators.

- Stochastic sources
- Distillation (perambulators*)



*) Merriam-Webster:
perambulator synonyms:
ambler, hiker, rambler, tramper, walker.

First Known Use: 1611

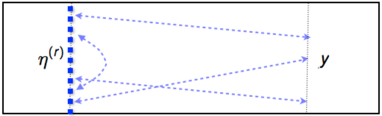
Stochastic sources: “all-to-all”

Source vectors $\eta^{(r)}$ with components $|\eta_x^{(r)}| = 1$, $[\eta_x^{(r)}]_R = 0$, $[\eta_x^{(r)} \eta_y^{(r)\dagger}]_R = \delta_{xy}$ (e,g, $\eta_x^{(r)} \in (1, \mathrm{i}, -1, -\mathrm{i})$)

$$G(y, \eta^{(r)}) = M^{-1}(y, x)\eta_y^{(r)} \quad \text{gives} \quad [G(y, \eta^{(r)})\, \eta_x^{(r)\dagger}]_R = G(y, x)$$

Variance reduction by noise dilution and other techniques

cf. J. Foley et al., Comput. Phys. Commun. 172, 145 (2005), hep-lat 0505023



Distillation method: "all-to-all"

(M. Peardon et al. (HSC), PRD 80, 054506 (2009))

- Set of source vectors = eigenvectors $v^{(n)}$ of the 3D (time slice) lattice Laplacian; Completeness relation: $\sum_n^{N_{all}} v_x^{(n)} v_y^{(n)\dagger} = \delta_{xy}$ with $N_{all} = N_s^3 N_c N_d N_f$
- solve for

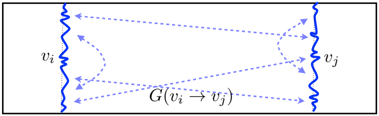
$$G(x,n) = M^{-1}(x,y) v_y^{(n)} \quad \to \text{ reconstruction; } \sum_n^{N_{all}} G(x,n) v_y^{(n)\dagger} = G(x,y)$$

- Better use "perambulators ": $v_x^{(m)\dagger} G(x,n) \equiv P(m,n)$

  Meson propagator example: (summation convention)

$$\mathrm{Tr}[M^{-1}(x,y)\Gamma_{src} M^{-1}(y,x)\Gamma_{snk}] \to$$
$$\mathrm{Tr}[M^{-1}(x,y) v_y^{(m)} v_z^{(m)\dagger} \Gamma_{src}(z,z') v_{z'}^{(n)} v_y^{(n)\dagger} M^{-1}(y,x) v_x^{(r)} v_u^{(r)\dagger} \Gamma_{snk}(r,r') v_{r'}^{(s)} v_y^{(s)\dagger}]$$
$$= \mathrm{Tr}[P(s,m)[v_z^{(m)\dagger}\Gamma_{src}(z,z') v_{z'}^{(n)}] P(n,r) [v_u^{(r)\dagger}\Gamma_{snk}(r,r') v_{r'}^{(s)}]]$$
$$= \mathrm{Tr}[P(s,m)\Phi_{src}(m,n) P(n,r) \Phi_{snk}(r,s)]$$

- Use $N \ll N_{all}$ (Gaussian smearing shapes)
- $P(n,m)$ need less memory than $G(x,y)$!
- Very flexible method, suitable for disconnected contributions



Leading parameters:

- Quark masses m_q
- Quark condensate $\Sigma \equiv \frac{1}{N_f} \langle \overline{\psi}\psi \rangle$
- Pion decay constant f_π

are related through Ward identities

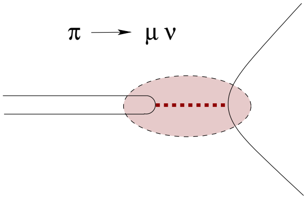
Pion decay constant and PCAC:
$$\partial_\mu A_\mu^{(r)a} = M_\pi^2 \, f_\pi \, \phi^{(r)a}$$

AWI (non-singlet axial Ward identity):
$$\partial_\mu A_\mu^{(r)a} = 2 \, m^{(r)} \, P^{(r)a} \; .$$

GMOR (Gell'Mann-Oakes-Renner relation):
$$f_\pi^2 \, M_\pi^2 = -m^{(r)} \, N_f \, \Sigma^{(r)}$$
with $\Sigma \equiv \frac{1}{N_f} \langle \overline{\psi}\psi \rangle$.

....can be obtained from (ratios of) correlation function of type $\langle AA \rangle$, $\langle AP \rangle$, $\langle PP \rangle$, etc.

For example: pion decay constant f_π.



From the coefficient of the asymptotic correlator:

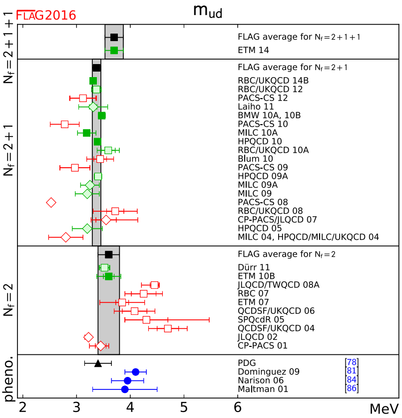
$$Z_A^2 \, \langle \, A_4^+(\vec{p}=\vec{0},t) \, A_4^-(0) \, \rangle \sim M_\pi \, f_\pi^2 \, \mathrm{e}^{-M_\pi \, t} \; .$$

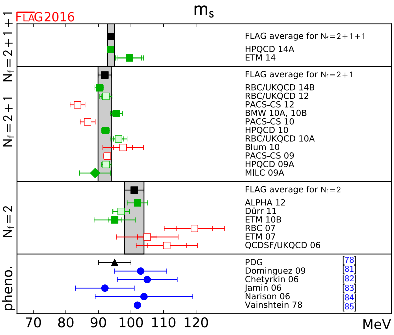
See: Flavor Lattice Averaging Group (FLAG) http://itpwiki.unibe.ch/flag/,
S. Aoki et al., Review of lattice results concerning low-energy particle physics, arXiv: 1607.00299

Covered topics:

- Quark masses
- Leptonic and semileptonic kaon and pion decay and $|V_{ud}|$ and $|V_{us}|$
- Low-energy constants
- Kaon mixing
- D-meson decay constants and form factors
- B-meson decay constants, mixing parameters and form factors
- The strong coupling α_s

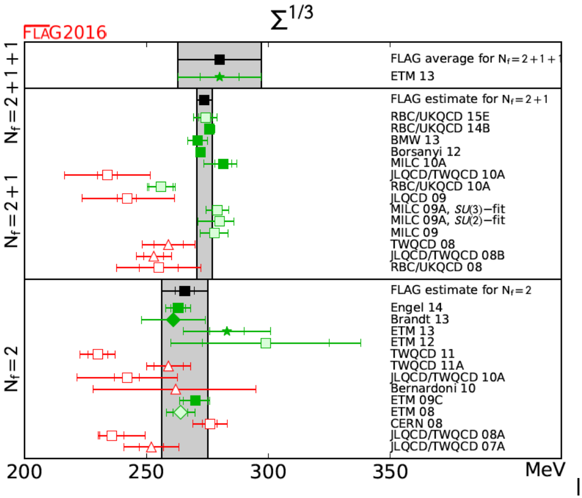
..quark masses





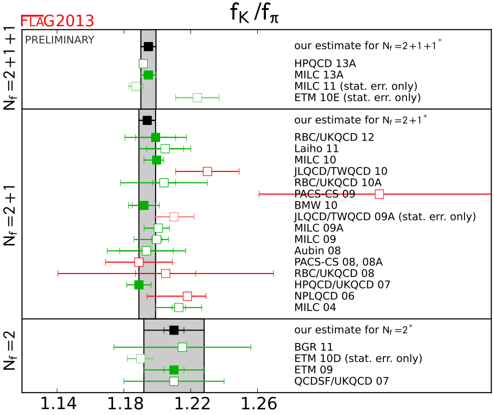
(FLAG) http://itpwiki.unibe.ch/flag/

...quark condensate



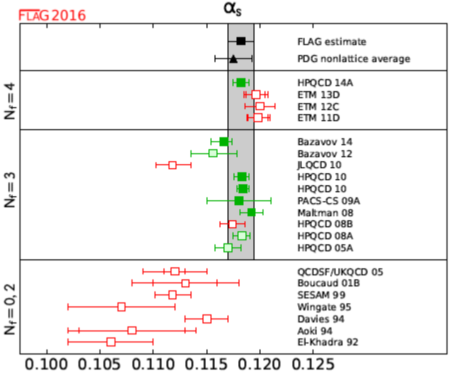
(FLAG) http://itpwiki.unibe.ch/flag/

...decay constants f_K/f_π

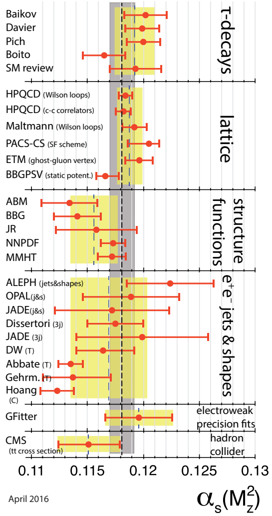


(FLAG) http://itpwiki.unibe.ch/flag/

...strong coupling α_s



(FLAG) http://itpwiki.unibe.ch/flag/



C. Patrignani et al. (Particle Data Group), Chin. Phys. C 40, 100001

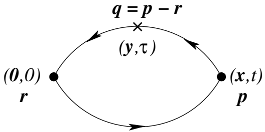
...Matrix elements

Example: Pion electromagnetic form factor

$$\langle \pi^+(\mathbf{p}_f)|\, V_\mu \,|\pi^+(\mathbf{p}_i)\rangle_{\rm cont} = (p_f + p_i)_\mu \, F_\pi(Q^2) \ ,$$

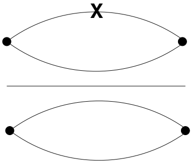
where $Q^2 = (p_f - p_i)^2 \equiv -t$ is the space-like invariant momentum transfer squared, and

$$V_\mu = \frac{2}{3}\, \overline{u}\, \gamma_\mu \, u - \frac{1}{3}\, \overline{d}\, \gamma_\mu \, d$$



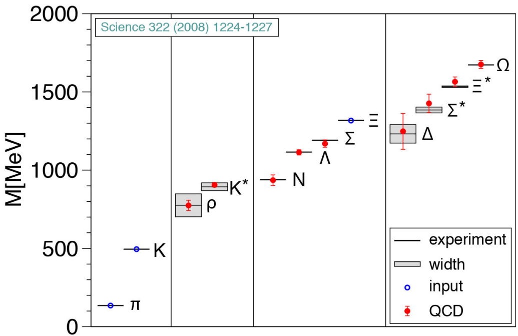
Method: ratio of correlation functions

$$\frac{\langle P(t;\mathbf{p})\, O(\tau;\mathbf{q})\, \overline{P}(0;\mathbf{r})\rangle}{\langle P(t;\mathbf{p})\, \overline{P}(0;\mathbf{p})\rangle}$$



(Sequential source method)

Example for ground state masses



Dürr et al..(BMW collab.)
Science 322, 1224-1227 (2008). arXiv:0906.3599 (Wilson fermions)

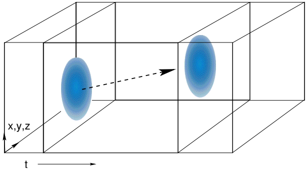
How is it done?
How to find also excited states?

Masses are measured through real space propagators of the form

$$C_X(\vec{p},t) = \langle X(\vec{p},\, t)\, \overline{X}(\vec{p},\, 0)\rangle \quad \text{with} \quad X(\vec{p},\, t) = \sum_{\vec{x}} \hat{X}(\vec{x},\, t)\, \mathrm{e}^{-\mathrm{i}\,\vec{x}\cdot\vec{p}}\ .$$

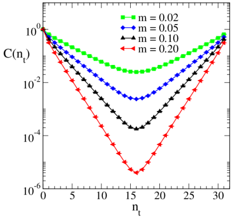
- Construct operators with correct Lorentz-, Dirac-, flavor-, and color symmetries ("interpolating field operators"), usually inspired by the quark model
- Example: Pion:
$$\pi^+ = \overline{d}(x)\gamma_5 u(x)$$
- Example: Simple nucleon-type operator:

$$N^{(i)} = \epsilon_{abc}\, \Gamma_1^{(i)}\, u_a \left(u_b^T\, \Gamma_2^{(i)}\, d_c - d_b^T\, \Gamma_2^{(i)}\, u_c \right)\ .$$



Correlation (2-point) function

$$C_X(\vec{p},t) = \langle X(\vec{p},\, t)\, \overline{X}(\vec{p},\, 0)\rangle$$



The slope is dimensionless:
m_{latt}=(lattice spacing a) x (physical mass M)

$\rightarrow$ comparison with experimental mass sets the scale a, other masses are then predictions

This works for ground states. We need to do better! See Section 6

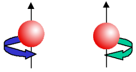
5. Chiral symmetry and fermions species

Continuum QCD

- Chiral transformation:

$$\psi' = \mathrm{e}^{\mathrm{i}\alpha\gamma_5}\psi\,, \quad \overline{\psi}' = \overline{\psi}\mathrm{e}^{\mathrm{i}\alpha\gamma_5}$$

  - leaves $\overline{\psi}D\psi$ invariant ($D = \gamma_\mu(\partial_\mu + \mathrm{i}A_\mu)$)
  - does not leave $\overline{\psi}\psi$ invariant



- Chirality projectors: $P_R = \frac{1}{2}(1+\gamma_5)$, $P_L = \frac{1}{2}(1-\gamma_5)$

$$\psi_L = P_L\psi\,, \quad \psi_R = P_R\psi\,, \quad \overline{\psi}_R = \overline{\psi}P_L\,, \quad \overline{\psi}_L = \overline{\psi}P_R$$

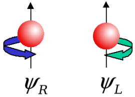
$$\overline{\psi}D\psi = \overline{\psi}_L D\psi_L + \overline{\psi}_R D\psi_R\,, \quad \overline{\psi}\psi = \overline{\psi}_L\psi_R + \overline{\psi}_R\psi_L$$

- The symmetry is (in continuum) manifest by

$$D\,\gamma_5 + \gamma_5\,D = 0$$

- Massless fermions have definite chirality.
- The condensate $\langle\overline{\psi}\psi\rangle$ is the order parameter of chiral symmetry breaking

- Massless u/d quarks ($N_f = 2$) $\rightarrow$ chiral symmetry $SU(2)_R \times SU(2)_L \times U(1)_V \times U(1)_A$.



- $U(1)_A$ broken by anomaly (non-invariance of fermion integration measure)

- $SU(2)_R \times SU(2)_L$ is spontaneously broken by QCD: $SU(2)_V$-multiplets + Goldstone bosons (pions)

Atiyah-Singer Index Theorem: topological charge of gauge field $\nu = n_L - n_R$.
(n.b.:Topological charge is a concept for differentiable manifolds, i.e. continuum; lattice implementation?)

Lattice QCD

Chiral symmetry is a problem for LQCD!

- The formulation should allow explicit chiral symmetry, such that it can be broken spontaneously!
- The Wilson action breaks chiral symmetry explicitly due to the term $\overline{\psi} U \psi$
- No-go theorem (Nielsen, Ninomiya, 1982):
  Lattice theories do not allow simultaneously chiral invariance, locality, and correct continuum behavior of quark propagators.
- Finally excavated (Hasenfratz):

$$D\,\gamma_5 + \gamma_5\,D = a\,D\,\gamma_5\,D$$

  Ginsparg-Wilson condition (1982!) for (quasi) chiral lattice fermions.
  Cont: zero modes are chiral modes
- Eigenvalue spectrum of D: only real modes can be chiral→ zero modes, Banks-Casher!
- "Lattice chiral symmetry" transformation (Lüscher): $\gamma_5 \to \hat{\gamma}_5 = \gamma_5\left(1 - \frac{a}{2}D\right)$
- The GWC is violated for simple Dirac operators (simple fermion actions)!

Lattice QCD

Chiral symmetry is a problem for LQCD!

- The formulation should allow explicit chiral symmetry, such that it can be broken spontaneously!
- The Wilson action breaks chiral symmetry explicitly due to the term $\overline{\psi} U \psi$
- No-go theorem (Nielsen, Ninomiya, 1982):
  Lattice theories do not allow simultaneously chiral invariance, locality, and correct continuum behavior of quark propagators.
- Finally excavated (Hasenfratz):

$$D\,\gamma_5 + \gamma_5\, D = a\, D\, \gamma_5\, D$$

  Ginsparg-Wilson condition (1982!) for (quasi) chiral lattice fermions.
  Cont: zero modes are chiral modes
- Eigenvalue spectrum of D: only real modes can be chiral$\rightarrow$ zero modes, Banks-Casher!
- "Lattice chiral symmetry" transformation (Lüscher): $\gamma_5 \rightarrow \hat{\gamma}_5 = \gamma_5\left(1 - \frac{a}{2} D\right)$
- The GWC is violated for simple Dirac operators (simple fermion actions)!

Lattice QCD

Chiral symmetry is a problem for LQCD!

- The formulation should allow explicit chiral symmetry, such that it can be broken spontaneously!
- The Wilson action breaks chiral symmetry explicitly due to the term $\overline{\psi} U \psi$
- No-go theorem (Nielsen, Ninomiya, 1982):
  Lattice theories do not allow simultaneously chiral invariance, locality, and correct continuum behavior of quark propagators.
- Finally excavated (Hasenfratz):

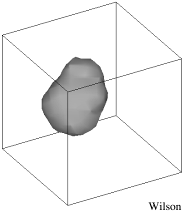
$$D\,\gamma_5 + \gamma_5\,D = a\,D\,\gamma_5\,D$$

  Ginsparg-Wilson condition (1982!) for (quasi) chiral lattice fermions.
  Cont: zero modes are chiral modes
- Eigenvalue spectrum of D: only real modes can be chiral$\rightarrow$ zero modes, Banks-Casher!
- "Lattice chiral symmetry" transformation (Lüscher): $\gamma_5 \rightarrow \hat{\gamma}_5 = \gamma_5 \left(1 - \frac{a}{2} D\right)$
- The GWC is violated for simple Dirac operators (simple fermion actions)!

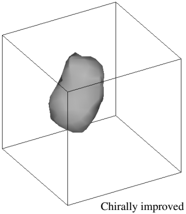
Eigenmodes and instantons

- Exact zero modes are chiral and "define" the topological sector.
- Non-GW-operators: real eigenmodes play this role.

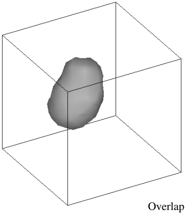
Iso-surfaces of eigenvector density $p_0(x) = \sum_{c,\alpha} v^*(c,\alpha,x)\, v(c,\alpha,x)$:



$(\lambda = 0.14)$



$(\lambda = 0.016)$

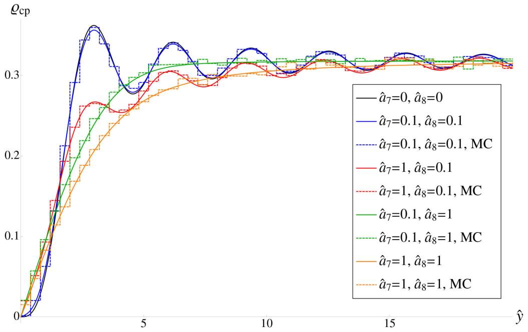


$(\lambda = 0)$

- Near zero modes (small real part, small imaginary part) define the density $\rho(m, V, \lambda)$ related (via Banks-Casher) to the condensate:

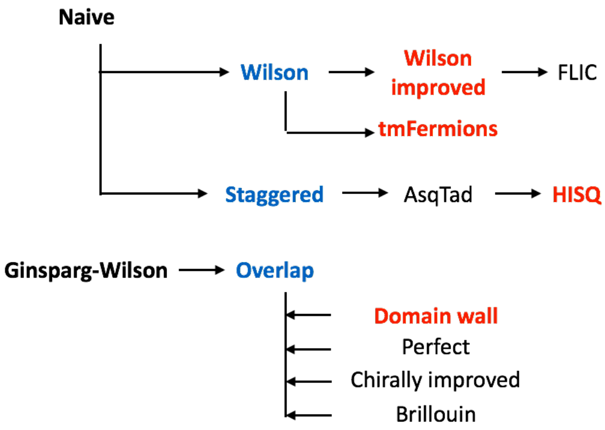
$$\sigma = -\lim_{m\to 0}\lim_{Im(\lambda)\to 0}\lim_{V\to\infty}\rho(m, V, \lambda).$$

- ChPT and RMT predict the shape of the distributions in universality classes.



Kieburg/Verbaarschot/Zafeiropoulos; arXiv:1307.7251 (2013)

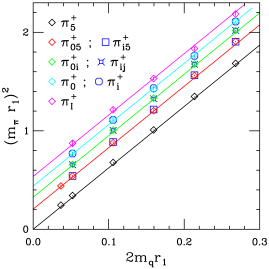
Fermion species



Abbreviations:
tm = twisted mass
AsqTad = a-squared tadpole improved staggered
HISQ = Highly Improved Staggered Quarks
FLIC = Fat-Link Irrelevant Clover

Staggered fermions

- Reduction from 16 down to 4 Dirac fermions (i.e. 16 Grassmann variables), distributed over the 16 sites of the hypercube
- Remnant chiral symmetry
- Asqtad: a^2 and tadpole improved
- 4th root trick: $(\det D)^{1/4}$ (QFT?) $\rightarrow$ tastes
- Simple implementation ☺, harder interpretation (taste splitting) ☹ $\rightarrow$ HISQ - Highly Improved Staggered Quarks



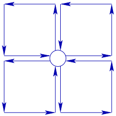
Squared pion mass as a function of the light quark masses (MILC,PoS LAT2006:163)

Wilson improved

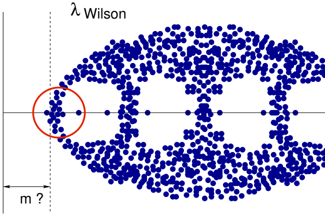
- Symanzik improvement program: $\mathcal{O}(a^2)$ improvement by clover leaf term

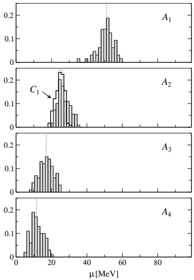
$$S_W + a^5 c_{\mathrm{SW}} \sum_x \overline{\psi}(x)\, \tfrac{\mathrm{i}}{4}\, \sigma_{\mu\nu}\, \hat{F}_{\mu\nu}\, \psi(x)$$

(Sheikoleslami/Wohlert), coefficient tuned non-perturbatively



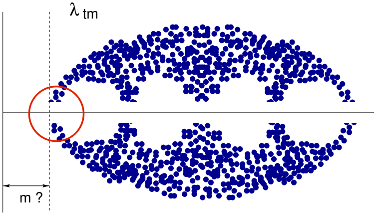
- Simple implementation
- Doubler modes
- Problem with small quark masses: Spurious low-lying eigenmodes of the Dirac operator





Twisted mass: tmQCD (Frezotti, Grassi, Sint, Weisz)

- Wilson + "twisted mass" i $\mu\,\overline{\psi}\,\gamma_5\tau_3\,\psi$
- $m = m_{\text{crit}},\ \mu > 0$ “maximal twist” is $\mathcal{O}(a)$ improved
- No spurious zero modes



- breaks parity and flavor

Overlap Dirac operator (Neuberger)

- Can be constructed explicitly ($a = 1$ for simplicity):

$$D(m=0) = (1 + \gamma_5\, sign(H)) \quad \text{with} \quad H = \gamma_5\, D_W(m < 0)$$

($\gamma_5 D_W$ is hermitian; other kernels also used)

- Sign function of an hermitian matrix?

$$H = \sum_\lambda \lambda\, |\lambda\rangle\langle\lambda| \quad \rightarrow \quad f(H) = \sum_\lambda f(\lambda)\, |\lambda\rangle\langle\lambda|$$

Thus

$$sign(H) = \sum_\lambda sign(\lambda)\, |\lambda\rangle\langle\lambda|$$

is very expensive (hardly possible).

Alternative:

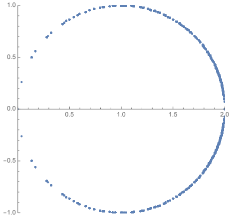
$$sign(H) = \frac{H}{\sqrt{H^2}}$$

approximated by Chebyshef polynomial series or rationals.

Overlap operator

- Exact Ginsparg-Wilson type
- Nice circular spectrum:

$$
\begin{aligned}
D\gamma_5 + \gamma_5 D &= D\gamma_5 D\\
\gamma_5 D\gamma_5 + D &= \gamma_5 D\gamma_5 D\\
D^\dagger + D &= D^\dagger D\\
\lambda^* + \lambda &= \lambda^*\lambda \to (\lambda-1)(\lambda^*-1) = 1 \to |\lambda - 1| = 1
\end{aligned}
$$



- exact zero modes
- spectral density related to condensate via Banks-Casher (and RMT studies):

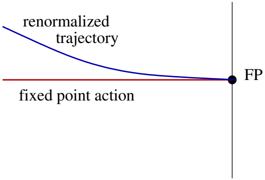
$$\langle\overline{\psi}\psi\rangle \propto \lim_{\text{Im}\lambda\to 0}\lim_{V\to\infty}\rho(\text{Im}\lambda, V)$$

- Allows to implement $n_f = 1$.
- 50-100 times more expensive than Wilson's operator.
- Problems with sector tunneling in HMC implementations.

Fixed Point action

Hasenfratz et al., Nucl. Phys. B 414 (1994) 785, Int. J. Mod. Phys. C 12 (2001) 691

A perfect action follows a renormalized trajectory without corrections to scaling. The fixed point action deviates from the renormalized trajectory; parametrized form with parameter-tuning based on blockspin transformations



Chirally Improved Dirac operator

Gattringer et al., Phys.Rev. D63 (2001) 114501, Nucl. Phys. B 597 (2001) 451

General ansatz for fermion action:

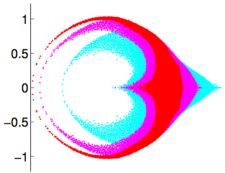
$$D_{mn} = \sum_{\alpha=1}^{16} \Gamma_\alpha \sum_{p \in \mathcal{P}^\alpha_{m,n}} c_p^\alpha \prod_{l \in p} U_l \, \delta_{n,m+p}$$

Path lengths truncated to length 4, parameters tuned to obey the GW-condition. Used for hadron spectroscopy (BGR collab.).

Brillouin operator

S. Dürr & G. Koutsou, Phys.Rev. D83 (2011) 114512, PoS LATTICE2016 (2016) 249

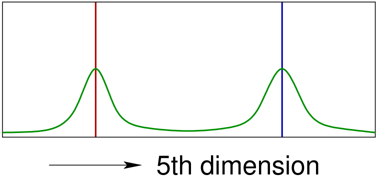
81 point stencil, tries to optimize rotational invariance, used for overlap kernel.



Spectrum of Brillouin op., different levels of APE smearing

Domain Wall

- Kaplan, Furman, Shamir: Introduced extra 5th dimension N_5
- Left-handed and right-handed part of the fermion is bound to the 4-dimensional interface walls.
- They decouple for $N_5 \to \infty$



In the limit one gets exact GW type: the Overlap operator (Neuberger)

Homework (5.1)

Prove that the Wilson Dirac operator (like most others, except the tm-operator) is γ_5-hermitian, i.e.,

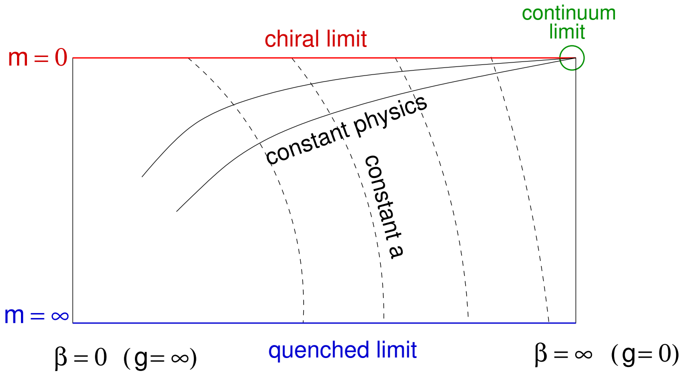
$$\gamma_5 D = (\gamma_5 D)^\dagger \ .$$

Homework (5.2)

Show that a Ginsparg-Wilson operator is "normal", i.e., it commutes with its hermitian conjugate: $[D, D^\dagger] = 0$. What does this imply for the eigenvalues and eigenvectors?

Phase diagram

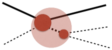
Phase diagram for fermions (idealized):



(Lines of constant physics: e.g., fixed f_K/m_K and m_π/m_K, or . . .)

Key points

- The Ginsparg-Wilson condition ensures lattice chiral symmetry.
- Simple (computationally less expensive) lattice Dirac operators violate the GWC.
- The overlap operator obeys the GWC but is very costly and numerically demanding.
- Today most "full" LQCD calculations on large lattices are for staggered, Wilson-improved, twisted mass, and domain wall actions.
- The eigenvalues of the Dirac operator provide information on instantons, the condensate and the mechanism of spontaneous chiral symmetry breaking.



6. Resonances and scattering

Spectroscopy

Ground state spectroscopy

is correct only for stable particles. Simple hadron approach qqq or qq is valid only below scattering threshold (“bound states” or “artificial bound states”)

Resonances and bound states

require inclusion of hadron-hadron channels in the calculation. Excited states spectroscopy and scattering amplitudes Multi-hadron approach: we need to extend the space of operators: (qq)(qq),(qqq)(qq), (qqq)(qqq)...

What do we need?

- Gauge configurations (with dynamical quarks)
- Quark propagators
- Hadron interpolators and propagators
- A method to extract higher energy levels
- Interpretation of the obtained energy levels

Do it yourself ☹ or go to

ILDG - International Lattice Data Grid

http://www.usqcd.org/ildg/

Correlation $C_N(t) = \langle N(t)\overline{N}(0)\rangle \sim \exp(-m_N t)$

- Example: Simple nucleon-type operator

$$N^{(i)} = \epsilon_{abc}\, \Gamma_1^{(i)}\, u_a \left(u_b^T\, \Gamma_2^{(i)}\, d_c - d_b^T\, \Gamma_2^{(i)}\, u_c \right) \; .$$

with the choices

	$\Gamma_1^{(i)}$	$\Gamma_2^{(i)}$
$i=1$	1	$C\gamma_5$
$i=2$	γ_5	C
$i=3$	i	$C\gamma_4\gamma_5$

(C is charge conjugation operator in Dirac space)

- Projected to definite parity with $P^{\pm}$

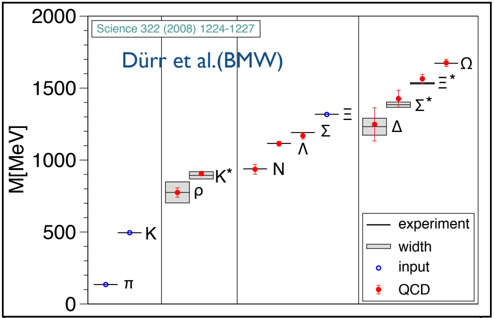
For further constructions (using lattice symmetry representations) see, e.g., Edwards et al., Phys.Rev. D84,074508 (2011) and Dudek et al., Phys.Rev. D85, 054016 (2012).

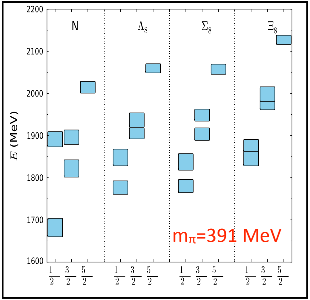
Milestones

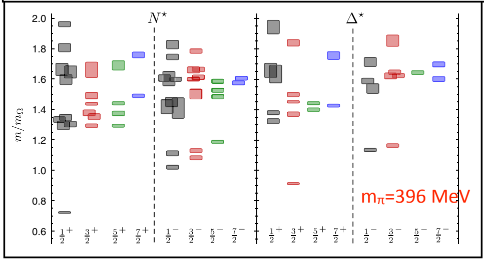
Single hadron approximation

BMW(2008)

HSC(2011, 2013)





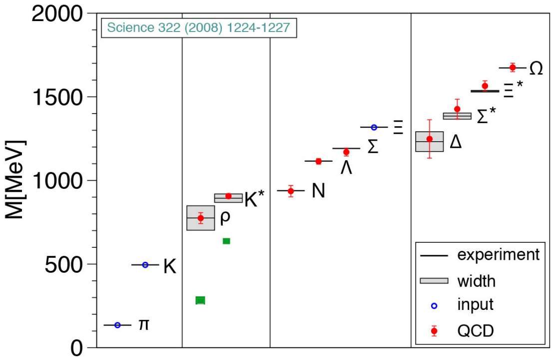


Edwards et al. (HSC) Phys.Rev. D87, 054506 (2013). Edwards et al. (HSC) PR D 84, 074508 (2011)

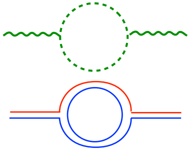
In the $\rho(772)(1^{--})$ channel the lowest intermediate state is the $\pi\pi$-system in (relative) p-wave.

$$m_\pi + m_\pi = 280 MeV \ll$$

$$m_\rho = 772 MeV$$



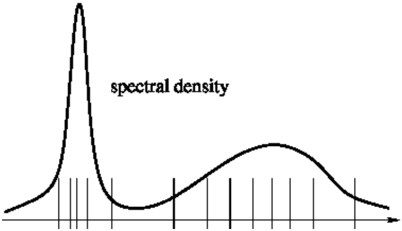
green dots added: physical $\pi\pi$- and $K\pi$-threshold



Why do we need to do better?

- Only a few hadrons are (under strong interactions) stable, most hadrons are resonances
- Finite volume: The spectral distribution is discrete!
- Energy levels are related to (resonance) phase shifts

$$\langle X(t)X^\dagger(0)\rangle = \int_{\omega_0}^{\infty} d\omega\ \rho(\omega) e^{-\omega\, t}$$



Approaches

Lattice QCD

solve lattice
regularised QFT
of quarks and gluons

compute hadron
propagators

discrete energy levels

Hybrid approaches

NLEFT
hadron EFT on a
lattice

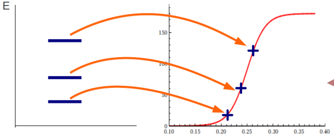
HAL-QCD
Use input from LQCD

Bethe-Salpeter eq.

QCD motivated continuum models

Eff. Hamiltonian
(ChEFT, HEFT,..)
constituent quarks
Unitarized ChPT
Bethe-Salpeter eq.

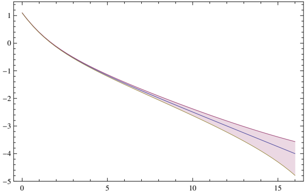
"latticise" by replacing
mom. integration
by lattice sum



Variational analysis

The correlation function is a sum of exponentials

$$\langle X(t)\overline{X}(0)\rangle$$
$$= \sum_n \langle X(t)|n\rangle\, e^{-m_n t}\, \langle n|\overline{X}(0)\rangle$$
$$\sim a_1\, e^{-m_1 t} + a_2\, e^{-m_2 t} + a_3\, e^{-m_3 t} + \ldots$$



Leading term with smallest mass: ground state (dominant at large t).

Higher mass states observed at smaller t

Fit to several exponentials is usually unstable!

"Variational" analysis = diagonalization (Michael, Lüscher/Wolff)

- Use several interpolators O_i
- Compute all cross-correlations

$$C(t)_{ij} = \langle O_i(t)\overline{O_j}(0)\rangle = \sum_n \langle 0|O_i|n\rangle\langle|O_j^\dagger|0\rangle \mathrm{e}^{-t\,M_n}\ .$$

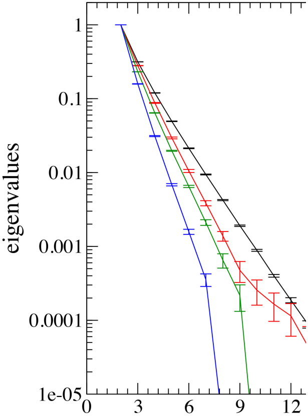
- Solve the generalized eigenvalue problem:

$$C(t)\,\vec{v}_i = \lambda_i(t)\,C(t_0)\,\vec{v}_i$$

- Then

$$\lambda_i(t) \propto \mathrm{e}^{-tM_i}\left(1 + \mathcal{O}\left(\mathrm{e}^{-t\Delta M_i}\right)\right)\ ,$$

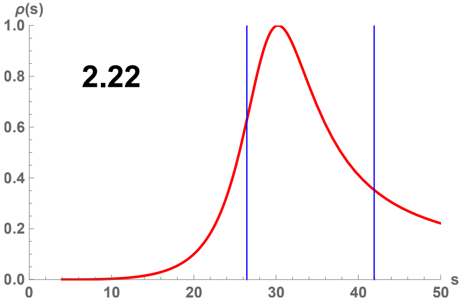
where ΔM_i is the mass difference between the state i and the closest lying state.
- The eigenvectors $\vec{v}$ are "fingerprints" of the state



Continuum vs. lattice

Correlation functions have discrete energy levels!

Example:
Spectral density of a simple resonance in continuum and the discrete energies for a lattice volume
(linear extent $m_\pi L = 2.22$, $s = (E/m_\pi)^2$)

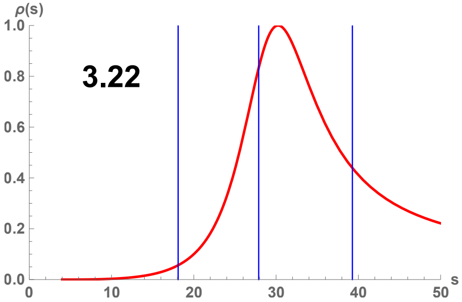


One cannot arbitrarily fix the energies: they are eigenvalues depending on the control parameters (volume, couplings,...).

Continuum vs. lattice

Correlation functions have discrete energy levels!

Example:
Spectral density of a simple resonance in continuum and the discrete energies for a lattice volume
(linear extent $m_\pi L = 3.22$,
$s = (E/m_\pi)^2$)

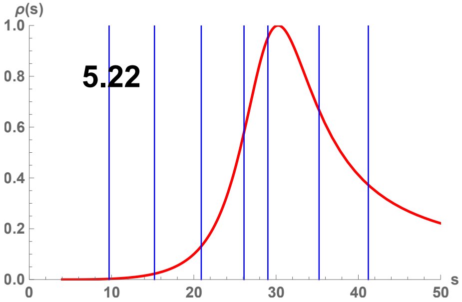


One cannot arbitrarily fix the energies: they are eigenvalues depending on the control parameters (volume, couplings,...).

Continuum vs. lattice

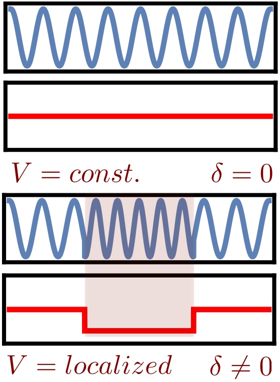
Correlation functions have discrete energy levels!

Example:
Spectral density of a simple resonance in continuum and the discrete energies for a lattice volume
(linear extent $m_\pi L = 5.22$,
$s = (E/m_\pi)^2$)



One cannot arbitrarily fix the energies: they are eigenvalues depending on the control parameters (volume, couplings,...).

Energy levels $\leftrightarrow$ phase shifts



$$e^{ipL} = 1 \longrightarrow p_n L = 2n\pi$$

$$e^{ipL+2i\delta(p)} = 1 \longrightarrow 2\delta(p_n) + p_n L = 2n\pi$$
$$\longrightarrow \cot\delta(p_n) = -\cot(p_n L/2)$$

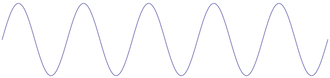
Solving the Helmholtz eq. for d=3 gives

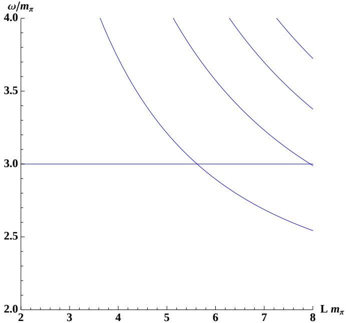
$$p_n \cot\delta(p_n) = c\mathcal{Z}_{00}\left(1; \left(\frac{p_n L}{2\pi}\right)^2\right)$$

Lüscher, CMP 105(86) 153, NP B354 (91) 531, NP B 364 (91) 237 without interaction. . .

M. Lüscher: CMP 105(86) 153, NP B354 (91) 531, NP B 364 (91) 237):
Energy levels are related to continuum phase shifts!

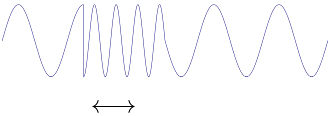
$$p_n \cot \delta(p_n) = c\mathcal{Z}_{00}\left(1; \left(\frac{p_n L}{2\pi}\right)^2\right)$$





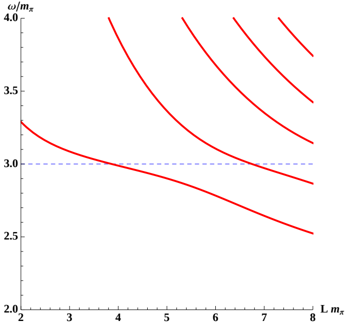
M. Lüscher: CMP 105(86) 153, NP B354 (91) 531, NP B 364 (91) 237):
Energy levels are related to continuum phase shifts!

$$p_n \cot \delta(p_n) = c\mathcal{Z}_{00}\left(1; \left(\frac{p_n L}{2\pi}\right)^2\right)$$



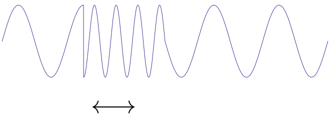
(localized interaction region)

with interaction...



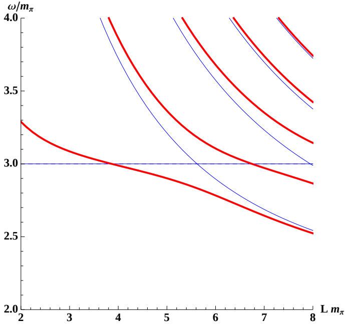
M. Lüscher: CMP 105(86) 153, NP B354 (91) 531, NP B 364 (91) 237):
Energy levels are related to continuum phase shifts!

$$p_n \cot\delta(p_n) = c\mathcal{Z}_{00}\left(1;\left(\frac{p_n L}{2\pi}\right)^2\right)$$



(localized interaction region)

both spectra superimposed



Analyticity and unitarity

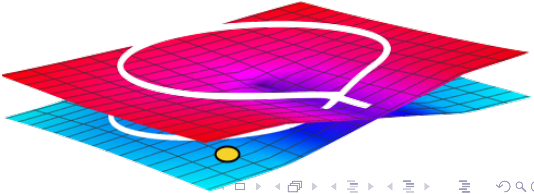
$$
\begin{aligned}
|S_\ell| &= 1 \\
S_\ell &= 1 + 2\mathrm{i}\rho\, t_\ell = \mathrm{e}^{2\mathrm{i}\delta_\ell} \\
t_\ell^{-1}(s) &= \rho(s)(\cot\delta_\ell(s) - \mathrm{i}) \quad \text{with} \quad s = E_{cms}^2
\end{aligned}
$$

(Phase space factor $\rho(s)$)

Analyticity: $t_\ell(s)$ is analytic up to cuts and poles:

- right-hand cut due to unitarity, left-hand cut due to exchange processes
- real axis below threshold: bound states; 2nd sheet above threshold: resonance

$t_\ell^{-1}(s) = 0 \quad \to$ pole in the complex plane



Elastic scattering

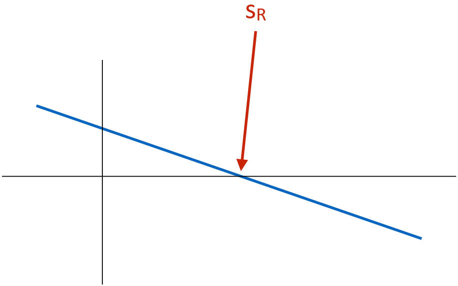
$t_\ell^{-1}(s) = 0 \quad \rightarrow$ pole in the complex plane

Partial wave amplitude t_ℓ

$$t_\ell^{-1}(s) = p \cot \delta_\ell(p) - \mathrm{i}p$$

$$k^{-1} = p \cot \delta(p)$$

$$k^{-1} \approx \frac{1}{a_0} + \frac{1}{2} r_0 p^2 \quad \text{for } p^2 \approx 0$$



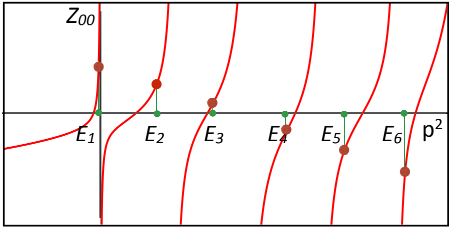
Elastic scattering

$t_\ell^{-1}(s) = 0 \quad \to$ pole in the complex plane

Partial wave amplitude t_ℓ

$$k^{-1} = p \cot \delta(p) \propto \mathcal{Z}_{00}\left(1; \left(\frac{pL}{2\pi}\right)^2\right)$$

$$k^{-1} \approx \frac{1}{a_0} + \frac{1}{2} r_0 p^2 \quad \text{for } p^2 \approx 0$$



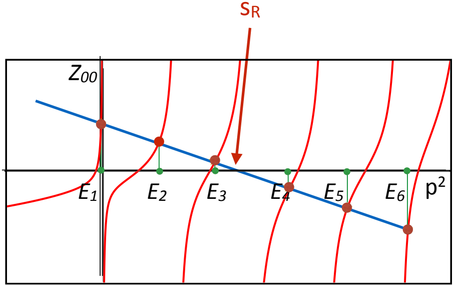
Elastic scattering

$t_\ell^{-1}(s) = 0 \quad \to$ pole in the complex plane

Partial wave amplitude t_ℓ

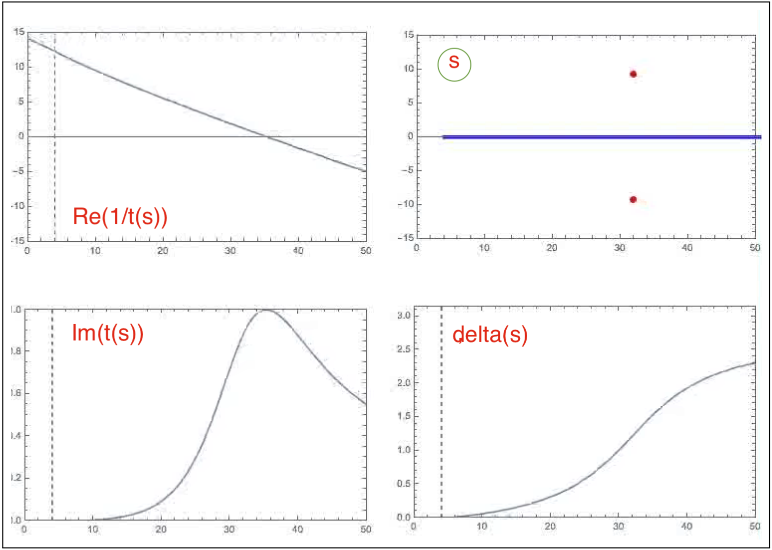
$$k^{-1} = p \cot\delta(p) \quad \text{for } p^2 > 0$$

$$k^{-1} \approx \frac{1}{a_0} + \frac{1}{2} r_0 p^2 \quad \text{for } p^2 \approx 0$$



Resonance or bound state

Resonance or bound state



Key points

- Most hadrons are “excited” states
- Exited states are unstable (no problem in quenched simulations)
- Energy spectrum volume dependent (cf. Lüscher) $\rightarrow$ allows to determine scattering lengths and phase shifts below the inelasticity threshold.
- Many states contribute to a quantum channel!

Homework (6.1)

Compute and plot the non-interacting energy values for a free pion-nucleon system in the N^3 timeslice (N is the linear extent in fm) for the range 2 fm$< N <$8 fm. For $L = 4$ fm: how many different energy level lie below 1.8 GeV?

Technical issues

- Operator basis complete enough?: more operators?
- we need more energy levels:
  - “moving frames”: new energy level for same set of gauge configurations

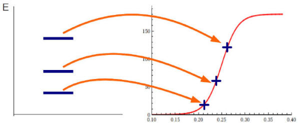
  - different boundary conditions
  - several volumes

- inelastic region: coupled channels, we need to combine different measurements, parametrisation, interpolation for K matrix elements

- Resonance pole position: analytic continuation (parametrize Re T^{-1}, disp.rel.; left hand cut?)

- Unstable decay products: 3-particle channels, e.g.

$$a_1(1260) \to \rho\pi \to \pi\pi\pi$$
$$b_1(1235) \to \omega\pi \to \pi\pi\pi\pi$$
$$N\pi \to (N f_0 \to N\pi\pi,\ N(1440) \to N\pi\pi,\ \Delta\pi \to N\pi\pi,\ N\rho \to N\pi\pi)$$



.... for scattering length and phase shift:

- Light quarks, elastic region

  $\pi\pi$ for $\ell = 0, 1, 2$ (f_0, ρ)
  πK for $\ell = 0, 1$ (κ, K^*)
  $\pi\rho$ and $\pi\omega$ (a_1, b_1)

- Light quarks, inelastic region

  $\pi\pi, K\overline{K}$
  $\pi K, \eta K$
  $\pi N, \pi\sigma$

- heavy-heavy and heavy light

  $\psi, \psi(3770), Z(3900), X(3872), \eta_c$
  $D\pi, DK, D^*K, BK, B^*K$

Example: ρ, $\pi\pi$ operators

$$\mathcal{O}_1^s(t) = \sum_{\mathbf{x},i} \frac{1}{\sqrt{2}}\, \bar{u}_s(x)\, A_i\gamma_i\, e^{i\mathbf{Px}}\, u_s(x) \;-\{u_s \leftrightarrow d_s\} \qquad (s=n,m,w)\,,$$

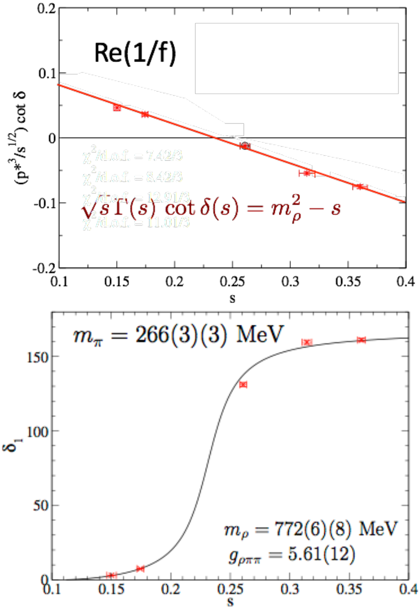
$$\mathcal{O}_2^s(t) = \sum_{\mathbf{x},i} \frac{1}{\sqrt{2}}\, \bar{u}_s(x)\, \gamma_t A_i\gamma_i\, e^{i\mathbf{Px}}\, u_s(x) \;-\{u_s \leftrightarrow d_s\} \qquad (s=n,m,w)\,,$$

$$\mathcal{O}_3^s(t) = \sum_{\mathbf{x},i,j} \frac{1}{\sqrt{2}}\, \bar{u}_s(x)\overleftarrow{\nabla}_j\, A_i\gamma_i\, e^{i\mathbf{Px}}\, \overrightarrow{\nabla}_j u_s(x) \;-\{u_s \leftrightarrow d_s\} \qquad (s=n,m,w)\,,$$

$$\mathcal{O}_4^s(t) = \sum_{\mathbf{x},i} \frac{1}{\sqrt{2}}\, \bar{u}_s(x)\, A_i\, \tfrac{1}{2}[e^{i\mathbf{Px}}\, \overrightarrow{\nabla}_i - \overleftarrow{\nabla}_i e^{i\mathbf{Px}}]u_s(x) \;-\{u_s \leftrightarrow d_s\} \qquad (s=n,m,w)\,,$$

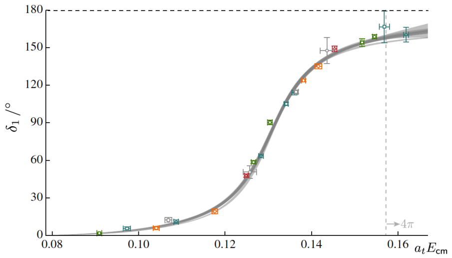
$$\mathcal{O}_5^s(t) = \sum_{\mathbf{x},i,j,k} \frac{1}{\sqrt{2}}\, \epsilon_{ijl}\, \bar{u}_s(x)\, A_i\gamma_j\gamma_5\, \tfrac{1}{2}[e^{i\mathbf{Px}}\overrightarrow{\nabla}_l - \overleftarrow{\nabla}_l e^{i\mathbf{Px}}]u_s(x) -\{u_s \leftrightarrow d_s\} \quad (s=n,m,w)\,,$$

$$\mathcal{O}_6^{s=n}(t) = \frac{1}{\sqrt{2}}[\pi^+(\mathbf{p_1})\pi^-(\mathbf{p_2}) - \pi^-(\mathbf{p_1})\pi^+(\mathbf{p_2})]\,, \qquad \pi^\pm(\mathbf{p_i}) = \sum_{\mathbf{x}} \bar{q}_n(x)\gamma_5\tau^\pm e^{i\mathbf{p_i x}} q_n(x)\,.$$

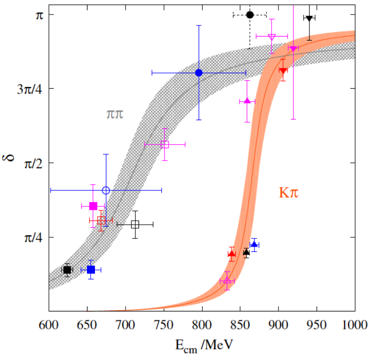


Early (2011) results for elastic $\pi\pi$ p-wave (ρ): $n_f = 2$, $m_\pi = 266$ MeV CBL, Mohler, Prelovsek, and Vidmar. Phys. Rev. D 84 (2011) 054503; Erratum PR D 89 (2014) 059903(E)

see also: X. Feng, et al.„ Phys. Rev. D 83, 094505 (2011). S. Aoki et al. (CS Collaboration), Phys. Rev. D 84, 094505 (2011).



D. J. Wilson et al., (HSC),PRD 92, 094502 (2015)
Coupled channels $\pi\pi$, $K\overline{K}$
$n_f = 2 + 1$, $m_\pi = 236$ MeV



G. Bali et al., PRD 93, 054509 (2016)
elastic $\pi\pi$ and πK scattering,
$n_f = 2$, $m_\pi = 150$ MeV

Further developments (s wave, πK,ηK, . . .): see D. Wilson at LATTICE 2017

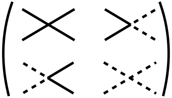
Beyond the elastic region: coupled channels

"..to boldly go, where.."

Extension to several coupled channels

Matrices T, Z:

$$\det\left[T^{-1} - Z\right] = 0$$



Bernard et al ., JHEP 1101 (2011) 019 [arXiv:1010.6018]

Briceno et al ., PR D 88, 034502 (2013) two nucleons

Briceno et al , PR D 88, 094507 (2013) moving multichannels

Briceno et al ., PR D 89, 074507 (2014) arbitrary spin

Hansen & Sharpe, PR D86 (2012) 016007[arXiv:1204.0826]

Briceno et al., PR D 91, 034501 (2015) $1 \rightarrow 2$ transitions

Meson-baryon scattering

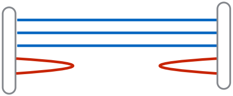
- Without annihilation

  Example: NN

  Example: pK^{+}

- With annihilation

  Example: πN
  neg.parity: 29 terms
  pos.parity: 114 terms



Baryons: Nπ

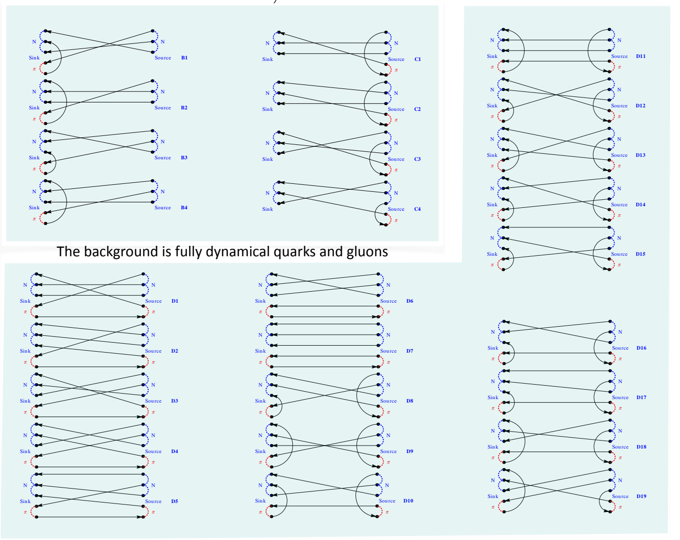
(negative parity)

CBL&Verduci, PRD87 (2013) 054502 [arXiv:1212.5055]

5-quark operators and 29 contraction terms

$N \to N\pi, N\pi \to N$

$N\pi \to N\pi$

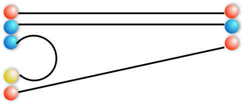


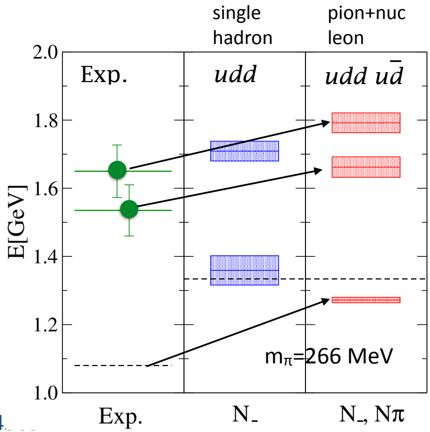
πN (neg.parity): Effect of open 2-hadron channel?

N*(1535),N*(1650)
Nπ negative parity

CBL&Verduci, PRD87 (2013) 054502
[arXiv:1212.5055]

needs annihilation terms





See also Kiratidis et al., PR D 91, 094…
(2015) [arXiv: 1501.07667]

Wanted: Coupled channel analysis (Nη, ΛK, Δπ)…

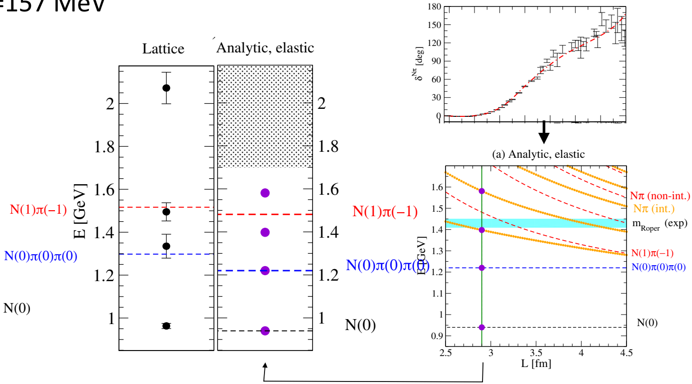
Beyond the single hadron approximation

CBL et al. PRD 95 (2017) 014510 ;
arXiv:1610.01422

Operator basis ($1/2^+$) allows for:

N, Nπ (p wave), Nσ (s wave)

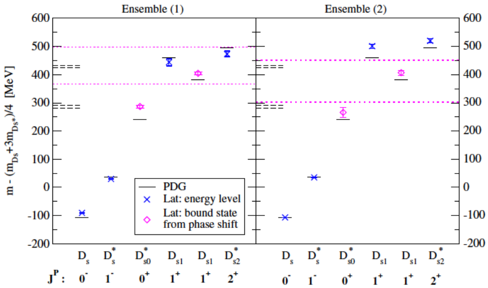
m_π=157 MeV



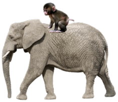
Example: Heavy-light system

Quark content $c\bar{s}$, $c(\bar{u}u, \bar{d}d)\bar{s}$: D_s, DK
($n_f = 2$ and $2+1$, $m_\pi = 266$ and 157 MeV

- DK as well as $\bar{s}c$ interpolating fields are used
- We identify D^*_{s0} ($J^P = 0^+$) as a bound state 37(17) MeV below DK threshold.
- The experimentally observed D^*_{s0}(2317) lies 40-50 MeV below DK threshold.

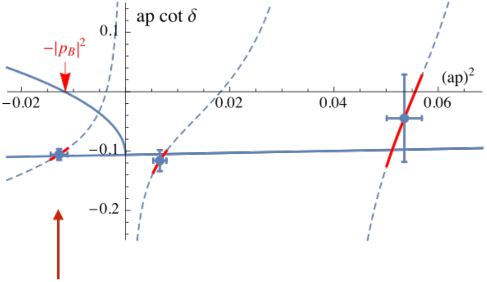


S. Prelovsek, L. Leskovec, CBL, D. Mohler, R. Woloshyn; arXiv:1308.3175



Quark content $c\bar{s}$, $c(\bar{u}u, \bar{d}d)\bar{s}$: B_s, BK
($n_f = 2$ and $2+1$, $m_\pi = 266$ and 157 MeV
Predicting positive parity B_s mesons

- BK scattering in $J^{PC} =^{++}$ near threshold
- BK as well as $\bar{s}b$ interpolating fields are used
- We predict a bound state 64(13)(19) MeV below BK threshold with $m(B_{s0}) = 5.711(13)(19)$ GeV
- Threshold scattering parameters obtained



D. Mohler et al., Phys:Lett. B 750 (2015) 17

Coupled channels formalism
Extension to 3-particle channels

But: No numerical lattice results yet!

see review by Briceno, Dudek, Young, arXiv: 1706.06223

Issues

Lattice operator basis: is it sufficient complete?

Coupled channels: need to combine different measurement, parametrisation, interpolation for K matrix elements

Resonance pole: analytic continuation (parametrize Re T^{-1}, disp.rel.; left h. cut?)

Unstable decay products:

$a_1(1260) \to \rho\pi \to \pi\pi\pi$

$b_1(1235) \to \omega\pi \to \pi\pi\pi\pi$

$N\pi \to \text{Roper} \to N\Delta \to N\pi\pi$

$\to N\rho \to N\pi\pi$

$\to N f_0 \to N\pi\pi$

Further reading

More

Topics	Lecturers (Affiliations)
Basics of EFTs & LGT	**C. B. Lang** (U. Graz) **A. Pich** (U. Valencia)
Basics in LGT algorithms	**A. Bazavov** (Michigan State U.)
Renormalization	**G. Martinelli** (La Sapienza U.) **C. Monahan** (Rutgers U.)
Introduction to chiral EFT & applications	**A. Pich** (U. Valencia) **E. Epelbaum** (U. Bochum)
Interface of ChPT & lattice	**S. Dürr** (U. Wuppertal) **J. Komijani** (TUM)
Heavy Quarks	**N. Brambilla, A. Vairo** (TUM) **S. Ryan** (Trinity College Dublin)
QCD at high density & temperature	**P. Petreczky** (BNL) **A. Vairo** (TUM)
Flavor physics & BSM	**G. Isidori** (U. Zürich) **A. Kronfeld** (Fermilab)
Nuclear physics from QCD	**S. Aoki** (YITP Kyoto) **W. Detmold** (MIT) **U. Meißner** (U. Bonn, FZ Jülich)
Soft-Collinear EFT & Future Lattice Frontiers	**Iain Stewart** (MIT)
New techniques	**O. Bär** (Humboldt U. Berlin) **M. Peardon** (Trinity College Dublin) **J. H. Weber** (TUM)

Further reading

I do not quote the standard texts on Quantum Field Theory (like Peskin/Schroeder or Ramond). For this please ask your favorite QFT lecturer.

- Lattice QCD specific web sites:
  http://www.scholarpedia.org/article/Lattice_gauge_theories
  https://arxiv.org/archive/hep-lat
- Lattice QCD specific monographs:
  - E. Seiler: Gauge Theories as a Problem of Constructive QFT and Statistical Mechanics, Vol. 159 of Springer Lecture Notes in Physics (Springer, 1982)
  - M. Creutz: Quarks, Gluons and Lattices (Cambridge Univ. Press, 1983)
  - H. J. Rothe: Lattice Gauge Theories - An Introduction (World Scientific, 1992)
  - I. Montvay and G. Münster: Quantum Fields on a Lattice (Cambridge University Press: 1997)
  - J. Smit: Introduction to Quantum Fields on a Lattice (Cambridge University Press: 2002)
  - J. Zinn-Justin: Quantum Field Theory and Critical Phenomena (Clarendon Press, Oxford, UK: 2002)
  - Thomas Degrand und Carleton Detar: Lattice Methods for Quantum Chromodynamics (World Scientific: 2006)
  - Christof Gattringer and Christian B. Lang: Quantum Chromodynamics on the Lattice - an Introductory Presentation (Springer: 2010)
  - Francesco Knechtli, Michael Günther, and Michael: Lattice Quantum Chromodynamics, Practical Essentials (Springer: 2017)

- Introductory lectures
  - Martin Lüscher, Computational Strategies in Lattice QCD, arXiv 1002.4232
  - Sinéad Ryan, INT Lectures on Hadron Spectroscopy, http://www.maths.tcd.ie/ryan/INT2012/
  - William Detmold, Hadron Interactions and Many-Body Physics, INT Summer School on Lattice QCD for Nuclear Physics, http://www.int.washington.edu/PROGRAMS/12-2c/Lectures.html
  - Anna Hasenfratz, Introduction to Lattice QCD, Summer School on Lattice QCD for Nuclear Physics, http://www.int.washington.edu/PROGRAMS/12-2c/Lectures.html
  - Christian Hoelbling, Lattice QCD: Concepts, techniques and some results, Acta Physica Polon. B45 no.12, 2143, 2014.
  - Daniel Mohler, Bound states on the lattice, lectures at IUTP 2017, http://physik.uni-graz.at/iutp2017/lecturenotes.php
- Other sources
  - Annual lattice proceedings, many of them at Proceedings of Science: https://pos.sissa.it/
  - HEP-LAT Preprint Server: https://arxiv.org/archive/hep-lat
- Software
  - openQCD: http://luscher.web.cern.ch/luscher/openQCD/
  - LQCD Software (SciDAC): https://www.usqcd.org/software.html