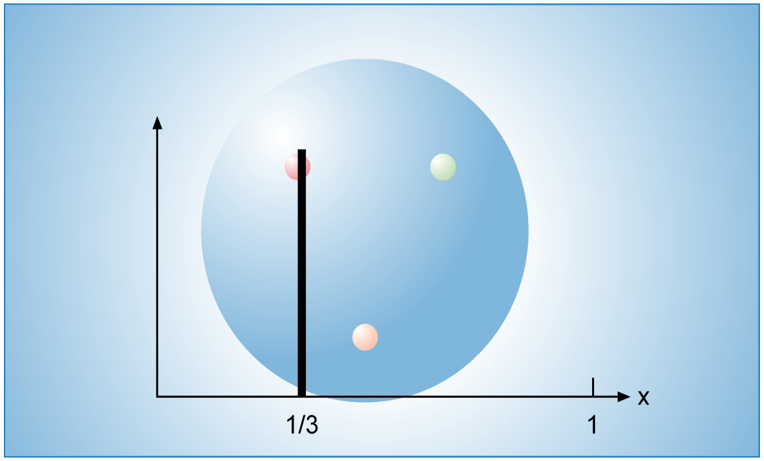
The Quest for Solving QCD: Simulating quark and gluon interactions on supercomputers

Karl Jansen

- **Introduction**
- **Status of present Lattice calculations**
- **Hadron structure on the lattice**
  - Moments of parton distribution functions
  - Spin and momentum of the nucleon
  - Direct calculation of parton distribution functions
- **Conclusion**

Quarks are the fundamental constituents of nuclear matter



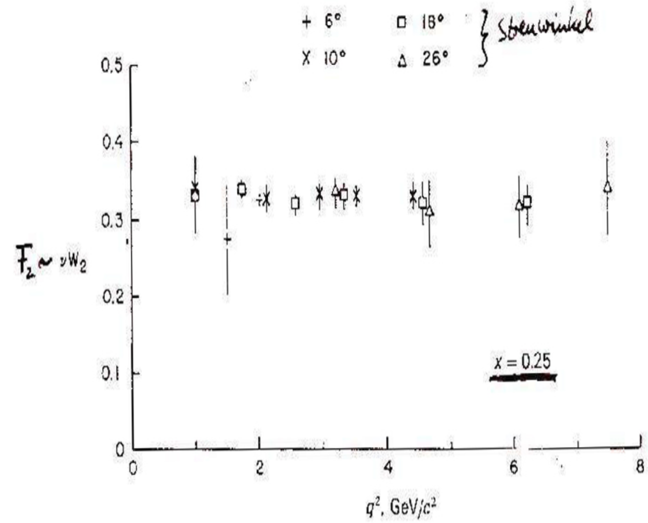


Fig. 7.17 νW_2 (or F_2) as a function of q^2 at $x = 0.25$. For this choice of x, there is practically no q^2-dependence, that is, exact "scaling". (After Friedman and Kendall 1972.)

Friedman and Kendall, 1972)

$f(x, Q^2)\big|_{x\approx 0.25, Q^2>10\mathrm{GeV}}$ independent of Q^2

(x momentum of quarks, Q^2 momentum transfer)

Interpretation (Feynman): scattering on single quarks in a hadron
$\rightarrow$ (Bjorken) scaling

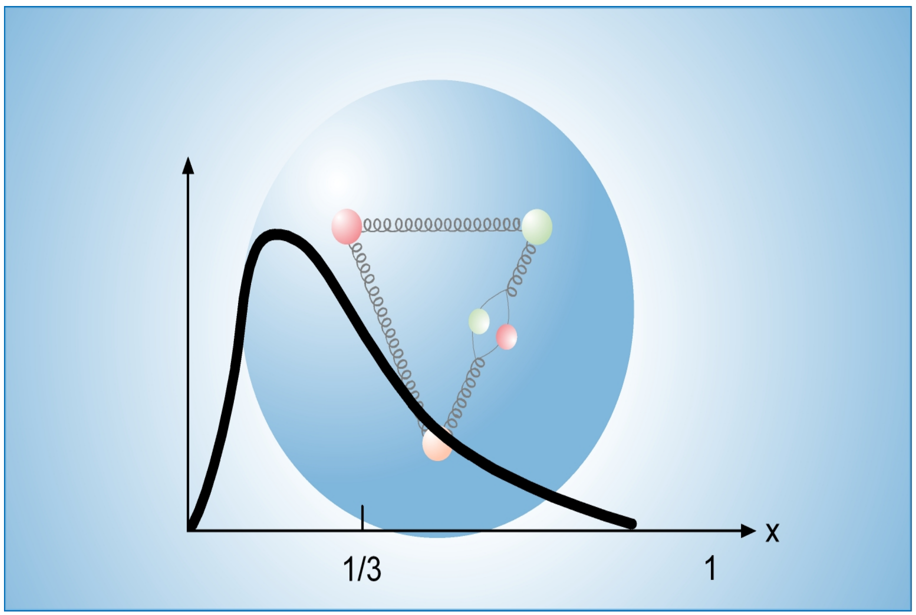
Quantum Fluctuations and the Quark Picture

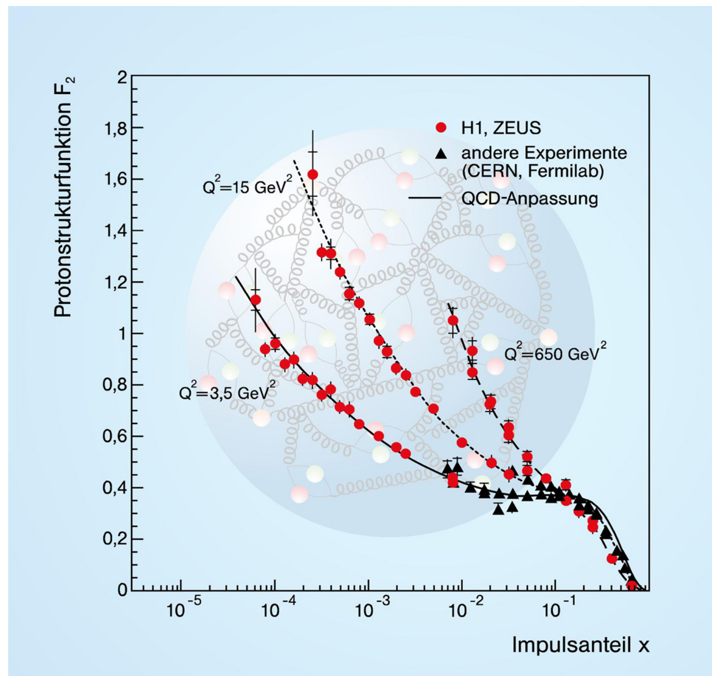
analysis in perturbation theory

$$\int_0^1 dx\, f(x,Q^2) = 3\left[1 - \frac{\alpha_s(Q^2)}{\pi} - a(n_f)\left(\frac{\alpha_s(Q^2)}{\pi}\right)^2 - b(n_f)\left(\frac{\alpha_s(Q^2)}{\pi}\right)^3\right]$$

– $a(n_f), b(n_f)$ calculable coefficients

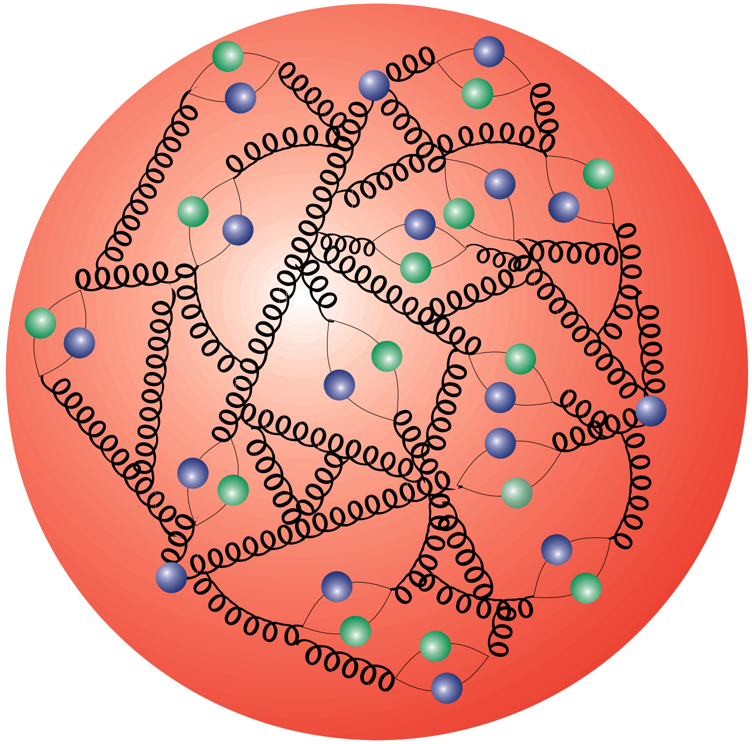
deviations from scaling $\rightarrow$ determination of strong coupling





Why we need lattice QCD

- situation becomes incredibly complicated



- value of the coupling (expansion parameter) $\alpha_{\mathrm{strong}}(1\mathrm{fm}) \approx 1$

$\Rightarrow$ need different ("exact") method

$\Rightarrow$ has to be non-perturbative
  $\rightarrow$ more than all Feynman graphs

- Wilson's Proposal: Lattice Quantum Chromodynamics

Lattice Gauge Theory had to be invented

$\rightarrow$ QuantumChromoDynamics

asymptotic freedom	confinement
distances $\ll 1\mathrm{fm}$	distances $\gtrsim 1\mathrm{fm}$
world of quarks and gluons	world of hadrons and glue balls
perturbative description	non-perturbative methods

Unfortunately, it is not known yet whether the quarks in quantum chromodynamics actually form the required bound states. To establish whether these bound states exist one must solve a strong coupling problem and present methods for solving field theories don't work for strong coupling.

Wilson, Cargese Lecture notes 1976

Schwinger model: 2-dimensional Quantum Electrodynamics

(Schwinger 1962)

Quantization via Feynman path integral (in Euclidean time)

$$\mathcal{Z} = \int \mathcal{D}A_\mu \mathcal{D}\Psi \mathcal{D}\bar{\Psi} e^{-S_{\rm gauge} - S_{\rm ferm}}$$

Fermion action

$$S_{\rm ferm} = \int d^2x \bar{\Psi}(x) \left[D_\mu + m \right] \Psi(x)$$

gauge covriant derivative

$$D_\mu \Psi(x) \equiv (\partial_\mu - i g_0 A_\mu(x)) \Psi(x)$$

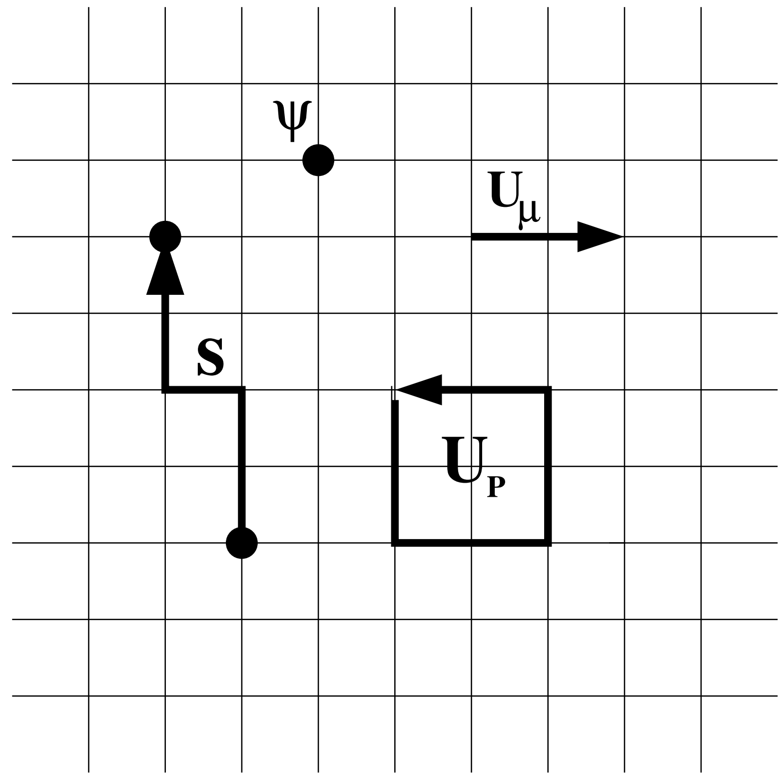
with A_μ gauge potential, g_0 bare coupling

$$S_{\rm gauge} = \int d^2x F_{\mu\nu} F_{\mu\nu} \ , \ F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)$$

equations of motion: obtain classical Maxwell equations

Lattice Schwinger model

introduce a 2-dimensional lattice with lattice spacing a



fields $\Psi(x)$, $\bar{\Psi}(x)$ on the lattice sites

$x = (t, \mathbf{x})$ integers

discretized fermion action

$$S \to a^2 \sum_x \bar{\Psi} \left[\gamma_\mu \partial_\mu - r \underbrace{\partial_\mu^2}_{\nabla_\mu^* \nabla_\mu} + m\right] \Psi(x)$$

$$\partial_\mu = \frac{1}{2} \left[\nabla_\mu^* + \nabla_\mu\right]$$

discrete derivatives

$$\nabla_\mu \Psi(x) = \frac{1}{a} \left[\Psi(x + a\hat{\mu}) - \Psi(x)\right] \ , \quad \nabla_\mu^* \Psi(x) = \frac{1}{a} \left[\Psi(x) - \Psi(x - a\hat{\mu})\right]$$

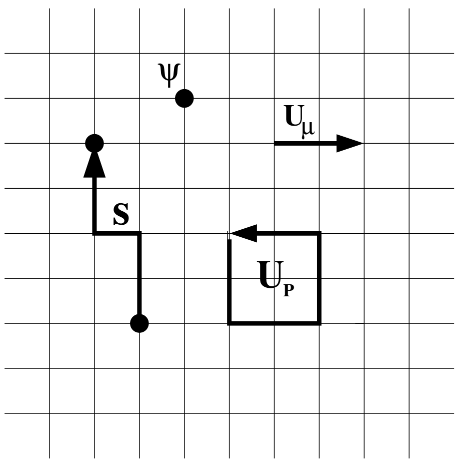
second order derivative $\to$ remove doubler $\leftarrow$ break chiral symmetry

Implementing gauge invariance

Wilson's fundamental observation: introduce parallel transporter connecting the points x and $y = x + a\hat{\mu}$:

$$U(x,\mu) = e^{iaA_\mu(x)} \in U(1)$$

$\Rightarrow$ lattice derivative: $\nabla_\mu \Psi(x) = \frac{1}{a}\left[U(x,\mu)\Psi(x+\mu) - \Psi(x)\right]$



$$U_p = U(x,\mu)U(x+\mu,\nu)U^\dagger(x+\nu,\mu)U^\dagger(x,\nu)$$

$$\rightarrow F_{\mu\nu}F^{\mu\nu}(x) \quad \text{for} \quad a \rightarrow 0$$

$$\boxed{S = a^2 \sum_x \left\{\beta(=\tfrac{1}{g_0^2})\left[1 - \mathrm{Re}(U_{(x,p)})\right] + \bar{\psi}\left[m + \tfrac{1}{2}\{\gamma_\mu(\nabla_\mu + \nabla^\star_\mu) - a\nabla^\star_\mu\nabla_\mu\}\right]\psi\right\}}$$

partition functions (path integral) with Boltzmann weight (action) S

$$\boxed{\mathcal{Z} = \int_{\text{fields}} e^{-S}}$$

Physical Observables

expectation value of physical observables $\mathcal{O}$

$$\underbrace{\langle\mathcal{O}\rangle = \frac{1}{\mathcal{Z}}\int_{\mathrm{fields}} \mathcal{O} e^{-S}}$$

$\downarrow$ lattice discretization

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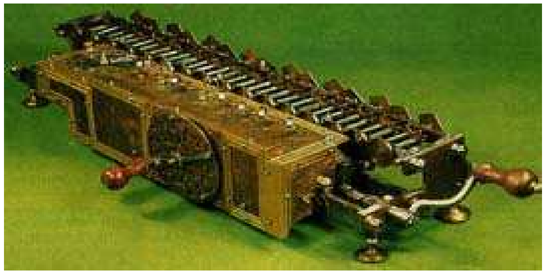
$\downarrow$



From the Schwinger model to quantum chromodynamics

- system becomes 4-dimensional:
  $[50 \cdot 50] \rightarrow [50 \cdot 50] \cdot 2500$

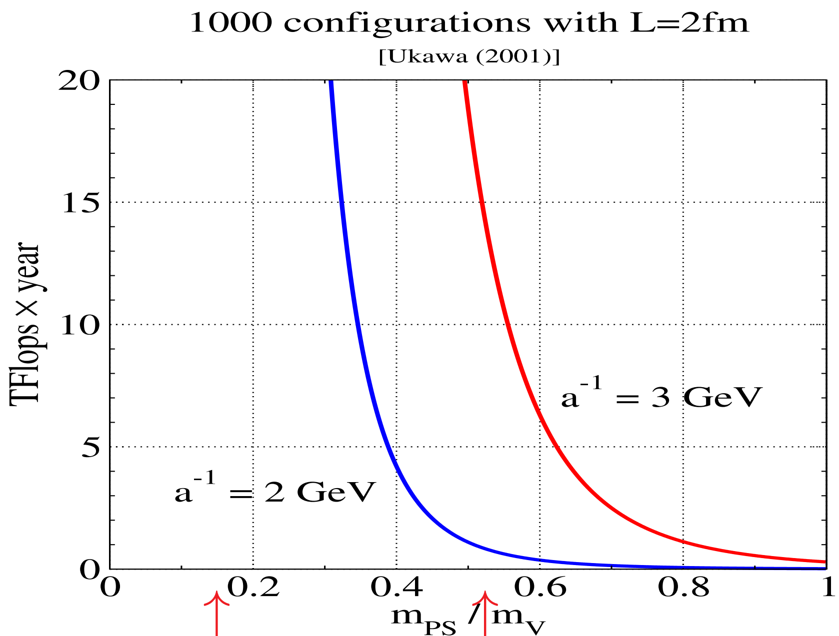
- gauge field $U(x,\mu) \in U(1) \rightarrow U(x,\mu) \in SU(3)$

- quarks receive 4 Dirac and 3 color components:
  $[50 \cdot 50] \rightarrow [50 \cdot 50] \cdot 30000$

- theory needs *non-perturbative* renormalization

The graph that wrote history: the "Berlin Wall"

see panel discussion in Lattice2001, Berlin, 2001



physical point

contact to χPT (?)

formula $C \propto \left(\frac{m_\pi}{m_\rho}\right)^{-z_\pi} (L)^{z_L} (a)^{-z_a}$

$$z_\pi = 6, \;\; z_L = 5, \;\; z_a = 7$$

"both a 10^8 increase in computing power AND spectacular algorithmic advances before a useful interaction with experiments starts taking place." (Wilson, 1989)

$\Rightarrow$ need of **Exaflops Computers**

Why are fermions so expensive?

- need to evaluate

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\bar{\psi}\{D_{\mathrm{lattice}}^{\mathrm{Dirac}}\}\psi} \propto \det[D_{\mathrm{lattice}}^{\mathrm{Dirac}}]$$

- bosonic representation of determinant

$$\det[D_{\mathrm{lattice}}^{\mathrm{Dirac}}] \propto \int \mathcal{D}\Phi^\dagger\mathcal{D}\Phi e^{-\Phi^\dagger\{D_{\mathrm{lattice}}^{-1}\}\Phi}$$

- need vector $X = D_{\mathrm{lattice}}^{-1}\Phi$

- solve linear equation $D_{\mathrm{lattice}}X = \Phi$

  D_{lattice} matrix of dimension $100\mathrm{million} \otimes 100\mathrm{million} \approx 12 \cdot 48^3 \cdot 96$
  (however, matrix is sparse)

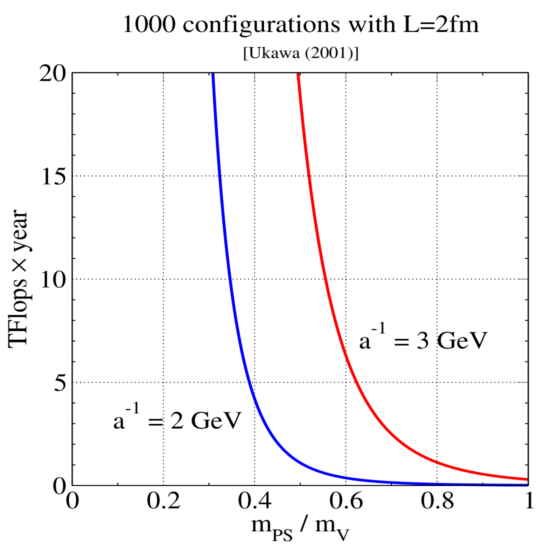
- number of such "inversions": $O(1000 - 10000)$ for one field configuration

- want: $O(1000 - 10000)$ such field configurations

A generic improvement for Wilson type fermions

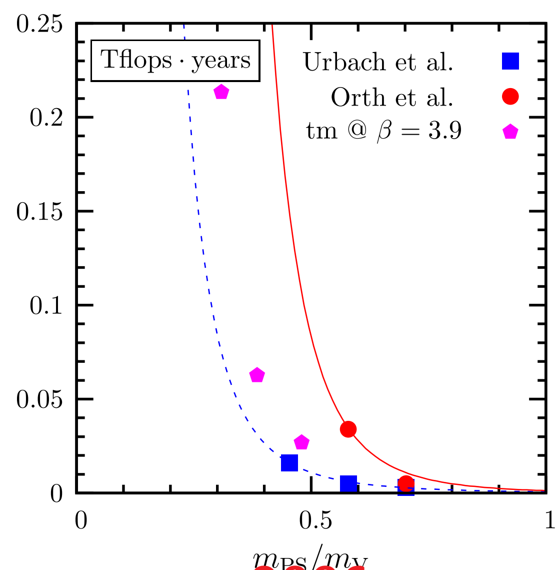
New variants of HMC algorithm
(here (Urbach, Shindler, Wenger, K.J.), see also RHMC, SAP)

- even/odd preconditioning
- (twisted) mass-shift (Hasenbusch trick)
- multiple time steps



2001

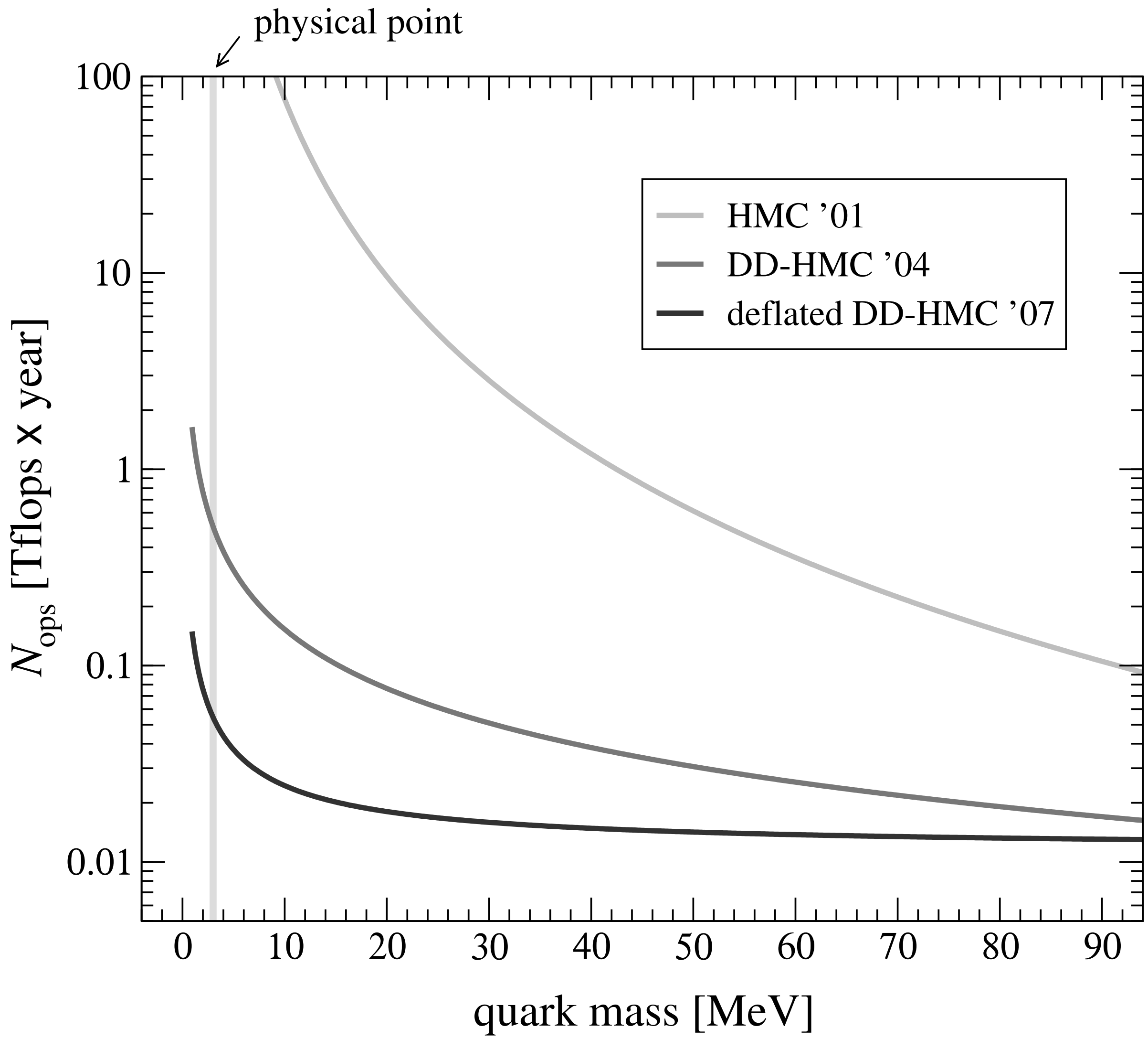
$\longrightarrow$



2006

– comparable to staggered
– reach small pseudo scalar masses $\approx 300\text{MeV}$

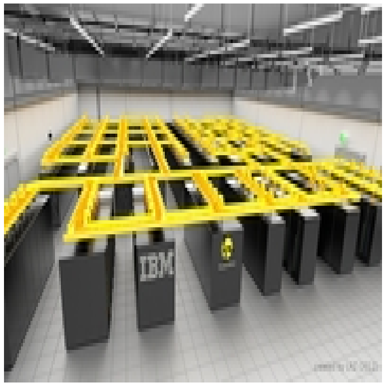
Recent pricture



German Supercomputer Infrastructure

- JUQUEEN (IBM BG/Q)
  at Supercompter center Jülich
  5 Petaflops

- HLRN (Hannover-Berlin)
  Gottfried and Konrad
  (CRAY XC30)
  2.6 Petaflops

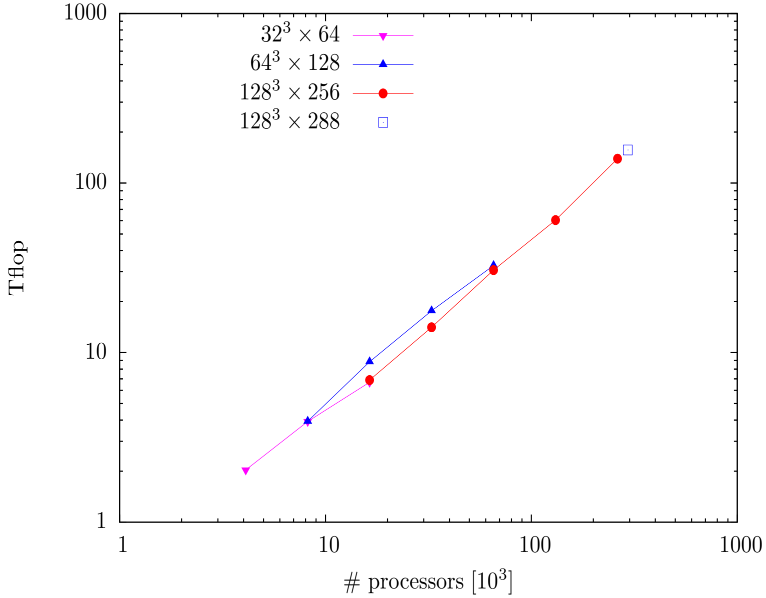


- Leibniz Supercomputer center Munich
  combined IBM/Intel system SuperMUC
  3 Petaflops

Computertime: through local calls, e.g. NIC, or Europe wide: PRACE → peer reviewed

Strong Scaling

- Test on 72 racks BlueGene/P installation at supercomputer center Jülich
- using tmHMC code

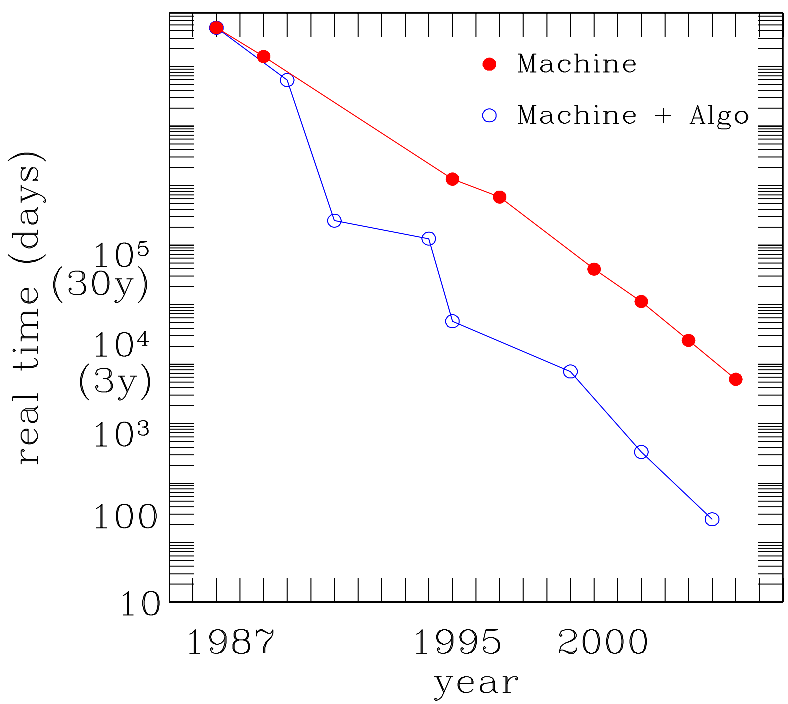


Computer and algorithm development over the years

Lattice physicists have invested a lot in algorithm development

supercomputer architectures show remarkable speedup

time estimates for simulating $32^3 \cdot 64$ lattice, 5000 configurations



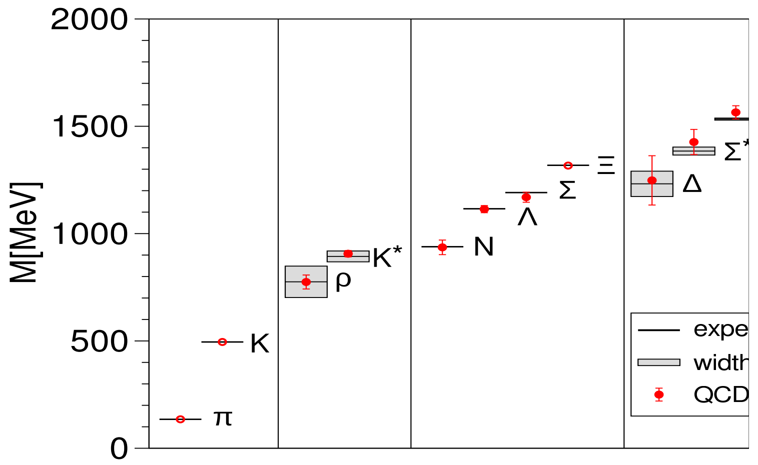
$\rightarrow$ algorithm development very important

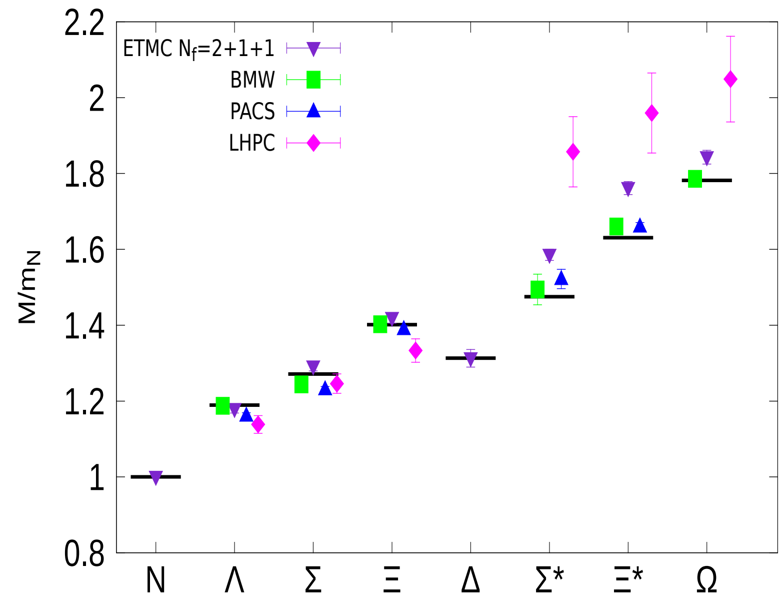
$\rightarrow$ typical architectures: **BG/L,P,Q, Intel, GPUs**

$\rightarrow$

The lattice QCD benchmark calculation: the spectrum

spectrum for $N_f = 2+1$ and $2+1+1$ flavours





first spectrum calculation BMW

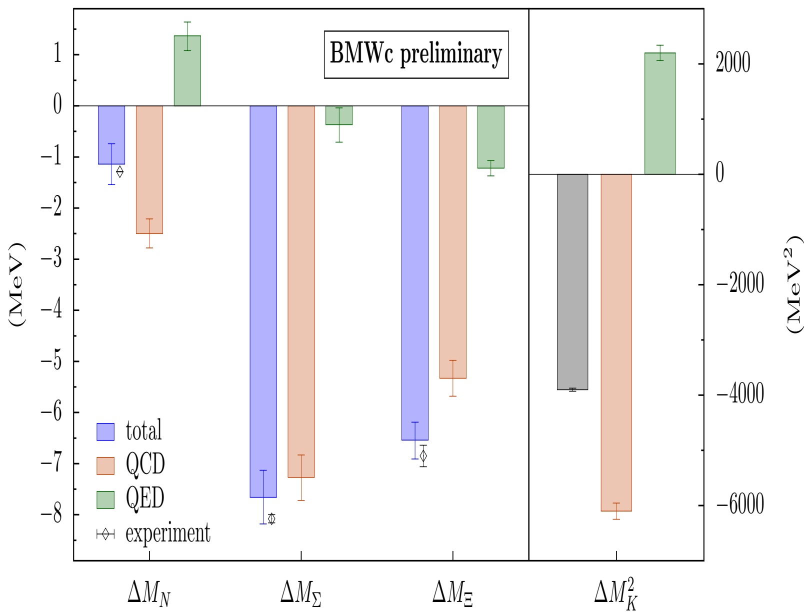
repeated by other collaborations

(ETMC: C. Alexandrou, M. Constantinou, V. Drach, G. Koutsou, K.J.)

- spectrum for $N_f = 2$, $N_f = 2+1$ and $N_f = 2+1+1$ flavours
  $\rightarrow$ no flavour effects for light baryon spectrum

Even isospin and electromagnetic mass splitting

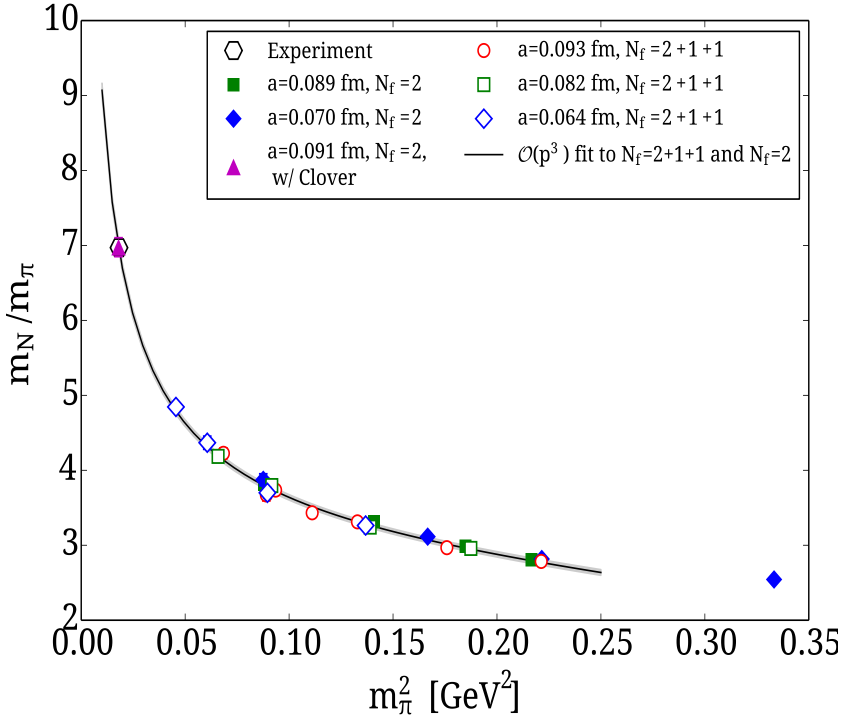
(BMW collaboration)



baryon spectrum with mass splitting

- nucleon: isospin and electromagnetic effects with opposite signs
- nevertheless physical splitting reproduced

Setting the scale



tune to $\dfrac{M_{\text{proton}}^{\text{phys}}}{M_{\text{pion}}^{\text{phys}}} = \dfrac{M_{\text{proton}}^{\text{latt}}}{M_{\text{pion}}^{\text{latt}}} = 6.95$

use proton mass: $a \cdot M_{\text{proton}}^{\text{phys}} = M_{\text{proton}}^{\text{latt}}$

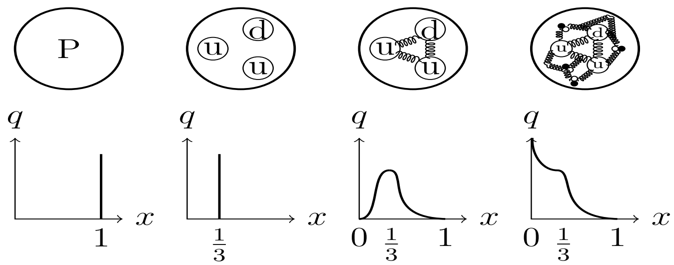
$\Rightarrow$ determine lattice spacing

$\Rightarrow$ using value of a other quantities have to come out right up to discretization effects

	M_{Ds}/M_K	M_{Ds}/M_D	f_K/f_π	f_{Ds}/f_D
lat.	3.96(2)	1.049(4)	1.197(6)	1.19(2)
PDG	3.988	1.0556(02)	1.197(06)	1.26(6)

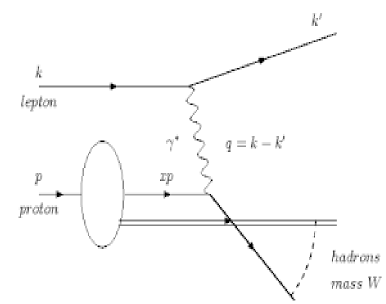
- with strange, charm quarks $\rightarrow$ need additional input
- repeat for smaller and smaller a $\rightarrow$ continuum limit

Hadron structure on the lattice



- parton distribution functions
- deep inelasic scattering experiments
- momentum fraction carried by quarks

(Bjorken variable) $x = \frac{Q^2}{2Pq}, \; Q^2 = -q^2$



Phenomenological analysis of PDFs

- worldwide data from deep inelastic scattering experiments **(e.g.: CERN, SLAC, DESY, Jlab)**

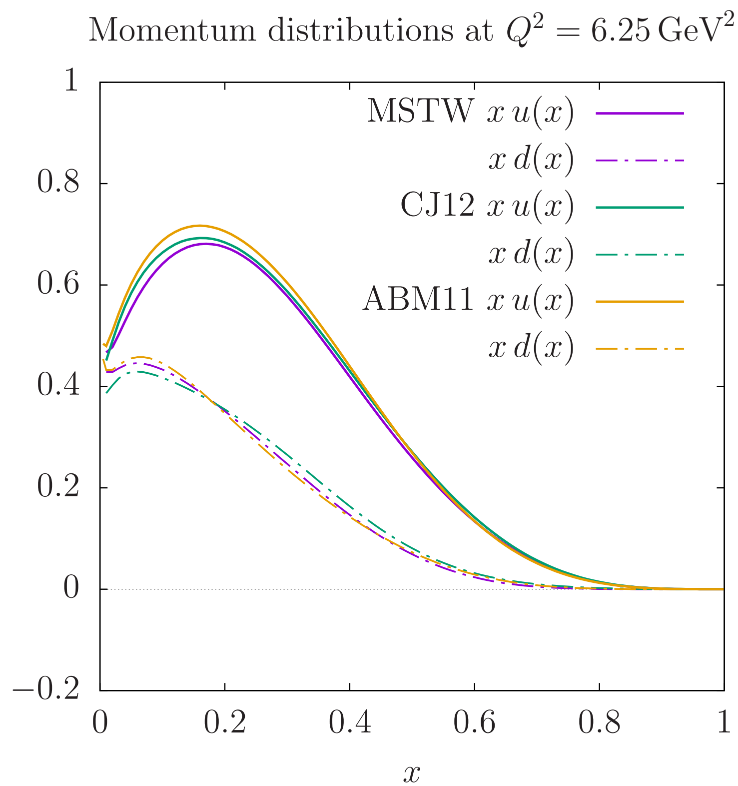
- fitting ansatz

$$xu(x) = A_u x^{a_u}(1-x)^{b_u} P_u(x)$$

$P(x)$ polynomial in x

- analysis not based on first principle calculation from QCD

- problem is of non-perturbative nature $\rightarrow$ lattice QCD



Problem on the lattice

- PDFs have form

$$q(x) = \int_{-\infty}^{\infty} \frac{d\xi^-}{4\pi} e^{-ix\xi^- P^+} \langle P|\bar{\psi}(\xi^-)\gamma^+ W(\xi^-,0)\psi(0)|P\rangle$$

- Wilson line $W(\xi^-,0) = e^{-ig\int_0^{\xi^-} A^+(\eta^-)\, d\eta^-}$
- dominated by area close to light cone $\xi^2 = \mathbf{x}^2 - t^2 = 0$
- this provides an issue on an Euclidean lattice where $\xi^2 = \mathbf{x}^2 + t^2 = 0$ is only fulfilled at a single point
- but, lattice can compute moments of PDFs: $\langle x\rangle_q = \int dx\, xq(x)$

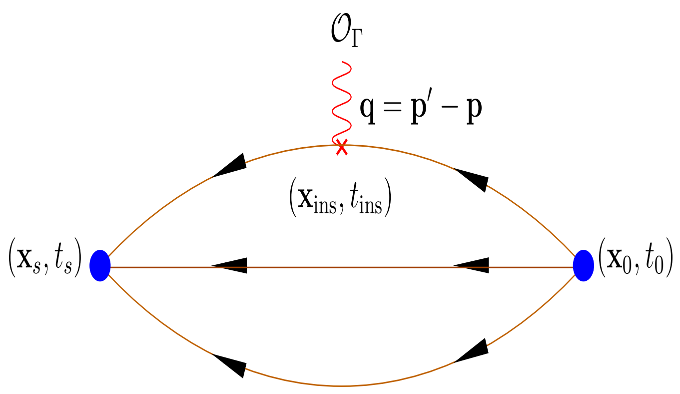
extraction of lattice moments

- nucleon 2-point function

$$G_{2\text{pt}}(t_s - t_0) = \langle J_\alpha(t_s)\bar{J}(t_0)\rangle \to e^{-M_{\text{nucleon}}(t_s-t_0)} \text{ for } t_s - t_0 \to \infty$$

- nucleon interpolating operator

$$J_\alpha(x) = \epsilon^{abc} u^a_\alpha(x)[u(x)^{\top b} C\gamma_5 d(x)^c]$$



- 3-point function

$$G_{3\text{pt}}(t_s - t_0, t_{\text{ins}}) = \Gamma\langle J_\alpha(t_s) O_\Gamma(t_{\text{ins}})\bar{J}(t_0)\rangle$$

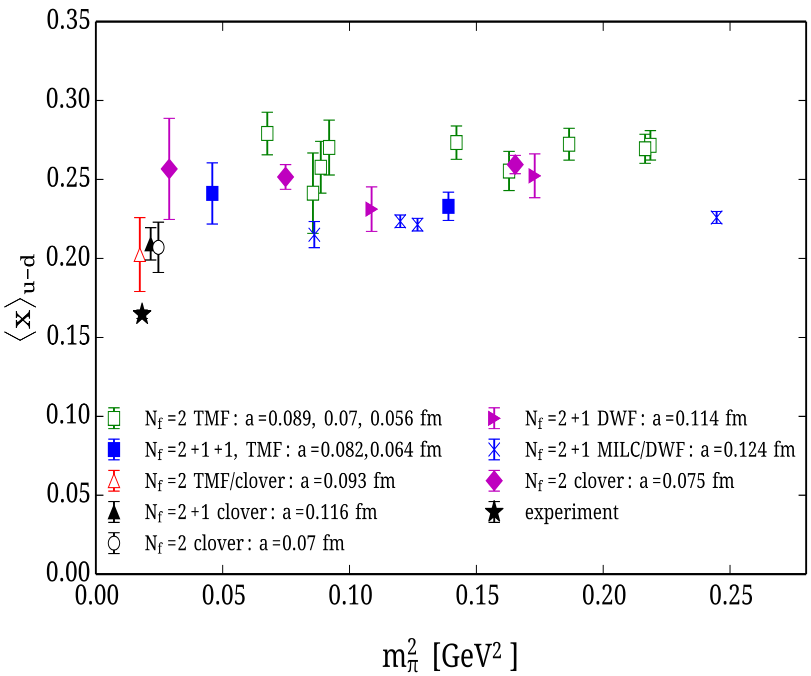
$$\to \langle O\rangle e^{-M_{\text{nucleon}}(t_s-t_0)}, \text{ for } t_s - t_0, t_{\text{ins}} \to \infty$$

- desired matrix element

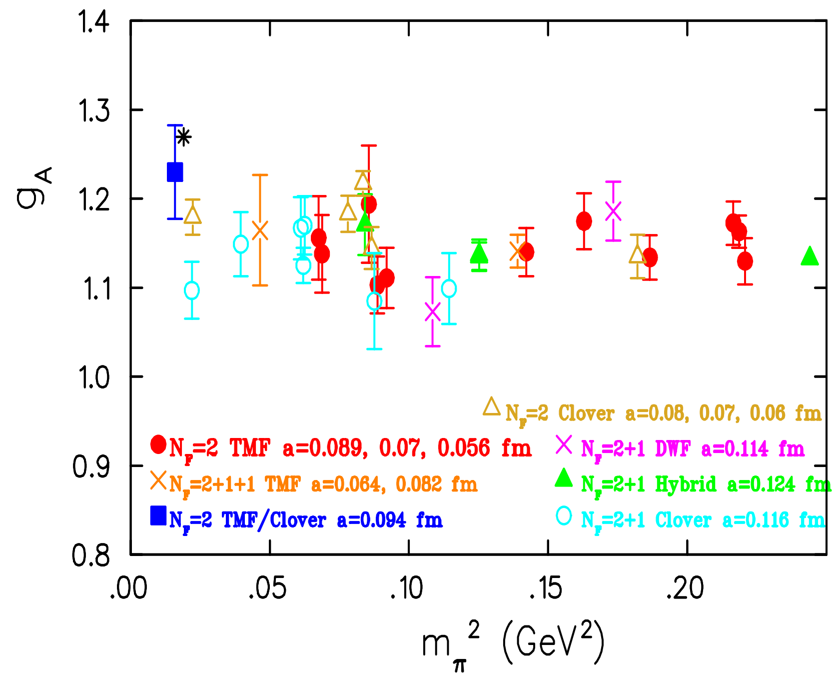
$$\frac{G_{3\text{pt}}(t_s-t_0,t_{\text{ins}})}{G_{2\text{pt}}(t_s-t_0)} \to \langle O\rangle, \text{ for } t_s - t_0, t_{\text{ins}} \to \infty$$

Moments of PDFs from the lattice

- moments $\langle x\rangle_q = \int dx\, x q(x)$
  - (unpolarized) quark distribution: $q(x) = q_\uparrow + q_\downarrow$
  - helicity distribution: $\Delta q(x) = q_\uparrow - q_\downarrow$
  - transversity distribution: $\delta q(x) = q_\top - q_\perp$



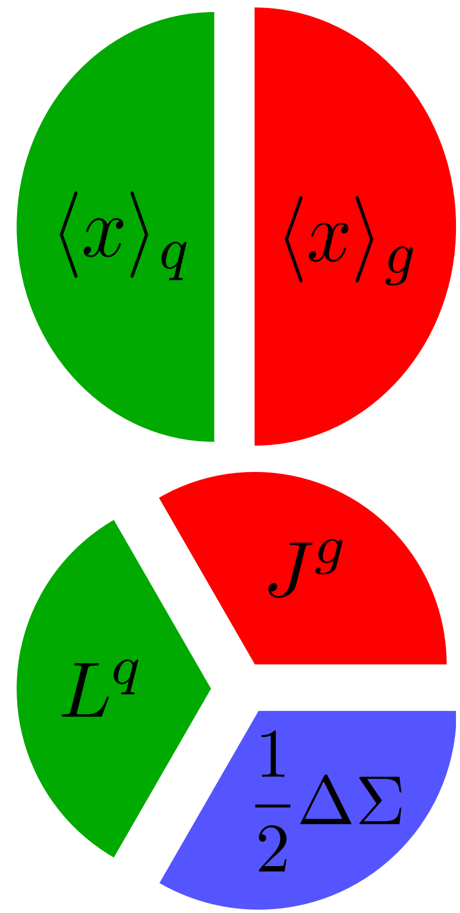
momentum fraction



axial charge

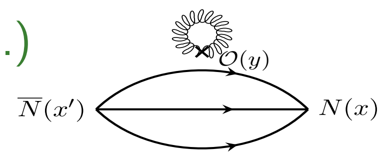
Spin of the nucleon

- momentum sum rule: $\sum_q \langle x \rangle_q + \langle x \rangle_g = 1$
  - experiment: $\sum_q \langle x \rangle_q \sim 0.6$
  - missing part completely covered by gluons?
- spin sum rule:
  $\frac{1}{2} = \frac{1}{2}\Delta\Sigma + L_q + J_g$
  - $\frac{1}{2}\Delta\Sigma$ quark spin
    L_q quark orbital angular momentum
    J_g gluon angular momentum
  - experiment: $0.13 < \frac{1}{2}\Delta\Sigma < 0.18$
- Here: computation of
  $\langle x \rangle_g$ and J_g



Gluon moment in the nucleon

(C. Alexandrou, M. Constantinou, K. Hadjiyiannakou,
H. Panagopoulos, C. Wiese, K.J.)



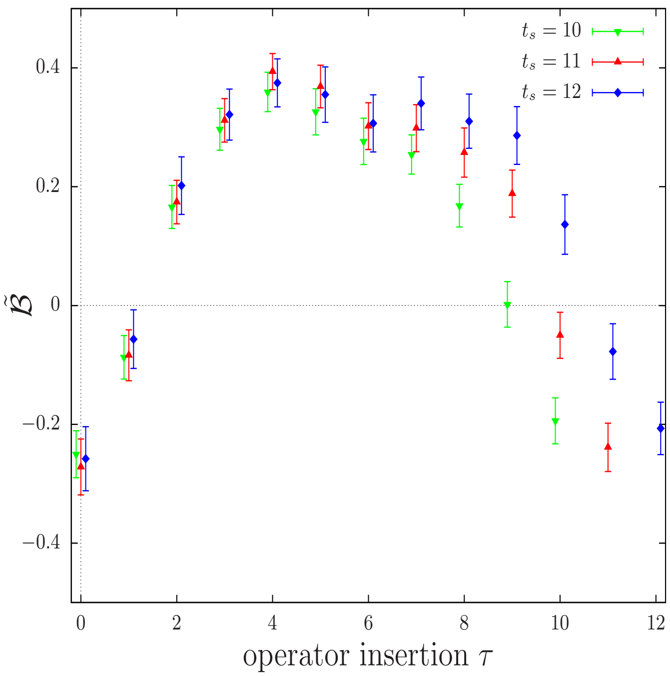
- gluon moment related to
  energy momentum tensor $T_g^{\{\mu\nu\}}$
  $\langle x \rangle_g = A_{20}^g$ with $\langle P | T_g^{\{\mu\nu\}} | P \rangle = 2A_{20}^g P^{\{\mu} P^{\nu\}}$

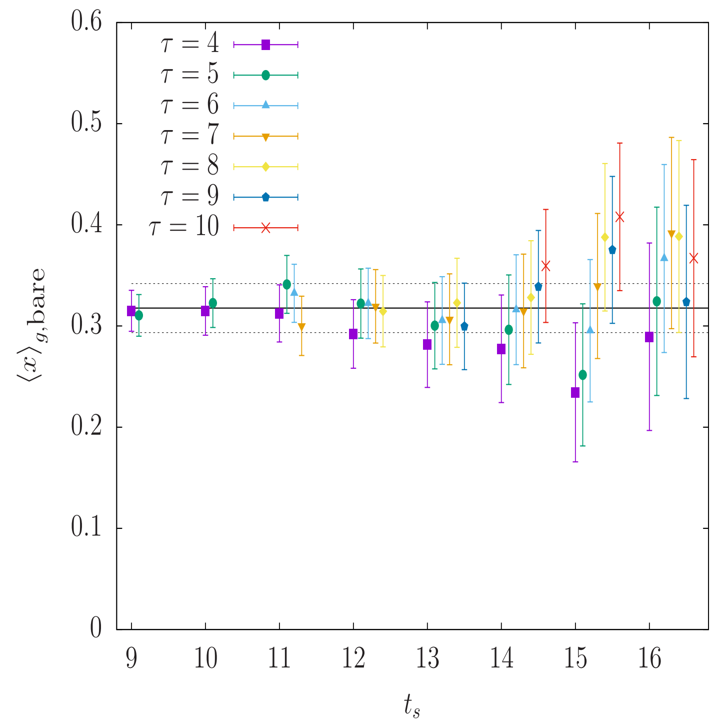
- gluon angular momentum related to
  $J_g = \frac{1}{2}(A_{20} + B_{20})$

- lattice: A_{20} computed from 3-point function
  - disconnected diagram
  - known to be very noisy
  - here: use $O(200.000)$ measurements (typically $O(1000)$ measurements)

The plateuax serach

- plateau behaviour only visible by special lattice techniques
  - HYP smearing
  - stochastic evaluation of 3-point function



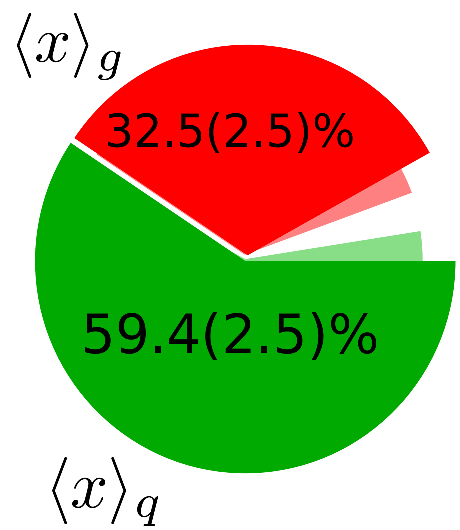


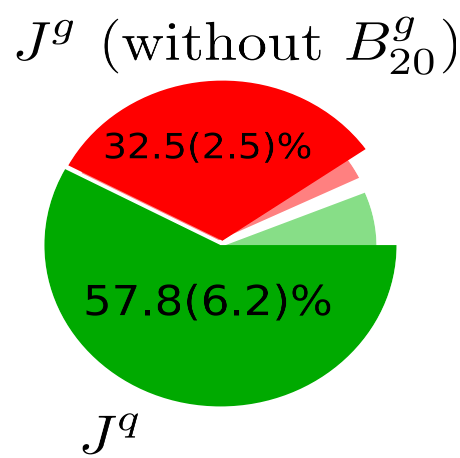
Result for gluon moment

- gluon moment at *physical* pion mass:
  $\langle x \rangle_{g,\mathrm{bare}} = 0.318(24)$
  $\longrightarrow$ Renormalization $\langle x \rangle_g = 0.325(25)$

- momentum and spin sum rules
  - $\langle x \rangle_{u+d+s} = 0.594(25)$
  - $J_{u+d+s} = 0.578(62)$

- missing systematic uncertainties
  - continuum and infinite volume limits
  - evaluation of B_{20}





Direct calculation of PDFs on the lattice

(C. Alexandrou, K. Cichy, V. Drach, E. Garcia-Ramos, K. Hadjiyiannakou, F. Steffens, C. Wiese, K.J.)

A feasibility study

- light cone operator

  $q(x) = \int_{-\infty}^{\infty} \frac{d\xi^-}{4\pi} e^{-ix\xi^- P^+} \langle P|\bar{\psi}(\xi^-)\gamma^+ W(\xi^-, 0)\psi(0)|P\rangle$

  $W(\xi^-, 0) = e^{-ig\int_0^{\xi^-} A^+(\eta^-)\, d\eta^-}$ (Wilson line)

- dominated by light cone $\xi^2 = \mathbf{x}^2 - t^2 = 0$

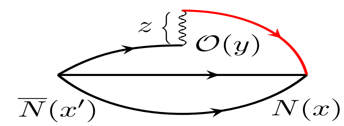
- Euclidean time lattice: $\xi^2 = \mathbf{x}^2 + t^2 = 0 \rightarrow$ not accessible

- new propodsal (Ji, 2013) quasi distribution

  $\tilde{q}(x, P_3) = \int_{-\infty}^{\infty} \frac{dz}{4\pi} e^{-izk_3} \langle P|\bar{\psi}(z)\gamma_3 W_3(z, 0)\psi(0)|P\rangle$

Relation of $\tilde{q}(x)$ and $q(x)$

- perturbative relation

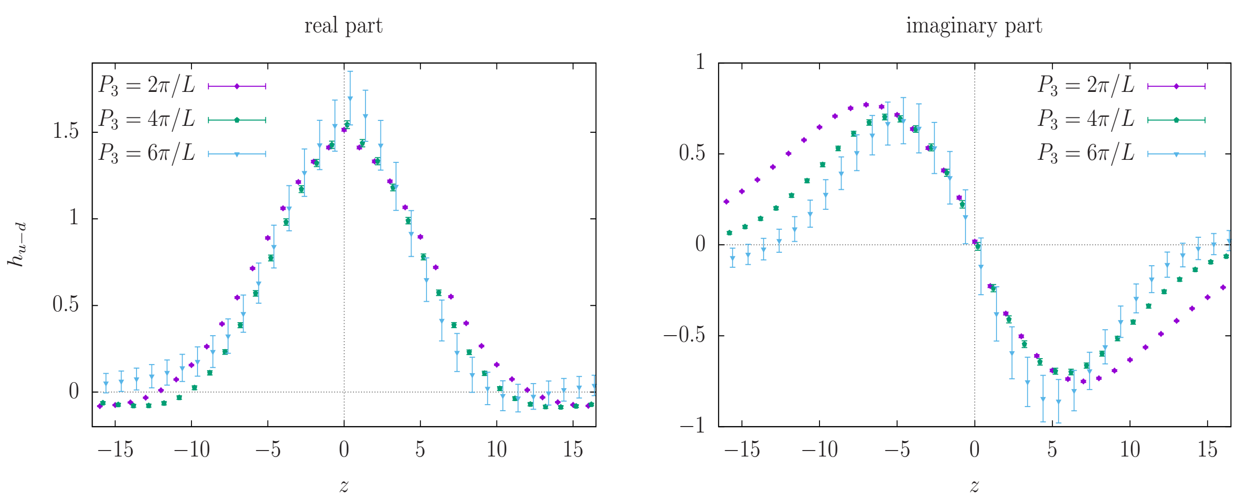


$$q(x,\mu) = \tilde{q}(x,\Lambda,P_3) - \frac{\alpha_s}{2\pi}\tilde{q}(x,\Lambda,P_3)\delta Z_F^{(1)}\left(\frac{\mu}{P_3},\frac{\Lambda}{P_3}\right)$$

$$-\frac{\alpha_s}{2\pi}\int_{-1}^{1} Z^{(1)}\left(\frac{x}{y},\frac{\mu}{P_3},\frac{\Lambda}{P_3}\right)\tilde{q}(y,\Lambda,P_3)\frac{dy}{|y|} + \mathcal{O}(\alpha_s^2)$$

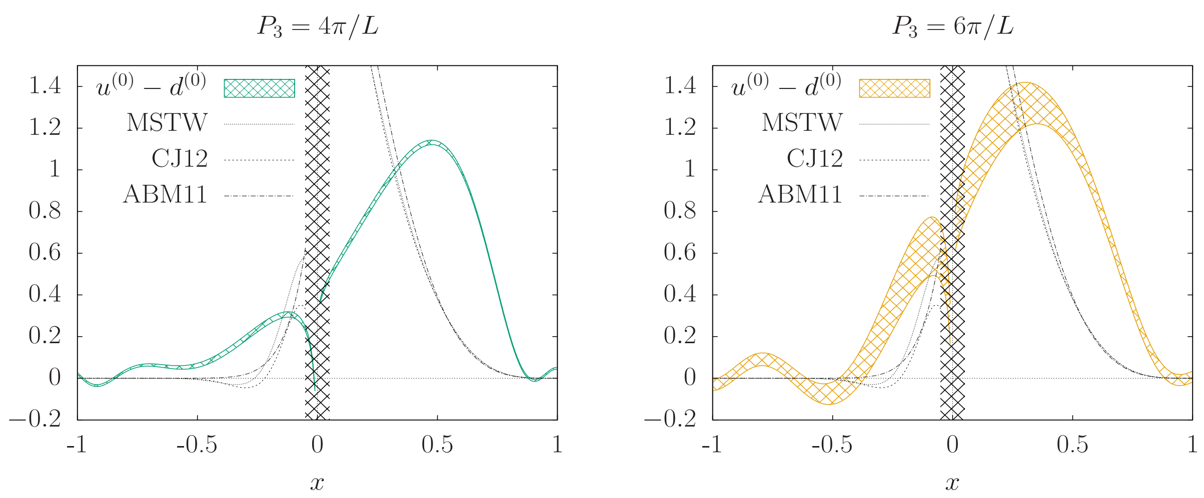
- needs $\Lambda/P_3 \ll 1$, $M_{\mathrm{nucleon}}/P_3 \ll 1$

- lattice operator: $\langle P|\overline{\psi}(z)\gamma_3 W_3(z,0)\psi(0)|P\rangle = \bar{u}(P)\gamma_3 h(P_3,z)u(P)$



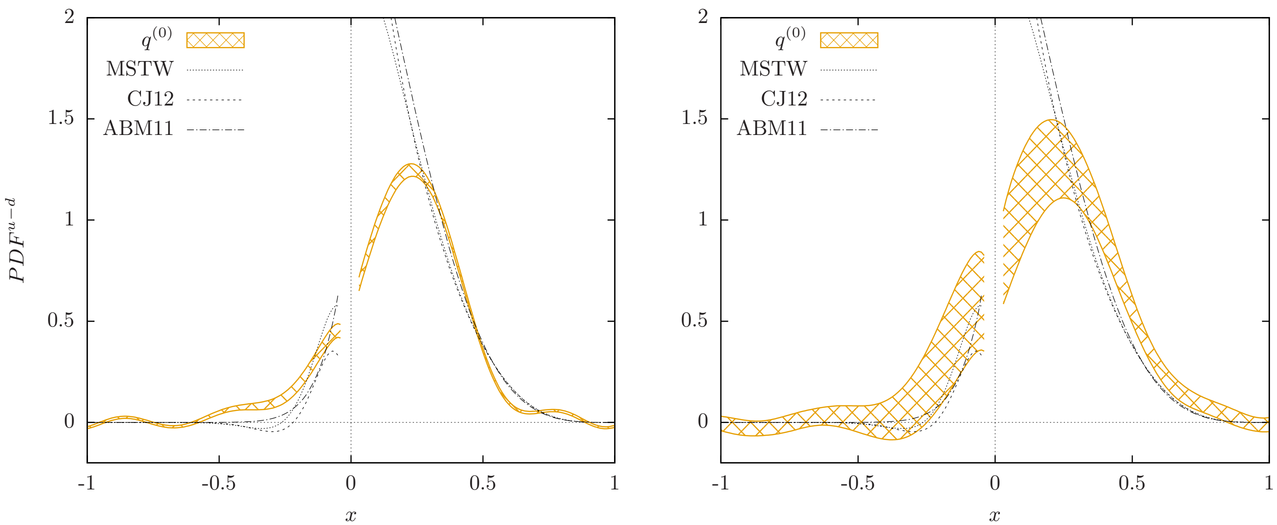
Relation of $\tilde{q}(x)$ and $q(x)$

- after target mass corrections
- matching of $\tilde{q}(x)$ and $q(x)$
- relating negative x region by crossing relation
  $\bar{q}(x) = -q(-x)$
- negative $x \Rightarrow \bar{d} - \bar{u}$



prospects and problems

- same calculation repeated for helicity and transversity distributions
- here not physical pion mass
- what if we would had higher momenta?



$P_3/4\pi/L$ $\qquad$ $P_3 = 6\pi/L$

a hypothetical setup: artificial larger momenta

- Fourier tranformation, matching and mass correction with $P_3 = 8\pi/L$
- very open: renormalization

Summary

- Progress in solving QCD with lattice techniques
  - dramatic algorithm improvements
  - new supercomputer architectures reaching $O(\mathrm{Petaflop})$
- have performed benchmark calculations in lattice QCD
  - Hadron spectrum from first principles
  - Electromagnetic and iso-spin mass splitting
- Hadron structure on the lattice
  - Moments of PDFs at the physical point
  - Progress towards understanding spin and momentum sum rules
  - First steps towards direct calculation of PDfs
- Major challenges
  - understand systematics, continuum and infinite volume limits, excited states
  - renormalization of PDFs


DB
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