

# From Random Numbers to the Physics of Hadrons

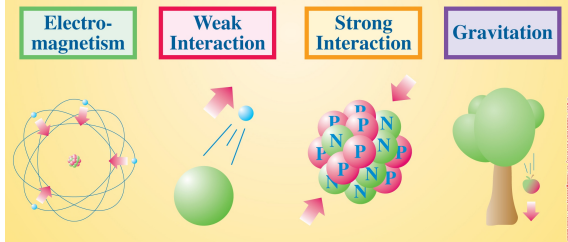
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April 3, 2019

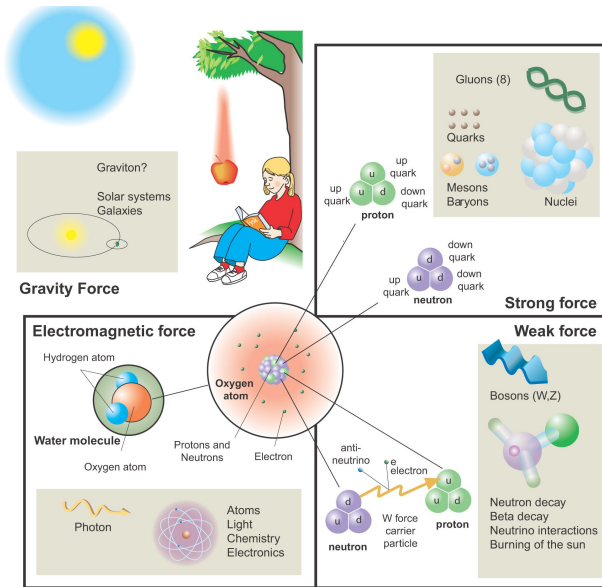
Perlen der Physik, Physikalisch-Astronomische Fakultät, FSU Jena

## The Four Fundamental Forces of Nature



Credits: Stichting Maharishi University of Management, the Netherlands

# Fundamental forces ... for physicists



Credits: [www.nobelprize.org](http://www.nobelprize.org)

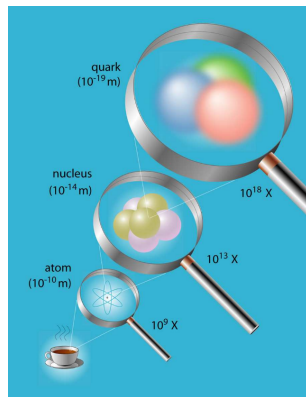
# What makes us confident about the existence of quarks?

## Fun facts:

- Neither quarks nor gluons ever observed as free particles (confinement)
- Only hadrons can be detected (bound states of quarks and gluons)
  - ▶ Mesons:  $\bar{q}q$ -states ( $\pi^{\pm 0}, K^{\pm}, \dots$ )
  - ▶ Baryons:  $qqq$ -states ( $p, n, \dots$ )
  - ▶ Anti-Baryons:  $\bar{q}\bar{q}\bar{q}$ -states ( $\bar{p}, \dots$ )
- Typical hadron size:  $\sim 1$  fm

## Wrap it up!

- Scattering experiments are our “magnifying-glass”
- Ab initio QCD calculation agree with experimental observations (will show you examples)



# Scattering experiments

## Elastic $e^- p \rightarrow e^- p$ scattering

(Considered as Coulomb scattering)

- both point-like particles
- no recoil of proton ( $\vec{p}' = 0$ )

## Rutherford Scattering

(point-like, spin-less particles, non-relativistic)

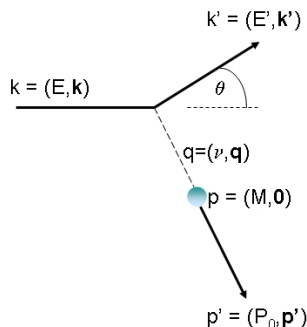
$$\frac{d\sigma}{d\Omega}_{\text{Rutherford}} = \frac{\alpha^2}{4E^2 \sin^4 \theta/2}$$

## Mott-Scattering

( $e^-$  with spin and relativistic)

$$\frac{d\sigma}{d\Omega}_{\text{Mott}} \simeq \frac{\alpha^2}{4E^2 \sin^4 \theta/2} \cos^2 \frac{\theta}{2}$$

Dirac-Scattering (both have spin-1/2)



# Scattering experiments

## Elastic $e^-p \rightarrow e^-p$ scattering

- Proton: extended object at rest (charge distributed, no recoil)

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma}{d\Omega}_{Mott} |F(\vec{q}^2)|^2$$

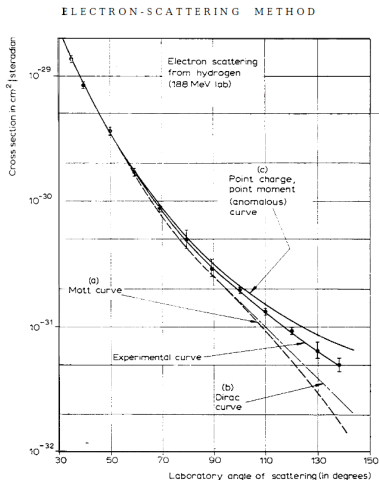
- $F(\vec{q}^2)$  form factor is Fourier transform of charge distribution

$$F(\vec{q}^2) = \int \rho(\vec{r}) e^{i\vec{q}\vec{r}} d^3r$$

- At low  $\vec{q}^2$ , deviations from 1 measure for proton charge radius

$$F(\vec{q}^2) \xrightarrow{\vec{q}^2 \simeq 0} 1 - \frac{1}{6} \vec{q}^2 \langle r^2 \rangle + \dots$$

- Experiment by Hofstadter 1954: First evidence **proton has a finite size** ( $\sim 0.74 \text{ fm}$ )



Hofstadter (Nobel lecture 1961)

# Scattering experiments

## Elastic $e^- p \rightarrow e^- p$ scattering

Rosenbluth-Formula (Lorentz-invariant)

$$\frac{d\sigma}{d\Omega} = \frac{\alpha^2}{4E^2 \sin^4 \theta/2} \frac{E'}{E} \left( \frac{G_E^2 + \tau G_M^2}{1 + \tau} \cos^2 \frac{\theta}{2} + 2\tau G_M^2 \sin^2 \frac{\theta}{2} \right) \quad \tau = -\frac{q^2}{2M_p^2}$$

- Electron ( $m_e = 0$ ) point-like, proton extended recoiling object, both have spin
- Two elastic form factors (functions of  $q^2$ )

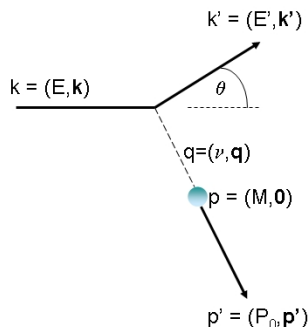
$$G_E(q^2) \xrightarrow{\tau \ll 1} \int e^{i\vec{q}\vec{r}} \rho(\vec{r}) d^3r \stackrel{(q^2=0)}{=} 1$$

$$G_M(q^2) \xrightarrow{\tau \ll 1} \int e^{i\vec{q}\vec{r}} \mu(\vec{r}) d^3r \stackrel{(q^2=0)}{=} 2.79$$

- 4-momentum transfer

$$q^2 = (k - k')^2 \stackrel{(m_e=0)}{\simeq} -4EE' \sin^2 \frac{\theta}{2}$$

- Anomalous magnetic moment of proton another evidence for not being point-like
- But: does not prove substructure

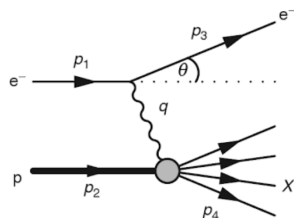


# High-energy scattering experiments

## Inelastic scattering

- Collision become inelastic when  $E_{e^-} > 1 \text{ GeV}$   
(SLAC, 1968:  $E_{e^-} = 5 - 20 \text{ GeV}$ )
- Invariant mass:  $p_4^2 = (p_2 + q)^2$   
(virtual photon:  $Q^2 = -q^2 > 0$ )
- Two degrees of freedom, e.g.,

$$x = -q^2 / (2p_2 \cdot q), \quad y = q \cdot p_2 / p_1 \cdot p_2$$



## Deep inelastic scattering ( $Q^2 \gg m_p^2 y^2$ )

$$\frac{d^2\sigma}{dx dQ^2} \simeq \frac{4\pi\alpha^2}{Q^4} \left[ (1-y) \frac{F_2(x, Q^2)}{x} + y^2 F_1(x, Q^2) \right]$$

## Observation

$$F_i(x, Q^2) \rightarrow F_i(x) \quad \text{Bjorken scaling}$$

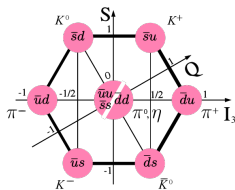
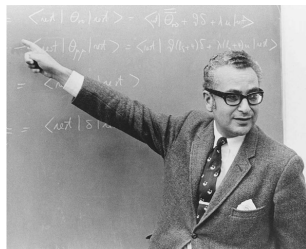
$$F_2(x) = 2F_1(x) \quad \text{Callan-Cross relation}$$

Photon scatters elastically from spin-1/2 constituent particles (partons) within proton

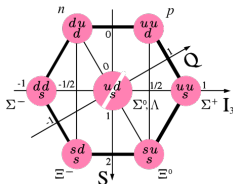


# Quark Modell — Eightfold Way of Gell-Mann (1962)

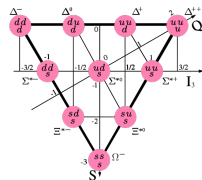
- Many hadrons are known (quantum number, masses)
- Fit to representations of  $SU_F(3)$  groups  
 $3 \otimes \bar{3}$  (mesons)  $3 \otimes 3 \otimes 3$  (baryons)
- If so, particles (quarks) forming fundamental representation must exist.



Spin-0 mesons (nonet)



Spin-1/2 baryons (octet)



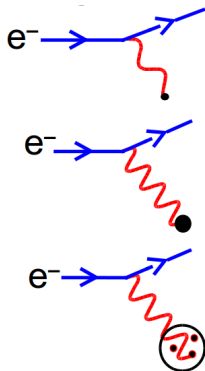
Spin-3/2 baryons (decuplet)

Today understood as flavor symmetry

## Scattering experiments: Summary

$e^- p \rightarrow e^- p$  scattering: nature of interaction of the virtual  $\gamma$  with proton depends on wavelength (or  $Q^2$ )

- Scattering at very low  $e^-$  energies ( $\lambda \gg r_p$ ) equivalent to scattering with point-like spin-less particle
- At low  $e^-$  energies ( $\lambda \sim r_p$ ) scattering equivalent to that from extended charged object
- At high  $e^-$  energies the wavelength ( $\lambda < r_p$ ) Scattering from constituent quarks (partons). Used to resolve sub-structure of proton.

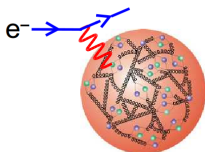


**Partonic picture** of proton result of SLAC deep inelastic scattering.

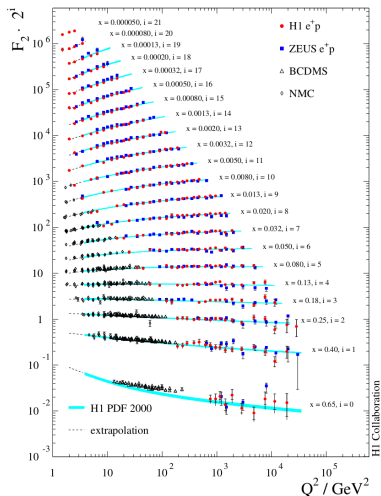
# Scattering experiments: Fast-forward many years

**At very high energies** ( $\lambda \ll r_p$ ):  
Proton looks like sea of quarks & gluons.

$$\frac{d^2\sigma}{dx dQ^2} \simeq \frac{4\pi\alpha^2}{2xQ^4} [1 + (1-y)^2] F_2(x, Q^2)$$



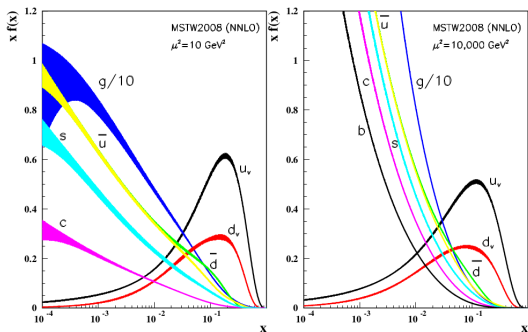
- $F_2$  not a delta-function  
(not all quarks have  $x = 1/3$ )
- Can calculate  $Q^2$ -dependence caused by  
dynamics of quarks and gluons



**QCD:** quarks have color charge and interact via colored gluons as described by QCD  
(theory of the strong interaction)

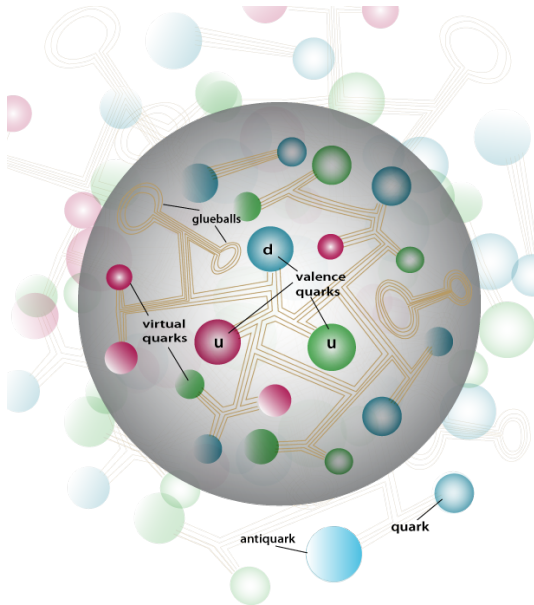
## Parton distribution function

Probability distribution of quarks and gluons in (fast moving) proton with momentum fraction  $x$



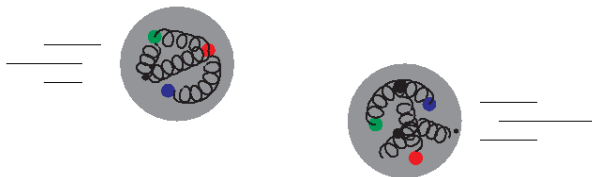
- Parton model: all quarks have  $x = 1/3 \rightarrow F_2 = \text{delta-function}$
- Extract  $f(x)$  from measurements of proton / neutron structure function
- Cannot predicted them from the theory (nonperturbative), only approximate
- deviations of parton distribution with  $Q^2$  well described by QCD

# Proton



# Strong-interaction process

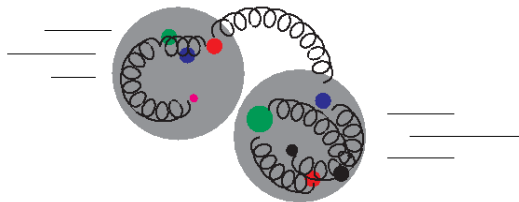
Animation of proton-proton collision



From Richard Ruiz <http://www.quantumdiaries.org/tag/qcd/>

# Strong-interaction process

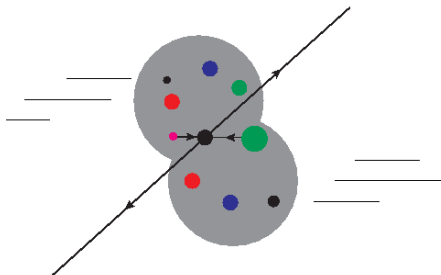
Animation of proton-proton collision



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# Strong-interaction process

Animation of proton-proton collision

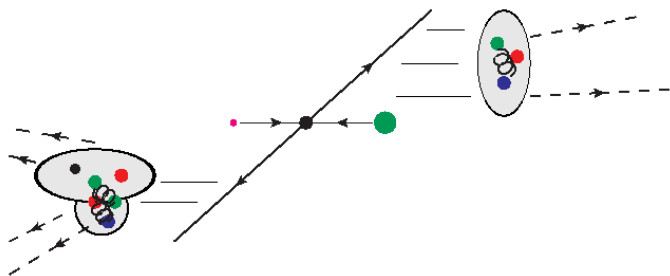


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# Strong-interaction process

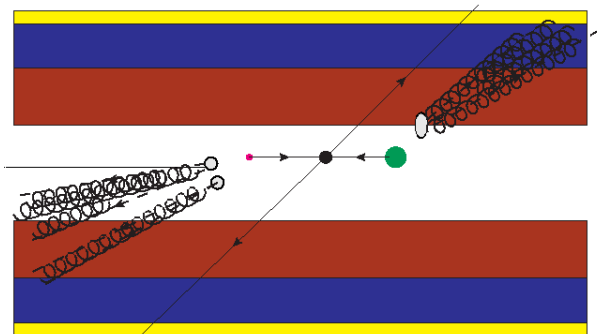
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# Strong-interaction process

Animation of proton-proton collision



From Richard Ruiz <http://www.quantumdiaries.org/tag/qcd/>



# Quantum Chromodynamic (QCD)

**Lagrange density** describes dynamics of quarks and gluons (Euclidean)

$$\mathcal{L}_{\text{QCD}} = \frac{1}{4} F_{\mu\nu}^a[A] F^{\mu\nu,a}[A] - \bar{\psi} (\gamma_\mu D_\mu[A] - m) \psi$$

- Field strength tensor:  $F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - g_s f^{abc} A_\mu^b A_\nu^c$
- **Gluons:**  $A_\mu^a$  (massless gauge bosons, color-charge  $\rightarrow$  self-int)
- **Fermions:**  $\psi_a^f, \bar{\psi}_a^f$  (quark and anti-quark)  
(Flavour:  $f = u, d, s, c, b, t$ , Color:  $a = r, g, b$ )
- invariant under gauge transformations

**Parameters** (scale & ren-scheme dependent, fixed through experiment)

- Strong coupling constant:  $g_s$
- Quark masses:  $m = \text{diag}(m_u, m_d, m_s, \dots)$

**Action** (Euclidean)

$$\mathcal{S}_{\text{QCD}} = \int d^4x \mathcal{L}_{\text{QCD}}$$

# Path integral formalism

## Quantization of a generic field theory

**Partition function** of a Euclidean QFT as a path integral (formally)

$$Z = \int D\Phi e^{-S(\Phi)}$$

- $\Phi$  denotes all fields of the theory,  $S(\Phi)$  is the action
- “formally” because integral may not be defined a priori
- $D\Phi$  integration over all paths

→ on a finite lattice with  $N$  sites:  $\int D\Phi \equiv \int \cdots \int \prod_{i=1}^N d\Phi_i$

**Expectation value** of an observable

$$\langle \mathcal{O} \rangle = \int D\Phi \mathcal{O}[\Phi] e^{-S(\Phi)}$$

# Path integral formalism

Sketch for QCD

## Partition function (formally)

$$Z = \int DA_\mu \int D\psi D\bar{\psi} e^{-(S_G+S_F)}$$

- $S_G$  ... Euclidean gauge action

$$S_G[A] = \frac{1}{4} \int d^4x F_{\mu\nu}^a[A] F_{\mu\nu}^a[A],$$

- $S_F$  ... fermion action:  $\psi^{(f)}$  where  $f = \{u, d, s, \dots\}$

$$S_F = \int dx^4 \bar{\psi} \underbrace{(\gamma_\mu D_\mu + m_0)}_{\text{"fermion matrix" } M} \psi \quad \text{where } D_\mu = \partial_\mu + ig_0 A_\mu$$

- "formally" because integral over  $DA$  not defined a priori (gauge invariance)
  - ▶ have to fix a gauge (perturbation theory)  $\rightarrow$  additional terms to action
  - ▶ physical observables independent of gauge
  - ▶ often covariant gauges (unique in the context of perturbation theory)

$$S_{\text{fix}} = \frac{1}{2\xi^2} (\partial_\mu A_\mu)^2 + (\partial_\mu \bar{\chi}) D_\mu \chi$$

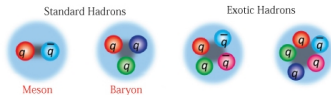
# Main difficulties (compared to QED calculations)

## High-energy physics experiments

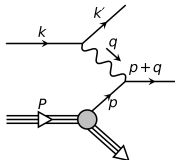
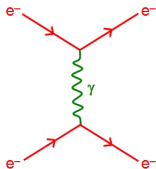
(perturbative regime of QCD)

- Strong coupling much larger ( $\alpha_s \sim 0.1$  vs.  $\alpha \sim 1/137$ )
- $\alpha_s$  constant grows for decreasing energy-momentum transfer
- Loop expansions much more involved (self-interactions of gluons)
- Hadrons are bound states (no free quark nor gluons ever observed)

- 1 Mesons:  $q\bar{q}$  ( $\pi^{\pm 0}, \dots$ )
- 2 Baryons:  $qqq$  ( $P, N, \dots$ )



- quarks and gluons interact strongly, and electro-weak with the other elementary particles



## Experimental Side

- Hadron properties
- Scattering experiments
- High-Temperature / density
- ...

## Theory

- Quantum Chromodynamic (QCD)  
(QFT of strong interaction)
- Effective Models  
(Chirale Perturbation, HQET, ...)
- ...

## Perturbative Methods

- extensive Loop-Calculations  
(algebraic, numerical)
- ...

## Non-perturbative Numerical Methods

- **Lattice QCD calculations**  
(Discretized QCD)
- Numerically solving coupled QCD equations (truncated QCD)
  - ▶ Bound-state equations
  - ▶ Dyson-Schwinger equations
  - ▶ Functional RG
- ...



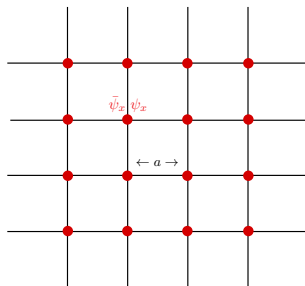
# Lattice regularization of QCD (LQCD)

## QCD action

$$S_{\text{QCD}} = \int d^4x \left[ -\frac{1}{2g_0^2} \text{Tr} F^2[A] + \sum_f \bar{\psi}_x^f (\not{D}[A] - m_0^f) \psi_x^f \right]$$

## Discretization of Euclidean space-time

- Introduce 4-dim lattice  $L^3 \times T$   
 $x = n a^4, \quad n \in \mathbf{Z}^4$
- Quark fields  $\psi, \bar{\psi}$  dwell on sites
- But: naive discretization of gluon field  $A_\mu(x)$  not gauge-invariant at finite  $a$



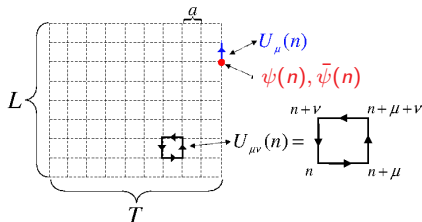
# Lattice regularization of QCD (LQCD)

introduced by K. Wilson (1974-77)

**Parallel transporter** between  $x$  and  $x + \hat{\mu}$

$$U_{\mu}(n) = \mathcal{P}e^{iag_0 \int_n^{n+\hat{\mu}} A_{\mu}(z) dz} \in SU_c(3)$$

Using "links"  $U_{\mu}(n)$  gives a **gauge-invariant** discretized action for any  $a$ .



**Example:** unimproved Wilson action

( $a \equiv 1$ )

$$S_{\text{LQCD}}^W = \overbrace{\beta \sum_{n, \mu < \nu} \left(1 - \frac{1}{3} \Re \text{Tr} \square_{n, \mu \nu}\right)}^{\text{gauge part}} + \overbrace{\sum_{n, m, f} \bar{\psi}_n^f M_{nm}^W[U, \kappa_f] \psi_m^f}^{\text{fermionic part}} \xrightarrow{a \rightarrow 0} S_{\text{QCD}}$$

- Fermion matrix:  $M_{nm}^W[U, \kappa_f] = \delta_{nm} - \kappa_f \sum_{\pm \mu} \delta_{m, n+\hat{\mu}} (1 + \gamma_{\mu}) U_{\mu}(n)$

- QCD Parameters:  $\beta \equiv 6/g_0^2, \quad \kappa_f \equiv 1/(2m_0^f - 8)$

Other (improved) discretizations possible, requirement:  $S_{\text{LQCD}} \xrightarrow{a \rightarrow 0} S_{\text{QCD}}$

**Expectation value** of an observable via path integral

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \prod_{n\mu} dU_{n\mu} \underline{d\bar{\psi}_n d\psi_n} \mathcal{O}[U, \bar{\psi}, \psi] e^{-(S_g[U] + S_f[U, \bar{\psi}, \psi])}$$

- No gauge-fixing needed! (compact gauge group)
- Integrate over quark fields exactly  $\implies$  modified action and integrand (non-local functional of links  $U$ )
- Left: **Master integral** for expectation value

$$\langle \mathcal{O} \rangle_{\beta, \kappa, L} = \frac{1}{Z} \int \prod_{n\mu} dU_{n\mu} F_{\mathcal{O}}[U] e^{-S_{\text{eff}}[U, \beta, \kappa]}$$

- Effective (partly integrated) action

$$S_{\text{eff}}[U; \beta, \kappa] = S_g[U; \beta] + \log \det M[U; \kappa]$$

# Lattice QCD calculation

## Monte-Carlo calculation

**Master integral** is very-high dimensional integral

$$\langle \mathcal{O} \rangle_{\beta, \kappa, L} = \frac{1}{Z} \int \prod_{n\mu} dU_{n\mu} F_{\mathcal{O}}[U] e^{-S_{\text{eff}}[U, \beta, \kappa]}$$

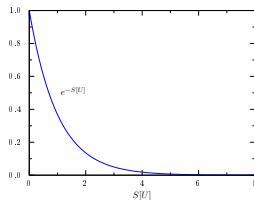
- Number of integration variables

$$(N_c = 3, N_d = 4)$$

$$64^3 \times 128 \times (N_c^2 - 1) \times N_d = 1\,073\,741\,824$$

$$16^3 \times 32 \times (N_c^2 - 1) \times N_d = 4\,194\,304$$

- Estimate integrals stochastically



**Monte-Carlo integration:** Sample links  $U$  with probability density

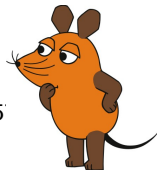
(“important sampling”)

$$P[U^{(i)}] = \frac{1}{Z} e^{-S_{\text{eff}}[U^{(i)}]} \quad \text{Markov chain: } U^{(1)}, U^{(2)}, \dots, U^{(N)} \in SU(3)$$

$$\text{Estimate for expectation value: } \bar{\mathcal{O}} \equiv \frac{1}{N} \sum_{i=1}^N \hat{\mathcal{O}}[U^{(i)}] \xrightarrow{N \rightarrow \infty} \langle \mathcal{O} \rangle_{\beta, \kappa, L}$$

# Monte-Carlo / Stochastic integration: How does it work?

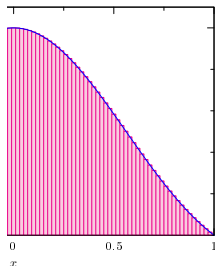
1-dim example



$$f(x) = (1 - x^2) \cdot e^{-x^2}, \quad I = \int_{-1}^1 f(x) dx = \frac{1}{e} + \frac{\sqrt{\pi}}{2} \text{Erf}(1) \simeq 1.1147035$$

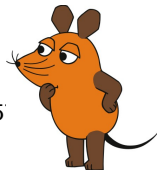
- Numerical integration with rectangular rule

$$I \simeq \sum_{i=1}^N f(x_i) \Delta x, \quad \Delta x = \frac{x_2 - x_1}{N}$$



# Monte-Carlo / Stochastic integration: How does it work?

## 1-dim example



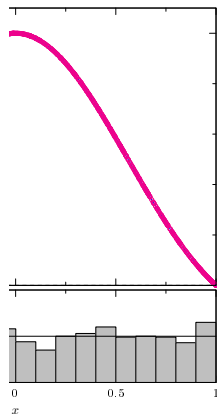
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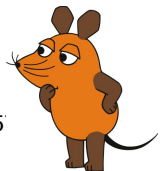
- Stochastic sampling of  $x_i \in [-1 : 1]$  with  $p(x) \propto 1$

$$I \simeq (x_2 - x_1) \cdot \frac{1}{N} \sum_{i=1}^N f(x_i) = (x_2 - x_1) \cdot \langle f \rangle_N$$



# Monte-Carlo / Stochastic integration: How does it work?

## 1-dim example



$$f(x) = (1 - x^2) \cdot e^{-x^2}, \quad I = \int_{-1}^1 f(x) dx = \frac{1}{e} + \frac{\sqrt{\pi}}{2} \text{Erf}(1) \simeq 1.1147035$$

- Numerical integration with rectangular rule

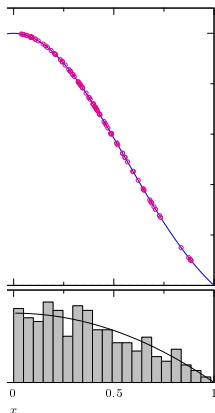
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- Stochastic sampling of  $x_i \in [-1 : 1]$  with  $p(x) \propto 1$

$$I \simeq (x_2 - x_1) \cdot \frac{1}{N} \sum_{i=1}^N f(x_i) = (x_2 - x_1) \cdot \langle f \rangle_N$$

- Improved Estimator: sample with  $p(x) \propto (1 - x^2)$

$$I \simeq (x_2 - x_1) \cdot \frac{1}{N} \sum_{i=1}^N p(x_i) \frac{f(x_i)}{p(x_i)} = (x_2 - x_1) \cdot \langle f/p \rangle_p$$



Efficiency: stochastic integration wins when dim > 10

# Systematics

**LQCD** comes with the same parameters as QCD  
(coupling, quark masses and volume)

$$\langle \mathcal{O} \rangle_{\beta, \kappa, L} = \frac{1}{Z} \int \prod_{n\mu} dU_{x\mu} F_{\mathcal{O}}[U] e^{-S_{\text{eff}}[U, \beta, \kappa]} = \left\langle F_{\mathcal{O}}[U^{(i)}] \right\rangle_{p(\beta, \kappa)}$$

**Parameters:**  $\beta \equiv 6/g_0^2$ ,  $\kappa_f \equiv 1/(2m_0^f - 8)$  tune them to “physical point”, e.g.,

$$\frac{aM_2}{aM_1}(\beta, \kappa) \xrightarrow{\beta, L \text{ large}} R_{21}(\kappa) \xrightarrow{\kappa^f \rightarrow \kappa_c^f} \frac{M_2^{\text{phys}}}{M_1^{\text{phys}}}$$

Access to lattice spacing via physical observable  $\rightarrow a = a(\beta, \kappa) \approx a(\beta)$

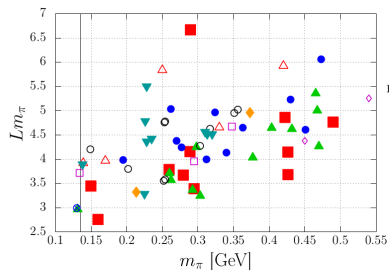
**Challenge:** Control over systematic error when extrapolating to physical point



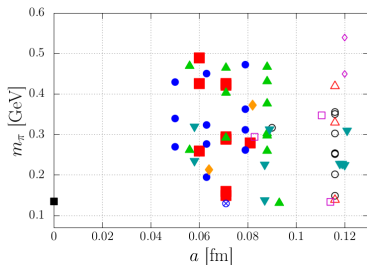
# Landscape of lattice simulations

## Status

- $N_f = 2, N_f = 2+1, N_f = 2+1+1$
- Lattice spacings:  $a \geq 0.04$  fm,      Volumes:  $L \leq 6$  fm



ROCD  $N_f = 2$     ■  
ETMC  $N_f = 2$     ▲  
Mainz  $N_f = 2$     ●  
QCDSF  $N_f = 2$     ⊗  
LHPC  $N_f = 2+1$     △  
RBC/UKQCD  $N_f = 2+1$     ○  
JLQCD  $N_f = 2+1$     ◇  
YQCD  $N_f = 2+1$     ▲  
PNDME  $N_f = 2+1+1$     ●  
ETMC  $N_f = 2+1+1$     ◇



compiled by S. Collins (Regensburg)

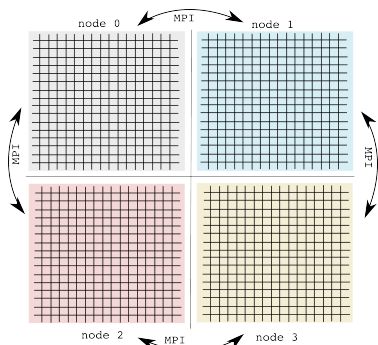
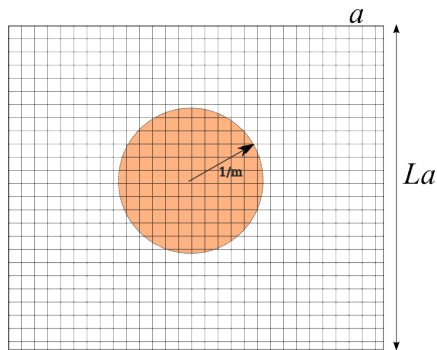
- Much progress in last ten years (algorithmic and computationally)
- Many lattice collaborations reach physical point (hadron masses)
- Safe extrapolation to continuum limit often remains (no always an issue)

## Calculations close to physical point very expensive

Monte-Carlo chain needs numerical inversion for every step:  $[\mathcal{D}(U) + m_f]^{-1}$

### Require

- Volume large enough: Lightest hadron is pion with  $m_\pi^2 \propto (m_u + m_d)$
- Lattice fine enough: discretization effects small



Rule of thumb:  $Lm_\pi \geq 4$

# Proton-Proton "Lattice QCD" accelerator

Lattice QCD often requires supercomputers and highly efficient codes



## Challenge and Progress in recent years

— Big computers are only one part of the success —

# Lattice QCD calculation

## Monte-Carlo calculation

**Master integral** is very-high dimensional integral

$$\langle \mathcal{O} \rangle_{\beta, \kappa, L} = \frac{1}{Z} \int \prod_{n\mu} dU_{n\mu} F_{\mathcal{O}}[U] e^{-S_{\text{eff}}[U, \beta, \kappa]}$$

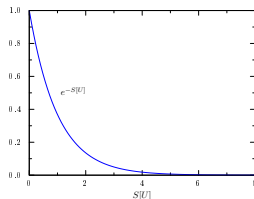
- Number of integration variables

$$(N_c = 3, N_d = 4)$$

$$64^3 \times 128 \times (N_c^2 - 1) \times N_d = 1\,073\,741\,824$$

$$16^3 \times 32 \times (N_c^2 - 1) \times N_d = 4\,194\,304$$

- Estimate integrals stochastically



**Monte-Carlo integration:** Sample links  $U$  with probability density  
(“important sampling”)

$$P[U^{(i)}] = \frac{1}{Z} e^{-S_{\text{eff}}[U^{(i)}]} \quad \text{Markov chain: } U^{(1)}, U^{(2)}, \dots, U^{(N)} \in SU(3)$$

**Estimate for expectation value:**  $\bar{\mathcal{O}} \equiv \frac{1}{N} \sum_{i=1}^N \hat{\mathcal{O}}[U^{(i)}] \xrightarrow{N \rightarrow \infty} \langle \mathcal{O} \rangle_{\beta, \kappa, L}$

# Main numerical challenge

Solving a linear system

For each  $U$  (varies strongly) solve **linear system** again, again and again

$$D(U) \cdot \vec{\psi} = \vec{b} \quad \rightarrow \quad \vec{\psi} = D^{-1}(U) \cdot \vec{b}$$

$D(U)$ : sparse matrix,  $\mathbb{C}^{12V \times 12V}$  elements, mostly zero

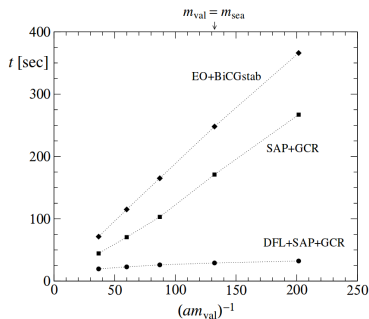
$\vec{b}$ :  $\mathbb{C}^{12V}$  elements, for  $V = 64^3 \times 128 \hat{=} 402\,653\,184$  elements

**Numerical solution** needed for:

- Monte-Carlo chain
- many observable  
(whenever quarks are part of the operator)

**Problem:**

- Simulation parameters  $\beta, \kappa$  directly connected to phys. parameters
- Physical limit very expensive  
(**"Critical slowing down"**)
- Reason: eigen vectors for smallest eigenvalues



# Standard-Trick: Präkonditionierung

## Solver

- typical: Krylov-space methods
- Number of iterations grows  $\propto 1/\lambda_0$

## Präconditioning

$$A \cdot \psi = b$$

$$LA \cdot R\psi = Lb$$

- if  $LAR \simeq \mathbb{I}$ , then  $LA \cdot \tilde{\psi} = \tilde{b}$  found fast and so  $\psi = R^{-1}\tilde{\psi}$
- additional numerical costs vs. reduction of number of iterations

## Typical methods used for lattice QCD

- Domain decomp. (checkerboard, DD, Hasenbusch trick)
- Multigrid (MG)
- Helps but can not to avoid "critical slowing down"

## Deflation

- Determination of Eigen space for smallest EV  $\lambda_0, \lambda_1, \dots$

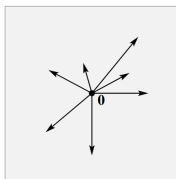
$$A\psi^{(n)} = \lambda_n b$$

- Find solution in remaining space (orthogonal to eigen space)
- helps a lot but similar expensive as original system

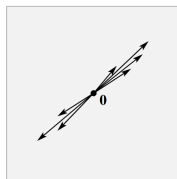
# Empirical fact

## Lowest EV for fermion matrix

- if reduced to small space region ( $4^4, 6^4$ ), build lower dimensional eigen space
- EV are local coherent, reason unknown, but seen empirically (maybe connected to  $\chi$ -Symmetry breaking in QCD)
- i.e. **approximation of eigen space sufficient** (inexact deflation)
- Combined with Domain-Decomposition (DD) or MG



incoherent



coherent

- Used in recent years in several algorithms, in particular AMG
- allows lattice QCD calculations at physical point (expensive but possible)



## Examples for typical lattice QCD calculations

## Typical observables

- Plaquette or other Wilson loops
- Chiral condensates
- Hadronic properties  
(e.g., masses, decay constants, form factors, structure functions. . . )
- Fundamental parameters of QCD (strong coupling, quark masses)
- . . .

## Will illustrate calculation of

- 1 Wilson loop: quark confinement
- 2 2-point functions: Hadron masses
- 3 3-point functions: Hadron structure

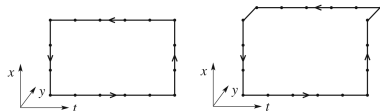
# Extracting Wilson loops

## Wilson loops

- Allow to estimate potential between (two) static color sources.
- Prototype of gauge-invariant observable (purely gluonic)
- Also used as operators for gluonic bound states (glueballs)  
(from exponential decay of correlation function)

## Wilson Loop on gauge field configuration $U$

$$W[U] = \text{Tr} \prod_{x, \mu \in \text{loop}(R, T)} U_{x\mu}$$



## Expectation value

$$\begin{aligned} \langle W \rangle_{R, T} &= \frac{1}{Z} \int DU W[U] e^{-S_{\text{eff}}[U]} = \frac{1}{N} \sum_{i=1}^N W[U^{(i)}] + O\left(\frac{1}{\sqrt{N}}\right) \\ &\propto e^{-tV(r)} \left(1 + O(e^{-t\Delta E})\right) \end{aligned}$$

# Static quark potential from expectation values of Wilson loops

## Static quark potential

$$V(r) = A + \frac{B}{r} + \sigma r$$

- Force between quarks is  $dV/dr$
- $A$  irrelevant
- 2<sup>nd</sup> term: Coulomb term with strength  $B$
- 3<sup>rd</sup> term: lin. rising potential  
 $\sigma$  is **string tension** ( $\approx 900$  MeV/fm)

## Linear rising potential:

energy rises the further quark and antiquark are pulled apart  
(quark confinement)

Lattice Data for quen. approximation  
(no sea quarks)

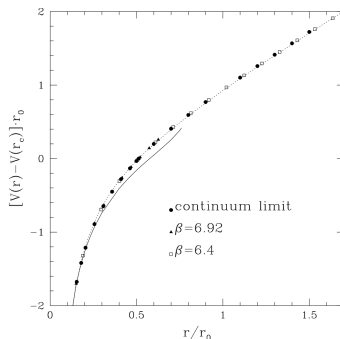


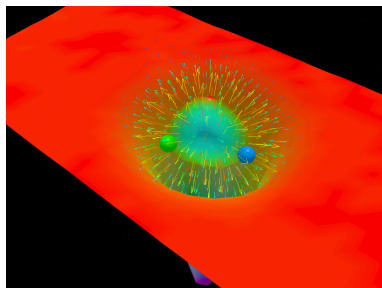
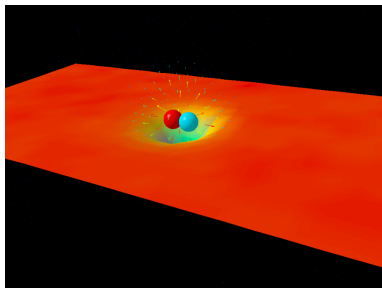
Figure : [Necco/Sommer, NPB622(2002)328] dashed line: bosonic string model, solid line pert. theory

# String formation

Meson and baryon fluxtubes (by Derek Leinweber)

See CSSM, Adelaide for animations

[www.physics.adelaide.edu.au/theory/staff/leinweber/VisualQCD/Nobel](http://www.physics.adelaide.edu.au/theory/staff/leinweber/VisualQCD/Nobel)



- Meson fluxtube (left)

[www.physics.adelaide.edu.au/theory/staff/leinweber/VisualQCD/Nobel/FluxTubeAnim2.gif](http://www.physics.adelaide.edu.au/theory/staff/leinweber/VisualQCD/Nobel/FluxTubeAnim2.gif)

- Baryon fluxtube (right)

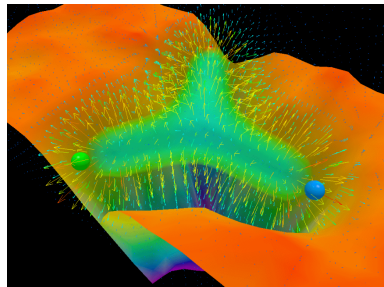
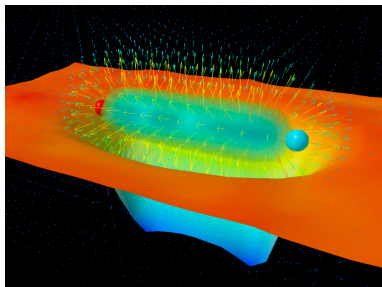
[www.physics.adelaide.edu.au/theory/staff/leinweber/VisualQCD/Nobel/VacuumRespAction16t32\\_Yshape8.gif](http://www.physics.adelaide.edu.au/theory/staff/leinweber/VisualQCD/Nobel/VacuumRespAction16t32_Yshape8.gif)

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- Meson fluxtube (left)

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- Baryon fluxtube (right)

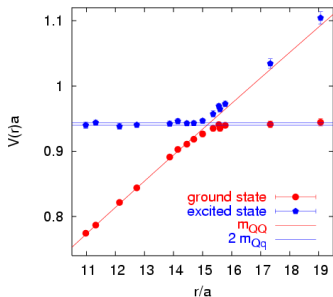
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# String formation and breaking

**Full QCD:** If QCD vacuum contains “sea quarks” (unquenched)

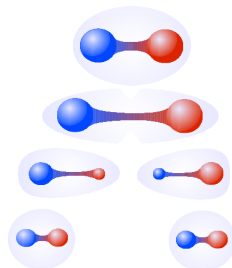
- creation of sea quark-antiquark pairs at sufficient energy
- flux tube breaks for large enough  $r$

## String-Breaking from Lattice QCD



SESAM-Collaboration: Bali et al. (2005)

Illustration:



# Extracting physics from LQCD calculations

## Typical observables

- Plaquette or other Wilson loops
- Chiral condensates
- **Hadronic properties**  
(e.g., masses, decay constants, form factors, structure functions. . . )
- . . .

## Will illustrate calculation of

- 1 Wilson loop: quark confinement
- 2 **2-point functions**: Hadron masses, decay constants
- 3 **3-point functions**: hadron structure, renormalization etc.



# Hadronic two- and three-point functions on the lattice

## 1 2-point correlation functions

$$C_{2pt}^h(\vec{p}, t) = \frac{1}{\sqrt{V_S}} \sum_{\vec{x}} e^{i\vec{x}\cdot\vec{p}} \langle \bar{h}(\vec{x}, t) h(\vec{0}, 0) \rangle_U \stackrel{(\vec{p}=\vec{0})}{=} |Z_0|^2 e^{-m_0 t} + |Z_1|^2 e^{-m_1 t} + \dots$$

## 2 3-point correlation functions

$$C_{3pt}^{\mathcal{O}}(\tau, t, \vec{p}, \vec{p}') = \frac{1}{\sqrt{V_S}} \sum_{\vec{x}} e^{i\vec{x}\cdot\vec{p}} e^{i\vec{z}\cdot\vec{\Delta}P} \langle h(t, \vec{x}) | \mathcal{O}(\tau, z) | \bar{h}(0, \vec{0}) \rangle_U \\ = \text{prefactor}(t, \tau, \vec{p}, \vec{p}') \otimes \langle H | \mathcal{O} | H \rangle + \dots$$

## • Interpolation operators $h$ have quantum number of hadron

▶ Proton:  $h_{p^+}(x) = \varepsilon^{abc} \{ u^{aT}(x) C \gamma_5 d^b(x) \} u^c(x)$

▶ Pion:  $h_{\pi^+}(x) = \bar{d}(x) \gamma_5 u(x),$   $x = (\vec{x}, t)$

## • Insertion operator $\mathcal{O}$ chosen wrt. desired **matrix element**

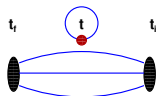
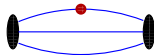
▶ Vector current:  $\bar{\psi} \gamma_\mu \psi$

▶ Axial-Vector current:  $\bar{\psi} \gamma_\mu \gamma_5 \psi$

# Illustration: Measurement of a three-point function on the lattice

Connected and disconnected contribution

Diagrams



On the Lattice

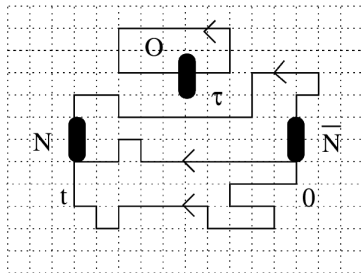
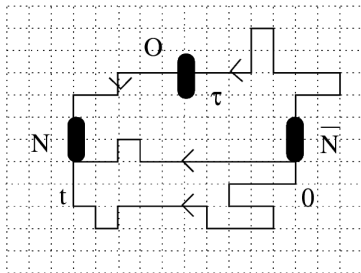


Figure : from R. Horsley (1999)

# Hadron masses from the lattice

[QCD works!](#)

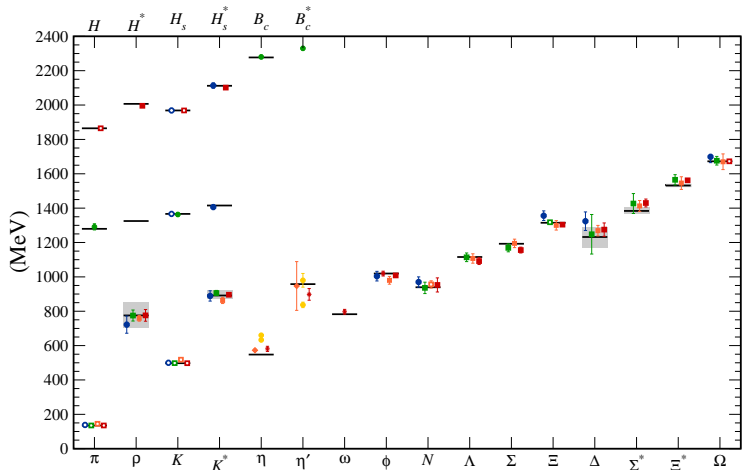


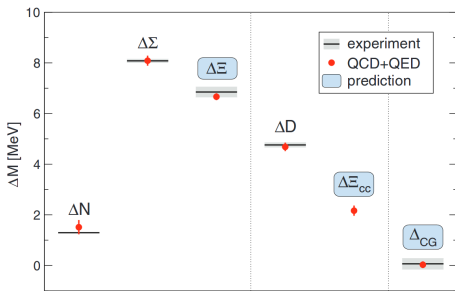
Figure : Hadron masses from lattice QCD: experimental vs. lattice QCD results

(MILC, PACS-CS, BMW, QCDSF und RBC&UKQCD).

From [Kronfeld 1203.1204].

# Hadron masses splitting from the lattice

Lattice QCD works also when adding QED effects!



	Mass splitting [MeV]	QCD [MeV]	QED [MeV]
$\Delta N = n - p$	1.51(16)(23)	2.52(17)(24)	-1.00(07)(14)
$\Delta \Sigma = \Sigma^- - \Sigma^+$	8.09(16)(11)	8.09(16)(11)	0
$\Delta \Xi = \Xi^- - \Xi^0$	6.66(11)(09)	5.53(17)(17)	1.14(16)(09)
$\Delta D = D^+ - D^0$	4.68(10)(13)	2.54(08)(10)	2.14(11)(07)
$\Delta \Xi_{cc} = \Xi_{cc}^{++} - \Xi_{cc}^+$	2.16(11)(17)	-2.53 (11)(06)	4.69(10)(17)
$\Delta_{CG} = \Delta N - \Delta \Sigma + \Delta \Xi$	0.00(11)(06)	-0.00 (13)(05)	0.00(06)(02)

Figure : Borsanyi et al., Science 347 (2015) 1452.

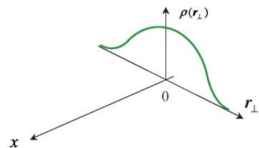
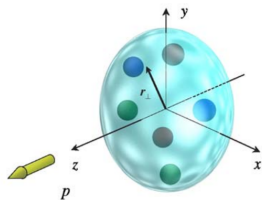
## Typical observables

- Plaquette or other Wilson loops
- Chiral condensates
- Hadronic properties  
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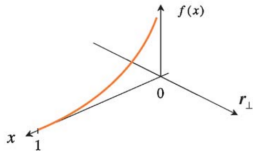
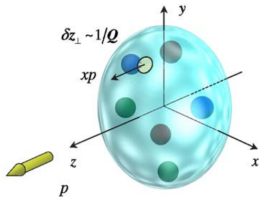
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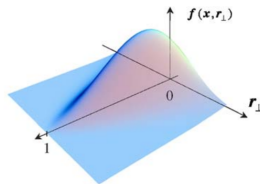
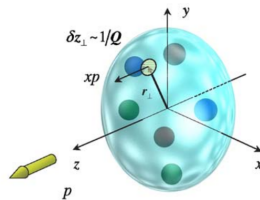
# Hadron structure functions



**Form factors:** Spatial distribution of charge and magnetization



**Parton distribution:** Distribution of momentum and spin



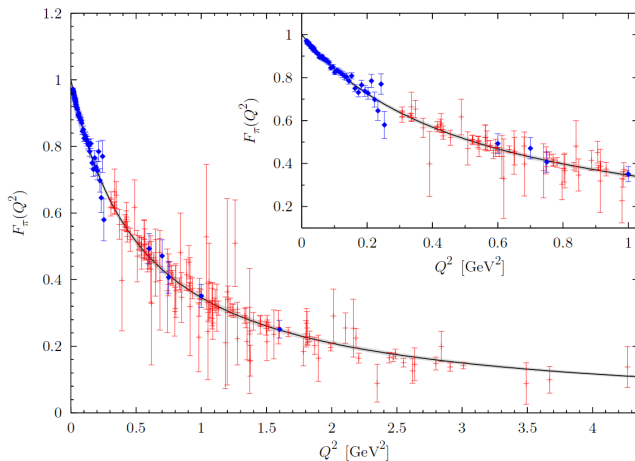
**Generalized parton distribution (GPDs):** correlated distribution of momentum, spin, charge

**Goal:** Determination of non-perturbative functions directly from QCD

- Form factors possible from lattice QCD
- GPDs, PDFs: only moments accessible so far (Ji'13: quasi-PDFs possible)

# Pion form factor

Experiment vs. Lattice



# Moments of Parton Distributions (PDFs)

## Nucleon parton distribution function

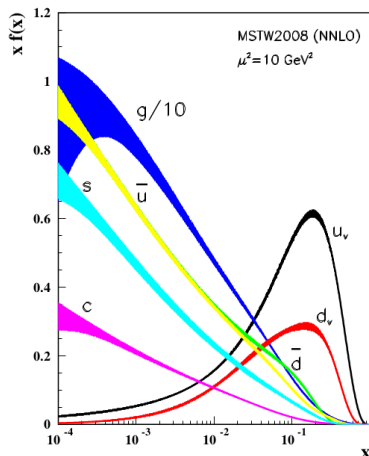
- Important for phenomenology
- Known for large range of  $x = [0, 1]$  (long. mom. fraction)
- Good knowledge for  $u$  and  $d$
- For other quarks not as good

## Lattice QCD

- Moments of nucleon PDF

$$\langle x^n \rangle_{(q)} = \int_0^1 dx x^n [q(x) + \bar{q}(x)]$$

- **New:** indirect access to  $q(x)$  itself





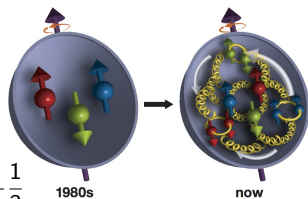
# Spin structure of the Nucleon

## Naive Parton model

- Nucleon spin = sum of valence quark spins

$$\frac{1}{2} = \frac{1}{2} \overbrace{(\Delta u_v + \Delta d_v)}^{\Delta\Sigma=1} \quad \text{where} \quad \Delta u_v = \frac{4}{3}, \Delta d_v = -\frac{1}{3}$$

- “Spin puzzle/crisis”:  $E_\mu$ -Collaboration (1989) found:  $\Delta\Sigma \approx 0.120$



## Modern view

- Valence quarks contribute only a fraction
- Significant contribution also from gluons and sea quarks
- Also important: Orbital angular momentum  $L$  of quarks and gluons

- Total spin: 
$$\frac{1}{2} = \frac{1}{2} \underbrace{(\Delta u + \Delta \bar{u} + \Delta d + \Delta \bar{d} + \Delta s + \Delta \bar{s})}_{\Delta\Sigma} + L_q + \Delta g + L_g$$

- Individual contributions can be calculated using lattice QCD

Bali et al., PRL108 (2012) 222001

$$\Delta s + \Delta \bar{s} = -0.020(10)(4)$$

$$\Delta\Sigma = \Delta u + \Delta \bar{u} + \Delta d + \Delta \bar{d} + \Delta s + \Delta \bar{s} = 0.45(4)(9)$$

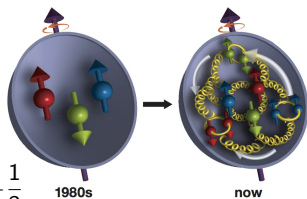
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- Total spin: 
$$\frac{1}{2} = \frac{1}{2} \underbrace{(\Delta u + \Delta \bar{u} + \Delta d + \Delta \bar{d} + \Delta s + \Delta \bar{s})}_{\Delta\Sigma} + L_q + \Delta g + L_g$$

- Moments of GPDs deliver total quark momentum

$$\frac{1}{2} = \frac{1}{2} \Delta\Sigma + L_q + \Delta g + L_g$$

# Extracting physics from LQCD calculations

## Typical observables

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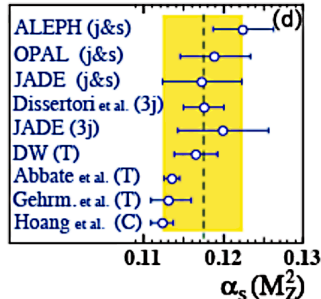
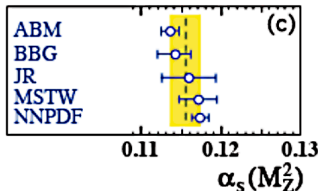
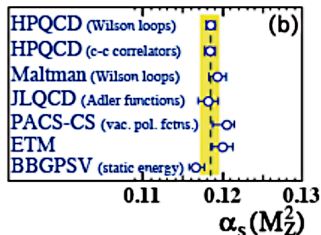
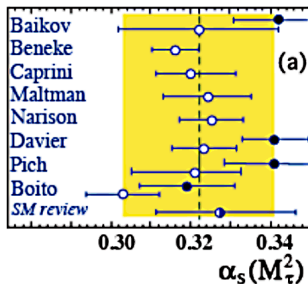
## Will illustrate calculation of

- 1 Wilson loop: quark confinement
- 2 2-point functions: Hadron masses
- 3 3-point functions: Hadron structure



# Strong coupling from QCD phenomenology and lattice QCD

Bethke (2015)



## Lattice QCD

- Provides numerical access to many quantities of strong interaction physics
- Systematically improvable, becomes QCD in the respective limits
- Needs usage of supercomputers and parallel programming
- Success nicely demonstrates correctness of QCD

— Thank you for your attention! —