Flavor physics from lattice QCD

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Flavour physics at LHC School
28. to 30. May 2025

Funded by
the European Union

My goals for these lectures

If everything works as planned, you will...

- understand why lattice QCD is a vital tool to make Standard Model predictions.
- have an idea what ingredients are needed for a full lattice QCD computation.
- be able to understand and identify the main sources of uncertainty when looking at a new lattice result.
- know what types of observables can be reliably computed on the lattice.

Please interrupt me and ask questions at any time!

Outline

1. Setting the stage
   - Why do we need lattice QCD?
   - How to formulate QCD on the lattice?
2. A guided tour through a lattice QCD computation
   - What steps are needed in a full lattice computation?
   - What are the dominant sources of uncertainty?
3. Flavor physics from lattice QCD
   - Standard Model parameters.
   - Heavy quarks on the lattice.
   - CKM matrix elements.

OUTLINE

1. Setting the stage
    - Why do we need lattice QCD?
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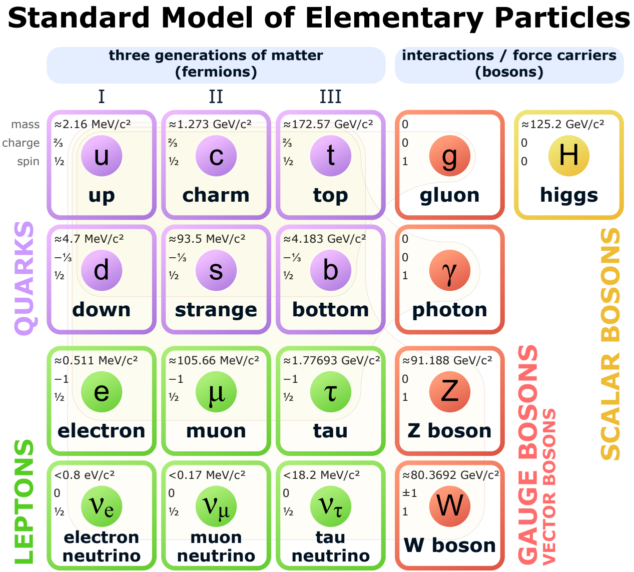
Motivation: Why do we need lattice QCD?

The search for physics beyond the Standard Model

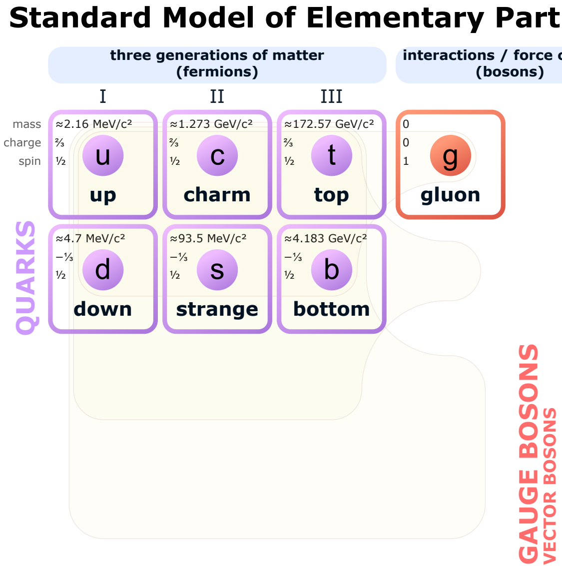
- The Standard Model of particle physics is incomplete.
- We are looking for BSM physics at the precision and intensity frontier.
- Accurate Standard Model predictions are required to take full advantage of experimental progress.

Hadronic uncertainties very often dominate the error budget

The Standard Model of particle physics



- A renormalizable field theory.
- Strong, electromagnetic and weak interactions mediated by gauge bosons.
- Three families of leptons (why?).
- six quark flavors (why?)



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- Three families of leptons (why?).
- six quark flavors (why?)
- We will focus on the theory of strong interactions—QCD.

Three types of interactions in the Standard Model

- Perturbation theory is a powerful tool.

$$\alpha + \underbrace{\alpha^2}_{\text{small}} + \underbrace{\alpha^3}_{\text{smaller}} + \underbrace{\ldots}_{\text{negligible?}}$$

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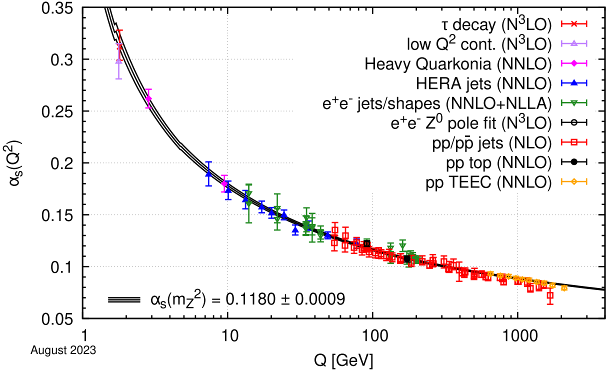
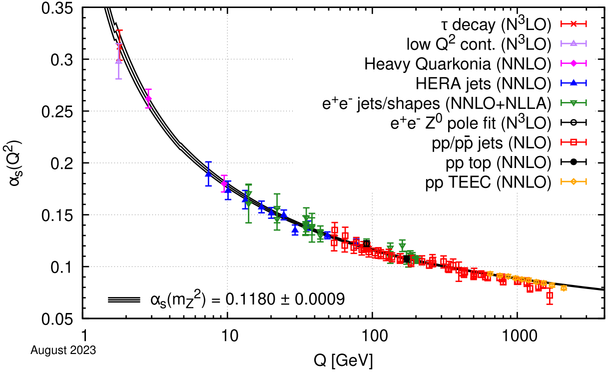
- Strong force, QCD
  - Force carrier: gluons
  - Coupling strength from 0 to $\mathrm{O}(1) \rightarrow$ perturbative expansion??



[PDG, 2024]

- The strong coupling constant $\alpha_\mathrm{s}(Q^2)$ runs with the energy Q.

The running coupling constant



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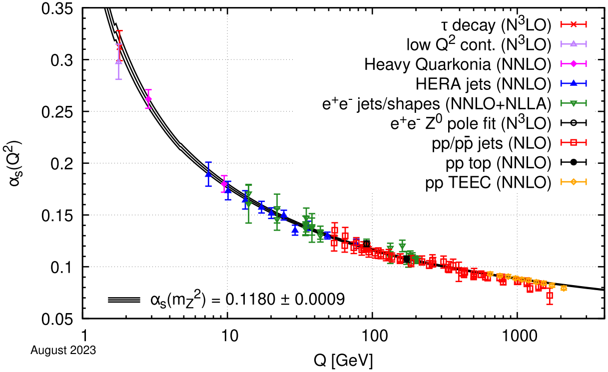

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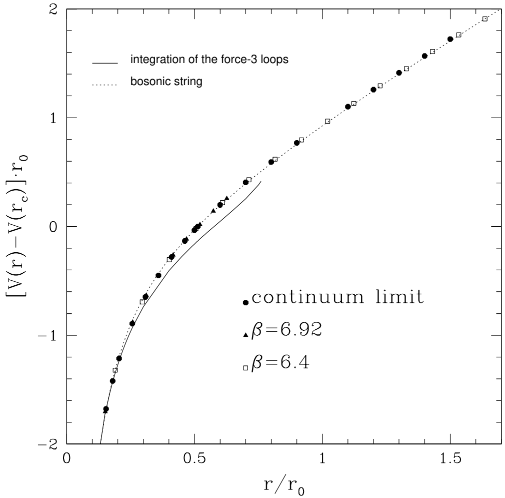
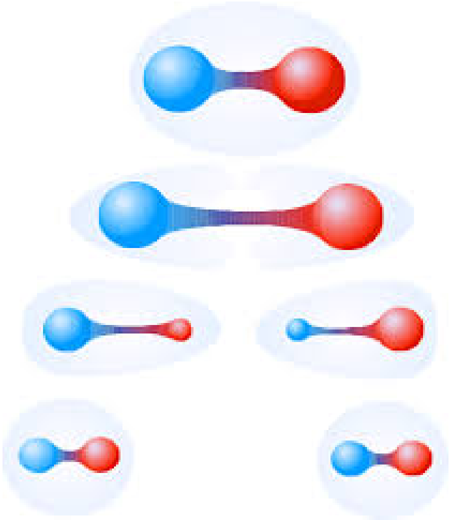
- At small energies $Q \sim \Lambda_{QCD}$ the coupling is strong:
  - non-perturbative physics
  - quarks are **confined**



- Quarks and gluons only appear in bound states.
- No strict proof for confinement so far. There is a US$1 million bounty!
- But there is numerical evidence from the lattice.

← The static quark potential in Yang-Mills theory [Necco and Sommer, hep-lat/0108008].

Non-perturbative QCD: Confinement



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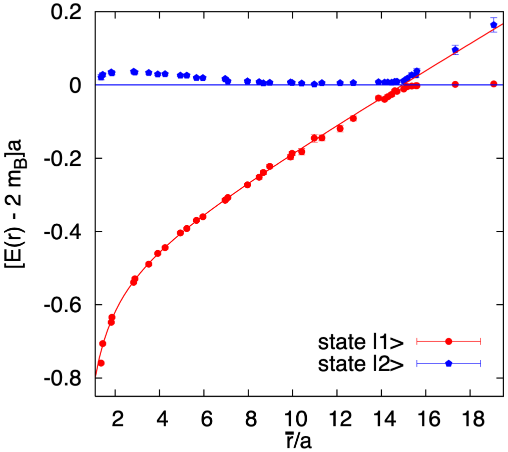

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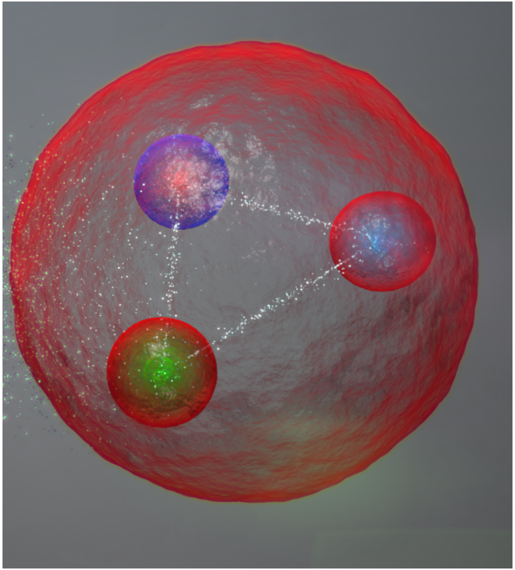
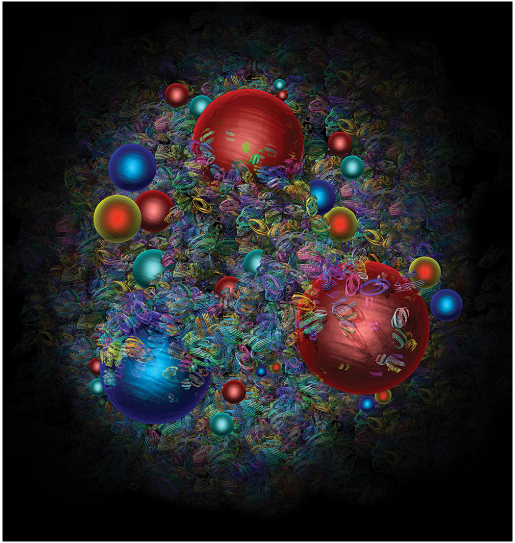
← String breaking in QCD [Bali et al., hep-lat/0505012].



- The proton is a bound state of three quarks.
- What is its mass?
  - up quark $m_\mathrm{u} \approx 2.2\,\mathrm{MeV}$
  - down quark $m_\mathrm{d} \approx 4.7\,\mathrm{MeV}$
  - proton $M_P \approx 938.3\,\mathrm{MeV}$
  - $2m_\mathrm{u} + m_\mathrm{d} \neq M_P \ldots$

based on https://cds.cern.ch/record/2034198

Non-perturbative QCD: the proton mass



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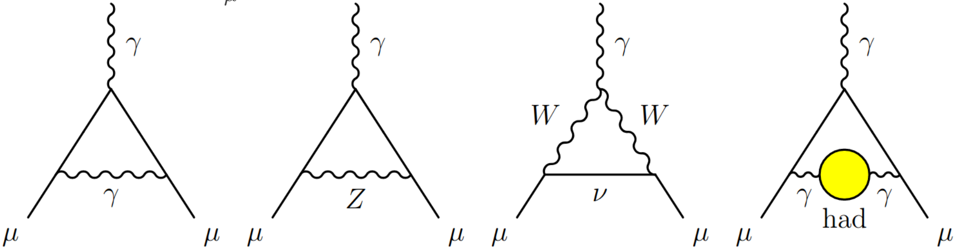
  - $2m_\mathrm{u} + m_\mathrm{d} \neq M_P \ldots$
- Confinement gives mass to protons!
- N. B. Computing the mass of a quark is non-trivial!

https://cerncourier.com/a/the-proton-laid-bare/

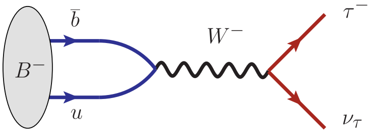
Leading contributions to a_μ: [PDG]

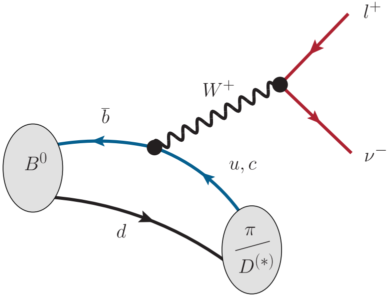


- (There was a) long-standing tension between SM and experiment for the anomalous magnetic moment of the muon [Aliberti et al., 2505.21476].
- SM prediction from QED, electroweak and hadronic contributions:

$$a_l^{\mathrm{SM}} = a_l^{\mathrm{QED}} + a_l^{\mathrm{EW}} + a_l^{\mathrm{had}} \quad \text{where} \quad a_l^{\mathrm{had}} = a_l^{\mathrm{hvp}} + a_l^{\mathrm{HLbL}} \,.$$

- Uncertainty of the SM prediction completely dominated by subleading a_μ^{hvp}.





- Computation of CKM matrix elements from

$$\Gamma_{\text{exp}} = |V_{ij}|(\text{WEAK})(\text{EM})(\text{STRONG})$$

relies on experimentally determined decay rates and hadronic quantities (decay constants, form factors) from lattice QCD.

Setting the stage

QCD

QCD

- QCD is based on the gauge group SU(3) : three colors
- Quarks carry a SU(3) color
- Anti-quarks also carry SU(3) (anti)-colors
- Gluons carry color and anticolor
- Gluons carry a color charge : different from QED (photon electrically neutral)
- Gluons interact with themselves.

QCD: The (classical) QCD action

- The Lagrange density of QCD can be expressed as

$$\mathcal{L}_{\text{QCD}} = \mathcal{L}_G + \mathcal{L}_F$$

$$= \underbrace{-\frac{1}{2}\text{Tr}[F_{\mu\nu}F^{\mu\nu}]}_{\text{gauge action}} \underbrace{+\sum_{f=1}^{N_f} \bar{\psi}_f(x)(i\not{D} - m_f)\psi_f(x)}_{\text{fermion action}}, \qquad \underbrace{\not{D} = \gamma^\mu[\partial_\mu - igA_\mu(x)]}_{\text{covariant derivative}}$$

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- Gluon fields A_μ and the Gluon field strength tensor

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f_{abc} A^b_\mu A^c_\nu \,,$$

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- Quark fields $(\psi_f)^a_\alpha$: $N_f = 6$ flavors $\mathrm{u, d, c, s, b, t}$ with spin index α, color index a.
- $N_f + 1$ free parameters: The quark masses m_f and the gauge coupling g.

- Basically all information on the quantum field theory can be extracted in terms of vacuum expectation values.

- Compute the vacuum expectation of an observable $\mathcal{O}$ from the path integral

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[\bar{\psi}, \psi, A]\, \mathcal{O}\, \mathrm{e}^{iS_{\mathrm{QCD}}[\bar{\psi},\psi,A]}\,, \qquad S_{\mathrm{QCD}} = \int \mathrm{d}^4x\, \mathcal{L}_{\mathrm{QCD}}[\bar{\psi}, \psi, A]$$

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  - The factor i introduces large oscillations $\rightarrow$ complicates integration!

Setting the stage

Discretizing QCD

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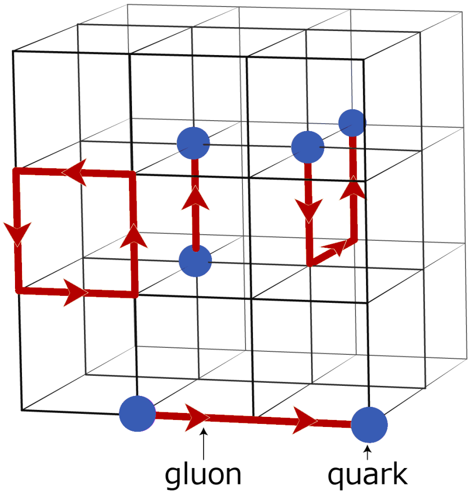
$\rightarrow$ recover QCD with $\lim\limits_{L\to\infty} \lim\limits_{a\to 0}$ after evaluating the path integral.



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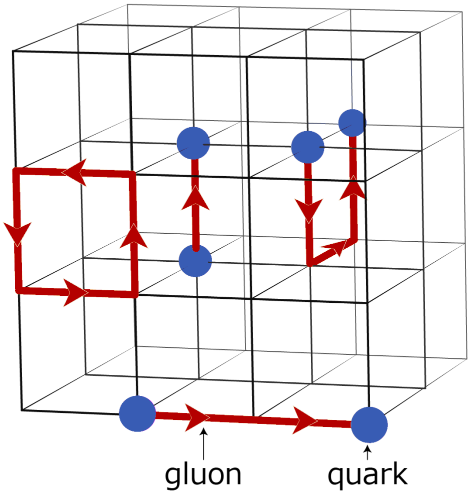

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  - parallel transporter: SU(3) matrices:

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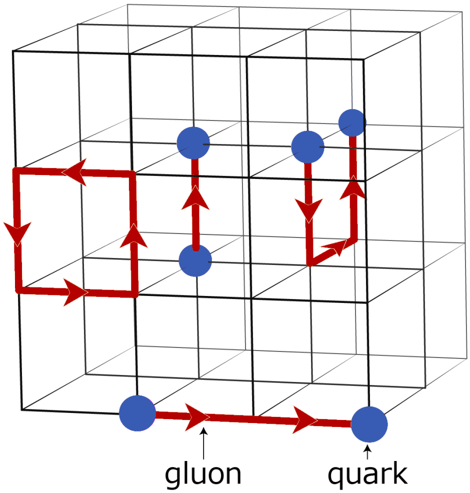

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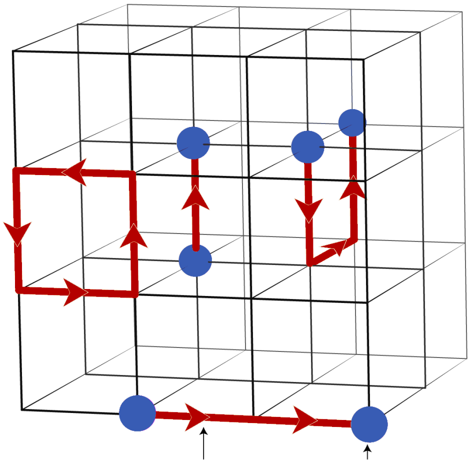

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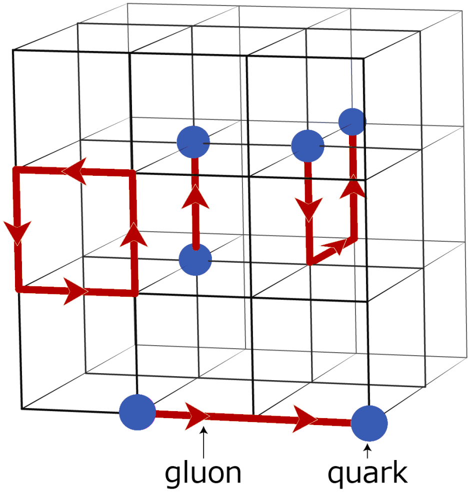

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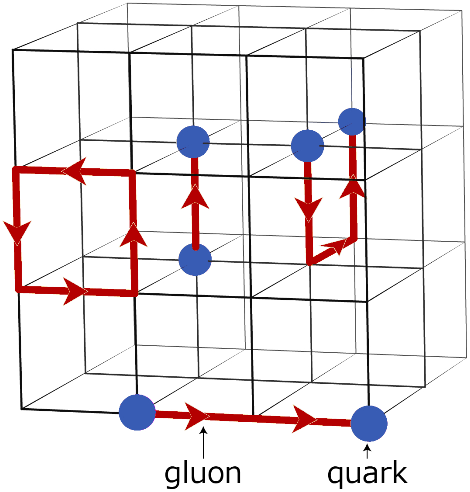

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  - **Gauge symmetry is preserved!**

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$$\partial_\mu f(x) \to \frac{1}{a}[f(x+a\hat{\mu}) - f(x)] + \mathrm{O}(a)\,, \qquad \partial_\mu f(x) \to \frac{1}{a}[f(x) - f(x-a\hat{\mu})] + \mathrm{O}(a)\,,$$

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better use the symmetric version (forward + backward)

$$\partial_\mu f(x) \to \frac{1}{2a}[f(x+a\hat{\mu}) - f(x-a\hat{\mu})] + \mathrm{O}(a^2)\,,$$

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need a gauge covariant derivative in practice:

$$\nabla_\mu \psi(x) = \frac{1}{a}[U_\mu(x)\psi(x+a\hat{\mu}) - \psi(x)]\,, \qquad \nabla^*_\mu \psi(x) = \frac{1}{a}[\psi(x) - U^\dagger_\mu(x-a\hat{\mu})\psi(x-a\hat{\mu})]\,,$$

→ The *naive* continuum limit has to agree with QCD!

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QCD ON THE LATTICE

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- Each action comes with advantages and disadvantages.

- The most relevant fermion actions approach QCD with $\mathrm{O}(a^2)$ cutoff effects:

Action	Advantages	Disadvantages
(root) Staggered	computationally very fast	rooting introduces non-locality
		unphysical bound states
		complicated Wick contractions
Wilson-Clover	computationally fast ($\times 10$)	breaks chiral symmetry
		requires extra work for a^2 scaling
Twisted-mass	computationally fast ($\times 10$)	breaks chiral symmetry
		violation of isospin
Domain wall	improved chiral symmetry	computationally expensive ($\times 100$)
Overlap	improved chiral symmetry	computationally expensive ($\times 100$)

Setting the stage

Evaluating the path integral

- Let's go back to the expectation value of $\mathcal{O}$, now at $a \neq 0$ and finite L

$$\langle\mathcal{O}\rangle(a,L) = \frac{1}{Z}\int \mathcal{D}[\bar{\psi},\psi,A]\,\mathcal{O}\,\mathrm{e}^{-S_{\mathrm{E}}[\bar{\psi},\psi,A]}\,,$$

where $S_{\mathrm{E}} = S_{\mathrm{G}} + S_{\mathrm{F}}$ is the Euclidean action of QCD.

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- Perform the Wick contractions to evaluate $\langle \mathcal{O} \rangle_{\mathrm{F}}$, e.g.,
$$\int \mathcal{D}[\bar{\psi}, \psi] \, \psi_i \bar{\psi}_j \mathrm{e}^{-S_{\mathrm{F}}[\bar{\psi}, \psi]} = - \left(D_W^{-1} \right)_{ij} \det D_W$$

The path integral on the lattice

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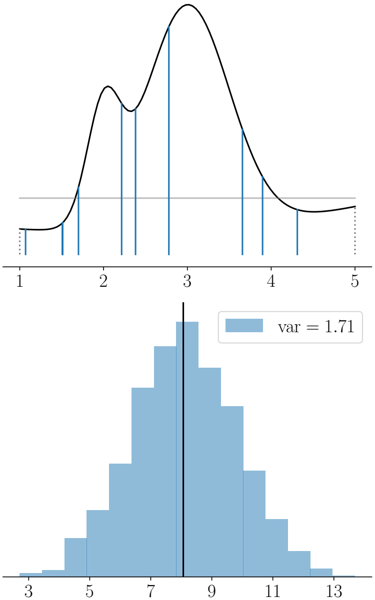
- Evaluate the path integral using **Monte Carlo methods**.



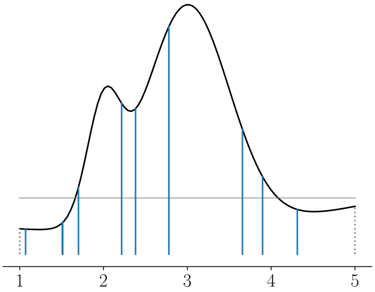
- General idea of Monte Carlo integration

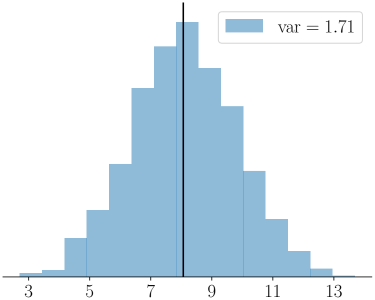
$$\frac{1}{b-a}\int_a^b \mathrm{d}x\, f(x) \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

with randomly chosen points x_i in the integration region.

- Works good if $f(x)$ is approximately constant.
- Unbiased estimator of the integral.

Monte Carlo integration





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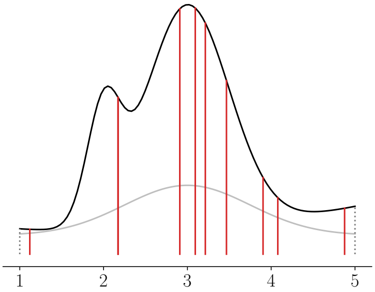
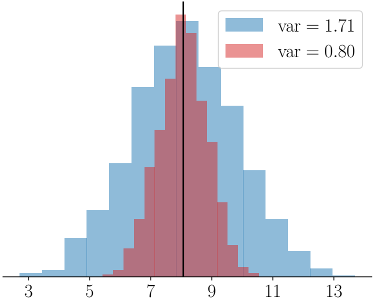
$$\int \mathrm{d}x\, f(x) = \int \rho(x)\mathrm{d}x\, \frac{f(x)}{\rho(x)} \approx \left[\frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{\rho(x_i)}\right]$$

- Choose points according to probability distribution $\rho(x)$ similar to the function to be integrated.

Monte Carlo integration





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3. Compute expectation values from averages over gauge ensembles

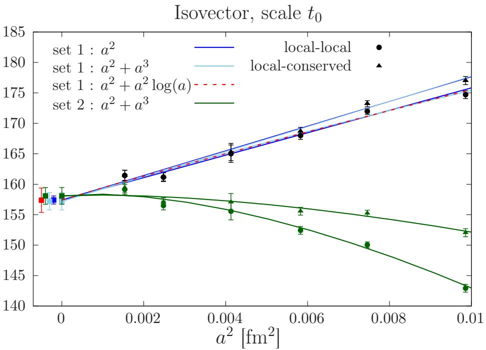
$$\bar{\mathcal{O}} = \frac{1}{N}\sum_{k=1}^{N}\langle\mathcal{O}\rangle_\mathrm{F}[U_\mu^{(k)}] = \langle\mathcal{O}\rangle + \mathrm{O}\left(\frac{1}{\sqrt{N}}\right)$$

   still at finite a and L.

Setting the stage

Approaching the physical point

To make predictions for QCD, we need to lift the regulators



[Cé et al. , 2206.06582]

Take the **continuum limit**:

- Simulate at several values of a.
- Take the continuum limit based on the known Symanzik expansion

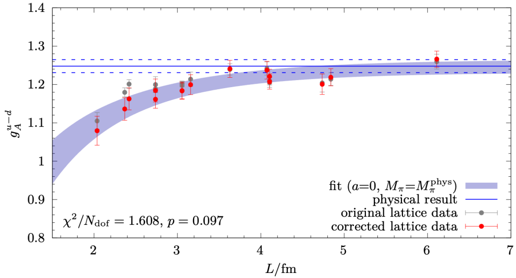
$$\mathcal{O} = \lim_{a\to 0} \left[\mathcal{O} + a^2 \mathcal{O}_2 + a^3 \mathcal{O}_3 + a^4 \mathcal{O}_4 + \dots \right]$$

$\to$ source of **systematic uncertainty**.

- Cutoff effects vanish **polynomially**.
- Optimal situation: a is small enough such that only $\mathrm{O}(a^2)$ is relevant.

APPROACHING THE PHYSICAL POINT: INFINITE VOLUME

To make predictions for QCD, we need to lift the regulators



[Djukanovic et al., 2402.03024]

Take the **infinite-volume limit**:

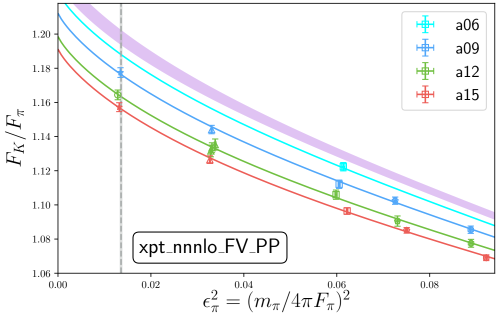
- Dominant finite-size effect due to pions wrapping around the torus.
- Chiral perturbation theory guides the finite-volume extrapolation

$$\mathcal{O} = \lim_{L\to\infty} \mathcal{O}\left[1 + \frac{c_1}{L^{3/2}} e^{-m_\pi L} + \ldots\right]$$

- Finite-volume effects vanish **exponentially**.
- Depending on the observable and the precision, it might be sufficient to fulfill

$$m_\pi L \geq 4$$

Some calculations use larger-than-physical light quark masses



[Miller et al., 2005.04795]

- Significantly cheaper (more on that later).
- Allows to afford smaller L.
- Chiral perturbation theory guides the chiral extrapolation, e.g.,

$$\mathcal{O}(m_\pi) = \mathcal{O}(0)\left[1 + c_1\,\frac{m_\pi^2}{8\pi^2 f_\pi^2} + \ldots\right]$$

- Combined chiral-continuum extrapolation.
- Many flagship calculations directly at physical masses nowadays.

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- The lightest dynamical degrees of freedoms are pions (not quarks!).
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  - Rule of thumb: small effects ($<\%$) if $m_\pi L \geq 4$.
  - Typical scale is $m_\pi \sim 140\,\mathrm{MeV}$.

$$\Rightarrow L \geq 6\,\mathrm{fm}$$

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  - For comparison: The proton radius is $\approx 0.9\,\mathrm{fm}$.
- The *dominant* cutoff effects are due to the largest energy scale
  - The charm quark has to be resolved such that $am_c \leq 0.5$.
  - Heavy scale is $m_c \sim 1.3\,\mathrm{GeV}$.

$$a^{-1} \geq 2.6\,\mathrm{GeV} \to a \leq 0.076\,\mathrm{fm}$$

How large, how fine?

$$a^{-1} \ll \text{relevant scales} \ll L^{-1}$$

- We fulfill this criterion with $L \geq 6\,\mathrm{fm}$ and $a \leq 0.076\,\mathrm{fm}$. $\rightarrow L/a \geq \frac{6}{0.076} \approx 80$

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A fine lattice in a small box is physics, a very coarse lattice in a large box is not!

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Most calculations use mass-degenerate up and down quarks

Have to include the effects of $\mathrm{O}\left(\frac{m_\mathrm{d}-m_\mathrm{u}}{\Lambda_\mathrm{QCD}}\right)$ and $\mathrm{O}\left(\alpha\right)$ when aiming for $< 1\%$ precision!

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The state of the art are $N_f = 2 + 1$ and $N_f = 2 + 1 + 1$ simulations.

Setting the scale

- Scale setting: How to relate the bare parameters of $\mathcal{L}_{\mathrm{QCD}}$ to a and m_π in MeV.
- Only dimensionless quantities can be computed: am_P, am_π, am_Ω, af_π, …
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- Determine the lattice spacing from physical input
  - From $am_\Omega(g_0)$ and m_Ω^{phys} we can determine

$$a(g_0) = \frac{am_\Omega(g_0)}{m_\Omega^{\text{phys}}}$$

  - The input should be cheap and precise on the lattice.
  - Other choices such as f_π lead to different values of

$$a'(g_0) = a(g_0) + \mathrm{O}(a^2) \qquad \text{with } a'(g_0) = \frac{af_\pi(g_0)}{f_\pi^{\text{phys}}}$$

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  - Fix m_{s} from $\left(\frac{am_{\mathrm{K}}}{am_\Omega}\right)^{\mathrm{lat}} = \left(\frac{m_{\mathrm{K}}}{m_\Omega}\right)^{\mathrm{phys}}$
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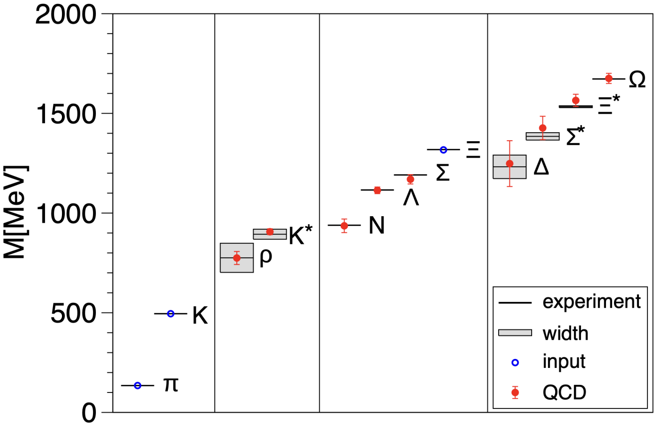
  requires careful tuning of the bare parameters.
- **All further output of the calculation is a prediction!**
- For instance, the prediction of the D meson decay constant:

$$f_{\mathrm{D}}^{\mathrm{phys}} = \left(\lim_{a\to 0} \frac{af_{\mathrm{D}}}{am_\Omega}\right) m_\Omega^{\mathrm{phys}}$$



- Postdicting the light QCD spectrum worked already 15 years ago [Dürr et al., 0906.3599].

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Sources of uncertainty

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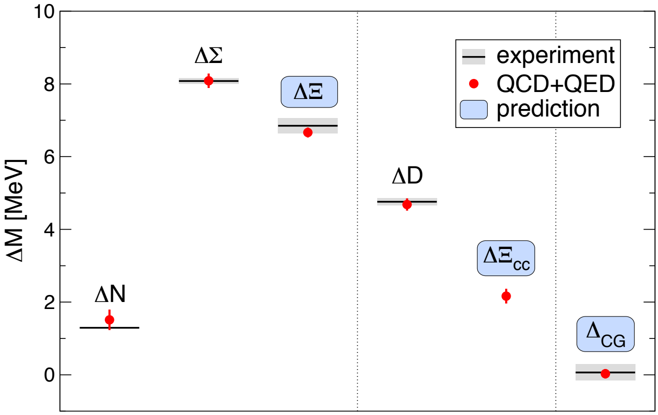
  - Extrapolate or interpolate to physical quark masses (based on χPT).
- Number of dynamical quark flavors N_f
  - Nowadays $N_f = 2 + 1$ or $N_f = 2 + 1 + 1$. This is sufficient.

- A number of observables now reaches below 1% precision.
- Have to include the effects of $\mathrm{O}\left(\frac{m_{\mathrm{d}}-m_{\mathrm{u}}}{\Lambda_{\mathrm{QCD}}}\right)$ and $\mathrm{O}\left(\alpha\right)$.

- A number of observables now reaches below 1% precision.
- Have to include the effects of $\mathrm{O}\left(\frac{m_{\mathrm{d}}-m_{\mathrm{u}}}{\Lambda_{\mathrm{QCD}}}\right)$ and $\mathrm{O}(\alpha)$.
- Formulating QED in finite-volume is challenging:
  - Long-range interactions don't like finite volumes with periodic boundary conditions [Patella, 1702.03857].
  - Finite-volume effects can be sizable and power-like [Hayakawa, Uno, 0804.2044].
  - Logarithmic infrared divergences arise when studying decays.

Isospin breaking on the lattice

- A number of observables now reaches below 1% precision.
- Have to include the effects of $\mathrm{O}\left(\frac{m_\mathrm{d}-m_\mathrm{u}}{\Lambda_\mathrm{QCD}}\right)$ and $\mathrm{O}(\alpha)$.
- Formulating QED in finite-volume is challenging:
  - Long-range interactions don't like finite volumes with periodic boundary conditions [Patella, 1702.03857].
  - Finite-volume effects can be sizable and power-like [Hayakawa, Uno, 0804.2044].
  - Logarithmic infrared divergences arise when studying decays.
- Two approaches are followed to include isospin breaking effects
  - Direct simulation of QCD+QED [CSSM/QCDSF/UKQCD] [RC*, 2212.11551].
  - Perturbative expansion in $\left(\frac{m_\mathrm{d}-m_\mathrm{u}}{\Lambda_\mathrm{QCD}}\right)$ and α allows to use isospin symmetric gauge ensembles at the cost of computing more diagrams [RM123, 1303.4896].



- Lattice QCD+QED allows to predict the splitting between neutron and proton from first principles [Borsanyi et al., 1406.4088].

Conclusions

Lattice QCD is not a model

$$\lim_{a\to 0}\lim_{L\to\infty}(\text{lattice QCD}) = \text{QCD}$$

- Lattice QCD is systematically improvable:
  larger statistic, smaller lattice spacings $\rightarrow$ improved accuracy and precision.
- Effective theories can guide extrapolations, but we work with QCD.
  We'll see a case where this is not the case.
- Lattice QCD computations are from first principles:
  All predictions are based on the QCD Lagrangian and the hadronic input to fix the $N_f + 1$ parameters.