Lattice QCD: an introduction

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Recommended resources

Most of the contents of this presentation have been extracted from the following introductory books:

- István **Montvay** & Gernot Münster, *"Quantum Fields on a Lattice"*, Cambridge Monographs on Mathematical Physics (1994).
- Christof **Gattringer** & Christian B. Lang *"Quantum Chromodynamics on the lattice"*, Lecture Notes in Physics, Springer (2010).
- M. **Creutz** *"Quarks, gluons and lattices"*, Cambridge Monographs on Mathematical Physics (1985).
- M. **Lüscher** notes at *Les Houches summer school* 1997.

youtube.com

Also M. Creutz lectures online at youtube.com. Links: I, II, III, and IV.

Outline

Lattice QCD: an introduction

Parts:

- I. The basics.
- II. Gauge and fermion fields.
- III. Phenomenology from lattice QCD.

Lattice QCD: an introduction

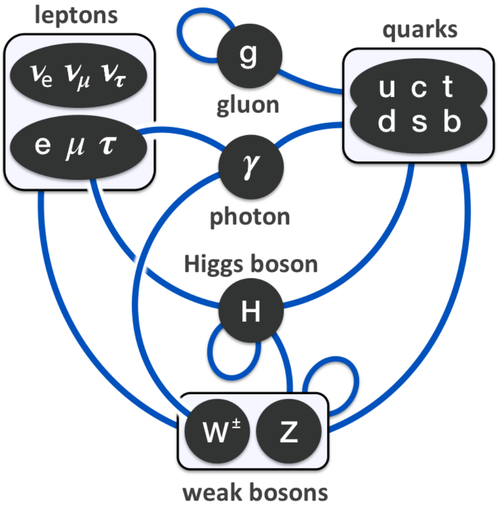
I. The basics.

Outline

1. Motivation: why lattice-QCD?

2. Scalar lattice field theory

The Standard Model



QCD

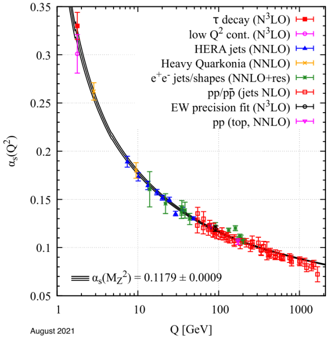
QCD Lagrangian depends on a few parameters: one coupling, α_s, and quark masses (m_u, m_d, m_s, m_c, m_b and m_t).

$$\mathcal{L}_{\mathrm{QCD}} = -\frac{1}{4} F_a^{\mu\nu} F_{\mu\nu}^a + \sum_{f=u,\cdots,t} \bar{\psi}_f \left(i \not{D} - m_f \right) \psi_f$$

α_s acquires a renormalization scheme dependent running with the momentum.

The running of $\alpha_s(\mu^2) = \frac{g^2(\mu^2)}{4\pi}$ is controlled by its RGE, $\frac{d\alpha_s}{d \ln \mu^2} = \beta(\alpha_s)$

It is usually expressed either by its RGE boundary condition, $\Lambda_{\overline{\mathrm{MS}}}$, or by its value at a reference scale, typically m_Z: $\alpha_{\overline{\mathrm{MS}}}(m_Z^2)$



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Emergent phenomena:

- Confinement.
- Hadron masses
- Spontaneous chiral symmetry breaking.

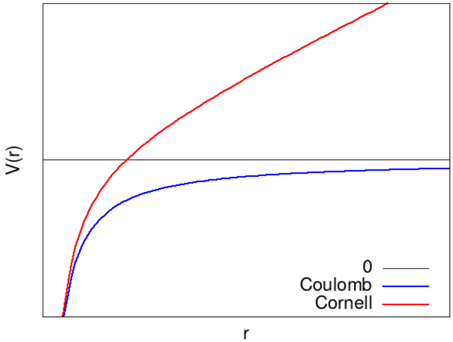
Require non-perturbative methods.

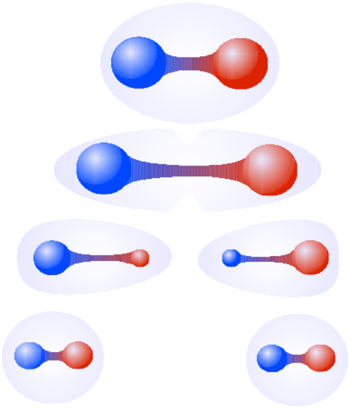
Cannot be described using α_s as an expansion parameter (perturbation theory).

Confinement and the linearly rising potential

Interaction potential among static quarks:

$$V(r) \sim -\frac{4}{3}\frac{\alpha_s}{r} + \sigma r$$





[Image from webific.ific.uv.es]

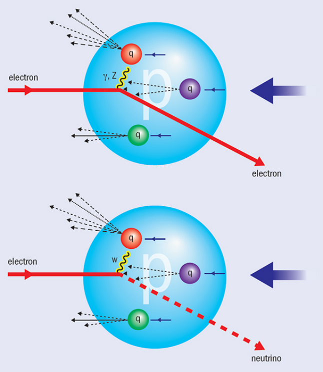
Confinement and the linearly rising potential

Quarks or gluons have never being observed isolated.

Particle Data Group:

> **Free Quark Searches**
>
> All searches since 1977 have had negative results.

[Particle Data Group]



[Image from cerncourier.com]

Initial and final states are hadrons, which are not the fundamental degrees of freedom of QCD!

Dimensional transmutation

The large-momentum running of the coupling is determined by

$$\alpha_s(\mu) \sim \frac{1}{\log(\mu/\Lambda)}$$

Perturbation theory provides the dependence on the Λ-parameter, but does not fix its value!

Dimensional transmutation

Masless QCD is a dimensionless theory, but a scale Λ emerges as a result of the interaction!

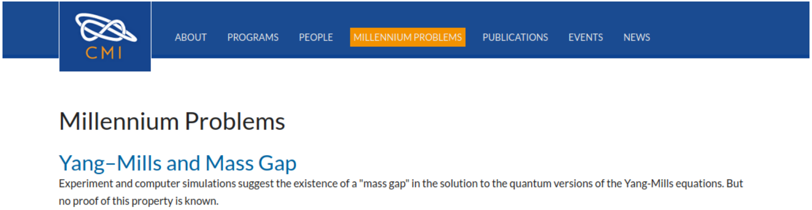
The coupling constant in gauge theories acquires a dependence on the renormalization scale encoded in the beta-function of the renormalization group.

Mass gap puzzle

Empirical finding: except pions (quasi-Nambu-Goldstone boson), light hadrons acquire a mass much larger than their corresponding quark masses!

For the lightest baryon, the proton:

$$\frac{m_{\mathrm{proton}}}{2m_{\mathrm{u}} + m_{\mathrm{d}}} \sim 100$$



Chiral limit

The $m_q = 0$ limit is dimensionless... but not so different from nature!

$$M_\pi = 0\,; \qquad \frac{M_\rho}{M_p} \sim \text{phys}$$

Chiral transformation

$$\psi \to e^{i\phi\gamma_5/2}\psi\,; \qquad \overline{\psi} \to \overline{\psi} e^{i\phi\gamma_5/2}$$

is a symmetry of the Lagrangian in the $m \to 0$ limit.

It allows to separate left- and right-modes $\psi_L = \frac{1-\gamma_5}{2}\psi\,, \qquad \psi_R = \frac{1+\gamma_5}{2}\psi$ as:

$$\begin{aligned} \overline{\psi}\not{D}\psi &= \overline{\psi}_L \not{D}\psi_L + \overline{\psi}_R \not{D}\psi_R \\ \overline{\psi} m\psi &= \overline{\psi}_L m\psi_R + \overline{\psi}_R m\psi_L \end{aligned}$$

Symmetry $\to$ Nambu-Goldstone bosons: $\pi^\pm$, π^0 $(m_\pi \approx 0)$.

Spontaneous chiral symmetry breaking

For massless quarks u and d quarks, $m_u = m_d = 0$, there is a chiral symmetry $SU(2)_L \times SU(2)_R$ in QCD.
is broken in QCD:

- spontaneously $\langle\overline{\psi}\psi\rangle$
- explicitly for $m_{u,d} \neq 0$.
- by the $U(1)$ anomaly (η' mass).

Chiral limit

Very rich phenomenology related to the chiral properties of QCD!

Gell-Mann–Oakes–Renner relation:

$$M_\pi^2 = (m_u + m_d)\frac{\langle\overline{\psi}\psi\rangle}{F_\pi^2}$$

shows that the pion mass is very sensitive to quark masses.

Take away message: Why lattice QCD?

Why non-perturbative methods?

- Perturbative expansions not useful in low-energy QCD.
- Only demonstration of confinement from QCD Lagrangian.
- QCD bound states not accessible in perturbation theory.
- Quarks and gluons do not correspond to the initial/final states.
- Flavour physics and new physics searches require precision QCD calculations.
- ..

Outline

1 Motivation: why lattice-QCD?

2 Scalar lattice field theory

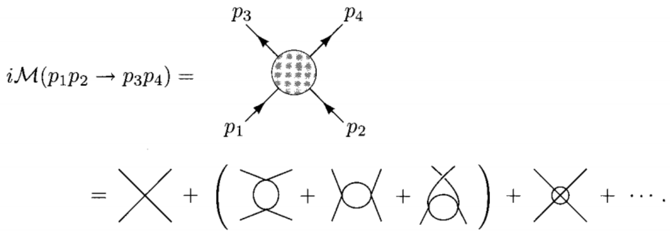
Green functions

Let us start with a real scalar field ϕ:

$$\mathcal{L}_\phi = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - U(\phi)\,; \qquad U(\phi) = \lambda\phi^4$$

Solving a QFT implies computing its Green functions:

$$\langle\mathcal{O}\rangle = \frac{1}{Z}\int[d\phi]\mathcal{O}(\phi)e^{-iS(\phi)} \quad \text{with} \quad S = \int d^4x\ \mathcal{L}_\phi$$



[Image from Peskin & Schroeder.]

Lattice formulation: Wick rotation

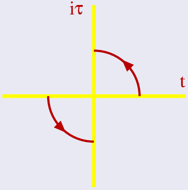
Path integral in imaginary time:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int [d\phi] \mathcal{O}(\phi) e^{-S(\phi)} \quad \text{with} \quad Z = \int [d\phi] e^{-S(\phi)}$$

is weighted by a real exponential, that can be used as a probability distribution.

The integral has ∞^∞ degrees of freedom... $\rightarrow$ requires a finite-discrete spacetime!

Wick rotation



$$t \rightarrow i\tau$$

Lattice formulation: discrete spacetime

The positions are discretized in a H4 lattice:

$$x_\mu = a n_\mu\,, \qquad n_\mu = 1, \cdots, N$$

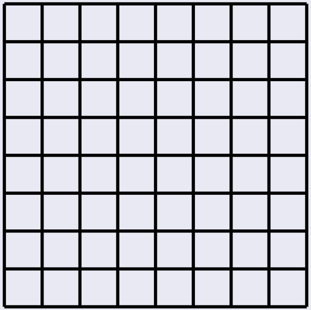
with a known as *lattice spacing*. The momentum-space is then limited to $|k_\mu| < \frac{\pi}{a}$.

With a number of degrees of freedom finite, the path integral:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int [d\phi] \mathcal{O}(\phi) e^{-S(\phi)} \to \frac{1}{N} \sum_{i=1}^{N} O_i$$

can be evaluated as a Monte Carlo sum.

A discrete lattice



Lattice formulation: discrete action

In order to write a **discrete action** we need:

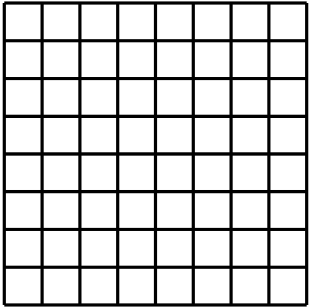
- a discrete derivative:

$$\partial_\mu \phi \to \frac{\phi_{x+\mu} - \phi_x}{a}$$

- some boundary conditions, e.g., *periodic*:

$$\phi_0 = \phi_{Na}\,, \quad \forall \text{directions}$$

The momenta are then discrete, $k = \frac{2\pi}{Na} n$ with $n = 0, 1, \cdots, N-1$ and p.b.c.



Regularization

The lattice field theories are regularized, the inverse lattice spacing a^{-1} working as a cutoff.

Lattice formulation: discrete action

With this we have a (free) discrete action:

$$S = \frac{a^2}{2} \sum_x \left[\left(8 - a^2 m^2\right) \phi_x^2 - 2 \sum_\mu \phi_x \phi_{x+\mu} \right]$$

Lattice formulation: discrete action

With this we have a (free) discrete action:

$$S = \frac{1}{2} \sum_x \left[\left(8 - \mu^2\right) \varphi_x^2 - 2 \sum_\mu \varphi_x \varphi_{x+\mu} \right]$$

where the lattice spacing a has been included in the definition of the dimensionless field $\varphi = a\phi$ and mass $\mu = am$.

Dimensionless

The action is dimensionless, the lattice spacing a is only fixed *a posteriori*, after comparison with **physical** quantities.

Different values of μ correspond to different lattice spacings a, for the same physical mass m.

Monte Carlo

Our purpose is to find field configurations $\{\varphi_x\}$ with probability distribution

$$P(\{\varphi_x\}) \propto e^{-S(\varphi)} .$$

Monte Carlo:

- Start with any initial configuration $\{\varphi_x^0\}$
- Propose some update strategy defined by a transition probability $P(\varphi_x \to \varphi'_x)$ satisfying detailed balance:

$$\frac{P(\varphi \to \varphi')}{P(\varphi' \to \varphi)} = e^{-\Delta S} \quad \text{with} \quad \Delta S = S(\varphi') - S(\varphi)$$

- Repeat the update process until convergence.

Monte Carlo

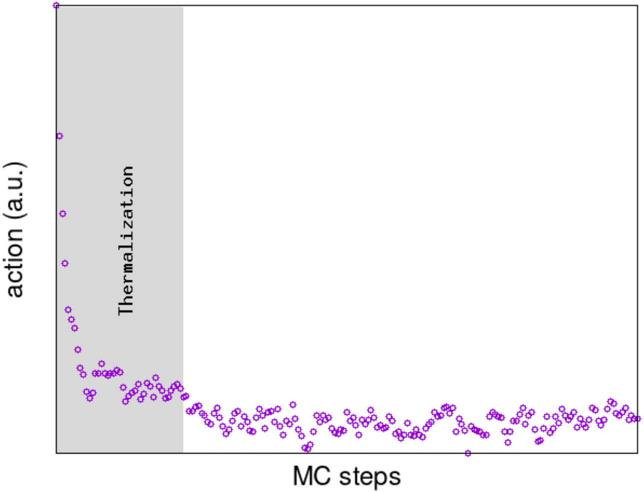
Within MC, the field value at each lattice site has to be updated.

Update strategies

- **Metropolis**: propose some new (random) field φ' and accept/reject with probability $P = max\left(1, e^{-\Delta S}\right)$.
- **Heatbath**: Choose φ' with probability $e^{-S(\varphi')}$ (independent of the old field φ). May be expensive, but guarantees acceptance.
- **Multi-hit metropolis**: as original Metropolis but make several hits for each site.
- **Overrelaxation**: chooses $\varphi' = \alpha - \varphi$ with $S(\varphi') = S(\varphi)$.

Monte Carlo generated configurations are necessarily correlated, i.e., a number of MC update sweeps is required to produce statistically pseudo-independent results (autocorrelation).

Monte Carlo



Once you have a set of configurations, you can compute any Green function of the theory as a Monte Carlo sum

$$\langle \mathcal{O} \rangle \quad \rightarrow \quad \frac{1}{N} \sum_{i=1}^{N} O_i$$

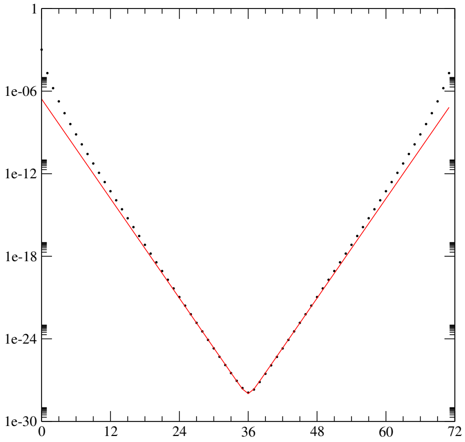
Autocorrelation

Only decorrelated configurations to be used in the average (for appropiate uncertainty evaluations).

Computing masses

For example, an operator $\mathcal{O} = J(\vec{x}, t)J^\dagger(\vec{0}, 0)$ that creates an state at $(\vec{0}, 0)$ and destroys it at $(\vec{x}, t)$:

$$
\begin{aligned}
C(t) &= \sum_{\vec{x}} \langle 0 | J(\vec{x}, t) J^\dagger(\vec{0}, 0) | 0 \rangle \\
&= \sum_{\vec{x}, P} \langle 0 | e^{Ht} J(\vec{x}, 0) e^{-Ht} | P \rangle \langle P | J^\dagger(\vec{0}, 0) 0 | \rangle \\
&= \sum_{P} c_P e^{-M_P t} \to c_0 e^{-M_0 t} \qquad \text{(large t)}
\end{aligned}
$$



The mass of the lightest particle is extracted from the asymptotic behavior of time-correlators.

Renormalization

For any Green function of the theory, $\widetilde{G}(p)$, one has to set a renormalization scheme so that:

$$\widetilde{G}_{R,\mu}(p) = \lim_{a\to 0} Z_G^{-1}(\mu, a)\widetilde{G}(p, a)$$

When $am \to 0$, the correlation length $\xi \sim 1/(am)$ diverges (criticality)... and one should warranty that

$$a \ll m^{-1} \ll L$$

Continuum limit

We are interested in the $a \to 0$ limit, where the spacing goes to zero and the momentum cutoff to infinity.

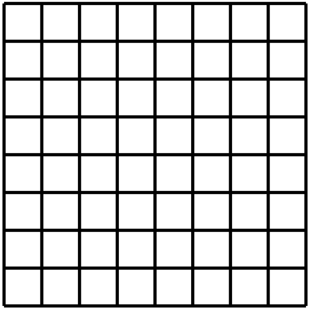
Thermodynamic limit

After calculations with different box sizes, one is interested in the $L \to \infty$ limit, corresponding to an infinite volume.

Take away message: lattice field theories

QFT in a lattice

- Wick rotation (imaginary time) $+$ lattice.
- Discrete action and boundary conditions.
- Preserve symmetries!
- Dimensionless (a fixed a posteriori).
- Monte Carlo
- Unphysical time evolution $\rightarrow$ masses.
- Continuum and thermodynamic limit.
- ...



Part II:

Lattice QCD: an introduction

Gauge and fermion fields.

Outline

3. Gauge fields
   - Yang-Mills action: gauge invariance
   - Parallel transporters & Wilson action
4. Fermion fields
   - Grasmann variables
   - Naive fermions: doublers
   - Nielsen-Ninomiya theorem
   - Chiral fermions
5. Monte Carlo for lattice-QCD
   - Updating the gauge fields
   - Hybrid Monte Carlo
   - Topology

Towards a discrete gauge action

The Yang-Mills action in Euclidean space is written as:

$$S_{YM} = \frac{1}{2g^2} \int d^4x \ \mathrm{tr}\left(F^{\mu\nu}(x) F_{\mu\nu}(x)\right)$$

where $F_{\mu\nu}$ is the field strength tensor:

$$F_{\mu\nu} = \sum_a F^a_{\mu\nu} T^a , \qquad F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g\ f^{abc} A^b_\mu A^c_\nu ,$$

A^a_μ is the gauge field, g the coupling and T^a the generators of the $SU(N_C)$ group.

The Yang-Mills action is invariant under local gauge transformations:

$$\begin{aligned} A_\mu &\to A'_\mu = \Omega_x A_\mu(x) \Omega^\dagger_x + ig \Omega_x \partial_\mu \Omega^\dagger_x , \\ F_{\mu\nu} &\to F'_{\mu\nu}(x) = \Omega_x F_{\mu\nu}(x) \Omega^\dagger_x \end{aligned}$$

where Ω_x is a $SU(N_C)$ group element associated to site x.

Towards a discrete gauge action

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A^a_μ is the gauge field, g the coupling and T^a the generators of the $SU(N_C)$ group.

Gauge invariance

The lattice action **has to** preserve gauge symmetry exactly, i.e., it cannot generate dimension-two terms in the gauge fields such as $A^a_\mu A^b_\nu$.

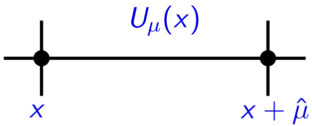
Towards a discrete gauge action

Wilson action

Kenneth Wilson showed in 1974 how to write a discrete action for a gauge group $SU(N_C)$ that is gauge invariant in a lattice using parallel transporters.

The continuum gauge transporter has the form:

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



In a lattice, the the lattice gauge transporter is associated to the link betweeen two neighboring sites x and $x+\hat{\mu}$.

$$U_\mu(x) = \exp(iaA_\mu(x))\,; \qquad A_\mu(x) = \sum_b A^b_\mu(x) T_b$$

where T_b are the $N_C^2 - 1$ generators of the $SU(N_C)$ Lie group.

Towards a discrete gauge action

Wilson action

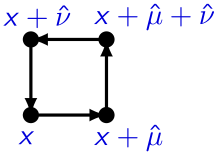
Kenneth Wilson showed in 1974 how to write a discrete action for a gauge group $SU(N_C)$ that is gauge invariant in a lattice using parallel transporters.

The link $U_\mu(x) \in SU(N_C)$ transforms under gauge transformations Ω_x as:

$$U_\mu(x) \quad \rightarrow \quad U'(x) = \Omega_x U_\mu(x) \Omega^\dagger_{x+a\hat{\mu}}$$

Wilson loop: the product of *links* along any closed path is gauge invariant, as $\Omega^\dagger_x = \Omega^{-1}_x$. The smallest **Wilson loop**, termed **plaquette**, is defined by:

$$\Pi_{\mu\nu}(x) = U_\mu(x) U_\nu(x+\hat{\mu}) U^\dagger_\mu(x+\hat{\nu}) U^\dagger_\nu(x)$$



Towards a discrete gauge action

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The plaquette $\Pi_{\mu\nu}(x)$ behaves for $a \to 0$ as:

$$Tr\left[\Pi_{\mu\nu}(x)\right] \approx N_C + \frac{a^4}{2} Tr\left[F_{\mu\nu}F^{\mu\nu}\right] + \mathcal{O}(a^5)$$

Homework

Show this limit by using the Campbell-Baker-Hausdorff formula ($e^X e^Y \approx e^{X+Y+\frac{1}{2}[X,Y]}$) and $A_\mu(x + a\hat{\mu}) = A_\mu(x) + a\Delta_\mu A_\nu(x)$...

Towards a discrete gauge action

Wilson action

Kenneth Wilson showed in 1974 how to write a discrete action for a gauge group $SU(N_C)$ that is gauge invariant in a lattice using parallel transporters.

From the plaquette, the Wilson gauge action is defined as:

$$S_W = \frac{\beta}{2N_C} \sum_x \sum_{\mu<\nu} \mathrm{Re}\,\mathrm{Tr}\left(1 - \Pi_{\mu\nu}(x)\right)$$

where for $SU(3)$, $\beta = 6/g_0^2$ to match the continuum action in the $a \to 0$ limit.

Improved versions of the action (in the sense of smaller lattice errors) can be constructed including larger Wilson loops (Symanzik's improvement).

Outline

3 Gauge fields
- Yang-Mills action: gauge invariance
- Parallel transporters & Wilson action

4 Fermion fields
- Grasmann variables
- Naive fermions: doublers
- Nielsen-Ninomiya theorem
- Chiral fermions

5 Monte Carlo for lattice-QCD
- Updating the gauge fields
- Hybrid Monte Carlo
- Topology

Fermions...

Quark fields are **Grasmann** variables (anticommute) and therefore cannot be described by numbers!

Instead, we will use the fact that the fermion action is a bilinear in the fermion fields:

$$S_{\text{fermionic}} = \int d^4x \; \mathcal{L}(\overline{\psi}, \psi) \to \sum_{xy} \sum_{\alpha\beta} \overline{\psi}_x^{\alpha} D_{xy}^{\alpha\beta} \psi_y^{\beta} \equiv \overline{\psi} D \psi$$

to integrate out the fermion field variables formally as:

$$\int [d\psi d\bar{\psi}] e^{-\overline{\psi} D\psi} = det(D)\,, \qquad \int [d\psi d\bar{\psi}] \psi_x \overline{\psi}_y e^{-\overline{\psi} D\psi} = D_{xy}^{-1} det(D)\,,$$

and so on.

Fermions...

Quark fields are **Grasmann** variables (anticommute) and therefore cannot be described by numbers!

For example, quark propagator will be given by:

$$\langle \psi_x \overline{\psi}_y \rangle = \frac{1}{Z} \int [dU][d\psi d\bar{\psi}] \psi_x \overline{\psi}_y e^{-S_{\text{gauge}} - \overline{\psi} D \psi} = \frac{\int [dU] D^{-1}_{xy} det(D) e^{-S_{gauge}}}{\int [dU] det(D) e^{-S_{gauge}}}$$

Quenched approximation amounts to set $det(D) = 1$ and the dynamical effect of fermion loops in the path integral is neglected...

Discretizing the fermionic action

Including a discrete derivative in the fermionic part of the action:

$$S = \sum_x \overline{\psi}_x \left(\partial_\mu \gamma_\mu + m\right) \psi_x$$

would generate terms like $\overline{\psi}_x \psi_y$, that is not gauge-invariant for $x \neq y$.

In order to build a gauge invariant action, we need to introduce a parallel transporter field $U_\mu(x)$ so that quark bilinears are gauge invariant written as:

$$\overline{\psi}_x \prod_{z \in \mathcal{C}_{xy}} U_\mu(z)\, \psi_y$$

where $\mathcal{C}_{xy}$ is a path that connects x to y. [Covariant derivative in the continuum]

Naive fermion discretization

The simplest discretization for the quark sector originates from a using a discrete derivative such as in the gluon sector:

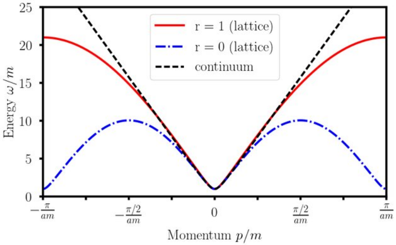
$$S_{\rm latt} = a^4 \sum_x \overline{\psi}_x \left(\gamma_\mu \frac{U_\mu(x)\Delta_\mu + \Delta^*_\mu U_\mu(x)^\dagger}{2} + m \right) \psi_x = a^4 \sum_{x,y} \overline{\psi}_x \, D_{xy} \, \psi_y$$

With this discrete action, the free quark propagator in momentum-space $S = D^{-1}$ results:

$$S_p = \frac{1}{i \sum_\mu \gamma_\mu \frac{1}{a} \sin(a p_\mu) + m}$$

which has poles not only for momenta $p = (0, 0, 0, 0)$, but also for $(\frac{\pi}{a}, 0, 0, 0)$, $(\frac{\pi}{a}, \frac{\pi}{a}, 0, 0)$, $(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}, 0)$, $(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a})$ and pp. In total there are **16 poles** termed doublers.

$|S^{-1}|$



Doublers and chirallity

The $m \to 0$ limit of QCD is invariant under

$$\psi \to e^{i\phi\gamma_5/2}\psi\,; \qquad \overline{\psi} \to \overline{\psi}e^{i\phi\gamma_5/2}$$

i.e.

$$\lim_{m\to 0}\,[D, \gamma_5]_+ = 0$$

The 16 poles that appear with a naive discretization behave as 8 left-handed + 8 right-handed fermions (commute with $P_\pm = \frac{1\pm\gamma_5}{2}$)

Doublers and chirallity

There is a deep connection between doubling problem and chirality!

Nielsen-Ninomiya ‘no-go’ theorem.

The problem of doublers is inherent to any lattice discretization of fermion fields.

No-go

[Nielsen, Ninomiya 1981] demonstrated that it is not possible to write a discrete fermion action that satisfy simultaneously:

- Invariant under space-time traslations.
- Quadratic in the fermionic fields.
- Local.
- Chirally symmetric.

There are different possibilities to overcome the difficulties derived from this theorem.

Wilson discretization

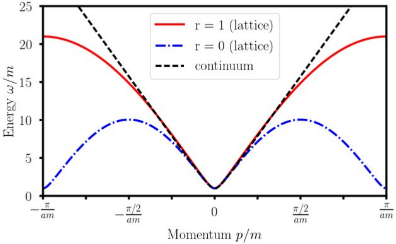
Wilson discretization introduces a term $a\Delta_\mu \Delta^*_\mu$ in the action:

$$S_{\text{latt}} = a^4 \sum_x \overline{\psi}_x \left(\gamma_\mu \frac{U_\mu(x)\Delta_\mu + \Delta^*_\mu U_\mu(x)^\dagger}{2} - r\Delta_\mu \Delta^*_\mu + m \right) \psi_x$$

which vanishes in the continuum limit.

The doublers acquire now a mass $\mathcal{O}(a^{-1})$ and therefore dissapear in the continuum limit:

$$S(p) = \frac{1}{i\sum_\mu \gamma_\mu \frac{1}{a}\sin(ap_\mu) + \frac{r}{a}\sum_\mu (1-\cos(ap_\mu)) + m}$$



Wilson discretization

Up to an irrelevant normalization factor, Wilson-Dirac action can be written as:

$$S_{\text{latt}} = \sum_{x,y} \overline{\psi}_x D_{x,y} \psi_y$$

with

$$D_{x,y} = 1 - \kappa H\,, \quad H = \sum_{\mu=\pm 1}^{\pm 4} (1-\gamma_\mu)\, U_\mu(x)\delta_{x+\hat{\mu},y}\,, \quad \kappa = \frac{1}{2am+8}$$

H and κ are referred to as *hoping* matrix and parameter resp.

Other discretizations

Most of the fermion discretizations use different strategies to tame the doubling problem:

- Staggered fermions (Kogut-Susskind)
- Twisted-mass Wilson fermions.

at the price of more time-consuming calculations.

More sophisticated fermion discretizations overcome the 'no-go' theorem by using the Ginsparg-Wilson relation:

$$[D, \gamma_5]_+ = aD\gamma_5 D \ .$$

The fermion discretizations that satisfy this relation, such as:

- Overlap
- Domain-Wall

have a remanent of the chiral symmetry (Ward-Takahashi identities).

Outline

3 Gauge fields
- Yang-Mills action: gauge invariance
- Parallel transporters & Wilson action

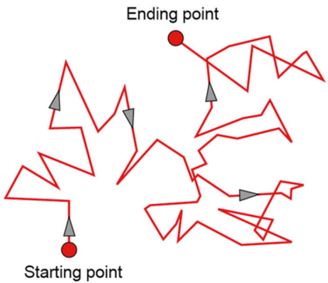
4 Fermion fields
- Grasmann variables
- Naive fermions: doublers
- Nielsen-Ninomiya theorem
- Chiral fermions

5 Monte Carlo for lattice-QCD
- Updating the gauge fields
- Hybrid Monte Carlo
- Topology

Quenched approximation

An update of the gauge fields (without quarks) can be done as in the scalar case:

- Start with any initial set of $SU(N_C)$ matrices, $\{U_\mu(x)\}$
- For each link x, μ propose a new matrix $U'_\mu(x)$ using
  - Metropolis
  - Heatbath
  - Overrelaxation
  - Microcanonical – Hamiltonian (U-Π)
  - ...
- Measure every n global updates (to avoid autocorrelation issues)



Grassmann variables

The path integral

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int [dUd\psi d\bar{\psi}] \mathcal{O}(U, \psi, \bar{\psi}) e^{-S(U,\psi,\bar{\psi})} \to \frac{1}{N} \sum_{i=1}^{N} O_i$$

is done in a Monte Carlo but while gauge fields are associated to links, quark fields anticommute, and cannot therefore be described by numbers!

Grassmann variables

The path integral

$$\langle \mathcal{O} \rangle \;=\; \frac{1}{Z}\int [dUd\psi d\bar{\psi}]\mathcal{O}(U,\psi,\bar{\psi})e^{-S(U,\psi,\bar{\psi})} \rightarrow \frac{1}{N}\sum_{i=1}^{N} O_i$$

is done in a Monte Carlo but while gauge fields are associated to links, quark fields anticommute, and cannot therefore be described by numbers!

Fermionic Gaussian integrals $\int [d\psi][d\bar{\psi}]e^{-\bar{\psi}D\psi} = det(D)$ imply that for each quark flavour:

$$\langle \mathcal{O} \rangle \;=\; \frac{1}{Z}\int [dU]\mathcal{O}(U,\psi,\bar{\psi})e^{-S_G(U)}det(D)$$

Hybrid Monte Carlo

Introducing the fermion determinant would imply that for any update of the gauge fields $\{U\} \to \{U'\}$, one has to evaluate $\det D[U]$ and $\det D[U']$, with the acceptance rate:

$$P \propto \frac{\det D[U']}{\det D[U]}$$

something that is computationally costly and very inefficient.

Instead, one can introduce a complex scalar field ϕ (termed *pseudo-fermion*), and write the Boltzmann weight factor as:

$$e^{-S_G} \det D = \int [d\phi^\dagger][d\phi] e^{-S_G + \phi^\dagger D^{-1} \phi}$$

with ϕ a bosonic (pseudo-fermion) field.

The effective action S_{eff}

$$e^{-S_G} \det D = e^{-S_{\text{eff}}}, \qquad S_{\text{eff}} = S_G - \log \det D$$

is real only if $\det D$ is positive.

- For a single quark flavour, we need a formulation with $\det D \geq 0$ to avoid sign problems!
- For a pair of degenerate quarks, $\det D_u \det D_d = (\det D)^2 \geq 0$

For $N_F = 2$, as $detD = \det D^\dagger$,

$$e^{-S_G} \det D^2 = \int [d\phi^\dagger][d\phi] e^{-S_G - \phi^\dagger (D^\dagger D)^{-1} \phi}$$

and

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int [dU d\phi^\dagger d\phi] \mathcal{O}(U, \psi, \bar{\psi}) e^{-S_G(U) - \phi^\dagger (D^\dagger D)^{-1} \phi}$$

Hybrid Monte Carlo

The effective action becomes non-local in this case!

$$S_{eff} = S_G + \phi^\dagger (D^\dagger D)^{-1} \phi$$

$(D^\dagger D)^{-1}$ is non-local, thus making the update process of the gauge link variables $\{U_\mu(x)\}$ and pseudo-fermion fields $\phi(x)$ computationally costly.

The acceptance for the Metropolis update process with this non-local action is negligible except for infinitesimal updates. A different approach is required.

Hybrid Monte Carlo

Hybrid Monte Carlo

For a scalar field, $S(\varphi)$ we can introduce an artificial Hamiltonian $\mathcal{H} = \frac{1}{2}\sum \Theta^2 + S(\varphi)$ with Θ the conjugate variable of φ. Then:

$$\langle O \rangle_\varphi = \frac{\int [d\varphi] O(\varphi) e^{-S}}{\int [d\varphi] e^{-S}} = \frac{\int [d\varphi][d\Theta] O(\varphi) e^{-\mathcal{H}}}{\int [d\varphi][d\Theta] e^{-\mathcal{H}}} = \langle O \rangle_{\varphi,\Theta}$$

as the Gaussian integral in Θ factors out.

Hybrid algorithms proceed in the following way:

- Choose some random conjugate momenta Θ with $P(\Theta) = e^{-\Theta^2/2}$
- Integrate the Hamilton's EOM for Θ, φ (microcanonical).
- Accept or reject the update with $P = min\left(1, e^{-\Delta\mathcal{H}}\right)$.

Hybrid Monte Carlo

Molecular Dynamics evolution is given by:

$$\frac{d\varphi}{d\tau} = \Theta\,, \quad \frac{d\Theta}{d\tau} = -\frac{d\mathcal{H}}{d\varphi} = -\frac{dS}{d\varphi}\,;$$

the artificial evolution-time variable τ is called the trajectory length.

With an exact integration scheme $\Delta H = 0$ and the acceptance of the update process

$$P = min\left(1, e^{-\Delta\mathcal{H}}\right) \to 1\,.$$

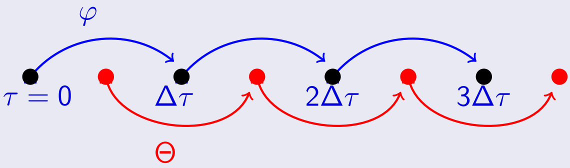
It can be shown that the update process satisfies *detailed balance*, and thus generates a Markov chain for φ.

Hybrid Monte Carlo

The equations of motion for this Hamiltonian can be integrated in discrete steps $\Delta\tau$ using a symplectic, reversible integrator (leapfrog).

Leapfrog integration:

Initial half-step: $\Theta_{\frac{\Delta\tau}{2}} = \Theta_0 - \left.\frac{dS}{d\varphi}\right|_0 \frac{\Delta\tau}{2}$



$$\begin{aligned} \varphi_\tau &= \varphi_{\tau-\Delta\tau} + \Theta_{\tau-\frac{\Delta\tau}{2}} \Delta\tau \\ \Theta_{\tau+\frac{\Delta\tau}{2}} &= \Theta_{\tau-\frac{\Delta\tau}{2}} - \left.\frac{dS}{d\varphi}\right|_\tau \Delta\tau \end{aligned}$$

Leapfrog integration has errors $O(\Delta\tau^3)$, for each step, allowing a high acceptance rate, which is controlled by the value of $\Delta\tau$.

Hybrid Monte Carlo for QCD

Introducing conjugate momenta P (for U) and π (for ϕ), one can write a Hamiltonian:

$$\mathcal{H}[P,\pi,U,\phi] = \frac{1}{2}\sum P^2 + \frac{1}{2}\sum \pi^\dagger \pi + S[U,\phi]$$

where the action S plays the role of a potential and

$$\frac{dP}{d\tau} = -\frac{dS}{dU}\,, \quad \frac{dU}{d\tau} = P\,; \quad \frac{d\pi}{d\tau} = -\frac{dS}{d\phi}\,, \quad \frac{d\phi}{d\tau} = \pi \quad .$$

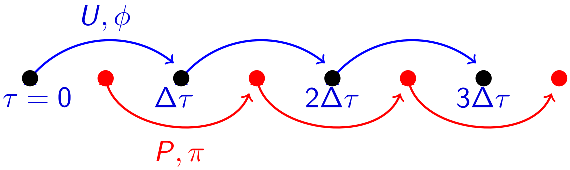
The process requires inverting $DD^\dagger$ at each step and computing D-derivatives, which make the whole process rather time-consuming...

Hybrid Monte Carlo Algorithm

The HMC pseudo-algorithm for QCD would be:

- **Init**: start with Gaussian fields χ and P. Compute $\phi = D\chi$ and integrate first half-step.
- **Integrate** the molecular dynamics trajectory (leapfrog).
- **Acceptance**: accept the update with probability $P = min\left(1, e^{-\Delta\mathcal{H}}\right)$.

Each one of these steps forms a *trajectory*. Each **trajectory** is determined by the initial set $\{\chi, P\}$ (ergodicity requires many trajectories...).



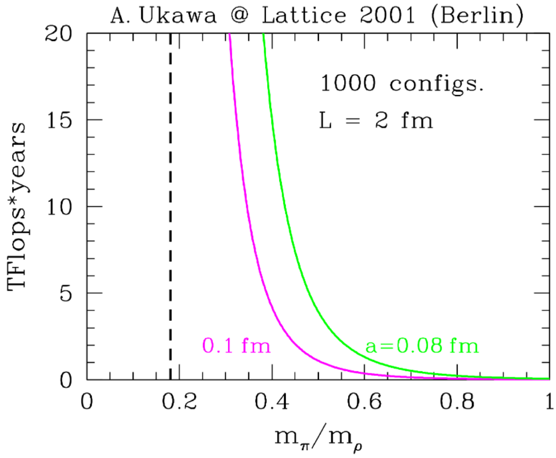
Berlin Wall Plot

The cost of unquenched lattice simulations grows when approaching continuum limit and physical point due to:

- Dirac matrix condition number increases as $m_q \to 0$ (larger times for inversion).
- Autocorrelation times increase.
- Step-size $\Delta\tau$ has to be reduced to maintain constant acceptance rates.

$$\text{Cost} \propto \left(\frac{m_\pi}{m_\rho}\right)^6 \cdot L^5 \cdot a^{-7}$$

making the physical point impossible to reach.



Strategies to tame the "Berlin Wall problem"

- Preconditioning with multiple time-scale integrations [Hasenbusch, 2001]

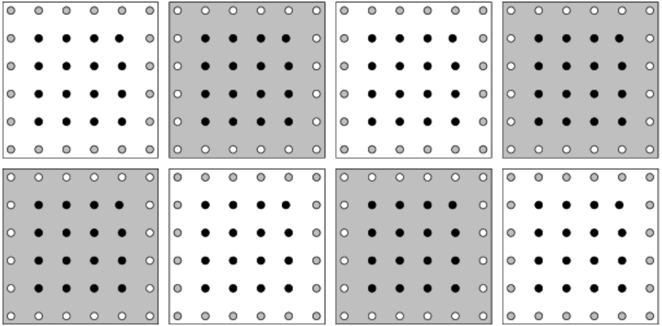
$$\det D^2 = \frac{\det D^2}{\det(D^2+\rho^2)} \cdot \det(D^2+\rho^2) \quad \rightarrow \quad S_{\text{eff}} = \underbrace{\psi^\dagger \frac{1}{D^2+\rho^2}\psi}_{\text{small } \Delta\tau} + \underbrace{\phi^\dagger \frac{D^2+\rho^2}{D^2}\phi}_{\text{large } \Delta\tau}$$

  Smaller forces in MD, separation of scales, compatible with other preconditioners (such as even-odd)...

- Deflated multi-grid solvers [Lüscher, 2007]

Strategies to tame the "Berlin Wall problem"

- Preconditioning with multiple time-scale integrations [Hasenbusch, 2001]
- Deflated multi-grid solvers [Lüscher, 2007]



Approximate the inverse D^{-1} in terms of its lowest eigenvectors, and use it as a preconditioner.

The axial anomaly

The axial singlet current $j^{5\mu} = \overline{\psi}\gamma_\mu\gamma_5\psi$ is conserved by in a massless Dirac Lagrangian,

$$\partial_\mu j^{5\mu} = 2im\overline{\psi}\gamma_5\psi$$

but the gauge symmetry implies the appearance of an anomalous term:

$$\partial_\mu j^{5\mu} = -\frac{g^2 N_F}{16\pi^2}\widetilde{F}_a^{\mu\nu}F_a^{\mu\nu}\,, \qquad \widetilde{F}_a^{\mu\nu} = \epsilon_{\mu\nu\rho\sigma}F_a^{\rho\sigma}$$

Gauge field configurations with $\langle\widetilde{F}_a^{\mu\nu}F_a^{\mu\nu}\rangle \neq 0$ produce an anomalous divergence of the axial current.

$\eta - \eta'$ puzzle

The axial anomaly is responsible for the mass difference between η and η' mesons.

Topology and zero modes

The anomalous term can be written as total divergence:

$$-\frac{N_F}{16\pi^2}\widetilde{F}^a_{\mu\nu}F^{\mu\nu}_a = \partial_\mu K^\mu$$

whose integral over the whole space vanishes except for topologically non-trivial configurations:

$$Q = \frac{1}{64\pi^2}\int d^4x\ \widetilde{F}^{\mu\nu}_a F^{\mu\nu}_a$$

Dirac zero modes $D\psi = 0$ can be chosen with defined chirality. Let us call the number of fermion zero modes with right n_+ and left n_-.

The **Atiyah–Singer Index Theorem** relates Q to the number of zero modes through:

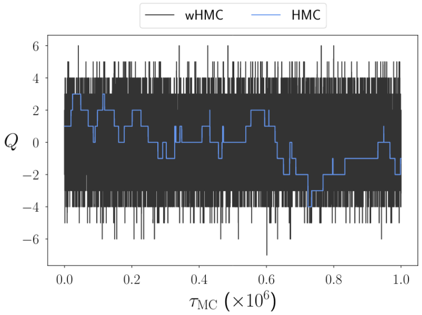
$$Q = n_+ - n_-$$

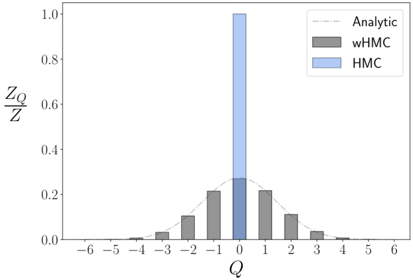
Topological freezing

Different topological sectors are difficult to sample in lattice-QCD calculations.

Topological freezing

Topological charge is difficult to sample correctly with HMC.





D. Albandea *et al.* 2111.05745

Some strategies to overcome this difficulty: open boundary conditions [Schaefer, 2011], or modified HMC through windings [Albandea, 2021].

$N_f = 0, 2, 2+1, 2+1+1, \cdots$

Lattice-QCD simulations can be done at different number of *dynamical* fermions:

$N_F = 0$: without dynamical quarks, the action is driven by the gauge sector solely [quenched lattice QCD]

$N_F = 2$: typical situation with degenerate u and d quarks. For years the challenge was to achieve physical pion masses.

$N_F = 2+1$: including s quark requires some modifications of the HMC algorithm.

$N_F = 2+1+1$: the dynamical role of c quark is small but sizable.

Price motivates collaboration

Fine lattices with realistic pion masses are possible, but expensive. It is done by large collaborations such as BMW, ETMC, MILC, UKQCD, RBC, HPQCD, ALPHA, ...

Open lattice-QCD collaborations

The prize of large-scale simulations close both to the physical pion mass and continuum limit has triggered the appearance of international collaborations such as

OPEN LATtice iniciative

Effort for the production and sharing of dynamical gauge field ensembles (2+1 flavour QCD gauge field ensembles produced with the stabilised Wilson fermion action) to study physical phenomena of the strong interaction.

OPEN LATtice initiative

ILDG

The International Lattice Data Grid (ILDG) was born with the aim of making the basic data sets from Lattice QCD simulations available to the international scientific community using defined standardized metadata and data formats.

Spanish lattice-QCD collaboration: latticeNET

Red Española de Lattice Gauge Theory: latticeNET

U. Zaragoza, Granada, Pablo de Olavide, Barcelona, Valencia, Autónoma de Madrid, IFIC, IFCA, IFT, . . .

Organized:

- Latticenet Meeting Jan. 2022 Zaragoza University.
- First LatticeNET workshop on challenges in Lattice field theory 2022, Sep 11 – Sep 17.
- LatticeNET School on Computing in HEP Exascale 2022, Sep 18 – Sep 24.
- . . .

Born in 2020 funded by the Ministry of Science and Innovation, has been renewed for two years (until 2024).

Take-away message: lattice QCD formulation.

Lattice QCD action:

- Gauge action (parallel transporters): plaquete, clover... Improvement program *a la* Symanzik
- Quark action much more involved, specially in the chiral limit.
- Preventing doublers introduce $\mathcal{O}(a)$ artifacts.
- Chiral fermions are much more expensive!

Monte Carlo:

- Dynamical simulations (non-local updates) done by Hybrid Monte Carlo.
- Key improvements (preconditioning) allow physical pion masses.
- Topology hard to sample correctly.
- Expensive MC runs.

Lattice QCD: an introduction

Phenomenology from lattice-QCD.

Outline

6. Fundamental physics from lattice-QCD
   - The static quark potential
   - Hadron spectrum
   - Strong coupling α_s
   - Muon $(g-2)$

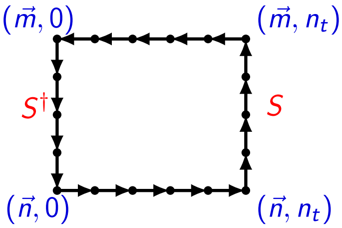
7. Hadron structure
   - The spectrum: decay constants
   - Scattering states: phase shifts
   - EM form factors, PDFs, GPDs,...

8. The phase diagram of QCD
   - Columbia plot
   - Finite temperature in the lattice
   - Finite μ in the lattice

Wilson loops

Wilson loop (gauge invariant)

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



In temporal gauge ($A_4 = 0$),

$$\langle L\rangle \;=\; \langle L\rangle_{\text{temp}} = \langle\, Tr\left(S(\vec{n},\vec{m},n_t)S^\dagger(\vec{n},\vec{m},0)\right)\rangle$$

and inserting a complete set of states,

$$\langle L\rangle \;=\; \sum_k \langle 0|S(\vec{n},\vec{m},0)|k\rangle e^{-n_t E_k}\langle k|S^\dagger(\vec{n},\vec{m},0)\rangle \sim e^{-n_t E_1}$$

with E_1 the energy of a static quark-antiquark pair placed at positions $\vec{n}$ and $\vec{m}$.

Wilson loops

Indeed, a Wilson line, $S(\vec{n}, \vec{m}, 0)$, corresponds to the infinite-mass limit of quark propagator. In the infinite mass limit ($\kappa \to 0$), the inverse of the Dirac operator

$$D_{x,y} = 1 - \kappa H \,, \quad H = \sum_{\mu=\pm 1}^{\pm 4} (1 - \gamma_\mu)\, U_\mu(x) \delta_{x+\hat{\mu},y} \,, \quad \kappa = \frac{1}{2am + 8}$$

is dominated by the shortest line among two sites, the Wilson line!

$$\lim_{\kappa \to 0} D^{-1}(\vec{n}, \vec{m}, 0) \sim \prod_{p,\mu \in \mathcal{C}} U_\mu(p) \sim S(\vec{n}, \vec{m}, 0)$$

where $\mathcal{C}$ is the shortest path that connects $(\vec{n}, 0)$ and $(\vec{m}, 0)$.

Thus, for Wilson loops:

$$\langle L(\vec{n}, \vec{m}) \rangle \sim e^{-a n_t V(\vec{n}-\vec{m})}$$

allows to obtain the static quark potential $V(r)$.

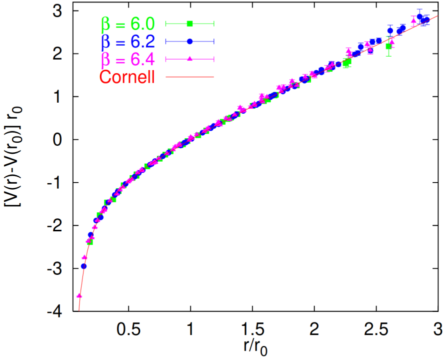
The potential shows a linearly rising behavior for large distances with $\sigma \approx (0.4\mathrm{GeV})^2$.

Confinement

The existence of a linear term in the inter-quark potential

$$V(r) = \frac{a}{r} + b + \sigma r$$

shows that QCD is a confining theory.



[Gunnar Bali, Phys.Rept. 343 (2001) 1]

Wilson loops

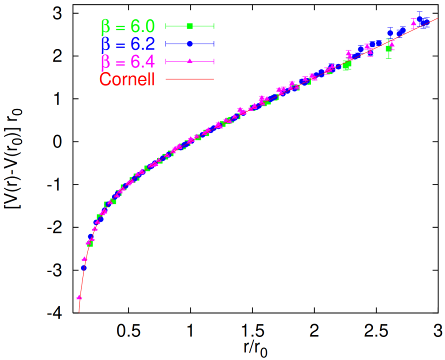
Sommer parameter

The sommer parameter, r_0, is defined by:

$$r^2 \frac{dV}{dr}\bigg|_{r=r_0} = 1.65$$

It allows for a relative calibration of lattice calculations at different β's, but we need to compute a dimensional quantity and compare with Nature to have the value of r_0 ($r_0 \approx 0.5\,\mathrm{fm}$).

Most contemporary callibrations use the Gradient Flow scales t_0 or ω_0 which have smaller uncertainty [M. Lüscher, JHEP 08 (2010) 071].



[Gunnar Bali, Phys.Rept. 343 (2001) 1]

If we build an operator J that satisfies $\langle 0|J|k\rangle \neq 0$ for a set of states $|k\rangle$,

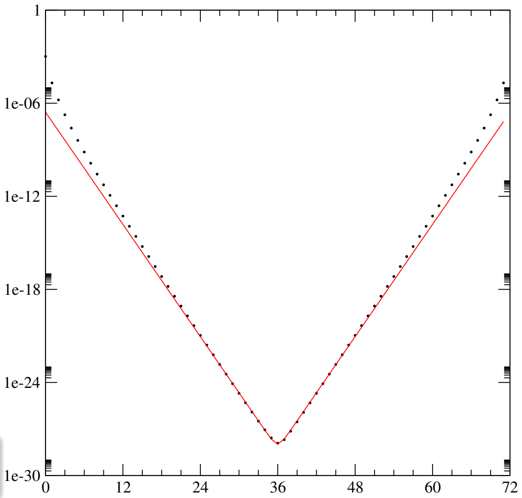
$$\langle J(n_t) J^\dagger(0)\rangle \quad = \quad \sum_k \langle 0|J|k\rangle e^{-E_k n_t} \langle k|J^\dagger|0\rangle$$

and then:

$$\lim_{n_t \to \infty} \langle J(n_t) J^\dagger(0)\rangle \quad \to \quad c_0 e^{-E_0 n_t}$$

with E_0 the mass of the lowest lying state (in units of a).

Excited states (beyond first exponential) are more difficult to extract...



Interpolating fields

For any hadron we need to search for an interpolating field based in the symmetries of the action, according to the quantum numbers of the state.

For **pions**, for example, we have $J = 0$, negative parity $P = -1$ and isospin $I = 1$, that can be built as:

$$\begin{aligned} J_{\pi^+}(\vec{n}, n_t) &= \overline{d}(\vec{n}, n_t)\, \gamma_5\, u(\vec{n}, n_t) \\ J_{\pi^-}(\vec{n}, n_t) &= \overline{u}(\vec{n}, n_t)\, \gamma_5\, d(\vec{n}, n_t) \end{aligned}$$

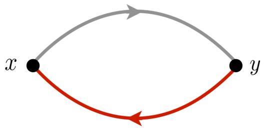
while for π^0 and η they would be:

$$\begin{aligned} J_{\pi^0}(\vec{n}, n_t) &= \frac{1}{\sqrt{2}} \left(\overline{u}(\vec{n}, n_t)\, \gamma_5\, u(\vec{n}, n_t) - \overline{d}(\vec{n}, n_t)\, \gamma_5\, d(\vec{n}, n_t) \right) \\ J_{\eta}(\vec{n}, n_t) &= \frac{1}{\sqrt{2}} \left(\overline{u}(\vec{n}, n_t)\, \gamma_5\, u(\vec{n}, n_t) + \overline{d}(\vec{n}, n_t)\, \gamma_5\, d(\vec{n}, n_t) \right) \end{aligned}$$

Interpolating fields

For charged pions, for example:

$$\begin{aligned} \langle J_\pi(x) J_\pi^\dagger(y)\rangle_{conf} &= \langle (\overline{u}\ \gamma_5\ d)_x\ (\overline{d}\ \gamma_5\ u)_y \rangle_{conf} \\ &= -\mathrm{tr}\left[\gamma_5 S(x,y)_d \gamma_5 S(y,x)_u\right]_{conf} \end{aligned}$$



and

$$\langle J_\pi(x) J_\pi^\dagger(y)\rangle = -\frac{1}{Z}\int [dU] \mathrm{tr}\left[\gamma_5 S(x,y)_d \gamma_5 S(y,x)_u\right] e^{-S_{\mathrm{gauge}}} \prod_{n_f} \det D$$

Then, pion mass is extracted from:

$$\lim_{t\to\infty} \sum_{\vec{x}} \langle J_\pi(x) J_\pi^\dagger(0)\rangle \sim e^{-m_\pi t}$$

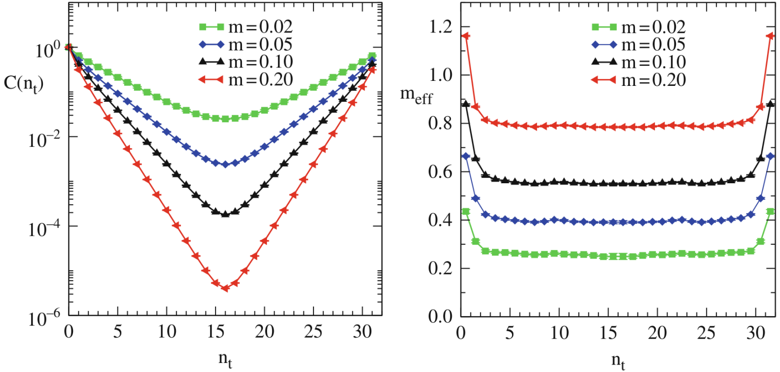
Extracting masses

With

$$C(t) \propto \cosh Mt$$

one can define an effective mass

$$aM_{\rm eff}(t) = \ln \frac{C(t)}{C(t+1)}$$



[Figure from C. Gattringer "Quantum Cromodynamics on the lattice"]

Calibrating the lattice and computing quark masses.

The lattice spacing is determined as:

$$a m_{\mathrm{phys}} = M_{\mathrm{latt}} \quad \to \quad a = \frac{M_{\mathrm{latt}}}{m_{\mathrm{phys}}}$$

for some dimensional parameter m.

If we think in QCD with $N_f = 2+1$ there are three parameters: g_0, m_{ud} and m_s that can be fixed using three measurements from the lattice (Eg. M_p, M_π and $M_K \dots$).

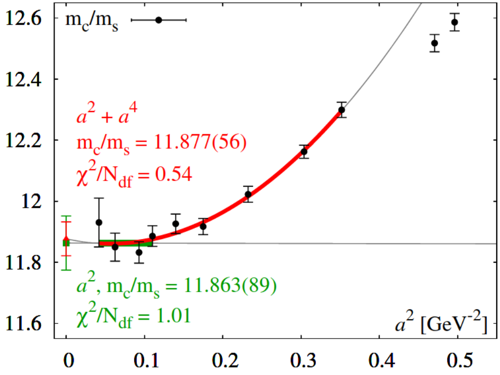
Continuum limit

For any other quantity, the limit $a \to 0$ has to be thoughtfully taken.

Nature is a bit more complicated, and precision measurements require taking into account heavy quark contributions and QED effects.

Continuum limit

Ratio m_c/m_s:



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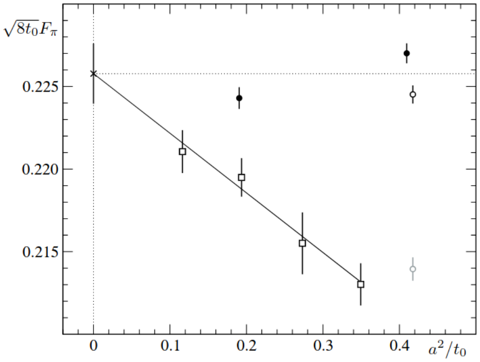
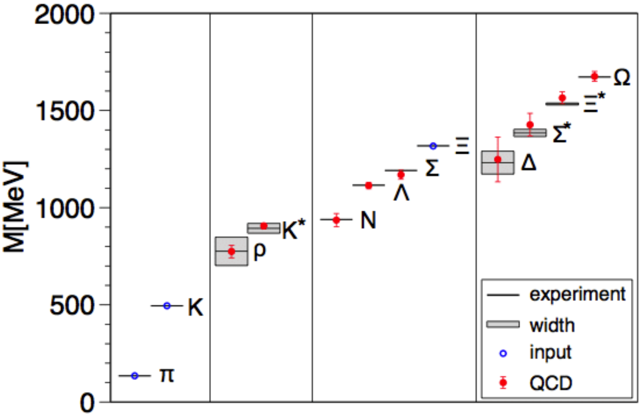
Pion decay constant F_π:



Comparison with improved actions, 1911.04533

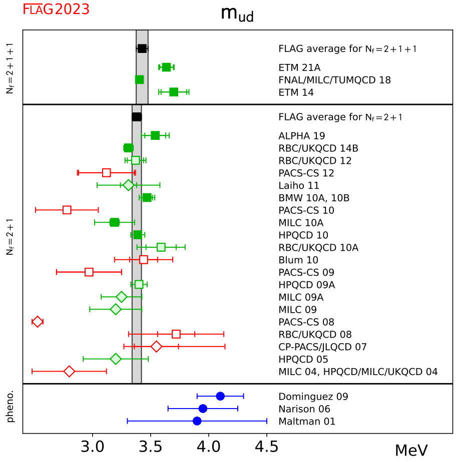
Light hadron spectrum

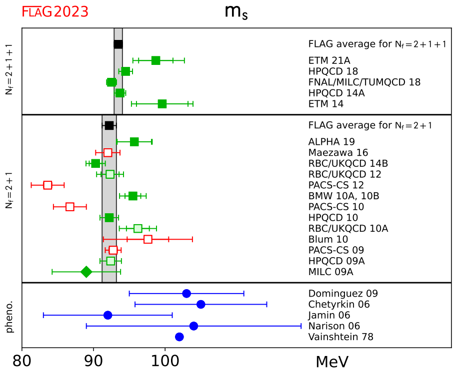


[Figure from S. Dürr et al., Science 322, 1224 (2008)]

Quark masses.

Report on lattice results related to pion, kaon, D-meson, B-meson, and nucleon physics with the aim of making them easily accessible to the nuclear and particle physics communities.

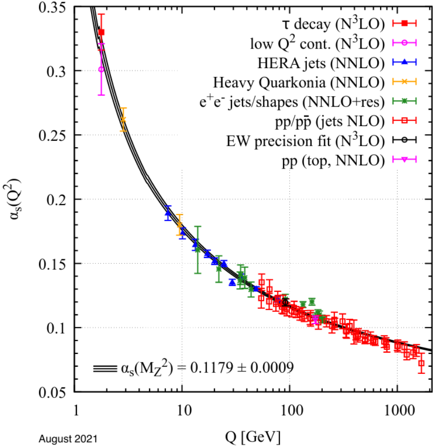




Strong coupling constant

The strong coupling acquires upon renormalization a runnning with the momenta controlled by its RGE:

$$\frac{d\alpha_s}{d\ln\mu} = \beta(\alpha_s)$$



Experimental HEP

The incertitude in α_s has a large impact over the analysis of the experients in colliders. For example, it dominates in the analysis of $H \to gg$ processes

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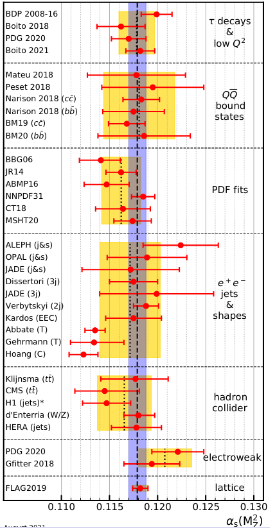


Strong coupling constant

Any observable $\mathcal{Q}(\mu^2)$ can be expanded in terms of α_s as:

$$\mathcal{Q}(\mu^2) = c_1\alpha_s(\mu^2) + c_2\alpha_s^2(\mu^2) + \cdots + \mathcal{NP}$$

both experimental and lattice estimates of $\mathcal{Q}(\mu^2)$ serve to fix $\alpha_s(\mu^2)$ in, for example, $\overline{\mathrm{MS}}$ scheme.

Experimental:

τ-decays, jets, DIS, structure functions... (See PDG)

Lattice:

Wilson loops, Schrodinger Functional method, Static potential, $q\bar{q}$ correlators, vertices, ...

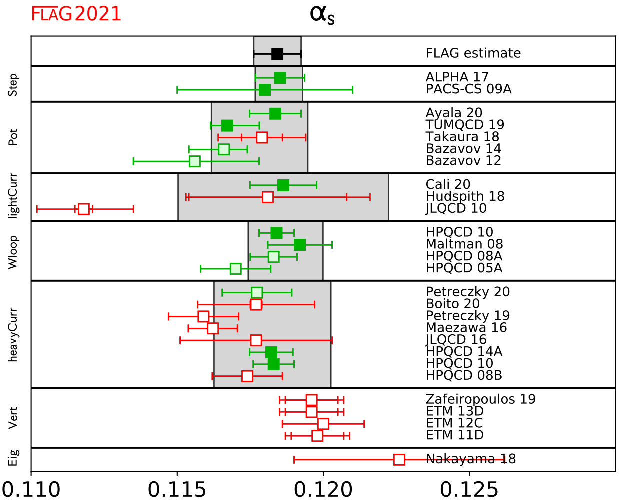
Strong coupling constant: lattice determinations.

Schrödinger Functional methods are specially well suited because they reach very high energies where NP contributions are negligible.

Current lattice + experimental average

$$\alpha_{\overline{\mathrm{MS}}}(m_Z) = 0.1184(8)$$

below 1% uncertainty.



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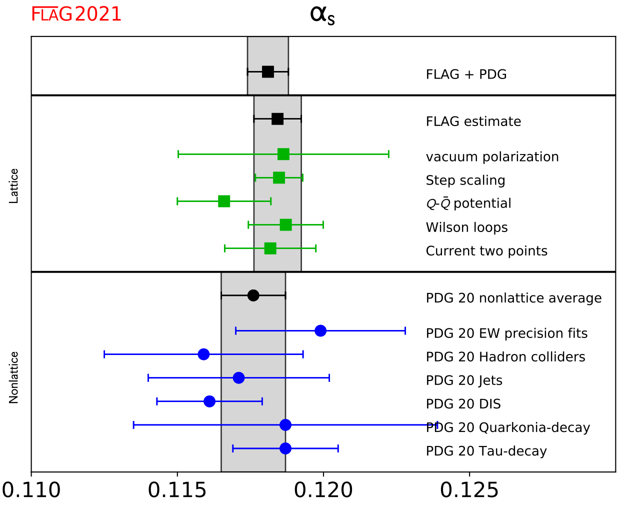


$(g-2)_\mu$

New physics?

Current measurements signal BSM physics in the muon anomalous magnetic moment

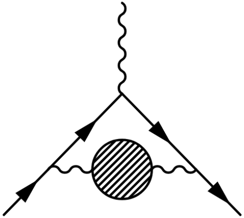
$$a = \frac{g-2}{2}, \qquad a_\mu^{\mathrm{SM}} = a_\mu^{\mathrm{QED}} + a_\mu^{\mathrm{weak}} + a_\mu^{\mathrm{had}}$$

with $\sim 4\sigma$ deviation between the SM result and the experimental one.

The hadronic contribution a_μ^{had} is dominated by the hadronic vacuum polarization

$$a_\mu^{hvp} = \left(\frac{\alpha}{\pi}\right)^2 \int_0^\infty dQ^2 \underbrace{f(Q^2)}_{\text{QED kernel}} \hat{\Pi}(Q^2)$$

with $\hat{\Pi}(Q^2)$ the polarization tensor.



(leading order)
hadronic vacuum polarization

HVP contribution to $(g-2)_\mu$

a_μ^{hvp} is evaluated in the lattice through:

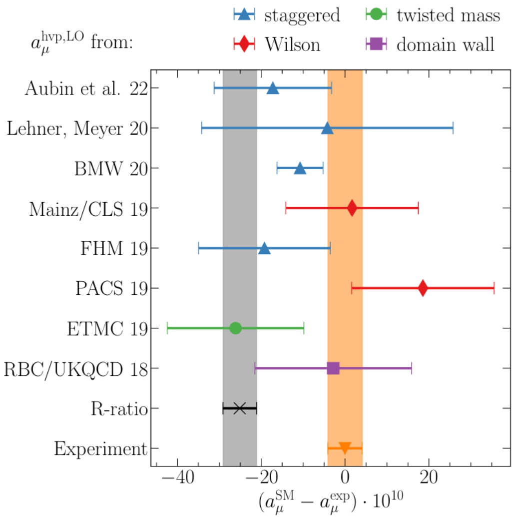
$$a_\mu^{hvp} = \left(\frac{\alpha}{\pi}\right)^2 \int_0^\infty dt \underbrace{\widetilde{K}(t)}_{\text{QED kernel}} G(t)$$

$$G(t) = -\frac{a^3}{3} \sum_{\vec{x}} \langle \vec{j}(\vec{x}, t) \cdot \vec{j}(\vec{0}, 0) \rangle$$

with the electromagnetic current:

$$j_\mu = \sum_f Q_f \bar{\psi}_f \gamma_\mu \psi_f$$

or evaluated using the R-ratio.



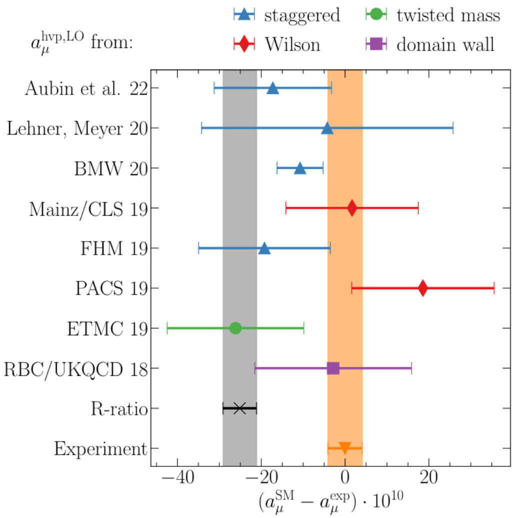
HVP contribution to $(g-2)_\mu$

The R-ratio determination uses

$$R(s) = \frac{\sigma_0(e^+e^- \to \text{hadrons})}{\sigma(e^+e^- \to \mu^+\mu^-)}$$

with center of mass energy $\sqrt{s}$ to compute a_μ^{hvp} as:

$$a_\mu^{hvp} = \frac{\alpha^2}{3\pi^2} \int_{m_\pi^2}^{\infty} ds \frac{K(s)R(s)}{s}$$

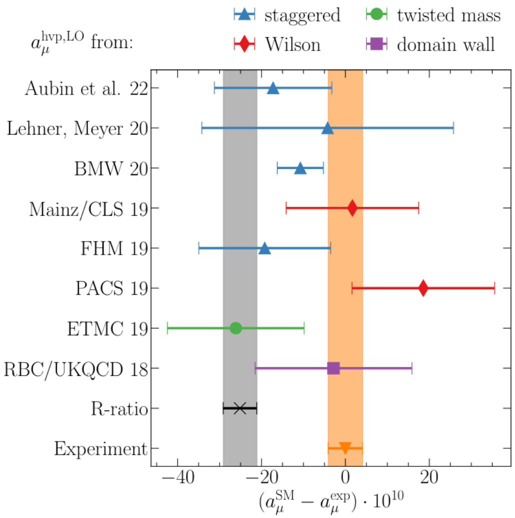


HVP contribution to $(g-2)_\mu$

Work to be done for a significant reduction of the dominant uncertainties:

- light ($u-d$) contributions (large-t behavior, ...).
- Finite-volume effects.
- Disconnected contributions.
- Isospin breaking terms.
- Continuum $a \to 0$ extrapolations.
- Scale setting.
- ...

See Kuberski's@lattice2023



Outline

6. Fundamental physics from lattice-QCD
   - The static quark potential
   - Hadron spectrum
   - Strong coupling α_s
   - Muon $(g-2)$

7. Hadron structure
   - The spectrum: decay constants
   - Scattering states: phase shifts
   - EM form factors, PDFs, GPDs,...

8. The phase diagram of QCD
   - Columbia plot
   - Finite temperature in the lattice
   - Finite μ in the lattice

Pion decay constant

Consider a flavor doublet $\psi = (u, d)$ ($N_F = 2$) and the flavor nonsinglet axial vector current:

$$A^a_\mu = \frac{1}{2}\overline{\psi}\gamma_\mu\gamma_5\tau^a\psi$$

and pseudoscalar interpolator:

$$P^a = \frac{1}{2}\overline{\psi}\gamma_5\tau^a\psi \ .$$

$\partial_\mu A^a_\mu$ has the same quantum numbers, and thus it works as an interpolating field for π.

F_Π

The $\pi \to e\nu_e$ decay constant F_π is given by

$$\langle 0|\partial_\mu A^a_\mu|\pi^b(\vec{p}=0)\rangle = \delta^{ab} M_\pi^2 F_\pi e^{-M_\pi t}$$

(with $F_\pi^{exp} = 92.4(3)\mathrm{MeV}$).

Pion decay constant

PCAC

The partial conservation of the axial current leads to the relation:

$$\langle \partial_0 A^a_\mu(x) P^a(0) \rangle = -2m_f \langle P^a(x) P^a(0) \rangle$$

with m_f the unrenormalized quark mass, known as the PCAC mass.

AWI

The Axial Ward identity allows to relate F_π, quark masses and the condensate through the Gell–Mann–Oakes–Renner (GMOR) relation:

$$F_\pi^2 M_\pi^2 = -m \langle \overline{u} u + \overline{d} d \rangle$$

Phase-shifts

Resonances...

We have seen how to obtain masses for asymptotic states. What about excited states, resonances, scattering, etc?

Phase-shifts

Resonances...

We have seen how to obtain masses for asymptotic states. What about excited states, resonances, scattering, etc?

Excited states are already hard to extract because

$$\sum_{\vec{x}} \langle J(x) J^\dagger(0) \rangle \sim c_0 e^{-E_0 t} + c_1 e^{-E_1 t} + c_2 e^{-E_2 t} + \cdots$$

- Ground state dominates for large-t.
- Excited states only accesible at small-t.
- Fits with several exponentials usually unstable.
- Using several interpolators and diagonalize...

Phase-shifts

Resonances...

We have seen how to obtain masses for asymptotic states. What about excited states, resonances, scattering, etc?

Scattering parameters are only accessible in the lattice as finite-volume effects (Luscher formalism) that establishes a relation between the finite-volume energy and the Low Energy parameters.

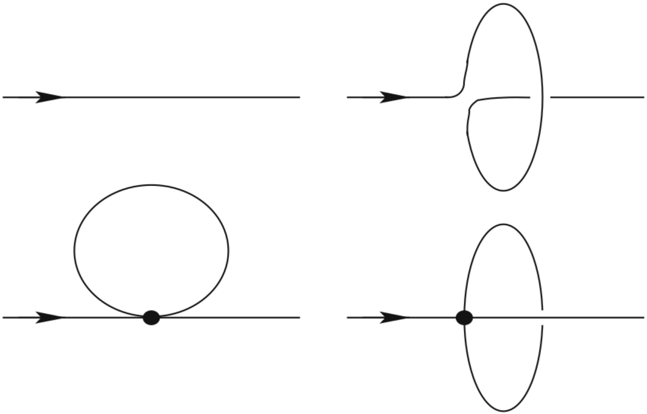
Finite volume effects:

- For stable particles are exponentially small $m - m(L) \sim e^{-mL}$.
- For scattering states there is a polynomial suppression $O(1/L^3)$.

Lüscher Nucl. Phys. B 354, 531 (1991) & Nucl. Phys. B 364, 237 (1991).

Lüscher mechanism

In a lattice with a finite spatial volume (assume periodic boundary conditions), particles can propagate across the borders:

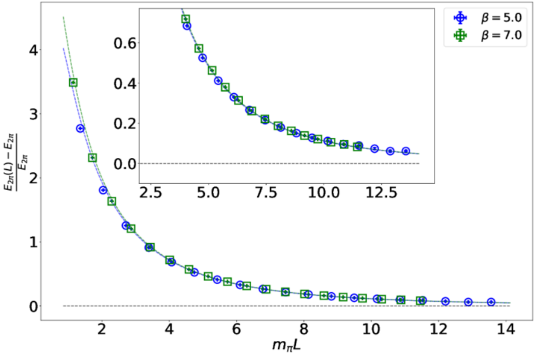


Lüscher mechanism

The ground-state energy for a pair of pions keeping just the s-wave scattering length a_0 contribution has the form:

$$W \approx 2M_\pi - \frac{4\pi a_0}{ML^3}\left(1 + c_1\frac{a_0}{L} + c_2\left(\frac{a_0}{L}\right)^2 + \cdots\right)$$

where the coefficients c_1 and c_2 are related to the lattice shape and generalized zeta function.

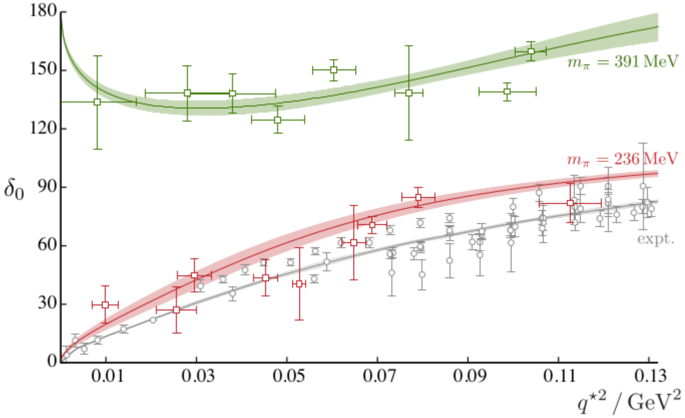


P. Bühlmann and U. Wenger. PoS 396 (2022).

Phase-shifts

The most widely studied cases are $\pi - \pi$ scattering in the p-wave $I = 1$ channel (ρ) or the $I = 0$ s-wave (σ).

The $I = 0$ s-wave channel has been very challenging because it implies *disconnected contributions*, and shows that the nature of the σ strongly depends on the pion mass, being a bound state for large pion masses.



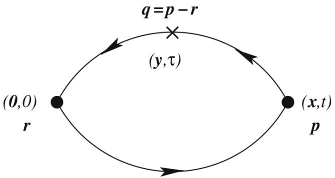
[Figure from R. Briceño *et al* 1706.06223]

EM form-factors

Electromagnetic form factors F can be evaluated from the matrix elements such as:

$$\langle \pi(p_f)|V_\mu|\pi(p_i)\rangle = (p_i + p_f)_\mu F^\pi(Q)$$

with $V_\mu = \sum_f Q_f \overline{\psi}\gamma_\mu\psi$ and $Q^2 = (p_i + p_f)^2$ the momentum transfer.

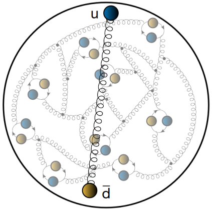


Pion mean charge radius can be extracted from its low-Q^2 behavior:

$$F^\pi(Q^2) = 1 - \frac{1}{6}\langle r^2\rangle Q^2 + \mathcal{O}(Q^4) \ .$$

Parton distribution functions

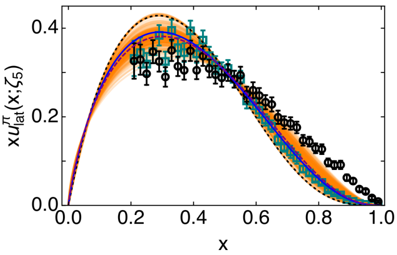
Deep inelastic scattering allows to gather information on the the internal structure of hadrons, such as their momentum distributions $q(x)$.



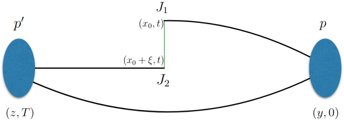
In the lattice, we cannot access the light-cone correlation functions, so one use their operator product expansion and evaluates their Mellin moments:

$$\langle x^n \rangle = \int dx \; x^n q(x)$$

2201.00884



- From Mellin moments one has to reconstruct $q(x)$.
- Pseudo-PDF from the lattice...



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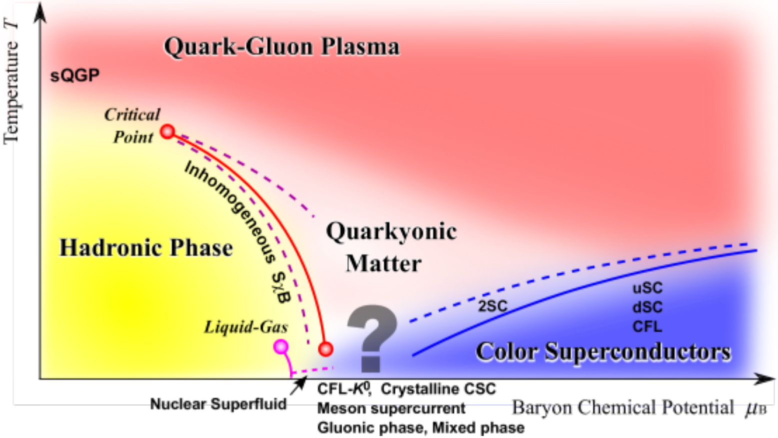
Exploring the phase diagram of QCD

The phase diagram of QCD is represented in the Columbia plot:

- At $T = 0$ there are both χSB and confinement (hadronic phase).
- Current studies at physical quark masses suggest a continuous crossover at low chemical potential up to a Critical Endpoint, being first order at larger μ's.



Finite T in the lattice

Quantum statistics' partition function $Z = tr\left(e^{-\hat{H}/T}\right)$ vs Euclidean evolution operator $e^{-\hat{H}t}$.

Finite T

The time extent of the lattice $\beta = N_t a$ plays the role of the inverse temperature.

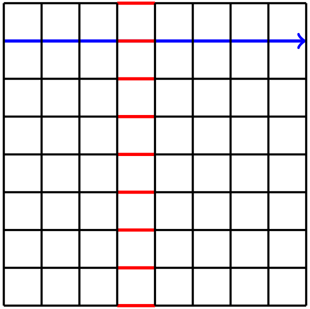
$$T = \frac{1}{\beta}$$

Finite T is obtained with a smaller lattice extent in the time-direction, typically with a smaller number of lattice points $N_t \ll N$. In Fourier-space, only energy levels multiple of $\Delta = 2\pi/\beta$ (**Matsubara frequencies**) are allowed.

Finite T in the lattice: Polyakov loop

Polyakov loop (or thermal Wilson line) is a Wilson loop closed along the T-direction boundary:

$$P = \mathrm{tr}\left[\prod_{j=0}^{N_T-1} U_4(\vec{m}, j)\right] \,, \qquad \langle P \rangle \sim e^{-F_q/T}$$

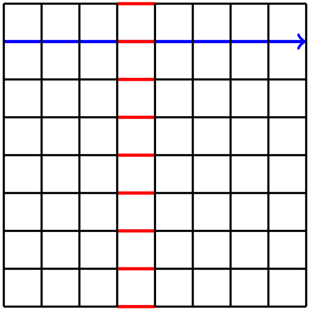


Center symmetry

Pure Yang-Mills in a finite lattice with PBC is invariant under a center symmetry, i.e., if all links in a given time-slice are multiplied by the elements of the SU(3) center symmetry z:

$$z = \left\{1, e^{2\pi i/3}, e^{-2\pi i/3}\right\}$$

Finite T in the lattice: Polyakov loop



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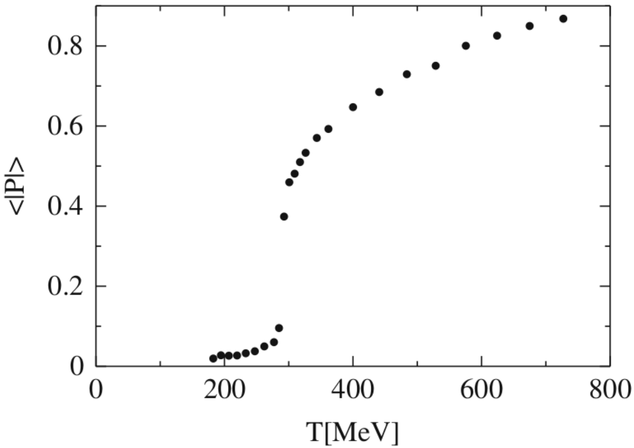
Order parameter

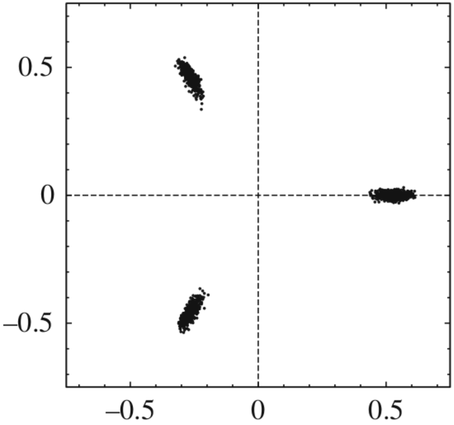
The deconfinement transition can be characterized in terms of the Polyakov loop:

- $\langle |P| \rangle = 0$; confined phase, $F_q \to \infty$.
- $\langle |P| \rangle \neq 0$; deconfined phase, F_q finite.

with F_q a quark's free energy.

Finite T in the lattice: Polyakov loop





Finite μ in the lattice

The thermodynamics of QFT's are conventiently described within the grand canonical ensemble by adding a term to the action

$$S \to S - \mu_f n_f$$

with $n_f = \overline{\psi}_f \gamma_0 \psi_f$ the quark numbers for each quark flavour f.

The partition function results:

$$Z = \int [dU][d\overline{\psi}][d\psi] e^{-S_{QCD} + \sum_f \overline{\psi}_f \gamma_0 \psi_f}$$

with thermodynamic properties computed as:

$$F = -T \ln Z \,, \quad P = \frac{\partial (T \ln Z)}{\partial V} \,, \quad Q_f = \frac{\partial (T \ln Z)}{\partial \mu_f} \cdots$$

[Philipsen, 2007]

Finite μ in the lattice

The Monte Carlo evaluation of the partition function encounters a **sign problem** because of the finite chemical potential.

Sign problem

Writing the modified Dirac operator (including the μ-term) as:

$$M(\mu) = \not{D} + m_f - \gamma_0 \mu_f$$

the determinant of M becomes complex, thus not allowing to use it in the importance sampling process. The problem is related to the γ_5-hermiticity of Dirac operator

$$M(\mu)^\dagger = \gamma_5 M(-\mu^*) \gamma_5$$

Some proposals such as reweighting, Taylor expanding around $\mu = 0$ or working at negative μ^2 and extrapolating to $\mu^2 > 0$ try to circumvent this problem.

Take away message: QCD phenomenology in the lattice.

QFT phenomenology

Modern calculations at $a \lesssim 0.1\mathrm{fm}$ and physical m_π.

- Static quark potential (confinement).
- Hadron spectrum.
- $\alpha_{\overline{\mathrm{MS}}}$
- $(g-2)_\mu$
- Decay constants
- Scattering LEPs
- Form factors, PDF, GPDs,...
- Finite T and Polyakov loop.
- Finite μ in the lattice...
- ...