From Quarks to Hadrons: Simulation of the vacuum in a femto-box

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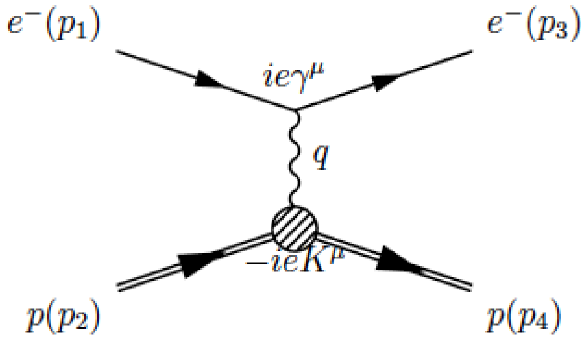
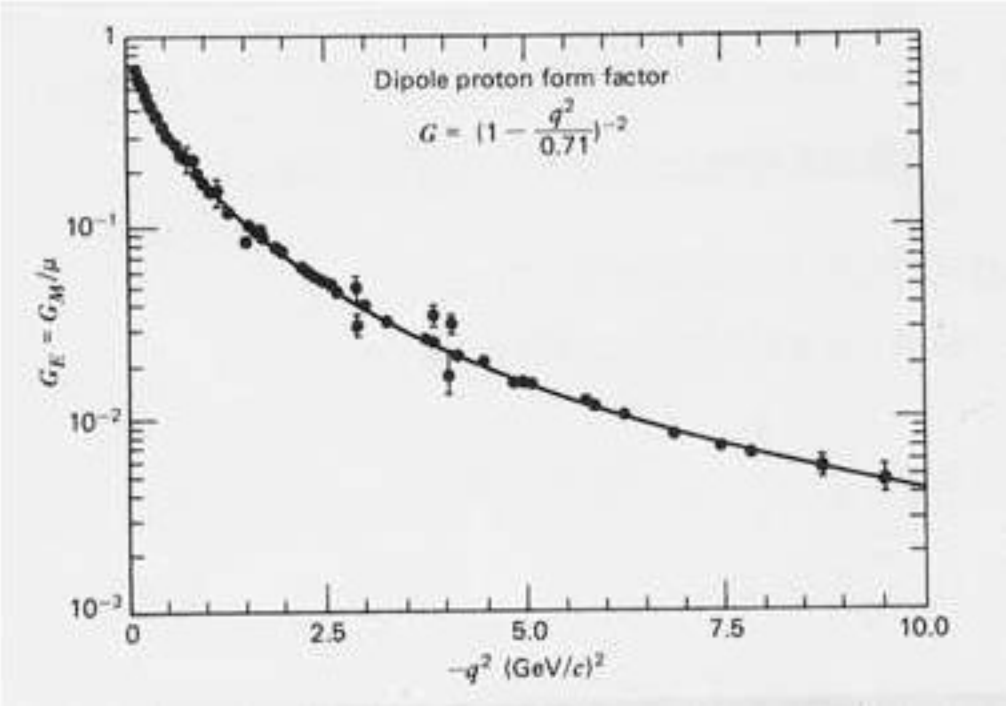
November 19, 2025

Historic overview

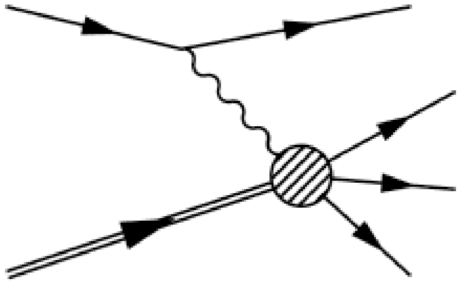
ep scattering = proton seems to have internal structure

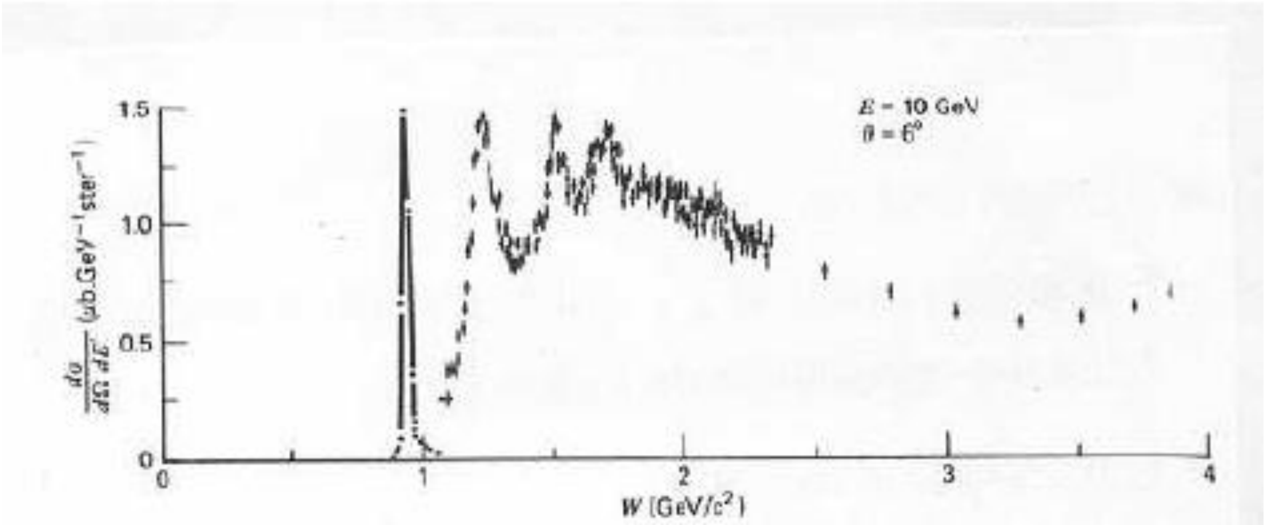




A proton extends as exp(- r/r_0); $r_0 \sim 1$ fm

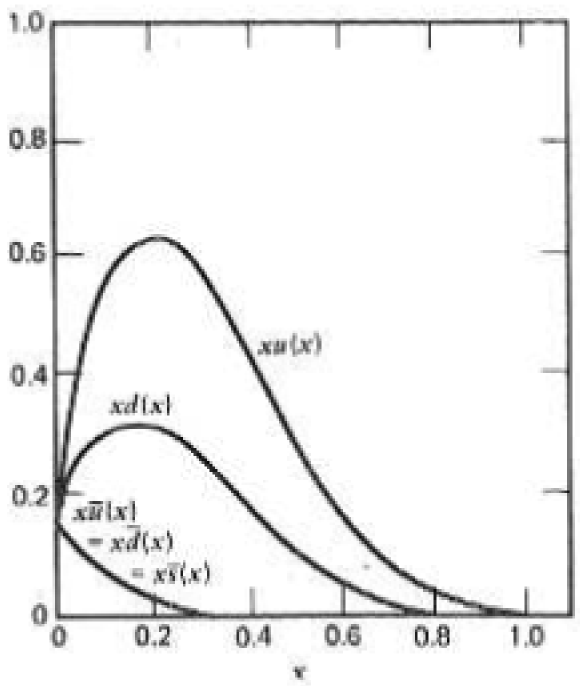
Generates resonances at higher energies:





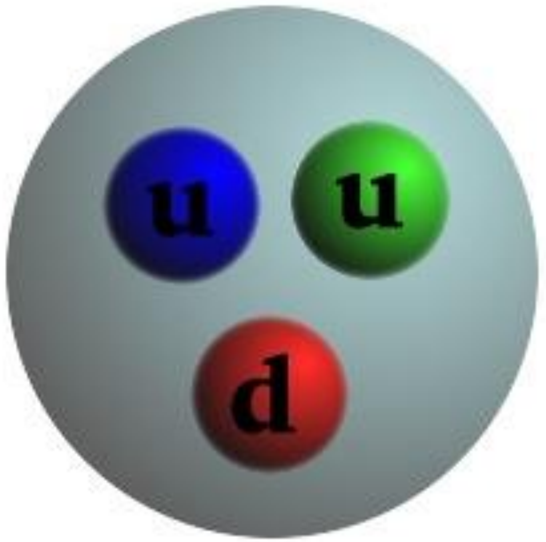
W: invariant mass of produced particles

At higher energies, electron looks like hitting a free “parton” inside proton.

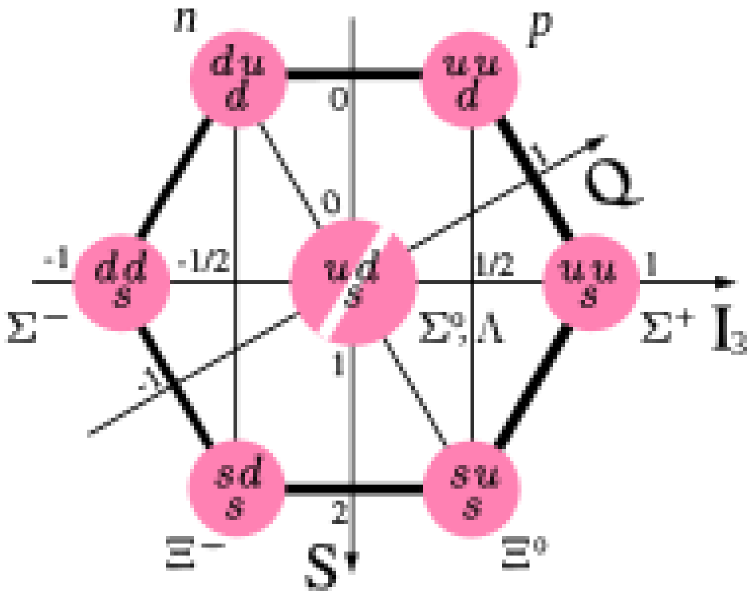


Each parton carries roughly 1/3 of proton’s momentum.

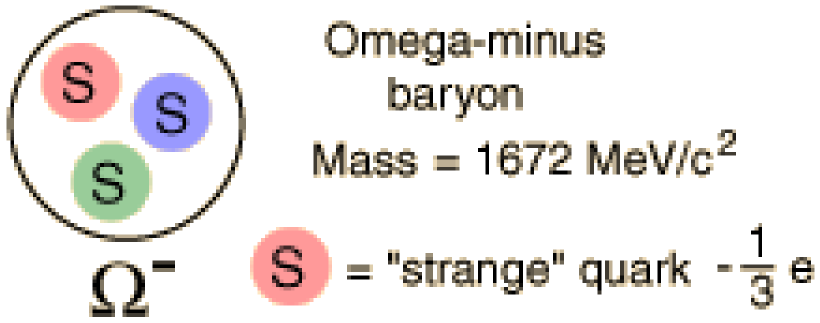
Three quarks: up, up, down



Can explain other baryons, as well.



Need to have three internal degrees of freedom
= color



Otherwise, forbidden by Pauli's exclusion principle.

Quarks

Requirements:

1. have fractional charge +2/3 e, -1/3 e

2. have internal degrees of freedom (=3)

3. may not appear as an isolated particle

4. (at high energy) behave as a free particle inside a proton

Model (or dynamics) to fulfill all of these ➔ QCD

Quantum Chromodynamics (QCD)

Dirac equation

QED
(for electron)

$$\left(\gamma^{\mu}\left(i\hbar\partial_{\mu}-\frac{e}{c}A_{\mu}\right)-mc\right)\psi=0$$

QCD
(for quark)

$$\left(\gamma^{\mu}\left(i\Box_{\mu}-gA_{\mu}\right)-mc\right)\psi=0$$

3x3 matrix — three degrees of freedom

Maxwell's equation

QED
(for photon)

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

$$\partial_\mu F^{\mu\nu} = j^\nu, \quad \varepsilon^{\mu\nu\rho\sigma}\partial_\mu F_{\nu\rho} = 0$$

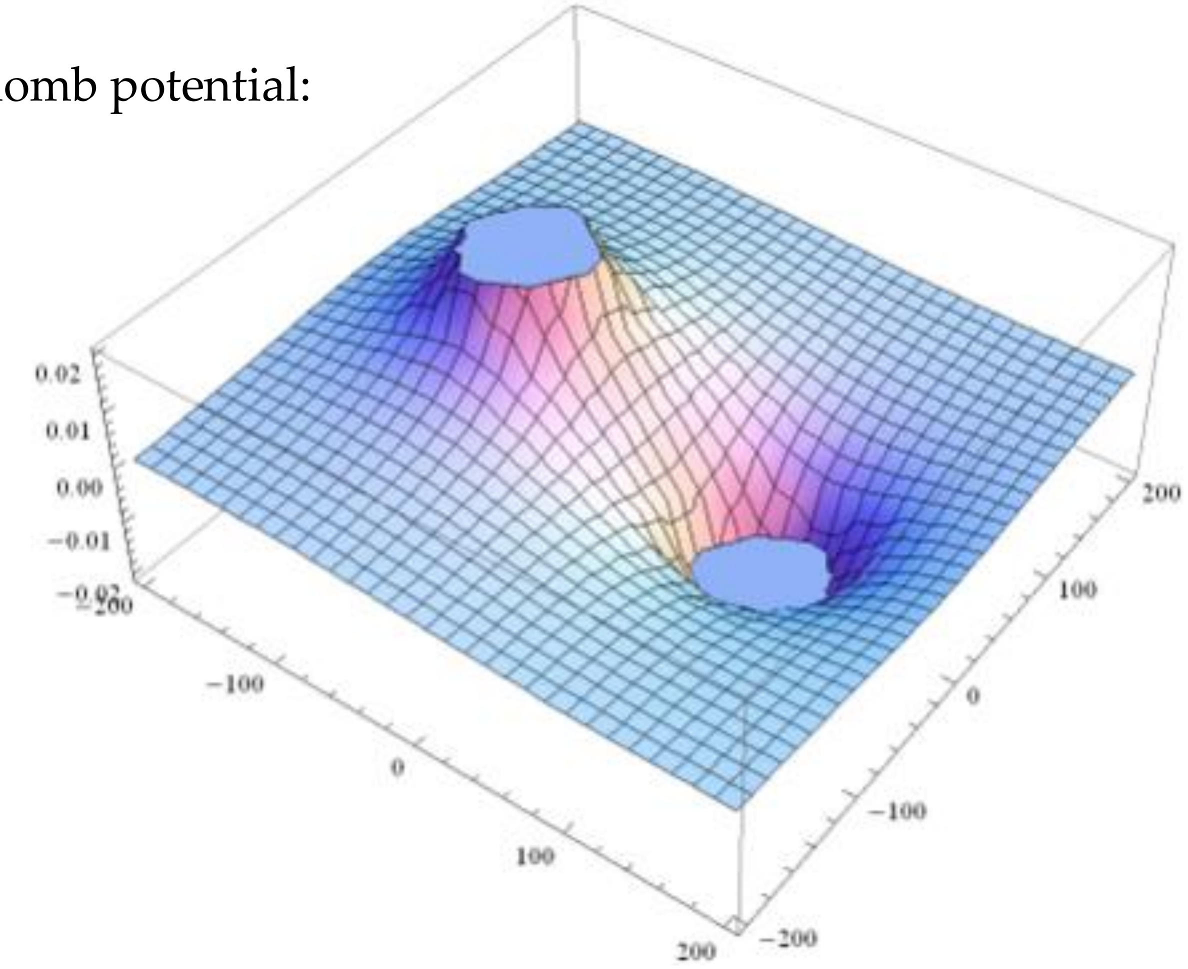
QCD
(for gluon)

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu]$$

$$(\partial_\mu + igA_\mu)F^{\mu\nu} = j^\nu, \quad \varepsilon^{\mu\nu\rho\sigma}(\partial_\mu + igA_\mu)F_{\nu\rho} = 0$$

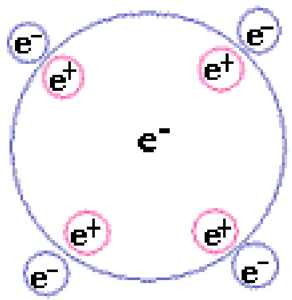
gauge field itself plays the role of a source

Coulomb potential:

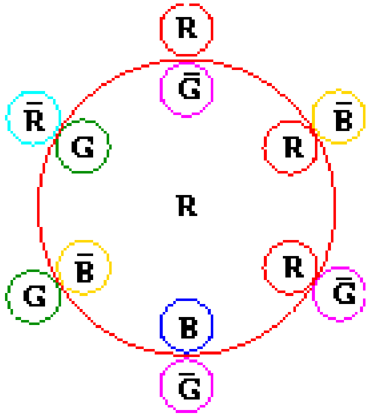


simply a sum of two sources; not the case for QCD!

Anti-screening



Vacuum polarization weakens the EM charge at long distances



Self-interaction enhances the color charge

Okay, let's carry out!

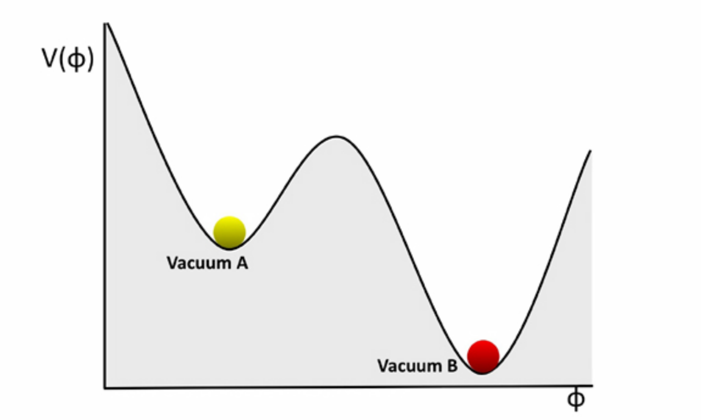
- Sounds easy?
  - Super-multiple integral…, actually infinitely many!

$$Z = \int [d\phi] e^{iS}; \; S = \int d^4 x \mathcal{L}$$

- Possible when the integral is known = Gaussian
  - Free field theory: $S \sim \phi^2$
  - Expansion around this simplest case = perturbation theory
  - Good approximation if the reality is sufficiently "free".

What is perturbation theory?

- Reduces to harmonic oscillator:
  - When the potential is complicated, try to expand around its bottom.

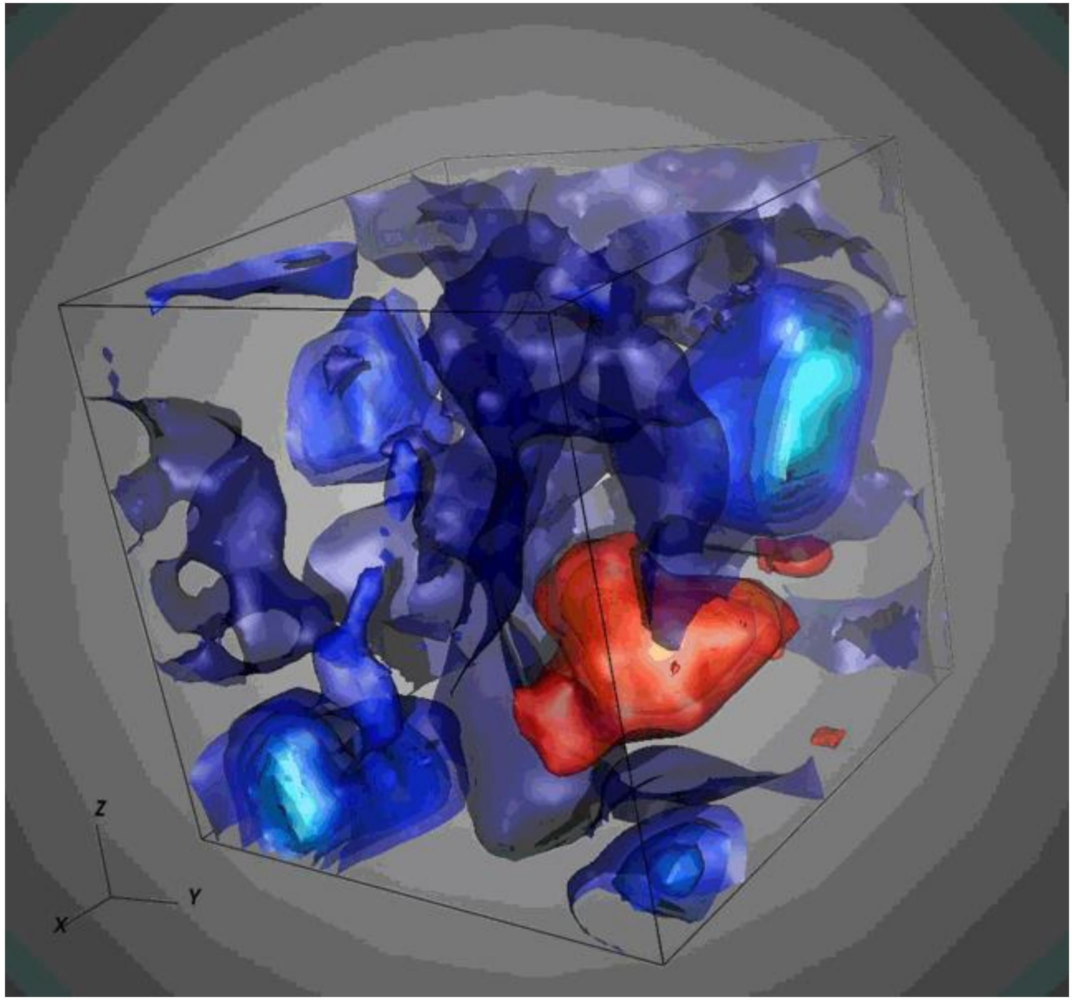


  - Good approximation if the field actually fluctuates around there.
  - If the fluctuation is bigger…, no way.

What is the *vacuum*?

- In QED,
  - $F_{\mu\nu}$=0 is the vacuum.
  - Photon is an excitation from there.

- In QCD,
  - More fluctuations. The vacuum is determined as the minimum of the "effective action", which is the free energy in the language of statistical mechanics.
  - But, not completely random either.
  - Particles represent the excitations on this "vacuum".


Z
Y
X

Correspondence

Statistical mechanics

- partition function; Hamiltonian

$$Z = \int [d\phi] e^{-H/T};\ H \sim \int d^3x \mathcal{H}$$

Quantum field theory

- partition function; action

$$Z = \int [d\phi] e^{iS};\ S = \int d^4x \mathcal{L}$$

- After the Wick rotation, it is made Euclidean

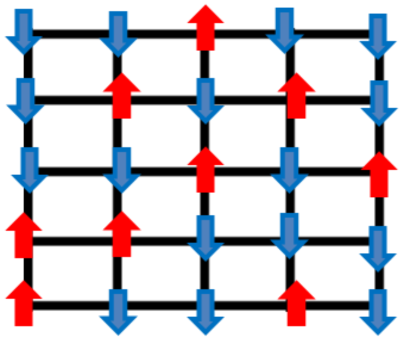
$$Z = \int [d\phi] e^{-S_E};\ S_E = \int d^4x \mathcal{L}$$

Monte Carlo simulation

Simple example

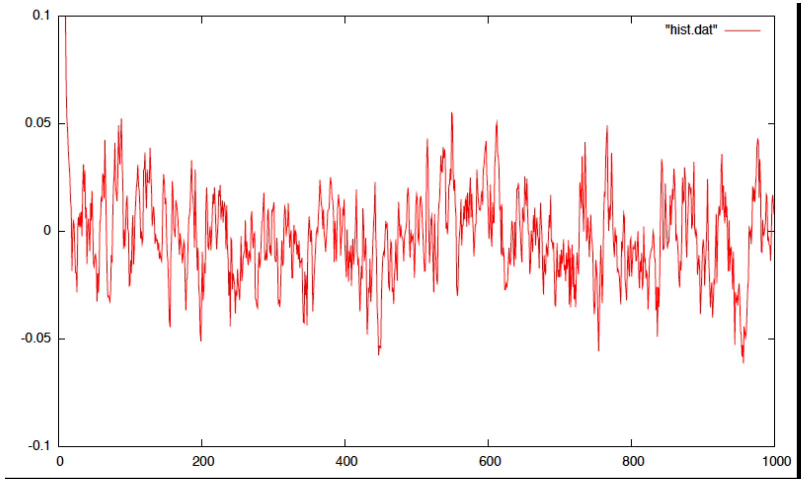
Ising model

$$Z = \sum_{\{s_i\}} \exp[-H\{s_i\}/T], \quad H\{s_i\} = -J \sum_{\{i,j\} \in n.n.} s_i s_j$$



How does the spontaneous magnetization emerge?

$$M = \frac{1}{L^2} \sum_i s_i$$

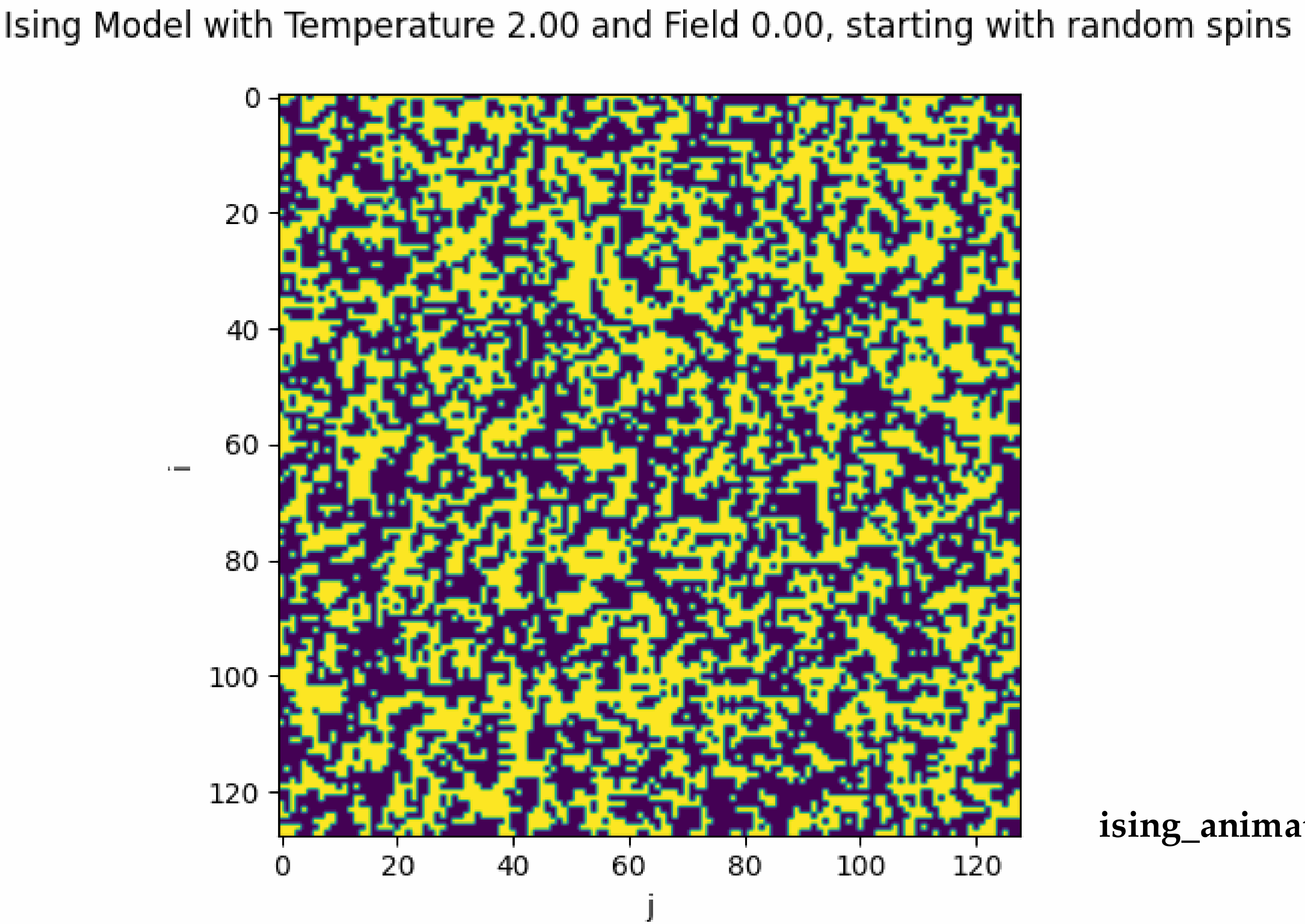


Monte Carlo method

Basic idea:

$$Z = \sum_{\{s_i\}} \exp[-H\{s_i\}/T], \quad H\{s_i\} = -J \sum_{\{i,j\} \in n.n.} s_i s_j$$

- The number of terms = $2^{(2L^2)}$. For L=100, it is $2^{20000} \sim 10^{2000}$. Impossible.
- Only some limited terms contribute to the sum:
  - T = 0: only those giving the minimum $H\{s_i\}$.
  - T = ∞: completely random.
- Pickup the relevant configurations only = MC



ising_animate

(intermediate) summary

- Quarks are inside nucleons; how do they look like?
- The theory is similar to QED (electromagnetism), but way more complicated.
- Tool to study = Monte Carlo simulation.

Lattice QCD

QCD calculation

Goes back to the Lagrangian and partition function

- SU(3) gauge theory
- plus, quarks (up, down, strange, …)

$$S = \int d^4x \left[-\frac{1}{4} \mathrm{Tr}\, F_{\mu\nu}^2 + \sum_f \bar{\psi}_f (\not{D} + m_f) \psi_f \right],$$

$$Z = \int [dA_\mu] \prod_f [d\psi][d\bar{\psi}] \exp\left[-S\right]$$

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g f^{abc} A_\mu^b A_\nu^c$$

$$D_\mu = \partial_\mu - igT^a A_\mu^a$$

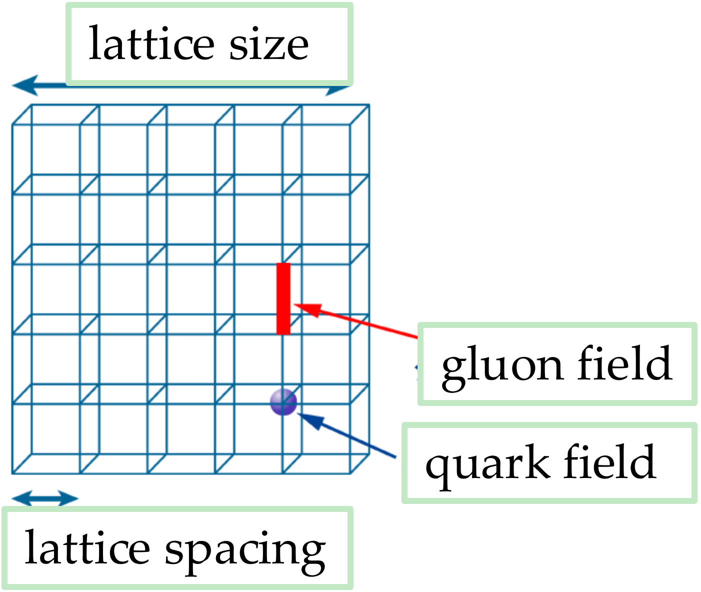
Non-Abelian nature

- Redefine on a 4D lattice

The lattice

<u>4D Lattice</u>

- of size $(L/a)^3x(T/a)$, typically 32^3x64 or 64^3x128.
- lattice spacing determined later with some input.



Gauge invariance

Gauge symmetry

- invariance under local SU(3) transformation
- guaranteed by introducing "link variables" (gauge field)

$\bar{\psi}(x)$ $\psi(x+\hat{\mu})$

$\bar{\psi}(x)V^\dagger(x)$ $V(x)U_\mu(x)V^\dagger(x+\hat{\mu})$ $V(x+\hat{\mu})\psi(x+\hat{\mu})$

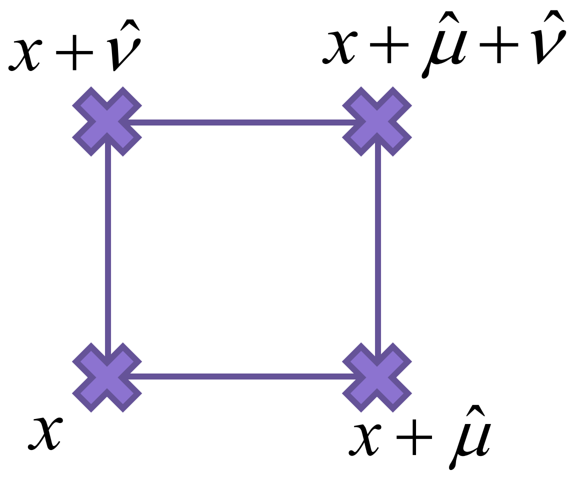
$$U_\mu(x) = \exp\left[igaA_\mu(x)\right] = 1 + igaA_\mu(x) + \dots$$

$$A_\mu(x) \to V(x)\left[A_\mu(x) + \frac{i}{g}\partial_\mu\right]V^\dagger(x)$$

Gauge field

- Built in the gauge link
  - SU(3) matrices
  - Gauge invariance guaranteed by connecting them.

$$U_\mu(x) = \exp\left[igaA_\mu(x)\right] = 1 + igaA_\mu(x) + \ldots$$



$$\mathrm{Tr}\left[U_\mu(x)U_\nu(x+\hat{\mu})U_\mu^\dagger(x+\hat{\nu})U_\nu^\dagger(x)\right]$$
$$\approx \mathrm{Tr}\left[e^{igaA_\mu} e^{iga(A_\nu + a\partial_\mu A_\nu)} e^{-iga(A_\mu + a\partial_\nu A_\mu)} e^{-igaA_\nu}\right]$$
$$\approx \mathrm{Tr}\left[e^{iga^2(\partial_\mu A_\nu - \partial_\nu A_\mu) - g^2a^2[A_\mu, A_\nu]}\right] = \mathrm{Tr}\left[e^{iga^2 F_{\mu\nu}}\right]$$
$$= \mathrm{Tr}[1] - \frac{1}{2} g^2 a^4 \mathrm{Tr}\left[F_{\mu\nu}^2\right] + \ldots$$

Gauge action

Should go back to the continuum, by taking $a \to 0$

$$S = \frac{6}{g^2} \sum_x \sum_{\mu<\nu} \left[1 - \frac{1}{3} \mathrm{Re}\,\mathrm{Tr} \left[U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x) \right] \right]$$

$$\to a^4 \sum_x \sum_{\mu<\nu} \mathrm{Re}\,\mathrm{Tr} \left[F_{\mu\nu}^2 \right]$$

$$= \int d^4x \, \frac{1}{4} \left(F_{\mu\nu}^a \right)^2$$

- Coupling constant $\beta = 6/g^2$
  - Corresponds to 1/kT in the statistical model.

Partition function

- Integrate over SU(3) variables U, rather than A

$$Z = \int [dU_\mu] \prod_f [d\psi][d\bar{\psi}] \exp\left[-S_g - \int d^4x \sum_f \bar{\psi}_f (D[U]+m_f)\psi_f\right]$$
$$= \int [dU_\mu] \prod_f \det(D[U]+m_f) \exp[-S_g]$$

- Fermion fields are anti-commuting, giving the determinant when integrated out

Apply the Monte Carlo method !?

Fermion determinant

- Too hard to evaluate
  - Determinant of a large matrix. Needs to obtain all the eigenvalues ~ N^3

$$\det(D[U]+m) = \prod_k (m + i\lambda_k[U])$$

- Rewrite in favor of bosons

non-local action

$$Z = \int [dU] \det(D[U]+m)^2 e^{-S_g}$$

$$= \int [dU][d\phi] e^{-S_g - \phi^\dagger (D[U]+m)^{-2} \phi} = \int [dU][d\phi] e^{-S_g - |(D[U]+m)^{-1}\phi|^2}$$

  - Reduces to the problem of matrix inversion. Hard, but more tractable.

Matrix inversion

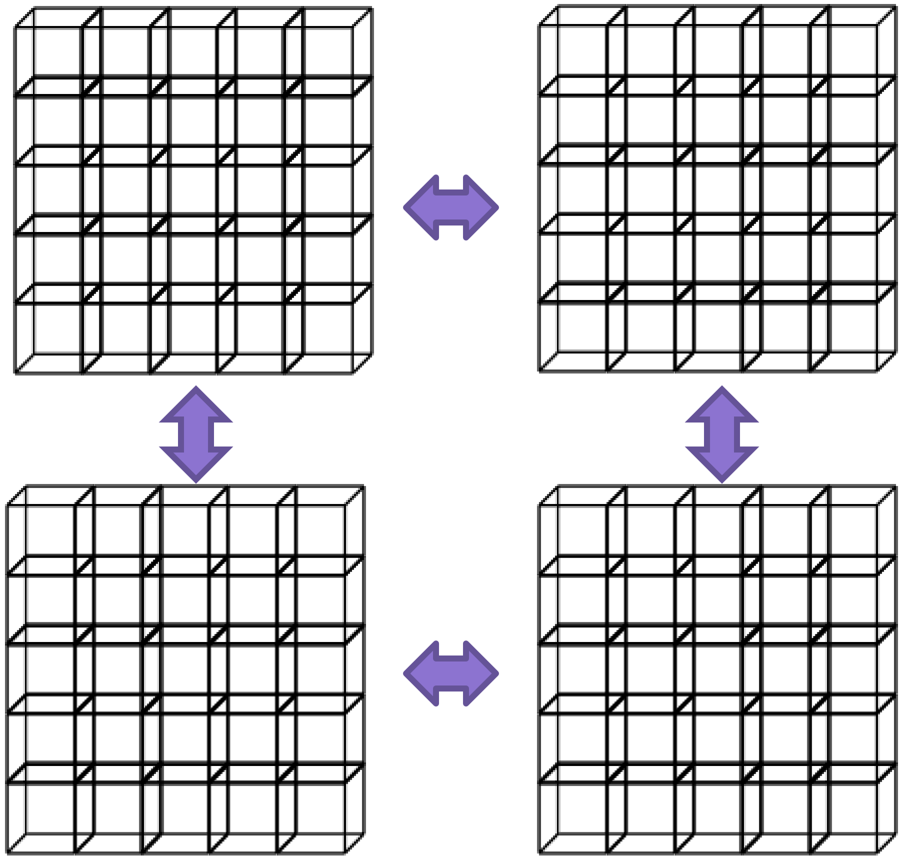
- Most time-consuming part in the LQCD calculations

$$\left(D[U]+m\right)x=b$$

  - $D[U]$: a 4D diffusion-like operator (typically nearest-neighbor)
  - In some cases, use 5D implementation for theoretical virtue
- 4D lattices:
  - Typical size: 64^3x128 x3(color)x4(spinor) = 400 M
  - 1 vector = 7 GB
- Iterative solver:
  - Conjugate Gradient (CG): typically 1,000-10,000 iterations per solve

Big computing

- Parallel computing
  - Conceptually straightforward. Each node is responsible for a small sub-lattice.
  - Not “easy” in practice.
- Code development
  - CPS, Chroma, MILC, …
  - QMP, QDP, QUDA, …
  - openQCD
  - Bridge++, Iroiro++
  - Grid/Hadrons



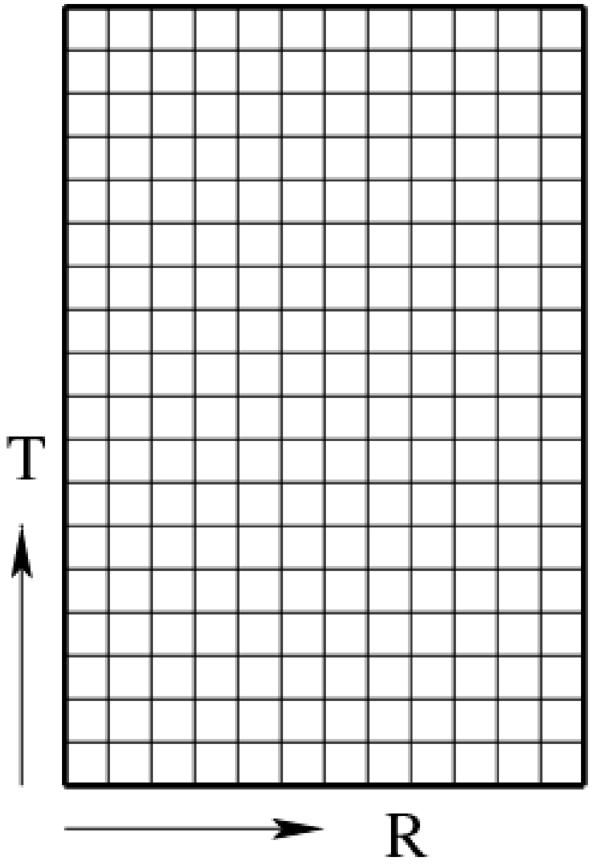
Supercomputer

- Fugaku computer (RIKEN Kobe)

  - General purpose (life, environment, material, etc). Running QCD, too
  - Next generation machine (Fugaku-NEXT) under development.

Basic applications

QCD potential

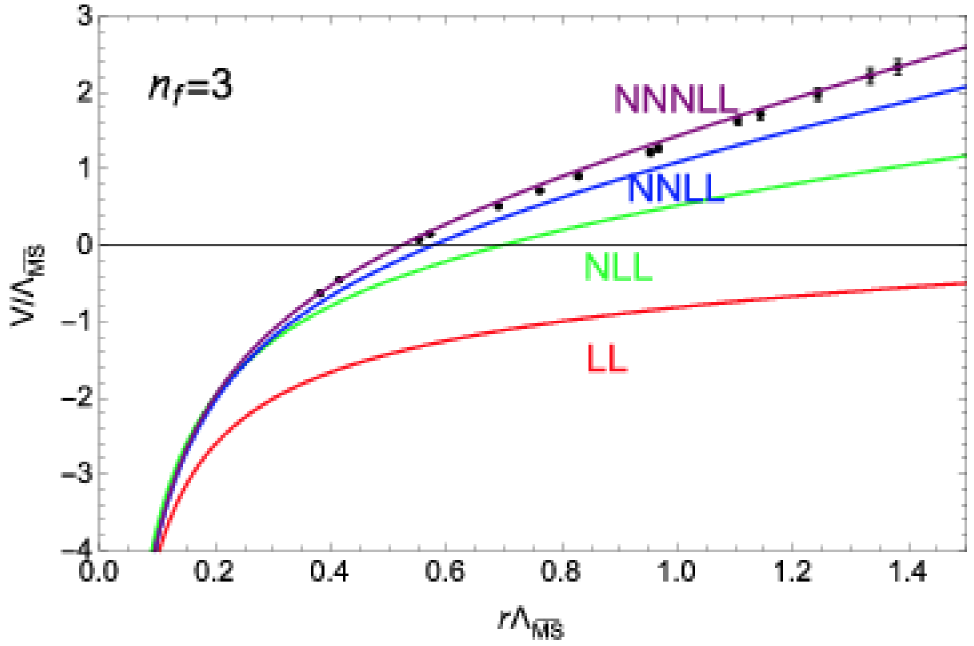


Energy of static QQbar system gives the potential $V(R)$

$$\sim \exp[-V(R)T]$$

Example (N_f=3):

Linearly rising potential at long distances = confinement

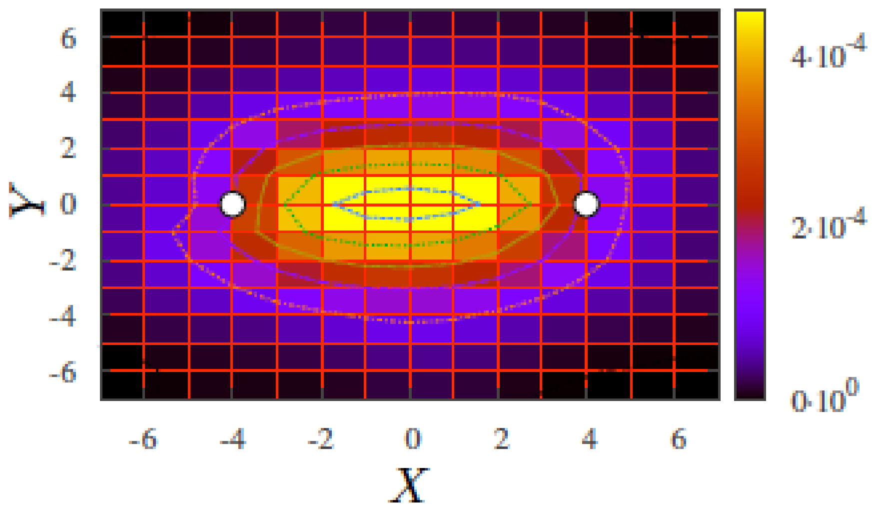


$\sim \sigma r$

Perturbative at short distances: $\sim C_F \dfrac{\alpha_s}{r}$

plot from Takaura et al. (2019)

Quark confinement



Restoration of chiral symmetry inside the flux-tube, Iritani (2015)

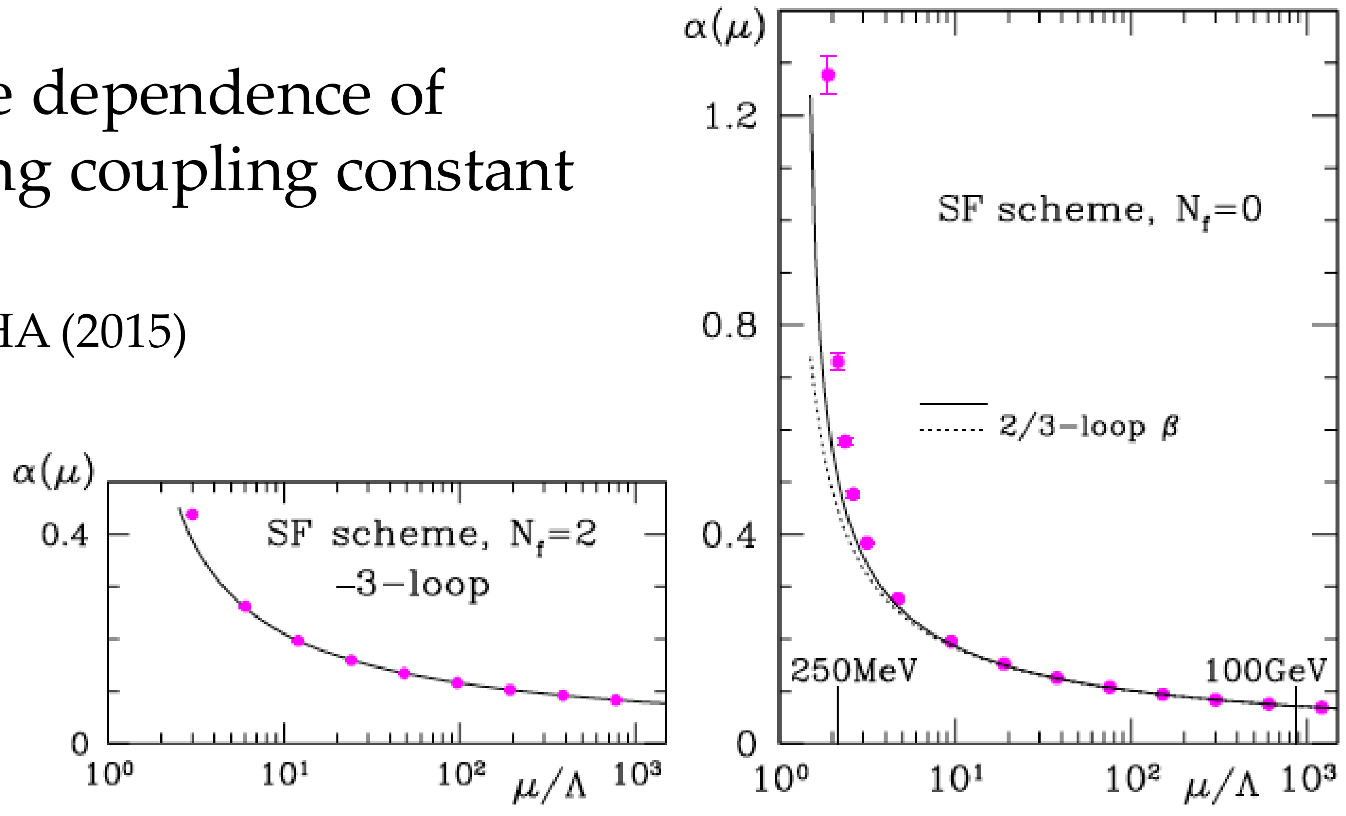
Flux-tube structure is generated between two color sources.

- Constant energy density of the flux-tube implies the linear potential.

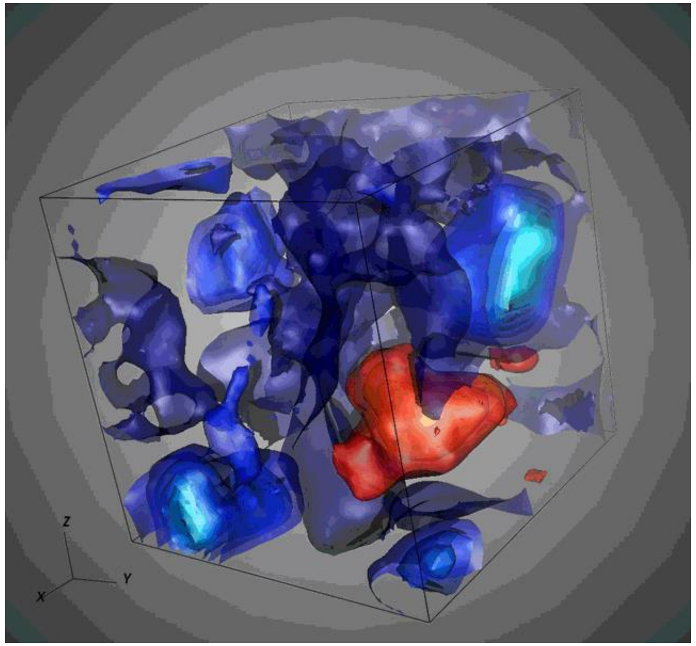
Asymptotic freedom

Scale dependence of
strong coupling constant

ALPHA (2015)



QCD vacuum?



Accumulation of near-zero eigenmodes of quarks leads to

- Chiral condensate

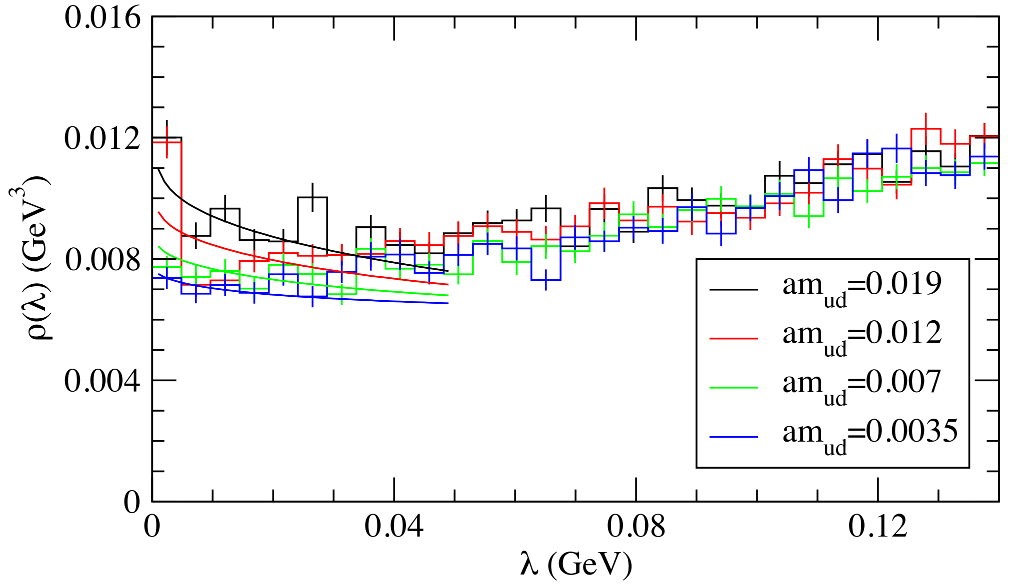
$$\langle \bar{q}q \rangle \neq 0$$

- Order parameter of the spontaneous chiral symmetry breaking.

Dirac spectrum

Eigenvalue distribution of $\not{D}$

$$-\langle \bar{q}q \rangle = \int_0^\infty d\lambda\, \rho(\lambda) \frac{2m}{\lambda^2 + m^2} = \pi\rho(0)$$



$$\Sigma = (270.0 \pm 4.9\ \text{MeV})^3$$

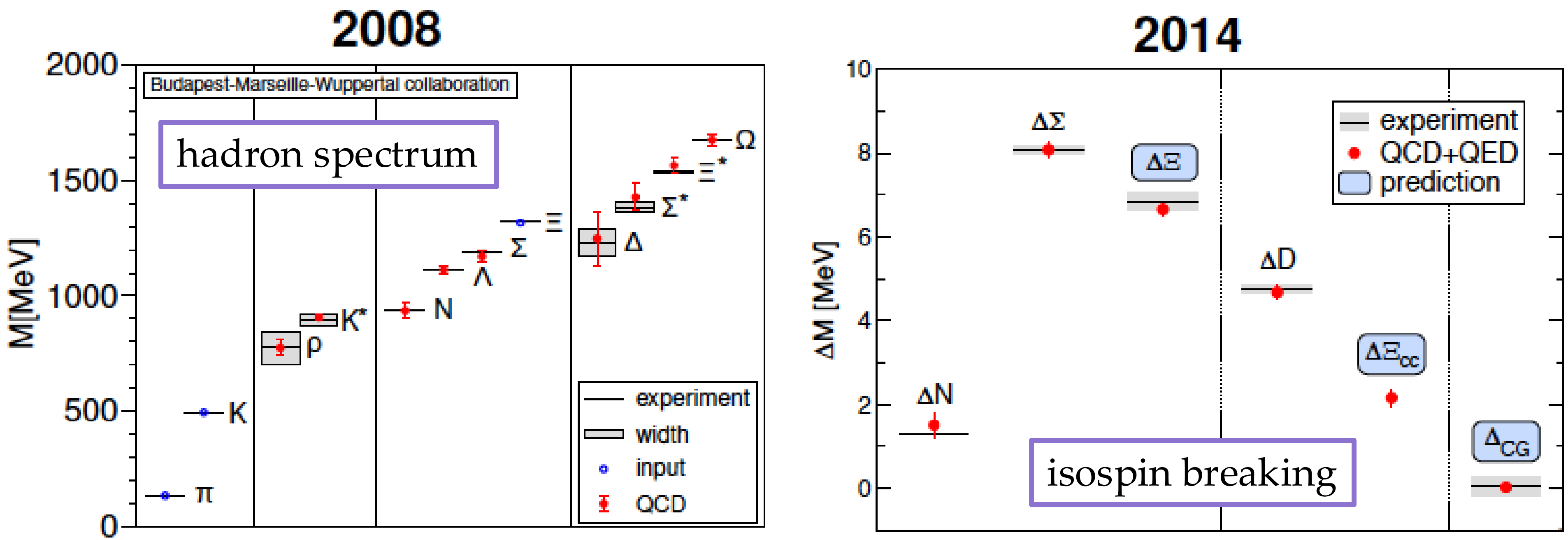
INPUT to LQCD

Parameters in QCD

- Strong coupling constant $\alpha_s(\mu)$
  - Fix the correspondence between the scale and coupling.
  - β is the relevant parameter to control the lattice spacing *a*.
- Light quark masses m_u, m_d, m_s
  - up and down are often assumed to be degenerate.
  - Tuned to reproduce π and K meson masses.
- Heavy quark masses m_c, m_b
  - Usually not in the sea, but changing.
  - Tuned to reproduce J/ψ and Υ masses.

All other quantities are OUTPUT.

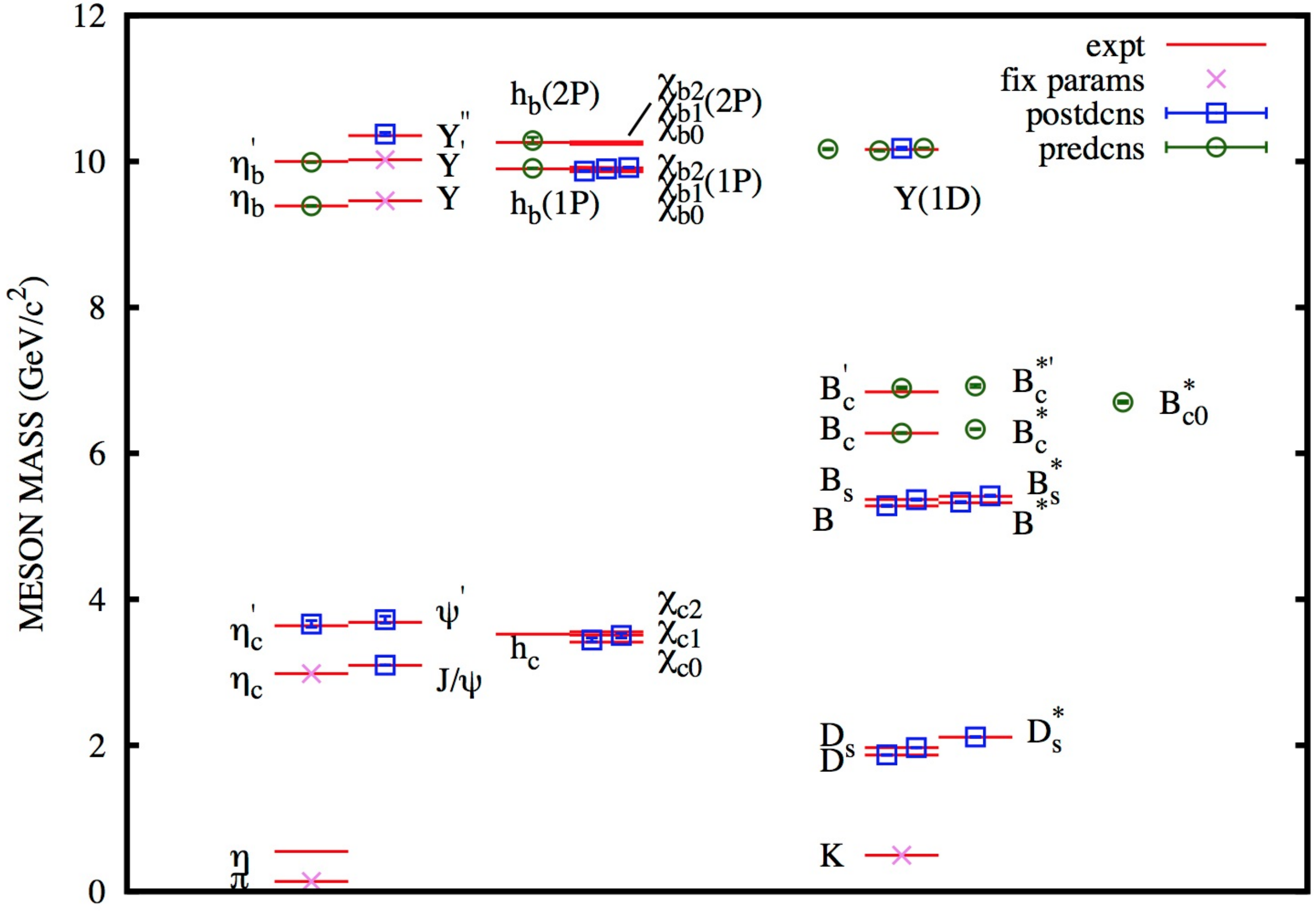
Hadron spectrum



Budapest-Marseille-Wuppertal collaboration, Science (2008, 2015)

Hadron masses

HPQCD (2012-2015)



Crucial question:

Can we expect to get correct solutions from them??

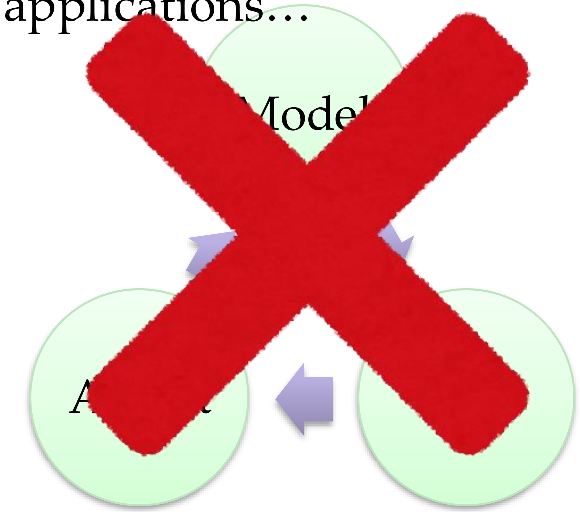
= What are the potential errors?

We believe it's right, because …

Firm theoretical framework = Quantum Field Theory

- Well-defined theory
  - Action (Lagrangian) and partition function
- Exact relations from symmetries
  - Ward-Takahashi identities
- Renormalization theory
  - Model itself is highly restricted.
  - "continuum limit" is unique.

In many other computational applications…



Understanding the errors

Understanding the errors

- Of course, there are practical limitations, which yield (sometimes significant) errors
  - Discretization effect, finite volume effect, statistical error…

- One may **theoretically** understand how the error behaves:
  - One should first confirm that the error is consistent with the expectation.
  - Then, eliminate it, e.g. by an extrapolation.

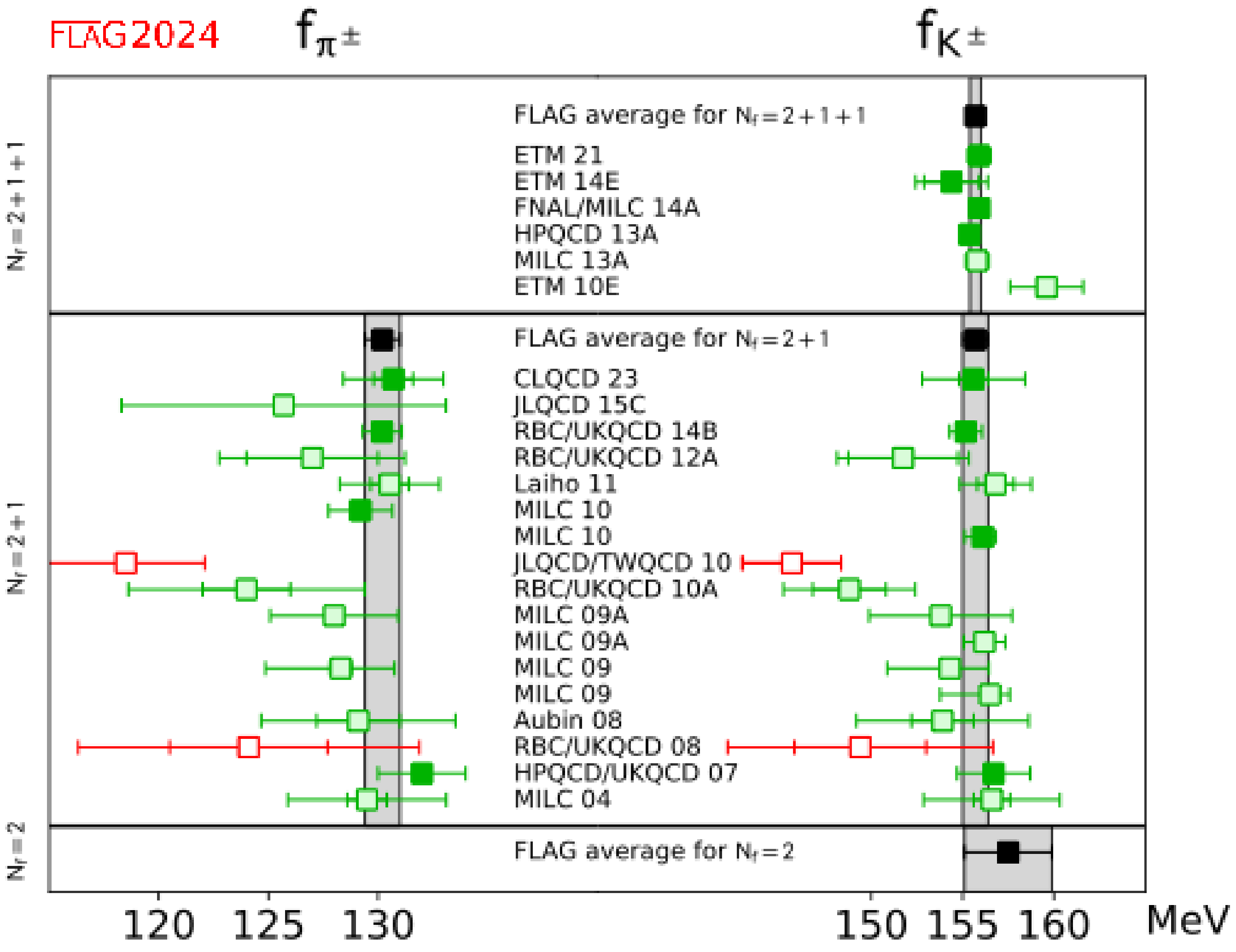
This is an ideal situation, though…

Systematic errors ~ Who cares?

Flavour Lattice Averaging Group (FLAG)

- Provides lattice average of various quantities
- Regularly updating: 2010, 2013, 2016, 2019, 2021, 2024
- Assesses the ability of controlling the systematic errors

FLAG 2024 Flavour Lattice Averaging Group


FLAG2024
$f_{\pi^\pm}$
$f_{K^\pm}$
FLAG average for $N_f=2+1+1$
ETM 21
ETM 14E
FNAL/MILC 14A
HPQCD 13A
MILC 13A
ETM 10E
FLAG average for $N_f=2+1$
CLQCD 23
JLQCD 15C
RBC/UKQCD 14B
RBC/UKQCD 12A
Laiho 11
MILC 10
MILC 10
JLQCD/TWQCD 10
RBC/UKQCD 10A
MILC 09A
MILC 09A
MILC 09
MILC 09
Aubin 08
RBC/UKQCD 08
HPQCD/UKQCD 07
MILC 04
FLAG average for $N_f=2$
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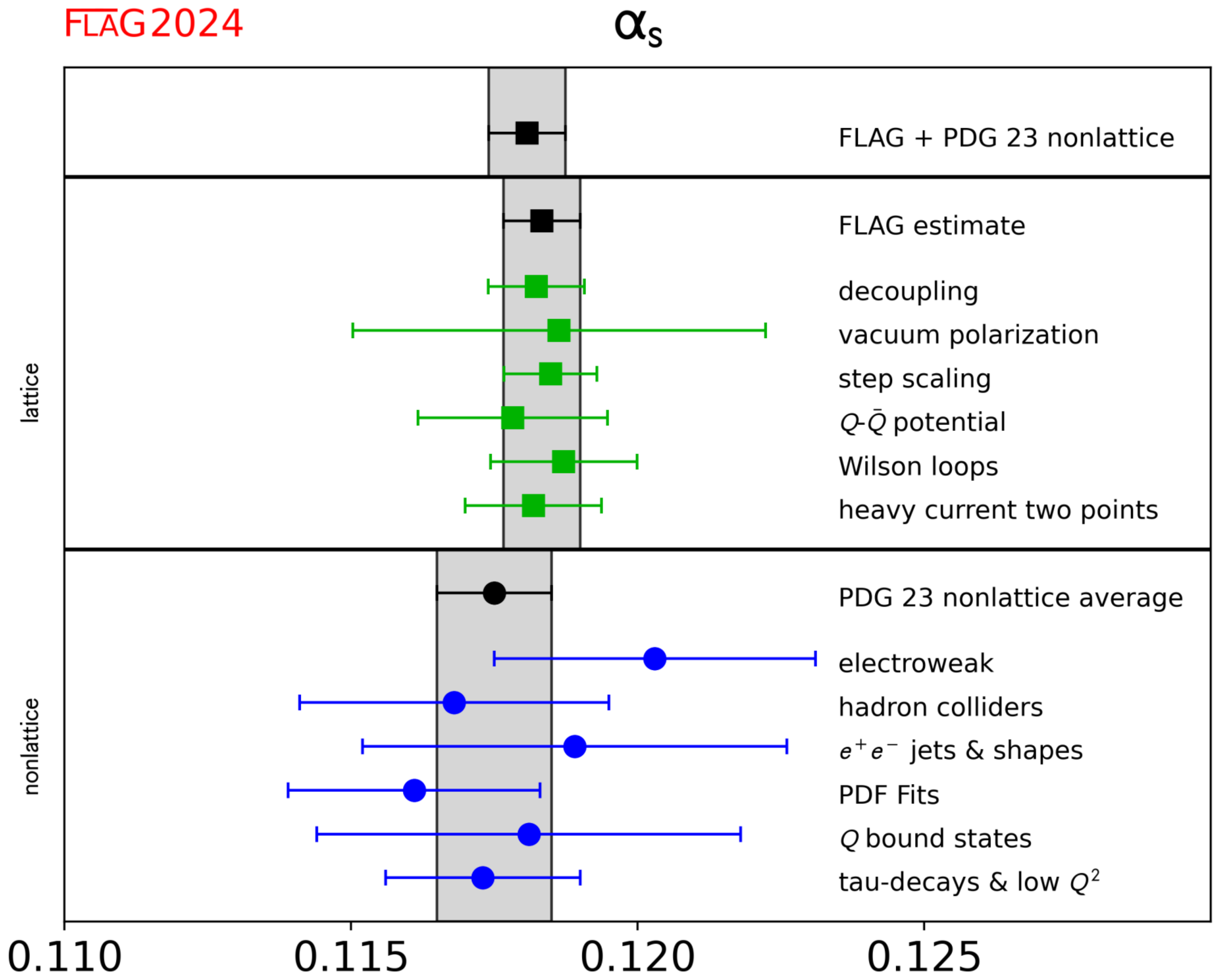
120 125 130
150 155 160
MeV


FLAG2024
αs
FLAG + PDG 23 nonlattice
FLAG estimate
decoupling
vacuum polarization
step scaling
Q-Q̄ potential
Wilson loops
heavy current two points
PDG 23 nonlattice average
electroweak
hadron colliders
e+e− jets & shapes
PDF Fits
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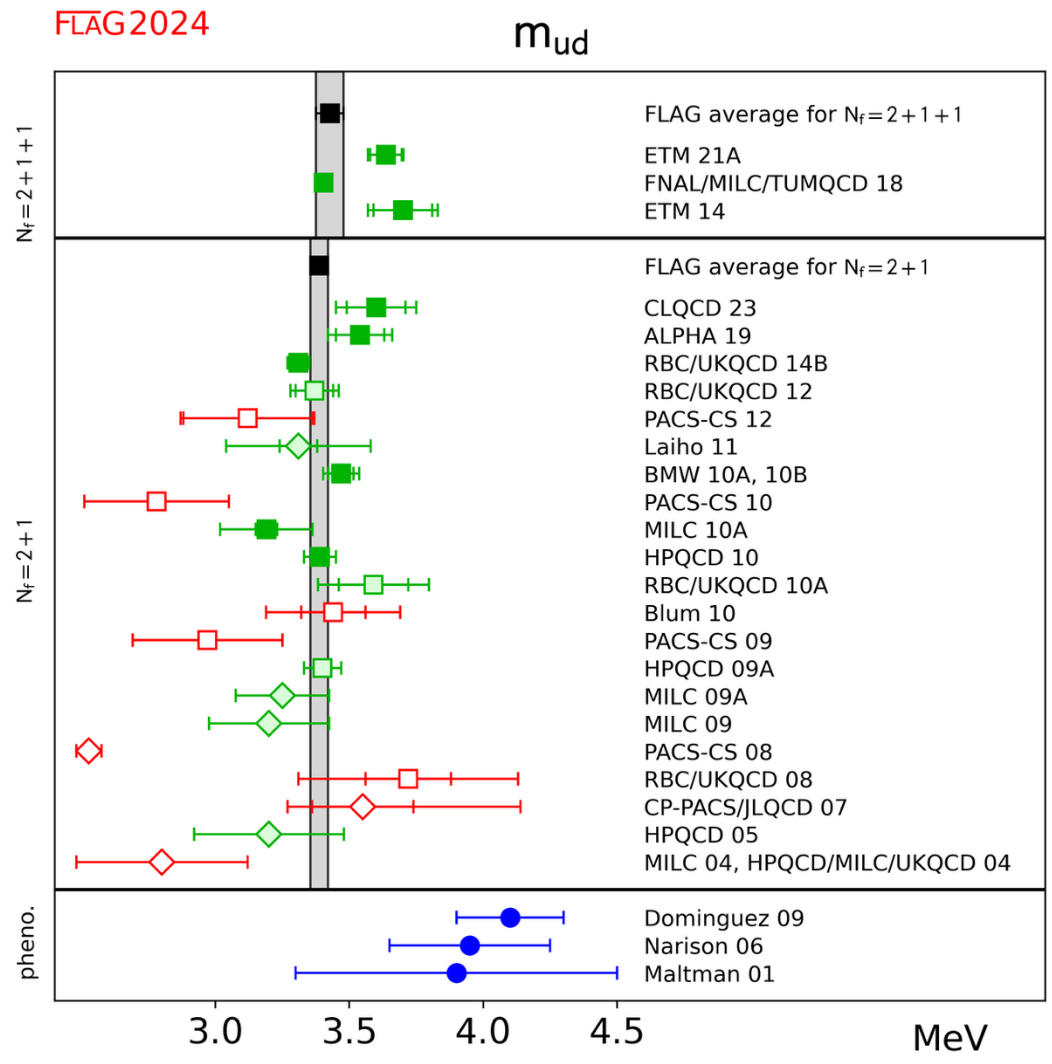
FLAG2024
m_{ud}
FLAG average for $N_f=2+1+1$
ETM 21A
FNAL/MILC/TUMQCD 18
ETM 14
FLAG average for $N_f=2+1$
CLQCD 23
ALPHA 19
RBC/UKQCD 14B
RBC/UKQCD 12
PACS-CS 12
Laiho 11
BMW 10A, 10B
PACS-CS 10
MILC 10A
HPQCD 10
RBC/UKQCD 10A
Blum 10
PACS-CS 09
HPQCD 09A
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
CP-PACS/JLQCD 07
HPQCD 05
MILC 04, HPQCD/MILC/UKQCD 04
Dominguez 09
Narison 06
Maltman 01
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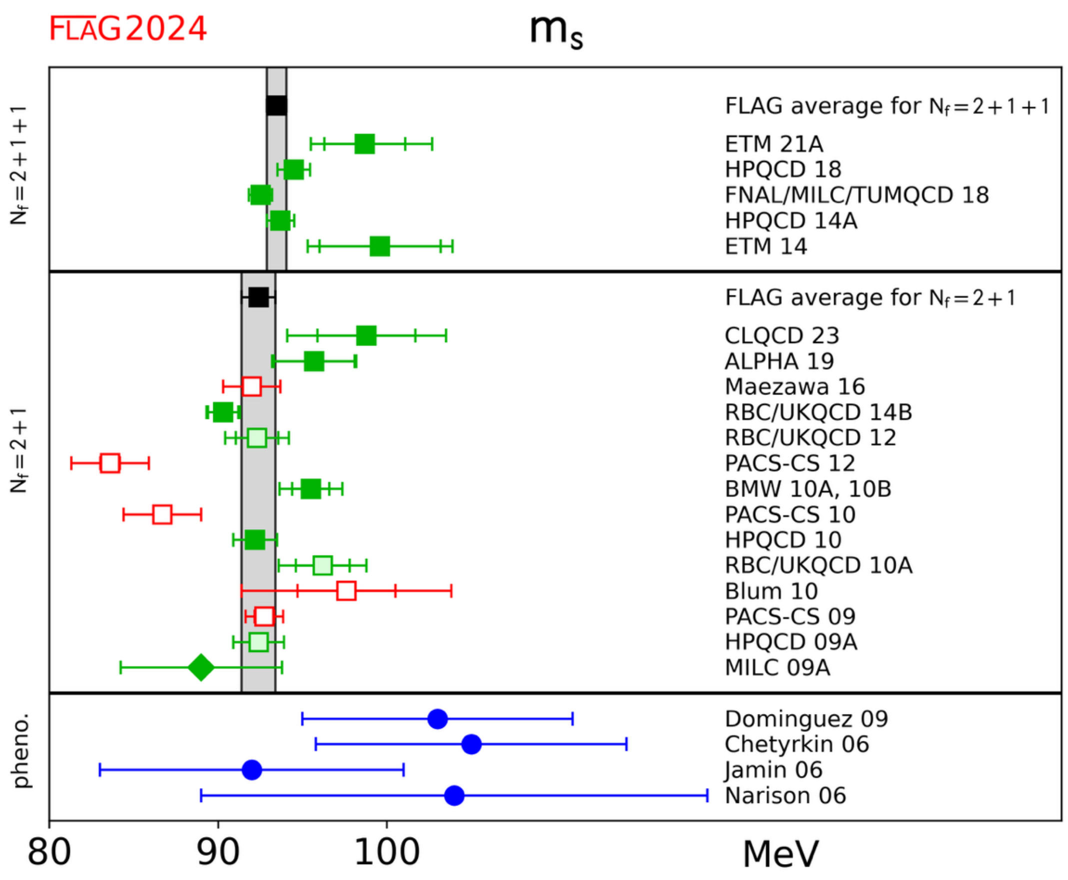
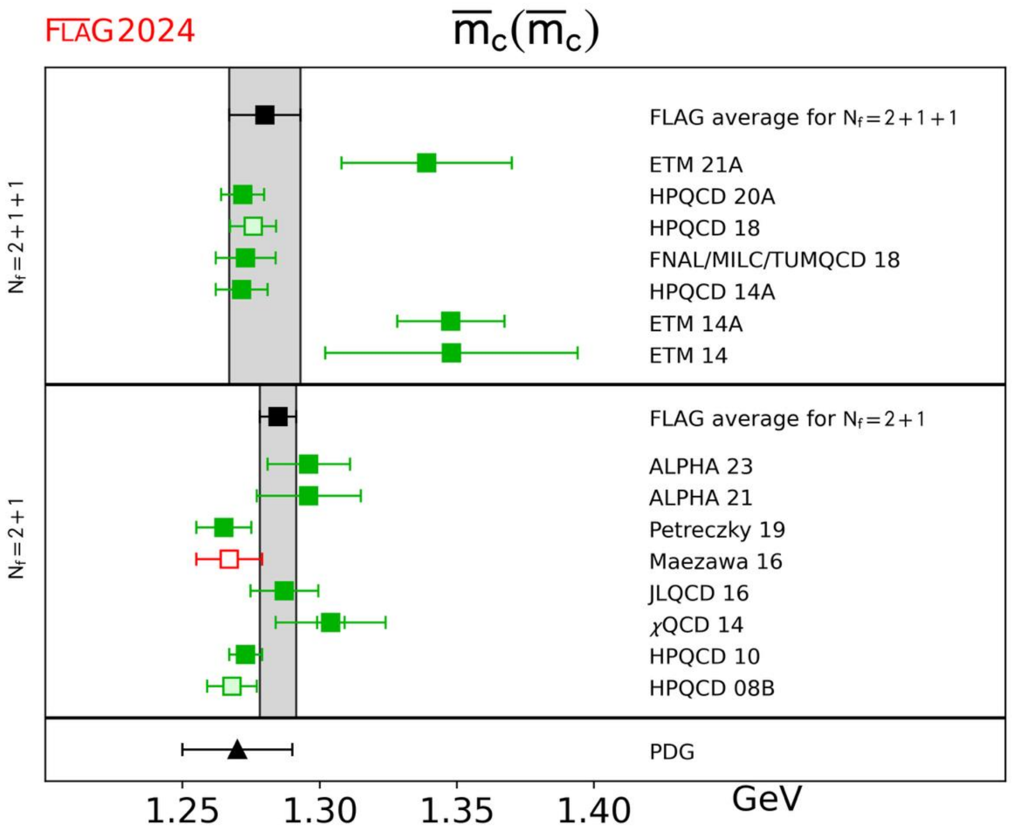
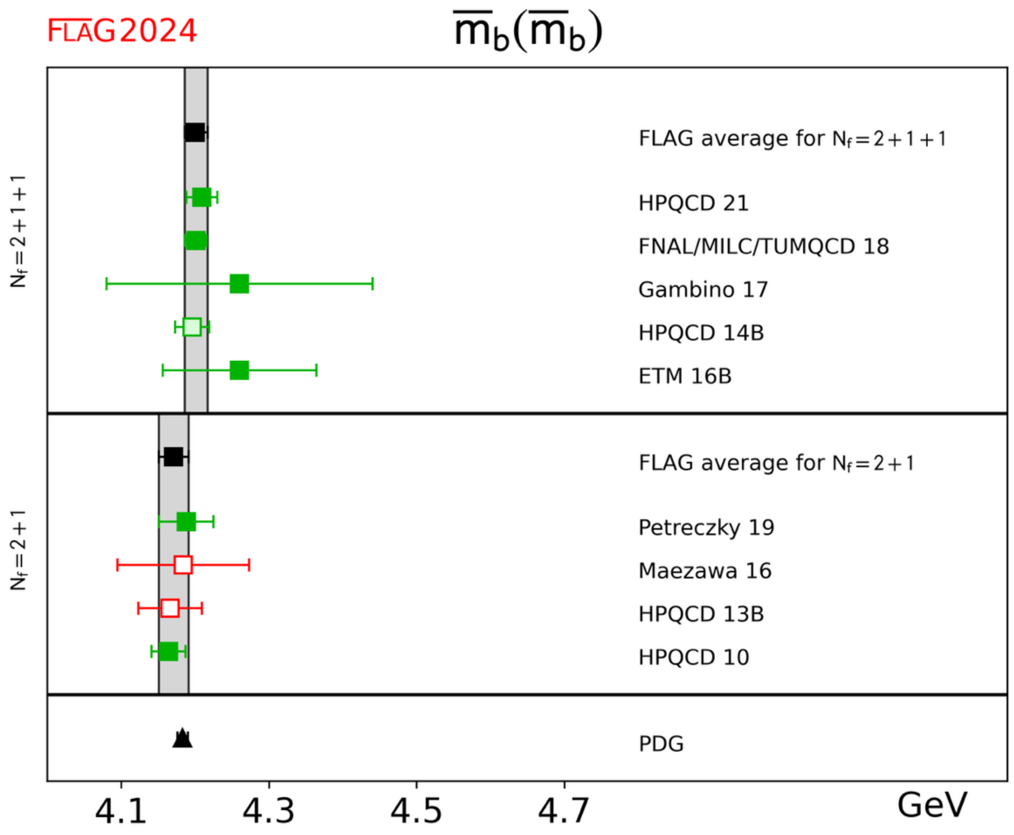
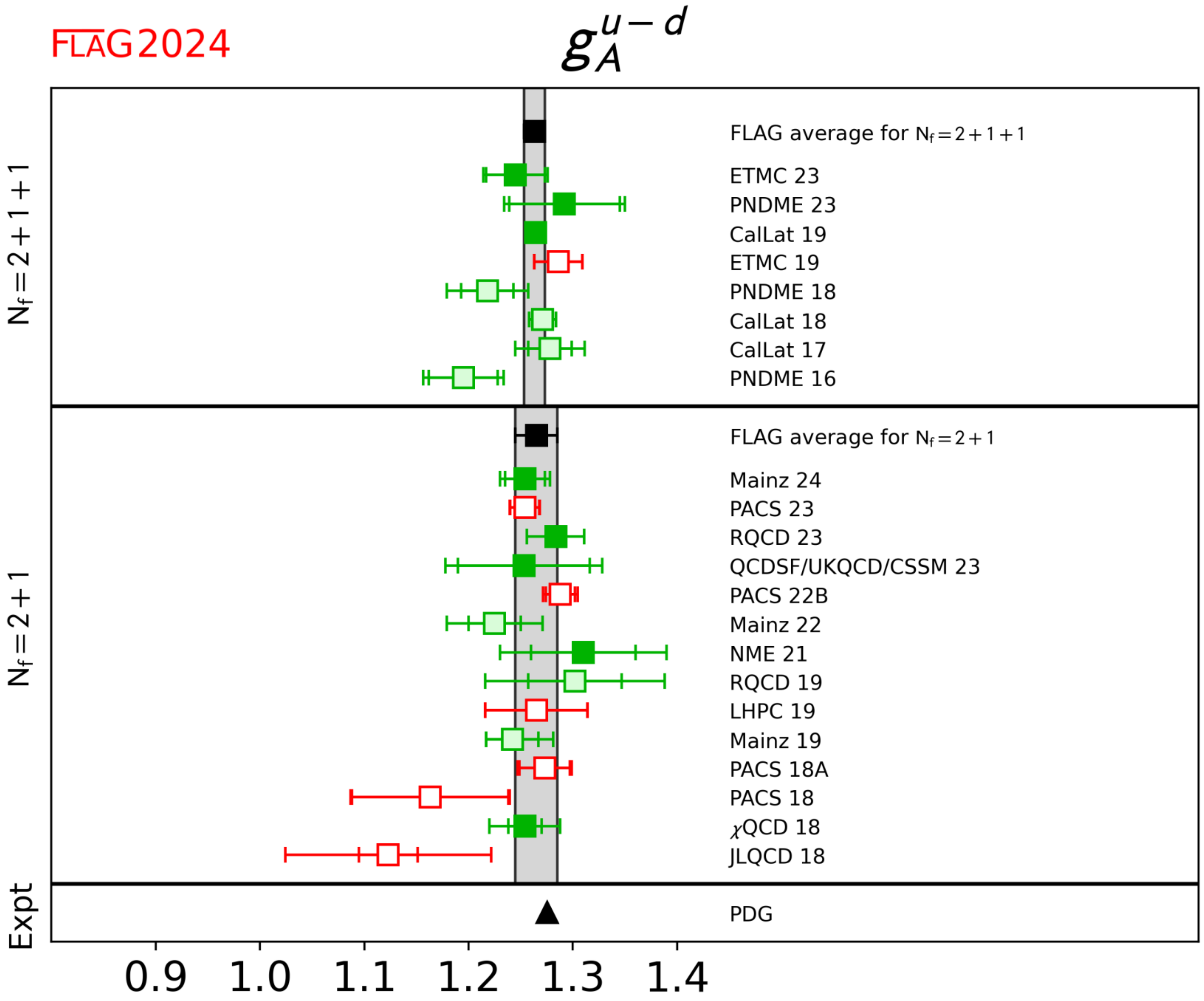
$N_f=2+1$
pheno.
3.0
3.5
4.0
4.5
MeV

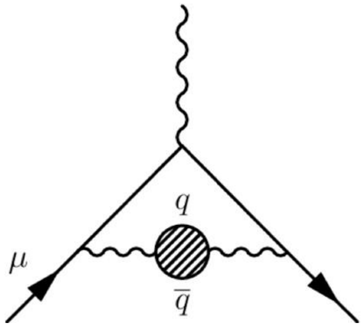

FLAG2024
m_s
FLAG average for $N_f=2+1+1$
ETM 21A
HPQCD 18
FNAL/MILC/TUMQCD 18
HPQCD 14A
ETM 14
FLAG average for $N_f=2+1$
CLQCD 23
ALPHA 19
Maezawa 16
RBC/UKQCD 14B
RBC/UKQCD 12
PACS-CS 12
BMW 10A, 10B
PACS-CS 10
HPQCD 10
RBC/UKQCD 10A
Blum 10
PACS-CS 09
HPQCD 09A
MILC 09A
Dominguez 09
Chetyrkin 06
Jamin 06
Narison 06
$N_f=2+1+1$
$N_f=2+1$
pheno.
80
90
100
MeV

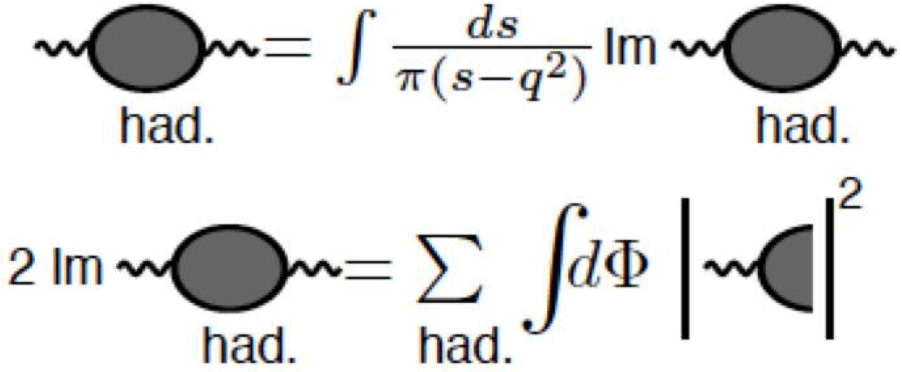

FLAG2024
$\overline{m}_c(\overline{m}_c)$
FLAG average for $N_f=2+1+1$
ETM 21A
HPQCD 20A
HPQCD 18
FNAL/MILC/TUMQCD 18
HPQCD 14A
ETM 14A
ETM 14
FLAG average for $N_f=2+1$
ALPHA 23
ALPHA 21
Petreczky 19
Maezawa 16
JLQCD 16
χQCD 14
HPQCD 10
HPQCD 08B
PDG
$N_f=2+1+1$
$N_f=2+1$
1.25
1.30
1.35
1.40
GeV

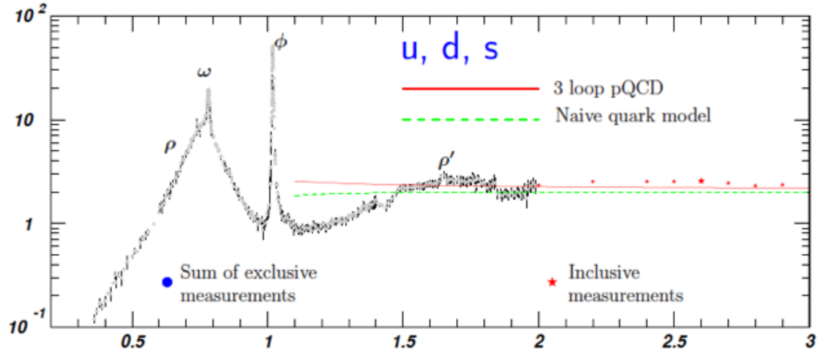

FLAG2024
$\overline{m}_b(\overline{m}_b)$
FLAG average for $N_f=2+1+1$
HPQCD 21
FNAL/MILC/TUMQCD 18
Gambino 17
HPQCD 14B
ETM 16B
FLAG average for $N_f=2+1$
Petreczky 19
Maezawa 16
HPQCD 13B
HPQCD 10
PDG
$N_f=2+1+1$
$N_f=2+1$
4.1
4.3
4.5
4.7
GeV


FLAG2024
g_A^{u-d}
FLAG average for $N_f = 2+1+1$
ETMC 23
PNDME 23
CalLat 19
ETMC 19
PNDME 18
CalLat 18
CalLat 17
PNDME 16
$N_f = 2+1+1$
FLAG average for $N_f = 2+1$
Mainz 24
PACS 23
RQCD 23
QCDSF/UKQCD/CSSM 23
PACS 22B
Mainz 22
NME 21
RQCD 19
LHPC 19
Mainz 19
PACS 18A
PACS 18
χQCD 18
JLQCD 18
$N_f = 2+1$
Expt
PDG
0.9
1.0
1.1
1.2
1.3
1.4

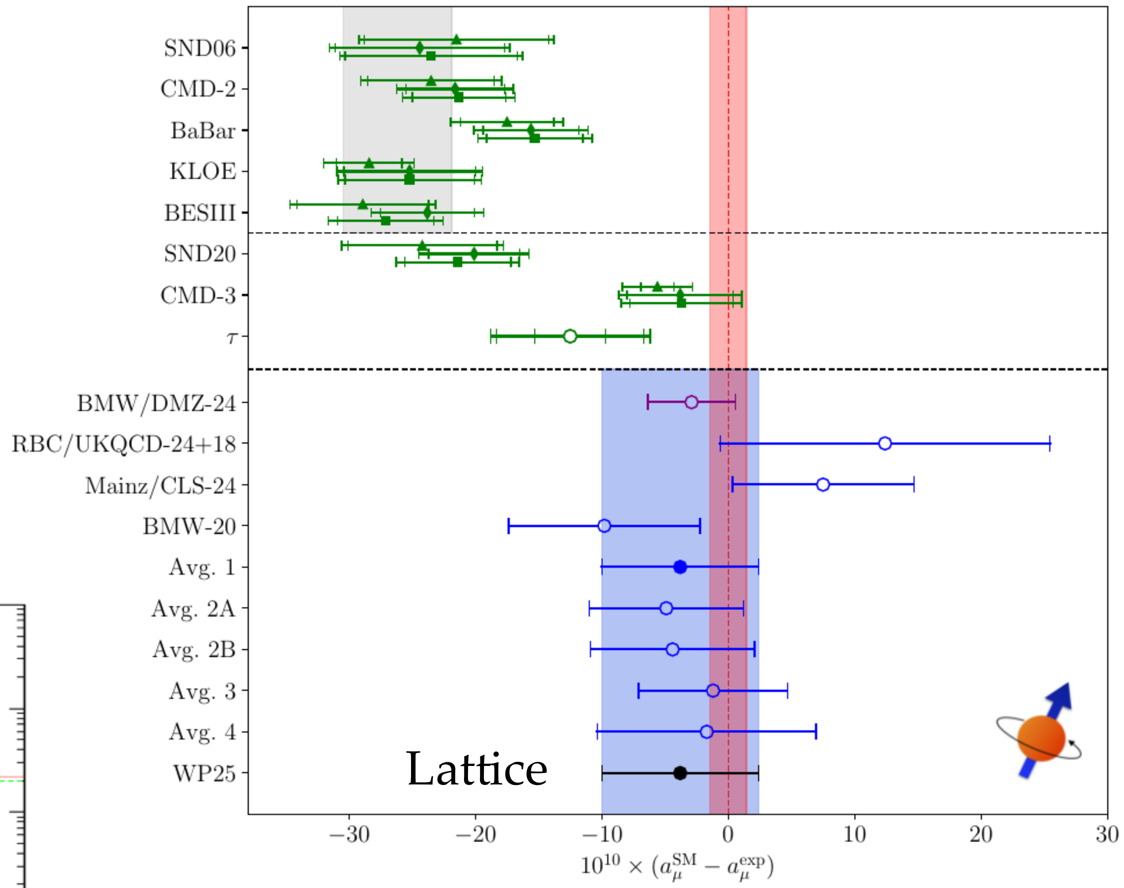
Muon g-2







White Paper: 2505.21476



Reasons to believe?

- Foundation is solid
  - QFT well-defined, Renormalizable theory
- Systematic errors
  - May be understood again using QFT.
  - Every efforts to control them going on.
- Statistical errors
  - Sometimes crucial, killing, fatal…