Synergy of HPC and Nuclear Physics to resolve long-standing puzzles: the proton spin & mass

Martha Constantinou

Temple University

The Cyprus Institute Seminar

March 16, 2021

Work within Extended Twisted Mass Collaboration (ETMC)

- **C. Alexandrou** Univ. of Cyprus/Cyprus Institute
- **S. Bacchio** Cyprus Institute
- **J. Finkenrath** Cyprus Institute
- **K. Hadjiyiannakou** Univ. of Cyprus/Cyprus Institute
- **K. Jansen** DESY, Zeuthen
- **G. Koutsou** Cyprus Institute
- **H. Panagopoulos** University of Cyprus
- **G. Spanoudes** University of Cyprus
- **A. Vaquero** University of Utah

Relevant publications:

- C. Alexandrou, S. Bacchio, M. Constantinou, K. Hadjiyiannakou, K. Jansen, G. Koutsou, A. Vaquero Aviles-Casco
  Phys. Rev. D 102 (2020) 054517, [arXiv:1909.00485]

- C C. Alexandrou, S. Bacchio, M. Constantinou, J. Finkenrath, K. Hadjiyiannakou, K. Jansen, G. Koutsou, H. Panagopoulos, G. Spanoudes
  Phys. Rev. D 101 (2020) 094513, [arXiv:2003.08485]

OUTLINE OF TALK

A. Introduction - Motivation

B. Hadron Structure from Lattice QCD

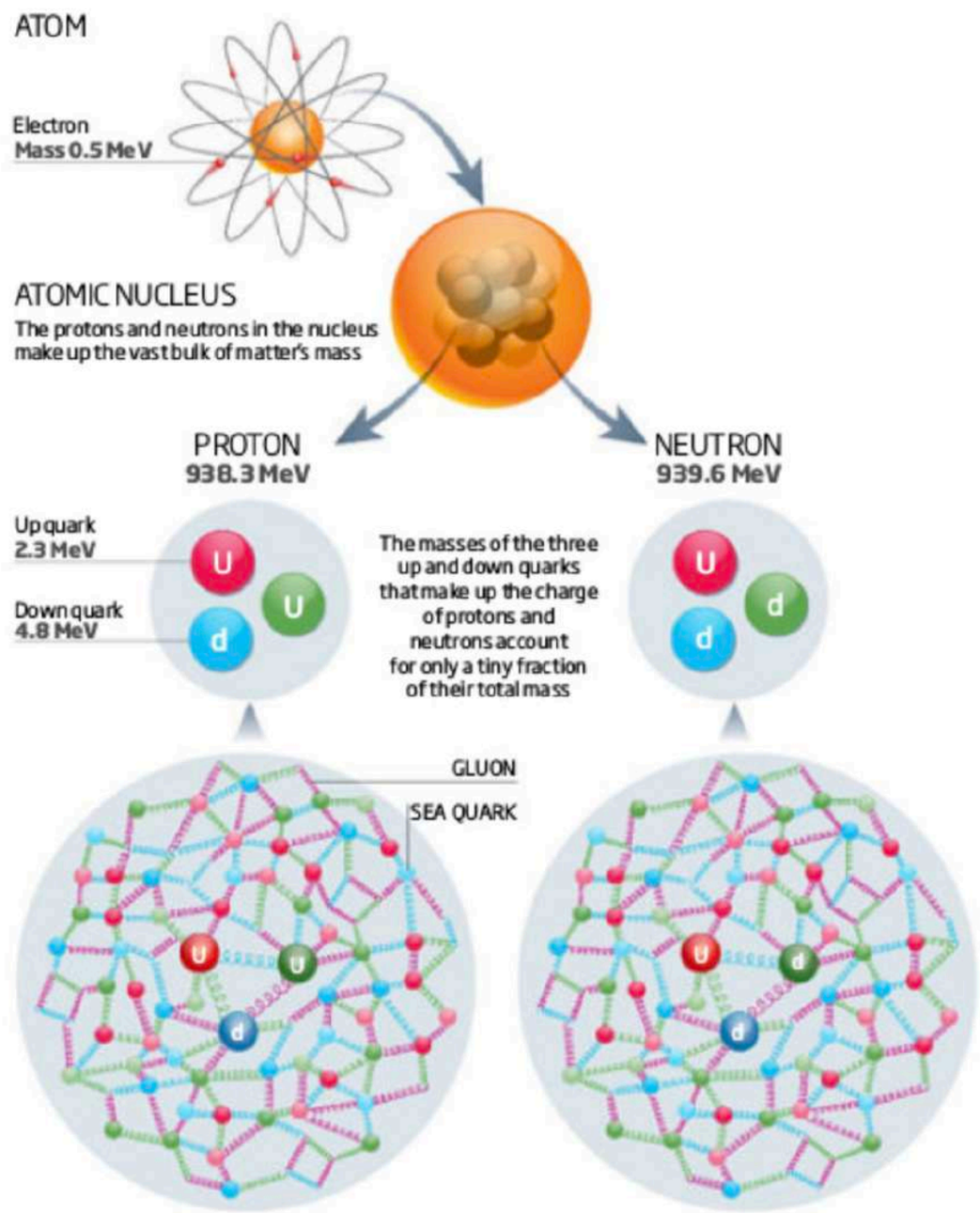
C. Proton spin

D. Proton mass

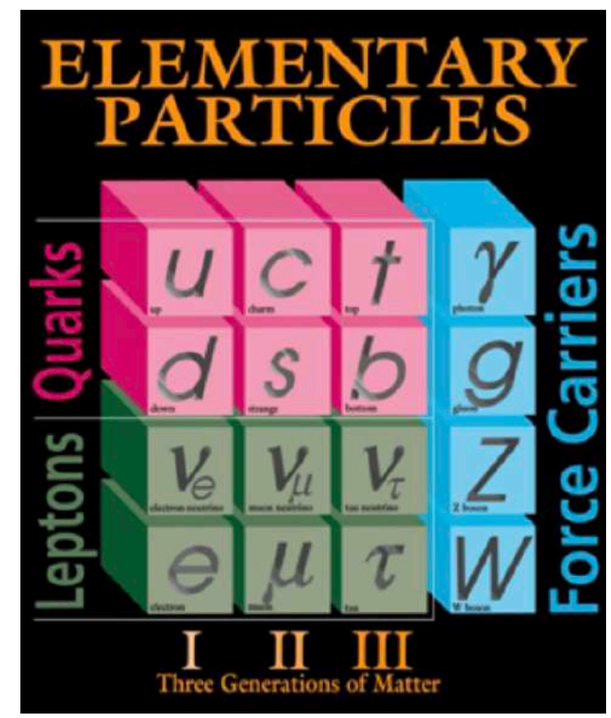
E. Summary

Quantum Chromodynamics (QCD)

Structure of Matter



- Theory of the strong interactions
- Fundamental constituents: quark and gluons



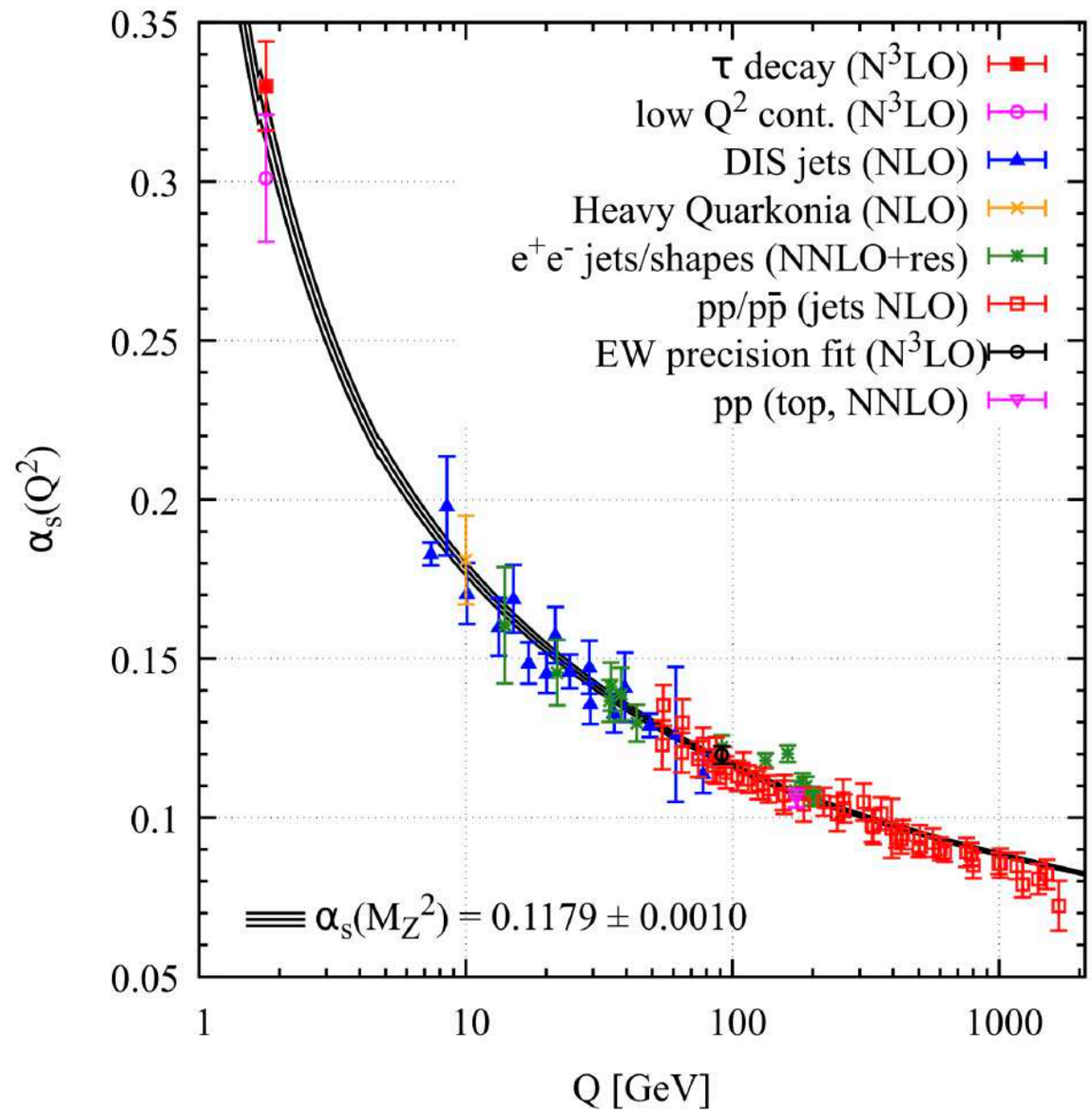
- Only a few parameters needed to describe QCD:
  quark masses & coupling constant

QCD is a unique theory

Coupling is not constant

- **At small distances (<<1 fm):**
  asymptotic freedom

- **At large distances (>1 fm):**
  confinement



Review of Particle Physics (2020)

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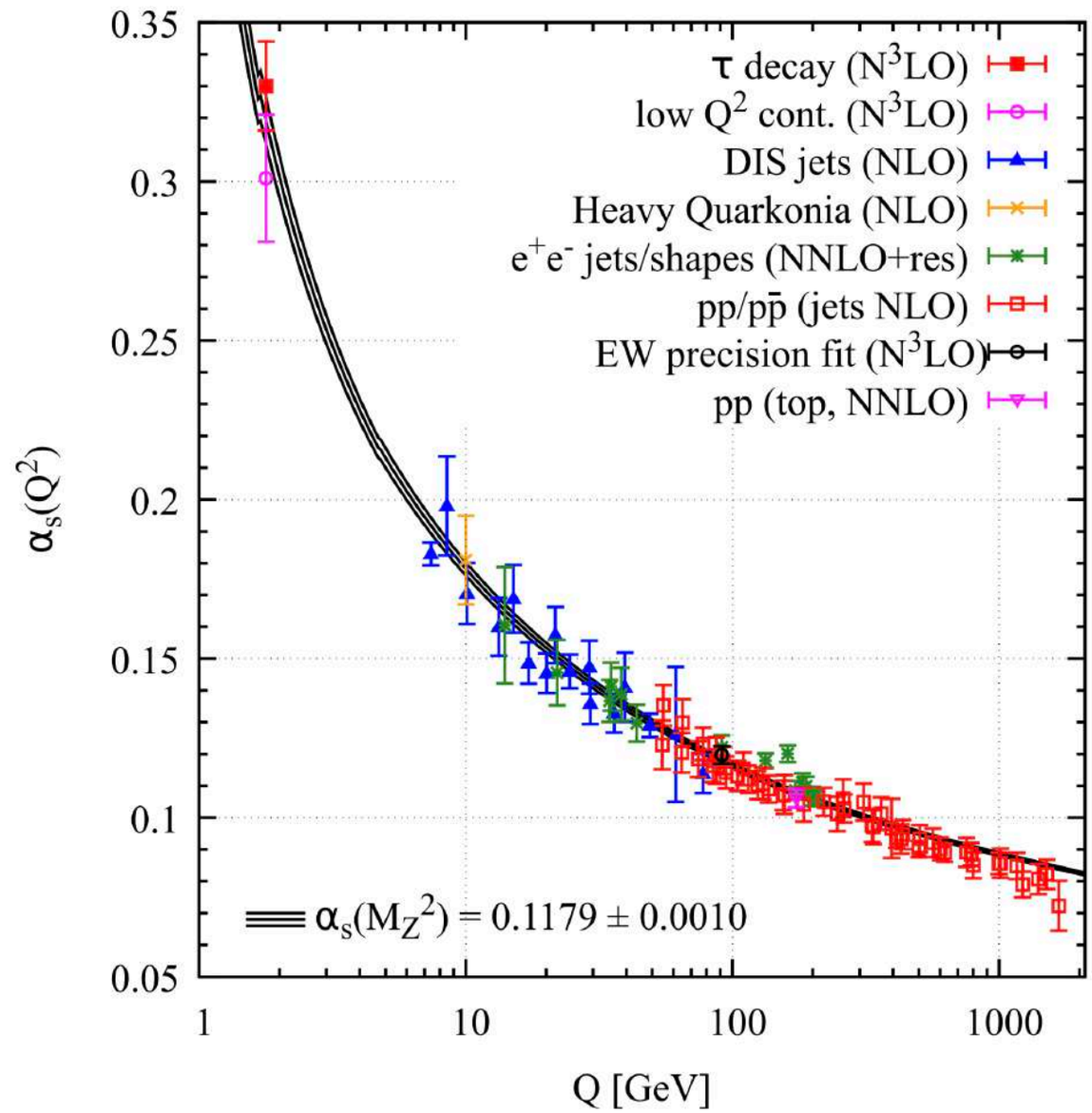

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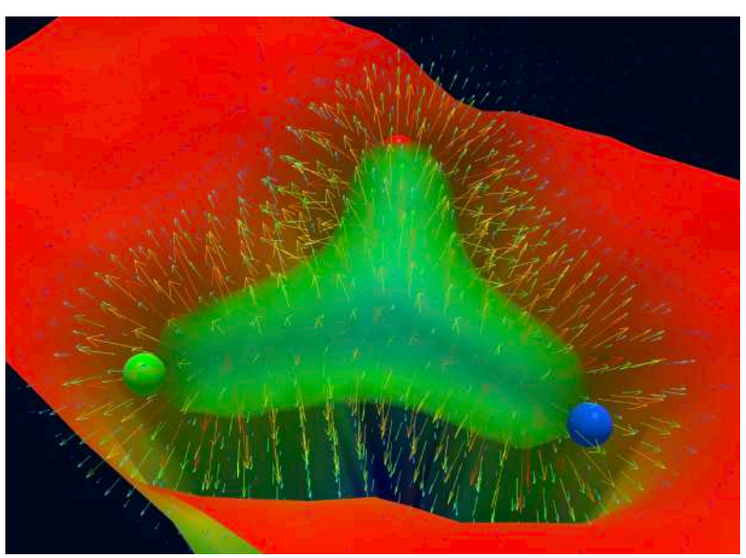
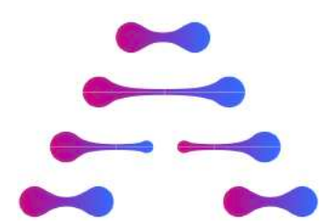


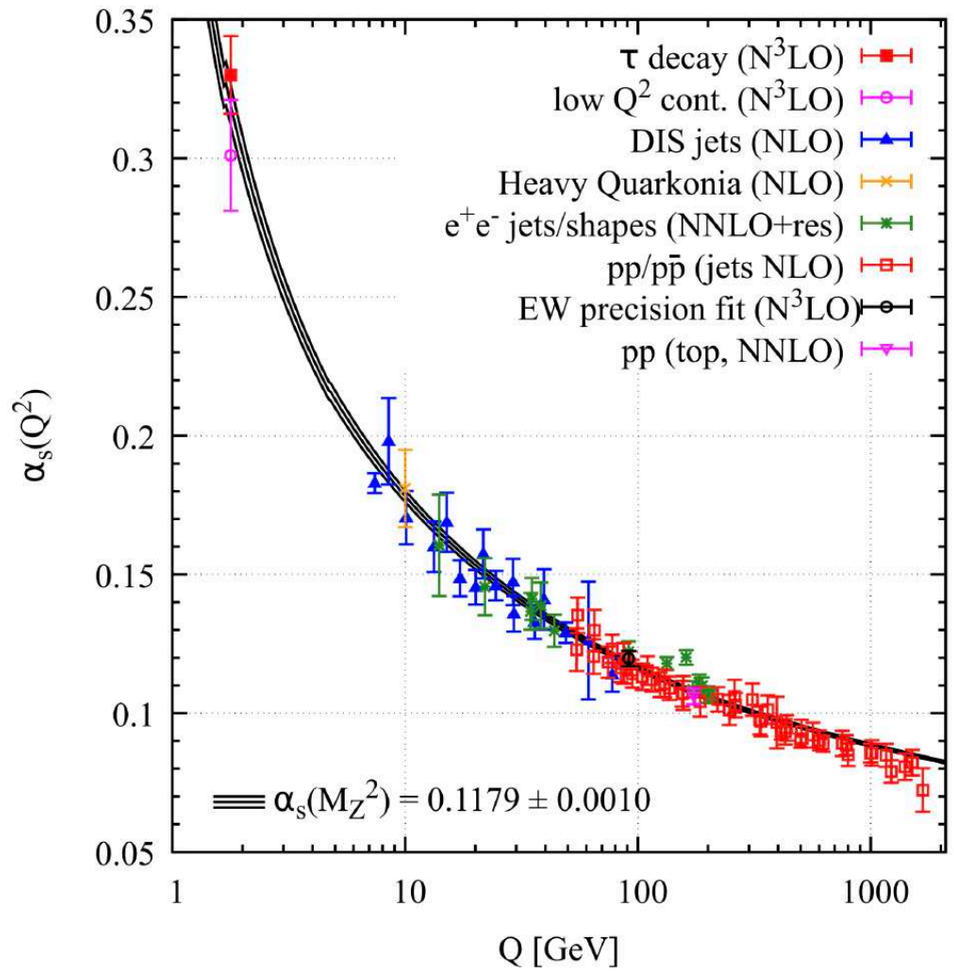
Credit: D. Leinweber

Flux tubes of QCD



Quark confinement

Computational



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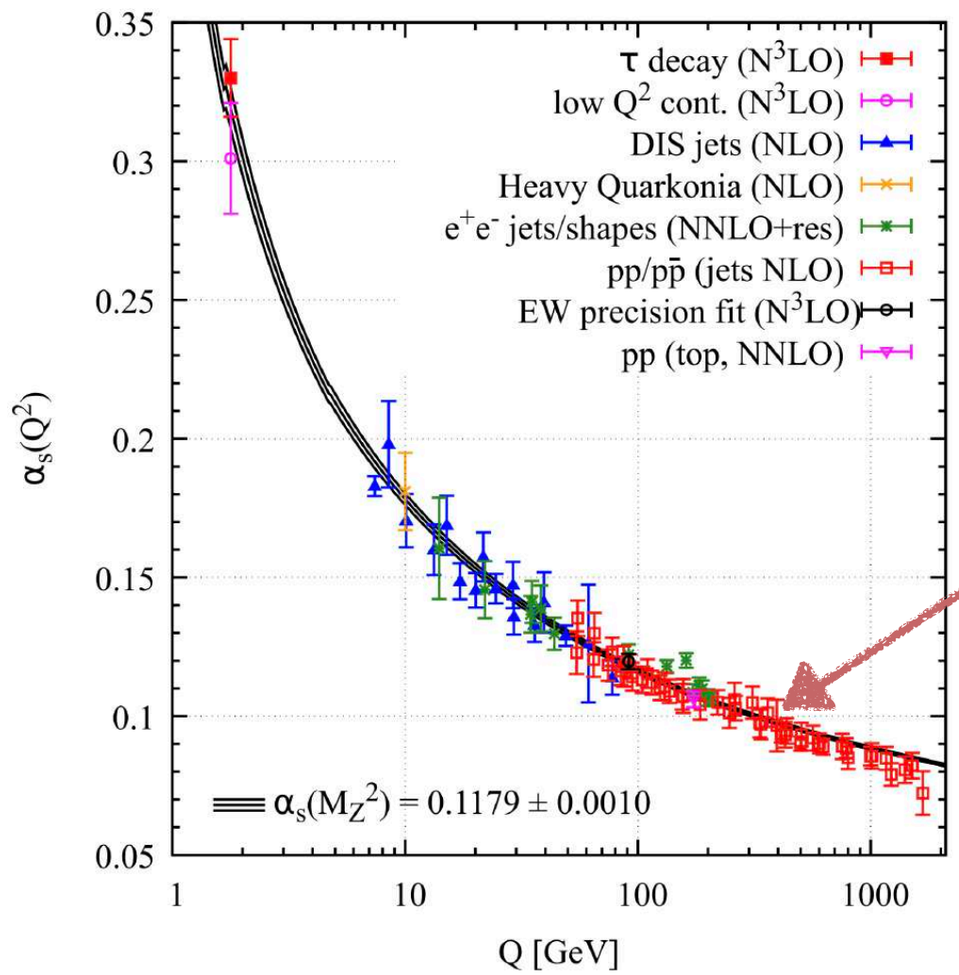

High energies

- perturbation theory

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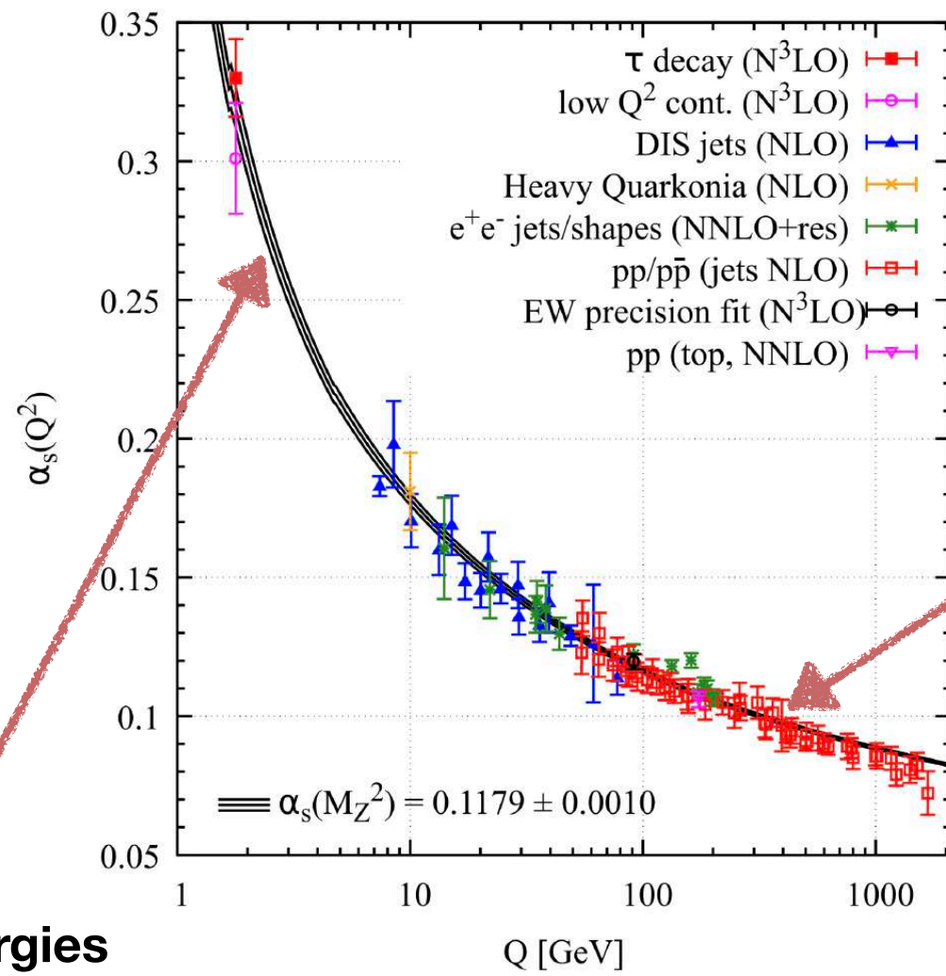


High energies

- perturbation theory

Low & intermediate energies

- Lattice QCD
(Large-scale numerical simulations)

- Chiral pert. Theory

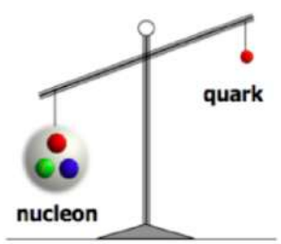
Mass Generation: Complex mechanism

Hydrogen Atom:

$$m_{hydr} = \underbrace{0.51MeV}_{m_{e^-}} + \underbrace{938.29MeV}_{m_{p^+}} - \underbrace{13.6eV}_{E_{binding}}$$

Proton:

$$m_p = 938.3MeV \qquad 2m_u + m_d = 9.1MeV$$



majority of mass generation is due to QCD dynamics

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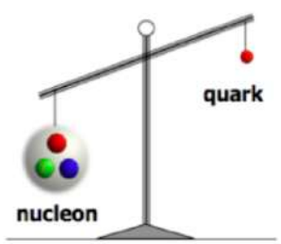

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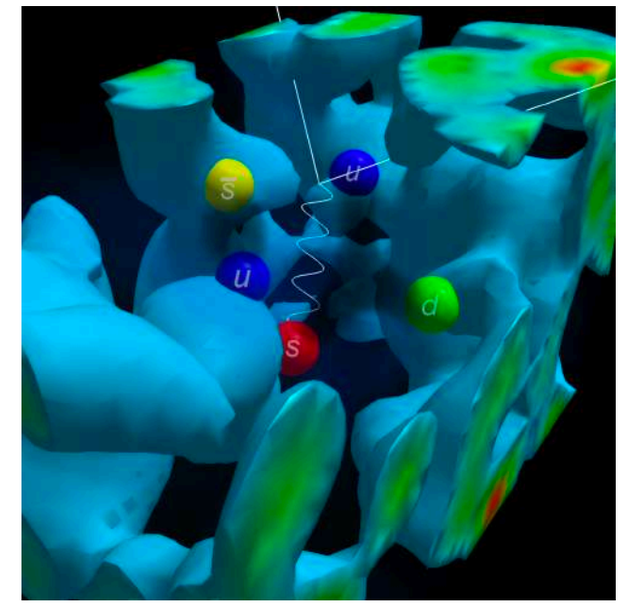

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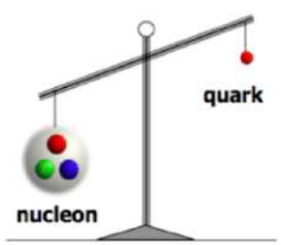

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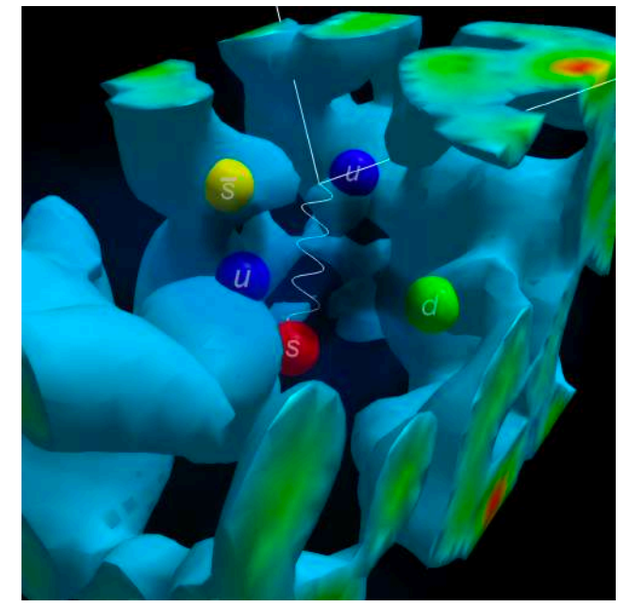

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QCD Lagrangian:

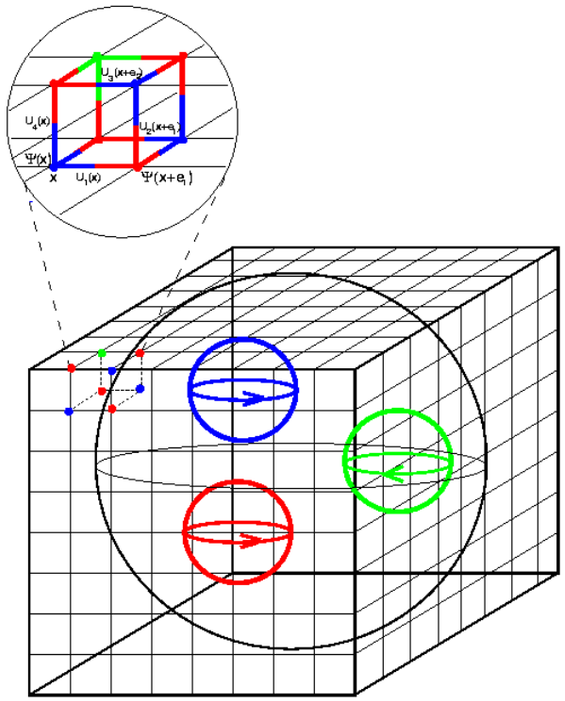
$$\mathscr{L}_{\mathrm{QCD}} = \sum_f \bar{\psi}_f \left(i\gamma^\mu D_\mu - m_f \right) \psi_f - \frac{1}{4} F^a_{\mu\nu} F^{a\,\mu\nu}$$

Describes strongly interacting matter in the universe

Very elegant BUT highly non-linear

Lattice formulation of QCD

Ideal first principle formulation of QCD
(simulations starting from original Lagrangian)



- ★ Space-time discretization on a finite-size 4-D lattice
- ★ Serves as a regulator:
  UV cut-off: inverse lattice spacing $\int_{-\infty}^{\infty} dp \;\rightarrow\; \int_{-\pi/a}^{\pi/a} \frac{dp}{2\pi}$
  IR cut-off: inverse lattice size $\int dp F(p) \;\rightarrow\; \sum_{n}^{N_{\max}} \frac{2\pi}{L} F(p_0 + \frac{2\pi n}{L})$
- ★ Removal of regulator $L \rightarrow \infty\,,\;\; a \rightarrow 0$

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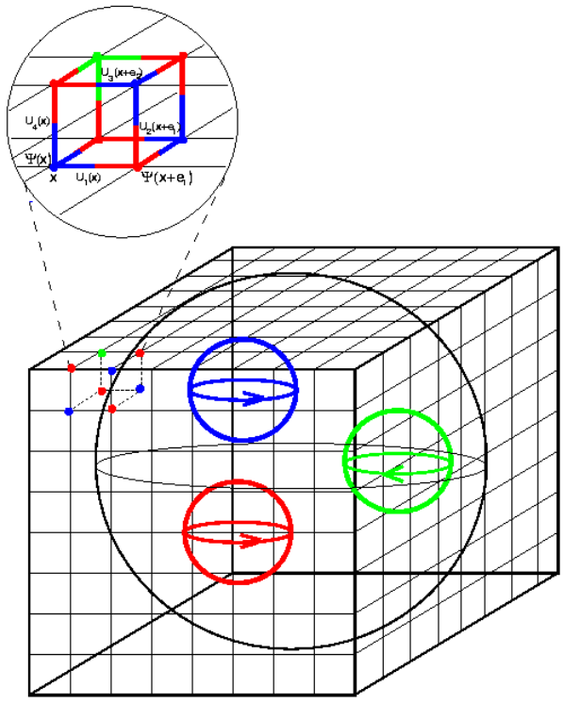

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Technical Aspects

- ★ Parameters (define cost of simulations):
  quark masses (aim at physical values)
  lattice spacing (ideally fine lattices)
  lattice size (need large volumes)
- ★ Discretization not unique:
  Wilson, Clover, Twisted Mass, Staggered, Overlap, Domain Wall, Mixed actions

Computational Challenges

★ **Parameters (define cost of simulations):**
quark masses (aim at physical values)
lattice spacing (ideally fine lattices)
lattice size (need large volumes)

★ **Billions of degrees of freedom:**
huge computational power
algorithmic improvements necessary

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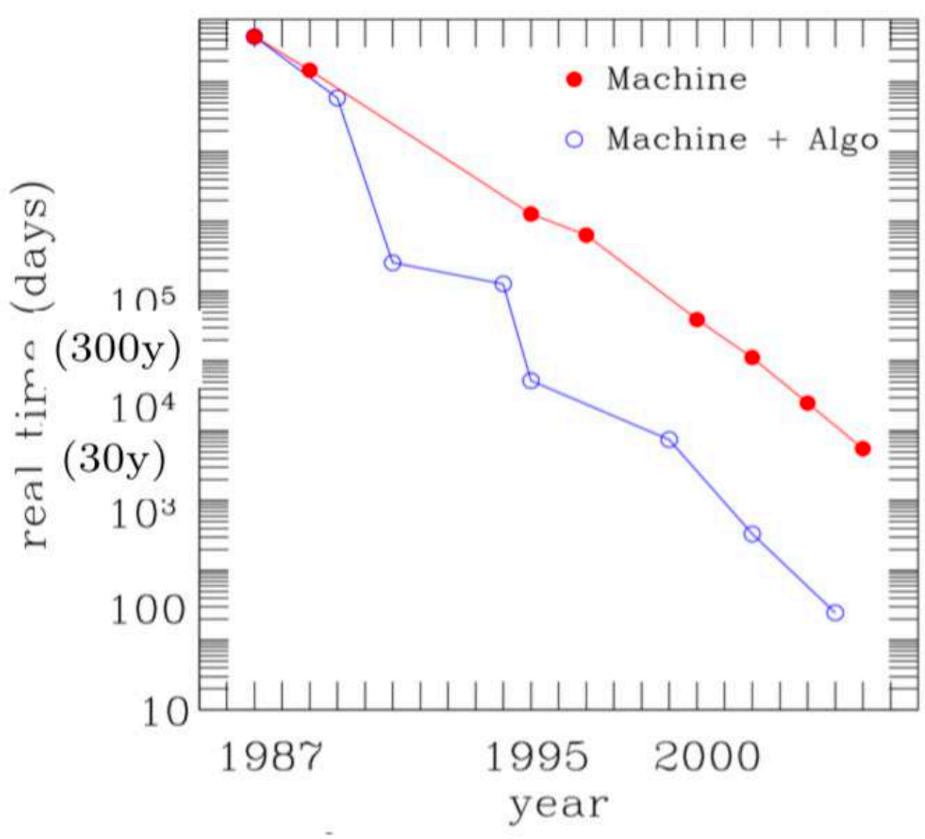

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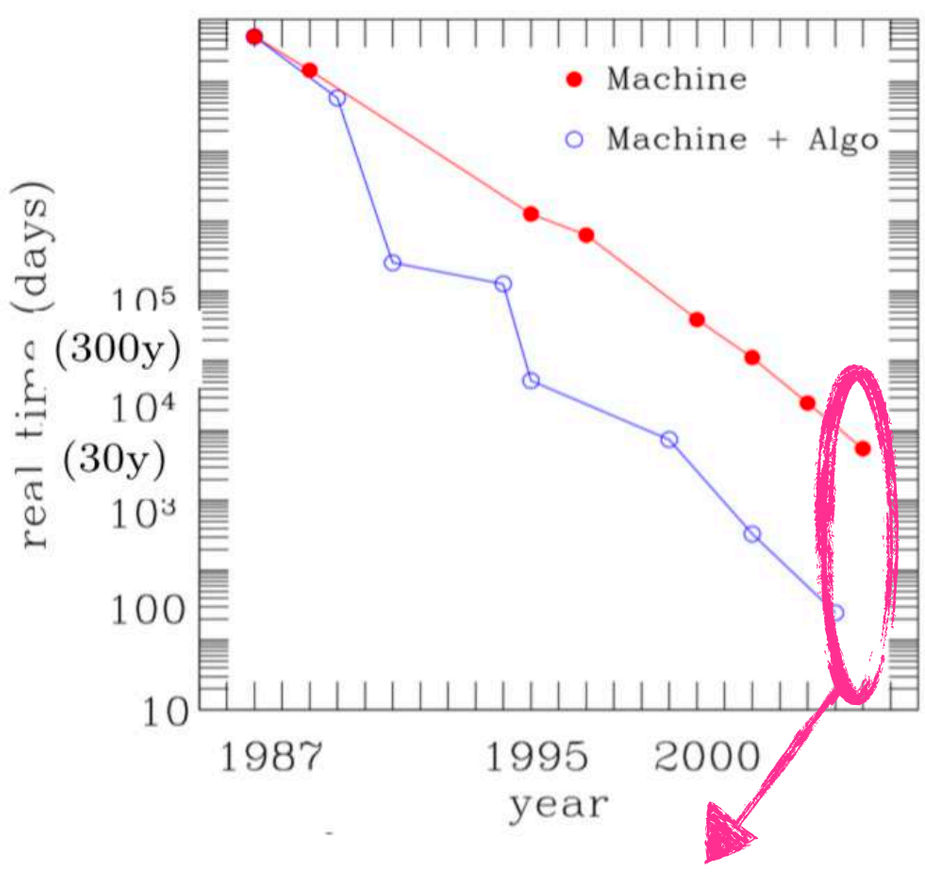

O(100) less cost

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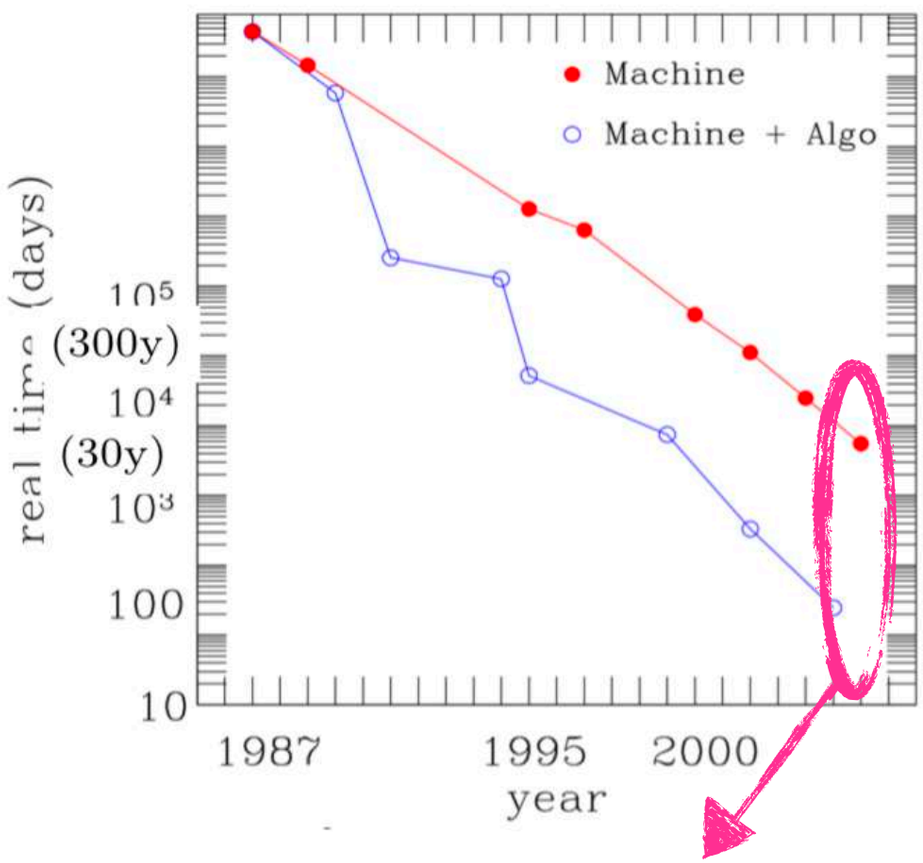

O(100) less cost

Cyclone, CaSToRC, Cyl

Argonne Nat. Lab

First exascale supercomputer

Computational Challenges

★ **Feynman Path Integral formulation**

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

★ **Fields ψ and U integrated (Monte Carlo)**
Direct calculation of path integral unfeasible

★ **Rotation to Euclidean space - integration of fermion fields**
Statistical mechanics methods

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U]\mathcal{O}(U,M^{-1})e^{-S_G[U]+\ln(\det(M[U]))}$$

★ **Calculation of observables, which are functions of the inverse of the fermion matrix M.**
- Sparse matrix
- Evaluated iteratively

★ **Matrix inversion: most common operation in calculations**

Computational Challenges

- ★ **Marcov-chain Monte Carlo process: generate representative configurations of U with probability following the theory**

$$p(U) = \frac{1}{Z}\int \mathcal{D}[\bar{\phi}]\mathcal{D}[\phi]e^{-S_G[U]-\bar{\phi}(M^+M)^{-1}\phi}$$

- ★ **Monte-Carlo process repeated $N \sim \mathcal{O}(100) - (1000)$ to control statistical uncertainties in observables $(1/\sqrt{N})$**

- ★ **Typical lattice sizes ($64^3 \times 128$, $96^3 \times 192$) contain $\mathcal{O}(10M) - (100M)$ of lattice points**

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HPC and parallel programing is necessary to perform calculations

- ★ **Generation of ~500 configurations for large lattices: $\mathcal{O}(100)$ M GPU-h**
  Observables (10,000 inversions) $\mathcal{O}(10)$ M GPU-h

Computational Challenges

- ★ Lattice QCD recognized as an important and transformative field

- ★ CaSToRC spearheads the software development
  - HPC in Life sciences, Engineering and Physics (HPC-LeaP)
    (Funded by EU Horizon)
  - Partnership for Advanced Computing in Europe (PRACE)
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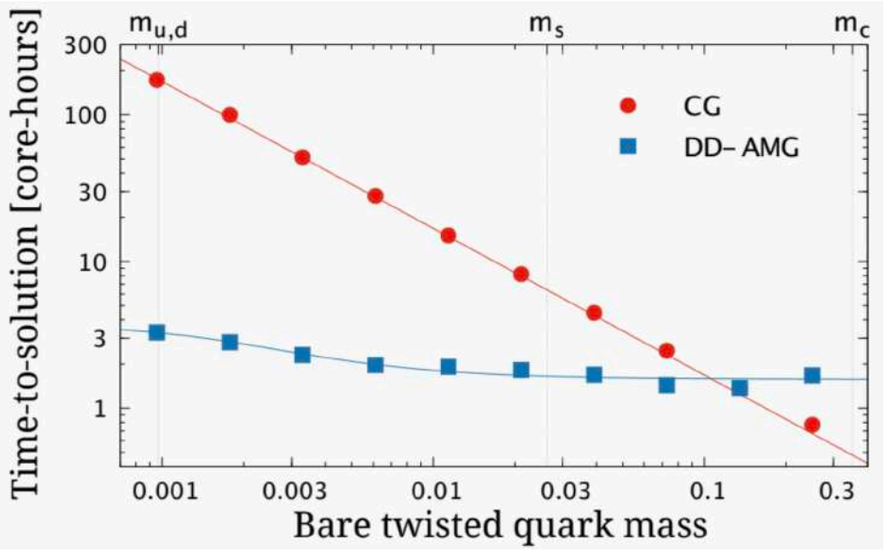
- ★ All scientists working on the Twisted Mass Lattice formulation



- ★ Multi-grid: Computational cost reduced by orders of magnitudes compared to other techniques (conjugate gradient, …)

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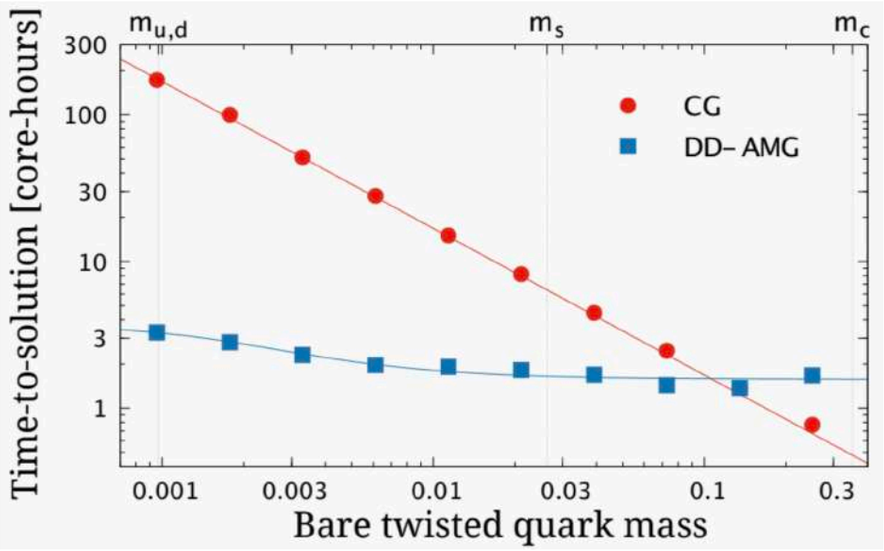

- ★ Multi-grid: Computational cost reduced by orders of magnitudes compared to other techniques (conjugate gradient, …)
- ★ ETMC worldwide leaders in lattice QCD calculations on the proton structure

Computational Challenges

- ★ **Being up-to-date with computer architecture and new methods is imperative**

Computational Challenges

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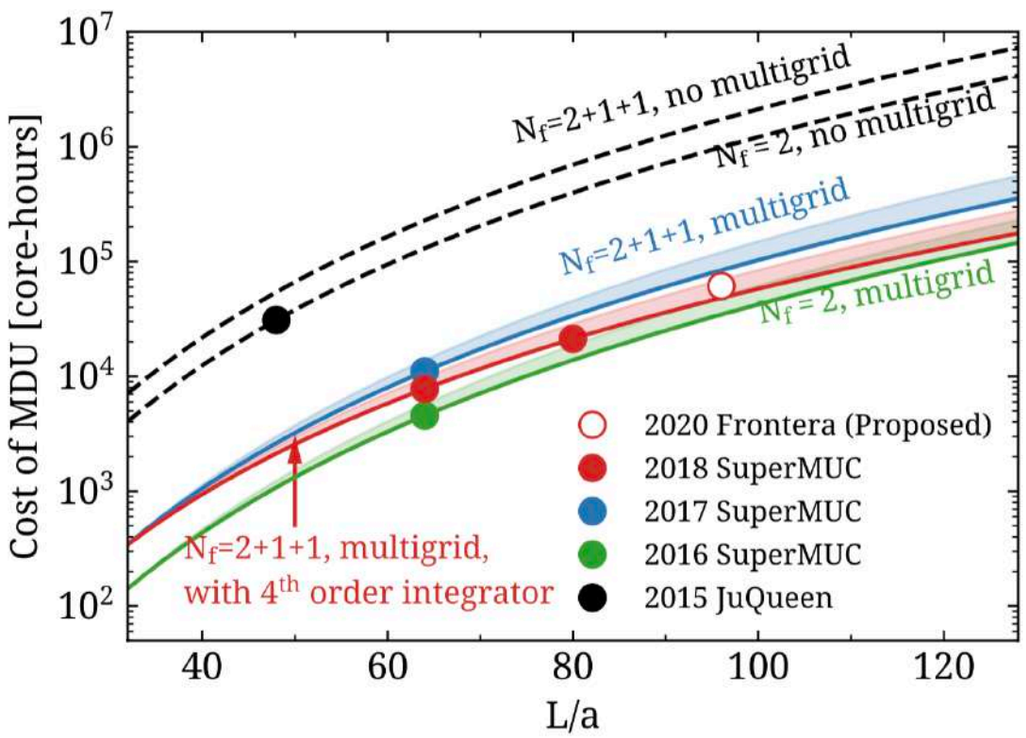
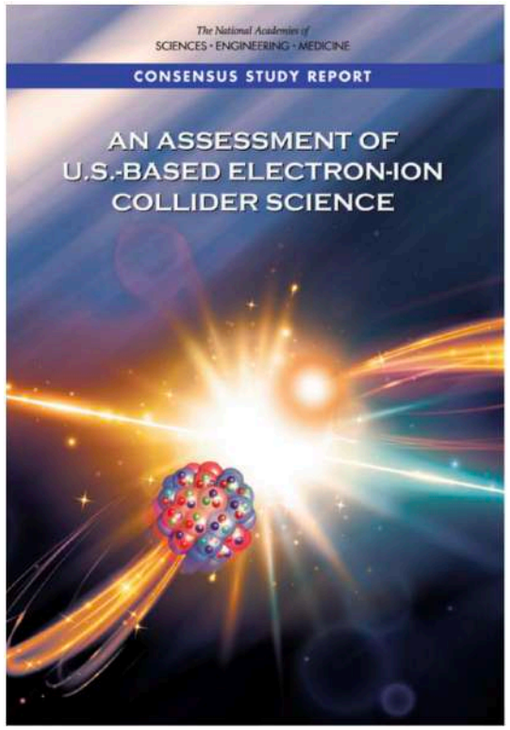


Recent improvements due to:
- **multi-grid solvers**
- **integration schemes**
- **computer architecture**

Advances of Lattice QCD are timely



Main Pillar of NAS
Assessment report for EIC

Finding 1: An EIC can uniquely address three profound questions about nucleons—neutrons and protons—and how they are assembled to form the nuclei of atoms:

- How does the mass of the nucleon arise?
- How does the spin of the nucleon arise?
- What are the emergent properties of dense systems of gluons?

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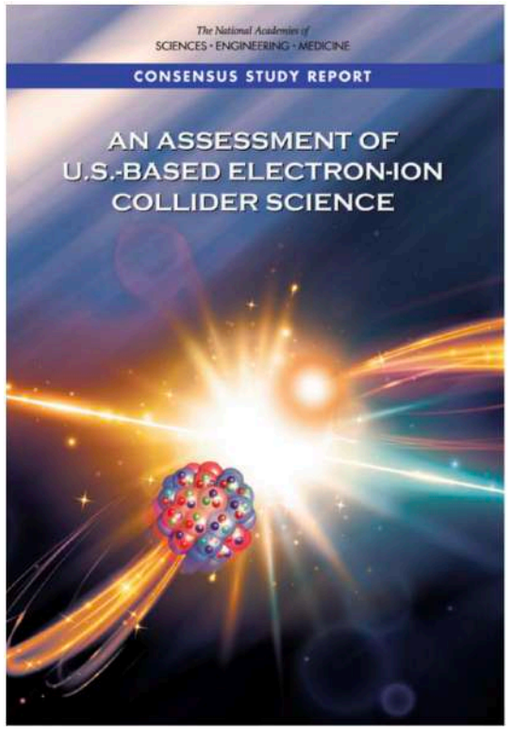

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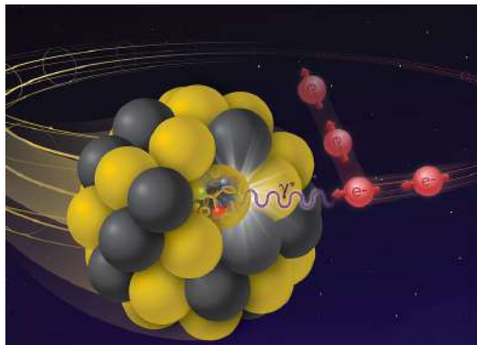
Lattice QCD is featured in the EIC Yellow Report
- 900-page document
- scientist from 151 Institutions

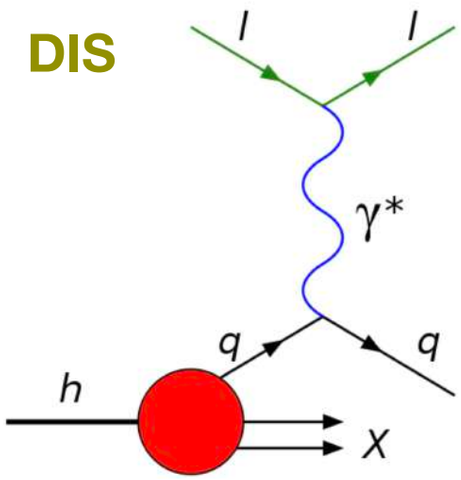
Lattice QCD can provide valuable input in understanding the proton mass and spin decomposition from *first principles*

Hadron Structure

- Structure of hadrons explored in high-energy scattering processes



Collisions @ EIC



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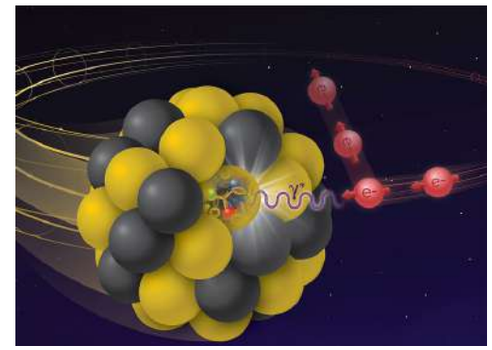

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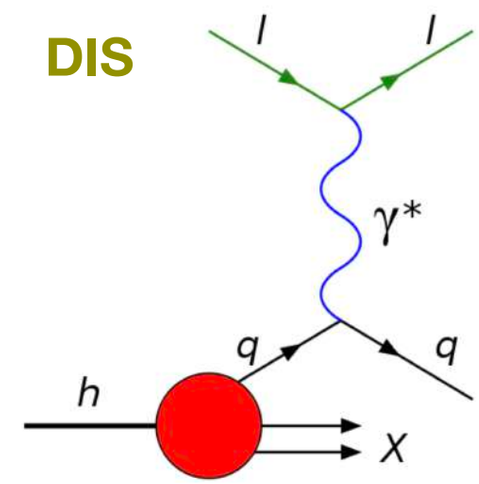
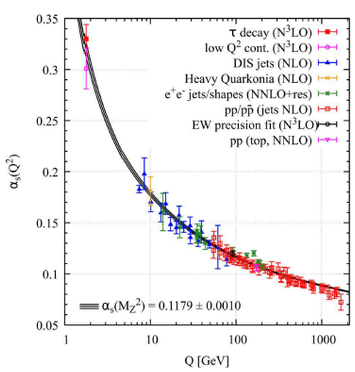


- Due to asymptotic freedom, e.g.



$$\sigma_{\rm DIS}(x,Q^2) = \sum_i \left[H^i_{\rm DIS} \otimes f_i\right](x,Q^2)$$

$$[a \otimes b](x) \equiv \int_x^1 \frac{d\xi}{\xi}\, a\left(\frac{x}{\xi}\right) b(\xi)$$

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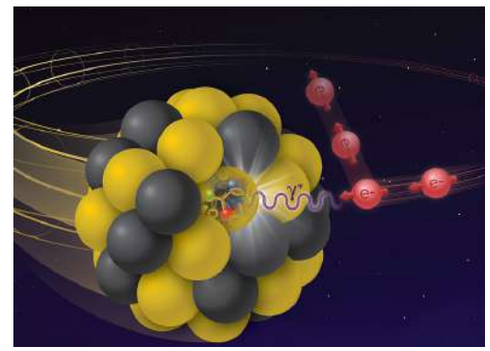

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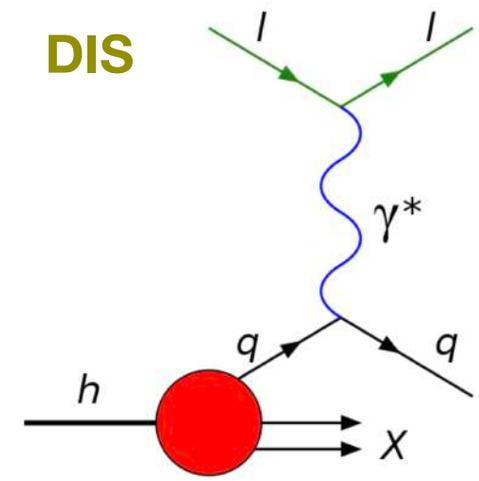

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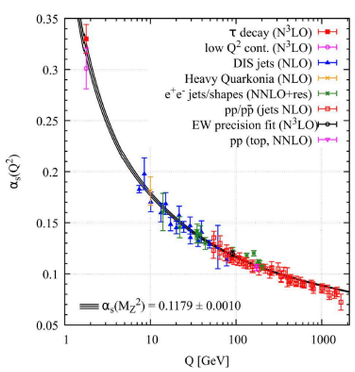

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Perturb. part
(process dependent)

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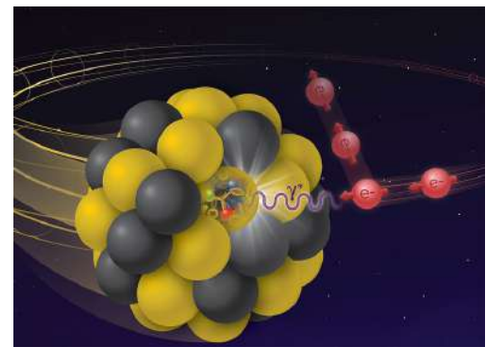

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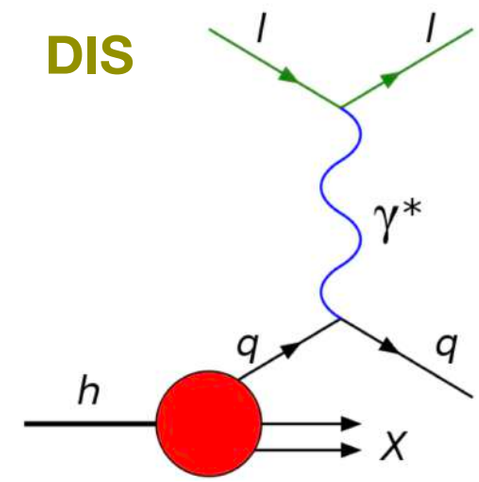

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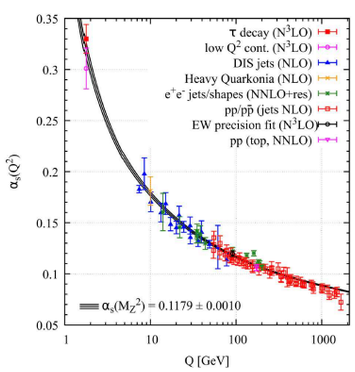

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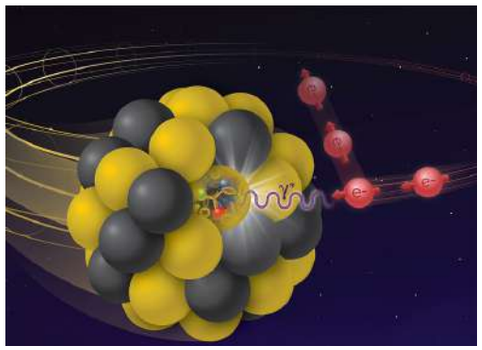
Perturb. part (process dependent)

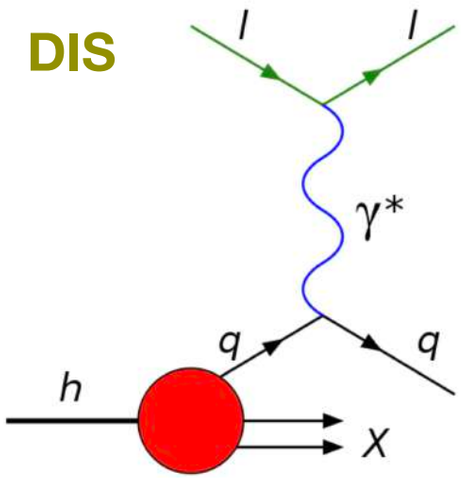
Non-Perturb. part (process "independent")

Hadron Structure

- Structure of hadrons explored in high-energy scattering processes



Collisions @ EIC



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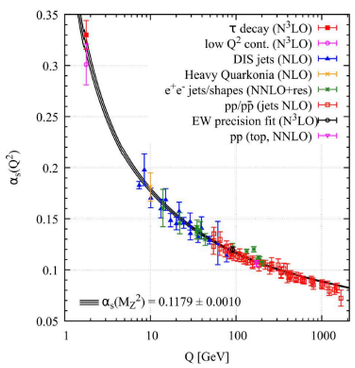

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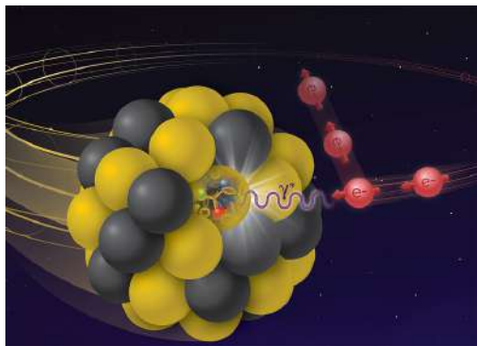

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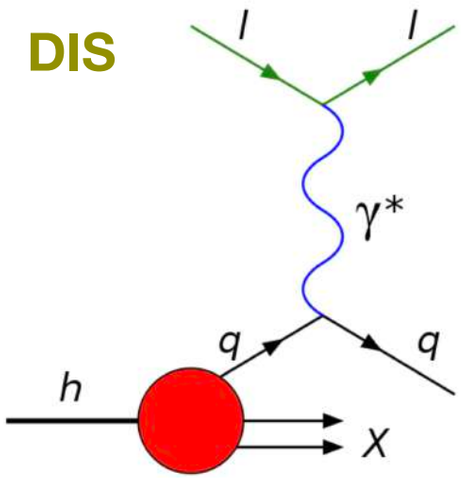

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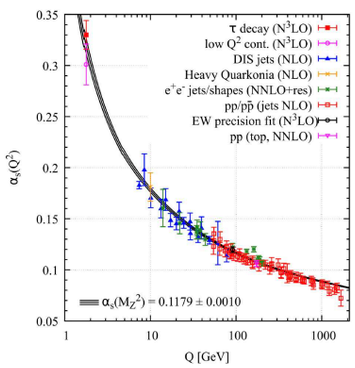

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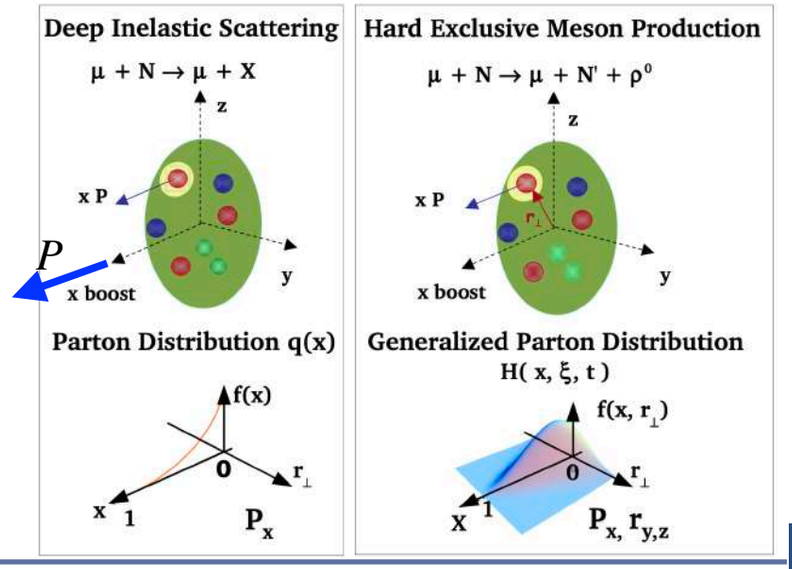

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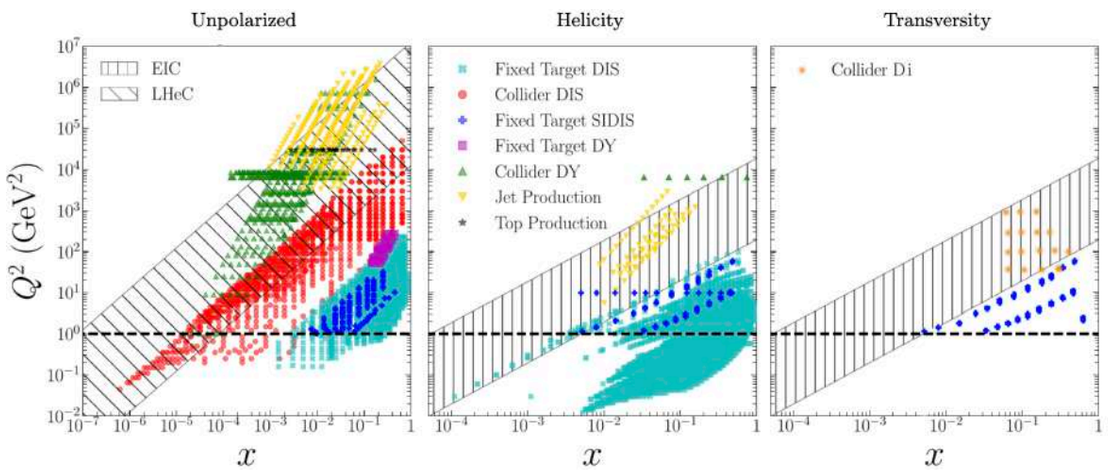
- ★ **Global fit analyses of DIS data: main source of information for PDFs**



[Ethier & Nocera, *Ann. Rev. Nucl. Part. Sci.* 70 (2020) 1, arXiv:2001.07722]

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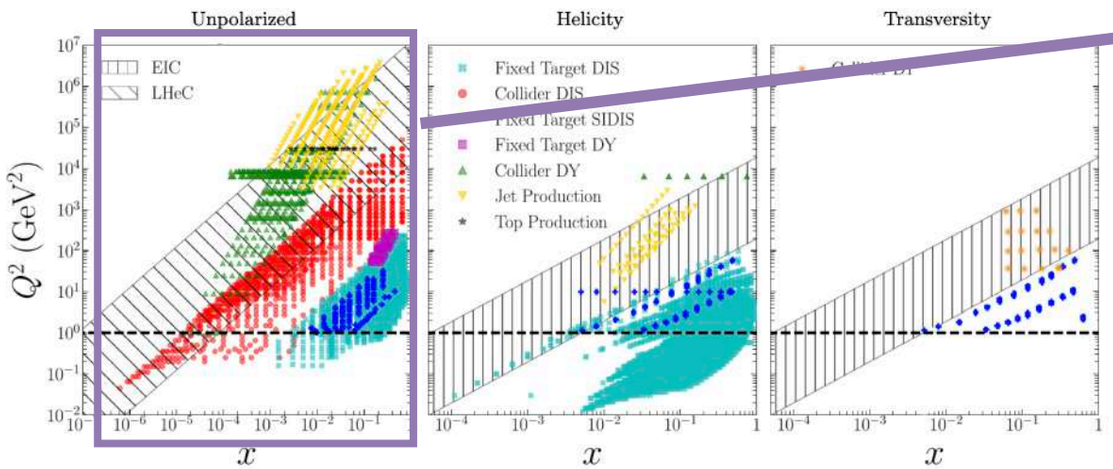

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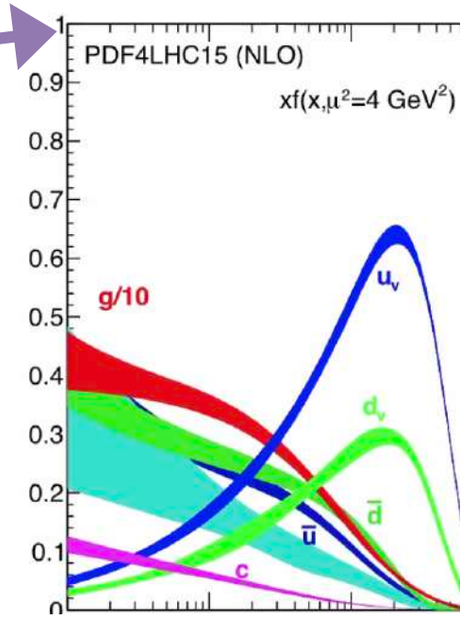

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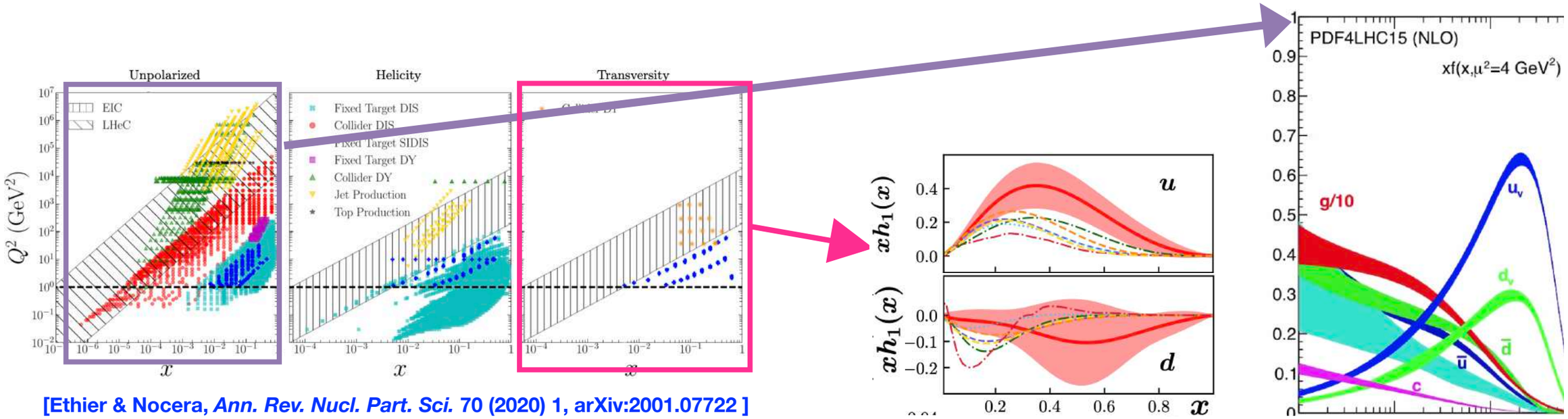

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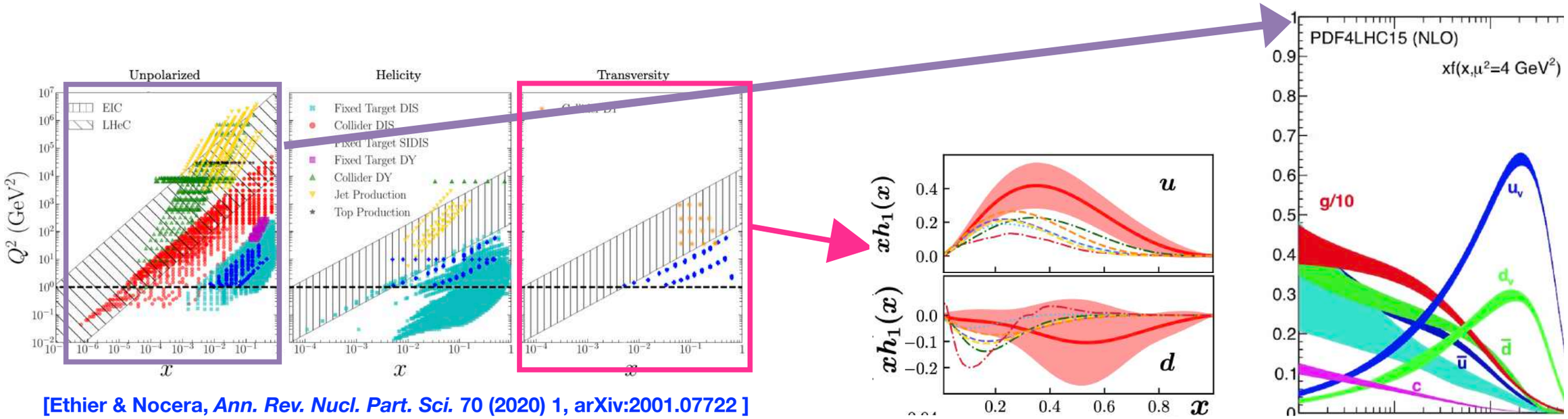

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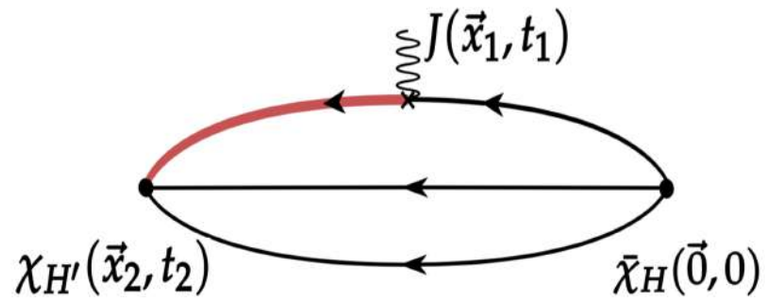
Calculation from first principle (lattice QCD) can help in the reliable extraction of physical quantities such as the proton spin and mass (related to PDFs)

Hadron Structure from Lattice QCD

Proton on the Lattice



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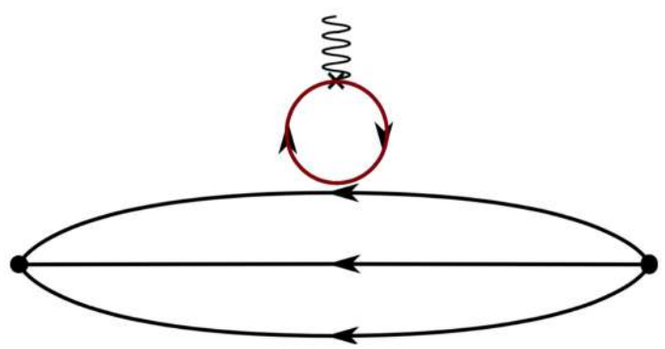
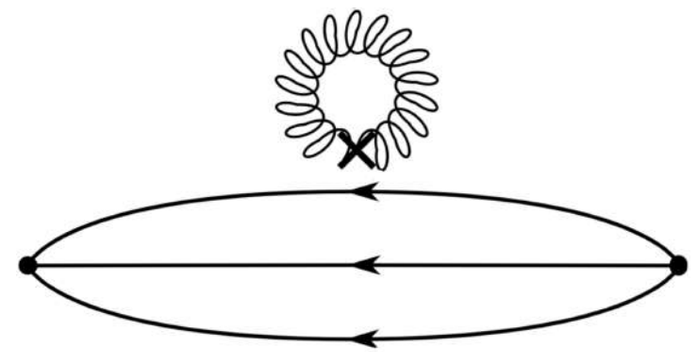


Disconnected
Quark loop



Disconnected
Gluon loop

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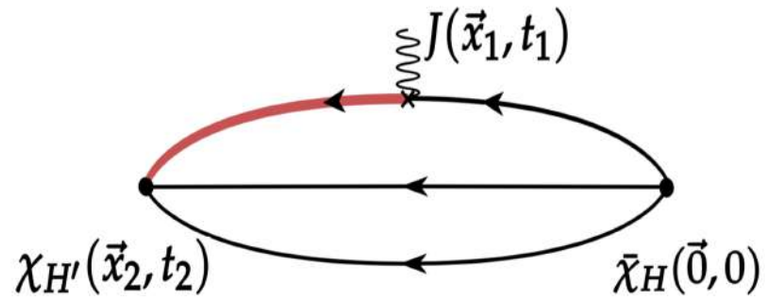

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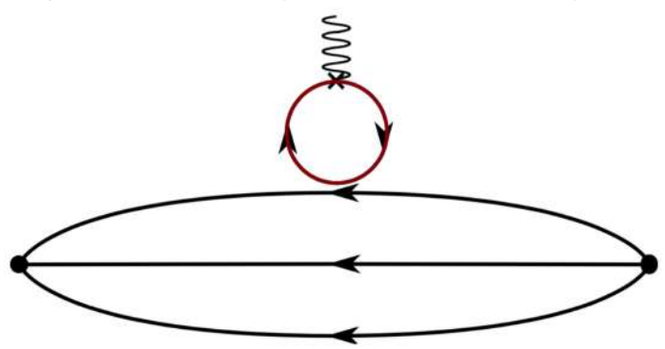

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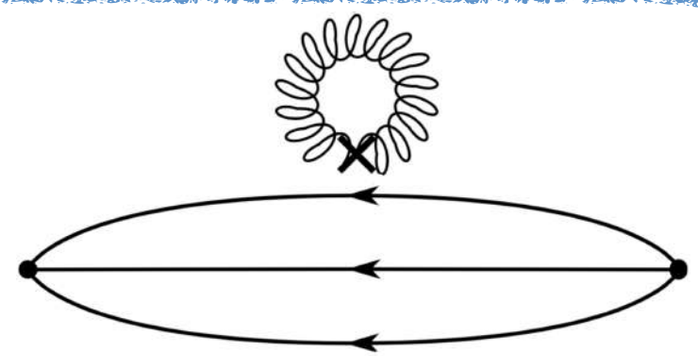

Disconnected
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Sizable contribution to spin and mass decomposition

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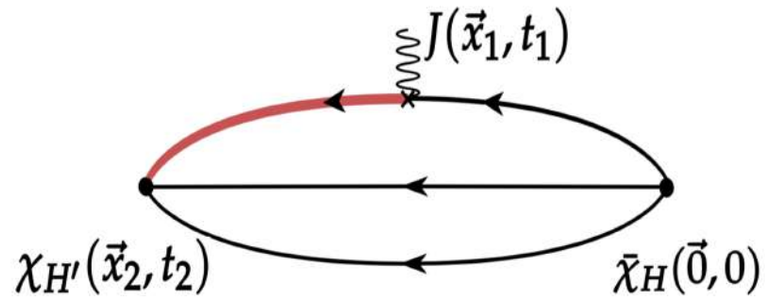

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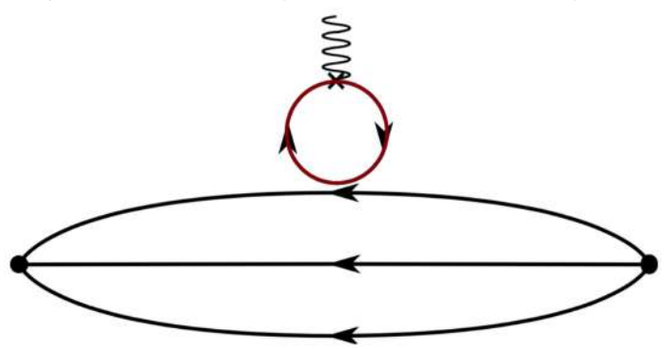

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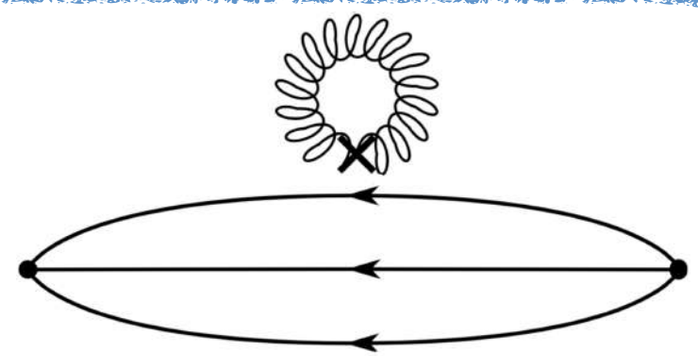

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Computationally very challenging!
Require at least an order of magnitude more computational resources

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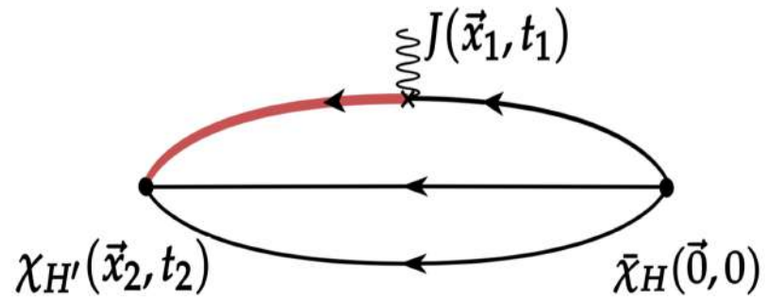

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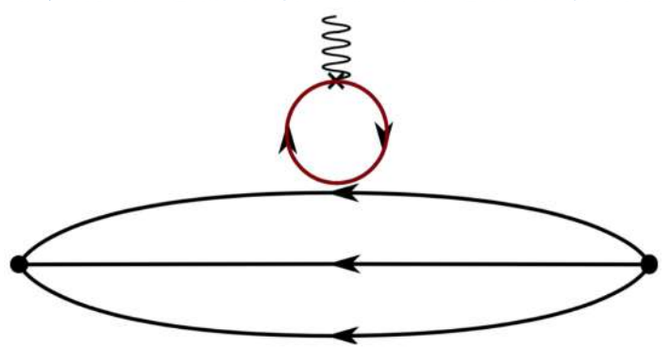

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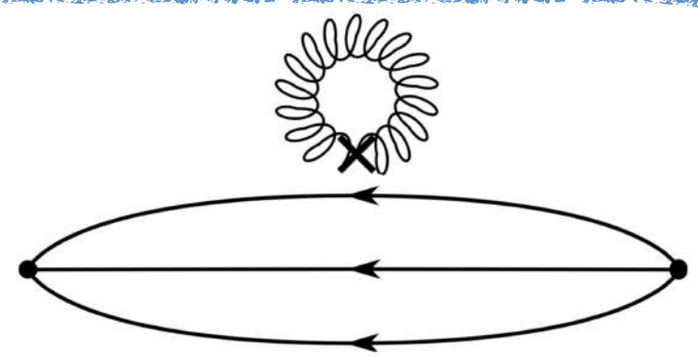

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Sizable contribution to spin and mass decomposition

Computationally very challenging!
Require at least an order of magnitude more computational resources

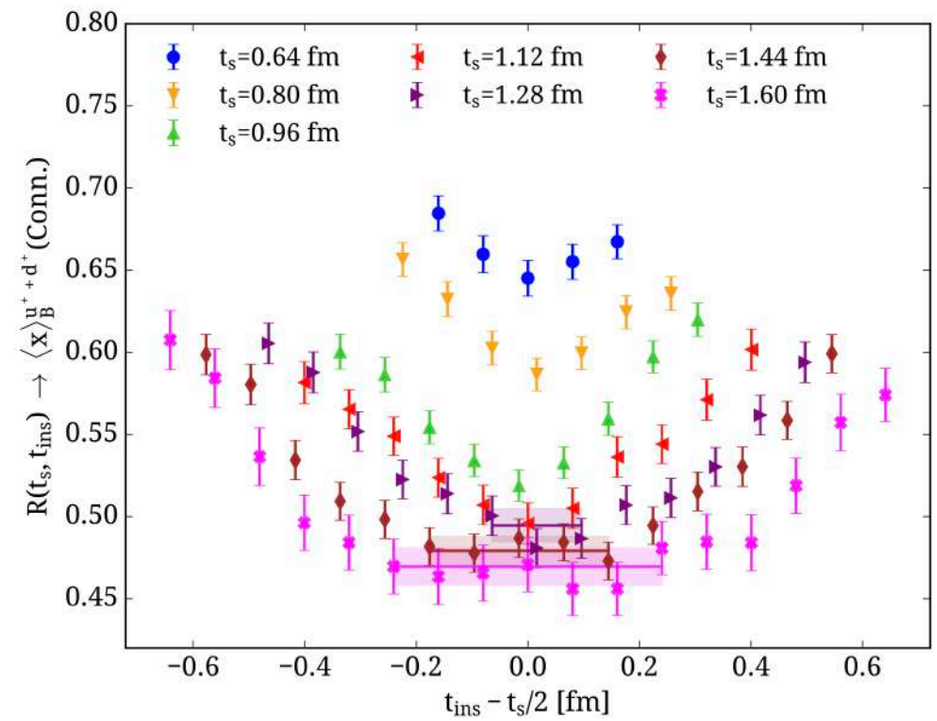
- Type of current insertion gives different part of proton mass & spin
- Extraction of each contribution has its own challenges
  (statistical and systematic uncertainties)

From lattice data to physical quantities

★ Calculation of matrix elements with appropriate operator

$$C^{2pt} = \langle N | N \rangle \qquad C^{3pt}_{\Gamma} = \langle N | \overline{\psi} \Gamma \psi | N \rangle$$

★ Isolation of ground state



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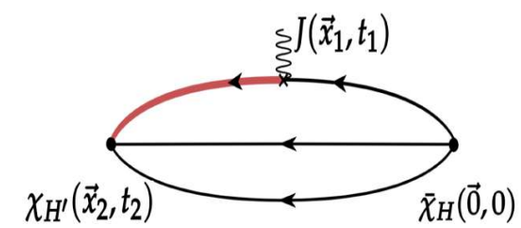

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$$\Pi^R_{\Gamma} = Z \Pi_{\Gamma}$$

★ Lattice results relate to measurable quantities

$$g_A = -2i\Pi^R_{\gamma^5\gamma^k}, \qquad < x >_q = -\frac{4}{3m}\Pi^R_{\gamma^0 D^0}$$

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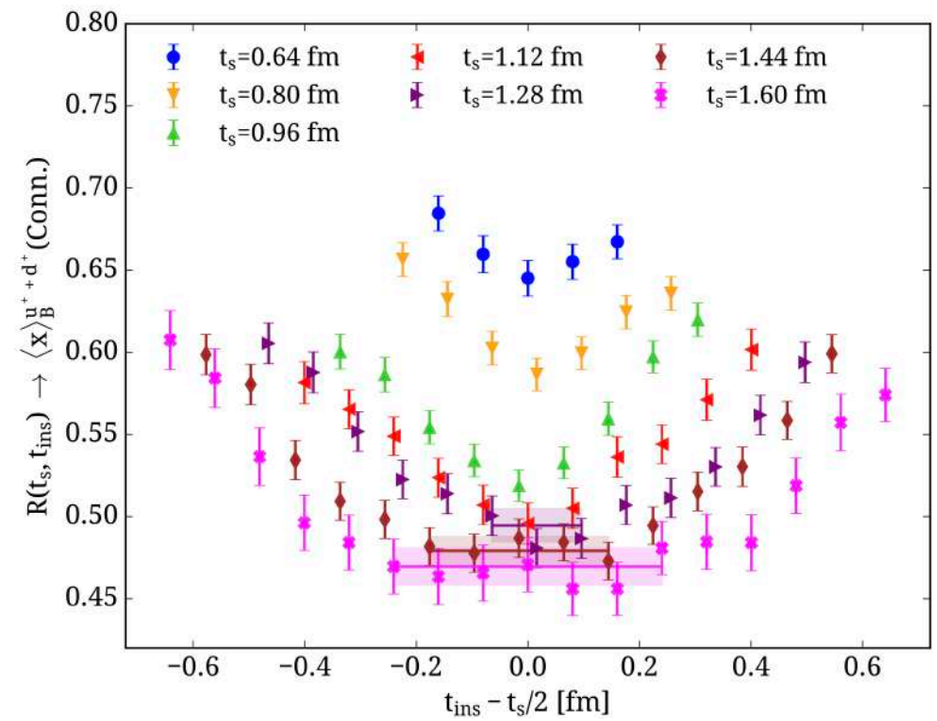

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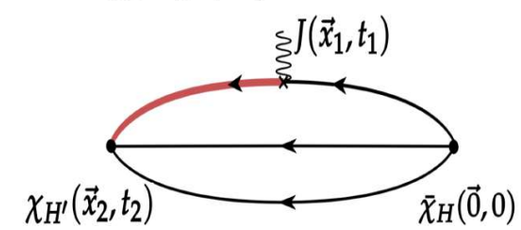

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Calculation Details

[C. Alexandrou et al., *Phys. Rev. D* 102 (2020) 054517, arXiv:1909.00485]
[C. Alexandrou et al., *Phys. Rev. D* 101 (2020) 094513, arXiv:2020]

Ensemble	$L^3 \times T$	m_N/m_π	$m_\pi L$	m_π [MeV]	L [fm]
$N_f = 2,\ \beta = 2.1,\ a = 0.0938(3)(1)$ fm					
cA2.09.48	$48^3 \times 98$	7.15(2)	2.98	130.3(4)(2)	4.50(1)
cA2.09.64	$64^3 \times 128$	7.14(4)	3.97	130.6(4)(2)	6.00(2)
$N_f = 2+1+1,\ \beta = 1.778,\ a = 0.0801(4)$ fm					
cB211.072.64	$64^3 \times 128$	6.74(3)	3.62	139.3(7)	5.12(3)

Connected

t_s/a	8	10	12	14	16	18	20
t_s [fm]	0.75	0.94	1.13	1.31	1.50	1.69	1.88
cA2.09.48	–	9264	9264	9264	47696	69784	–
cA2.09.64	–	–	5328	8064	17008	–	–
t_s [fm]	0.64	0.80	0.96	1.12	1.28	1.44	1.60
cB211.072.64	750	1500	3000	4500	12000	36000	48000

★ Tsink in 0.64 fm - 1.6 fm for large-volume ensemble

Disconnected

Flavor	$N_{\rm def}$	N_r	$N_{\rm Had}$	$N_{\rm sc}$	$N_{\rm inv}$
light	200	1	512	12	6144
strange	0	1	512	12	6144
charm	0	12	32	12	4608

(N_{cnf} = 750)

★ Quark loops:
- spin-color dilution
- deflation (light quark)
- hierarchical probing

★ Gluon loops:
- Stout Smearing

Proton Spin

Proton spin “puzzle”

DIS experiment (1988) shows surprising results for proton spin

”... $g_1(x)$ for the proton has been determined and its integral over x found to be 0.114±0.012±0.026, in disagreement with the Ellis-Jaffe sum rule. ...These values for the integrals of g_1 lead to the conclusion that the total quark spin constitutes a rather small fraction of the spin of the nucleon.”

[J. Ashman et al., Phys. Lett., vol. B206 (1988) 364]

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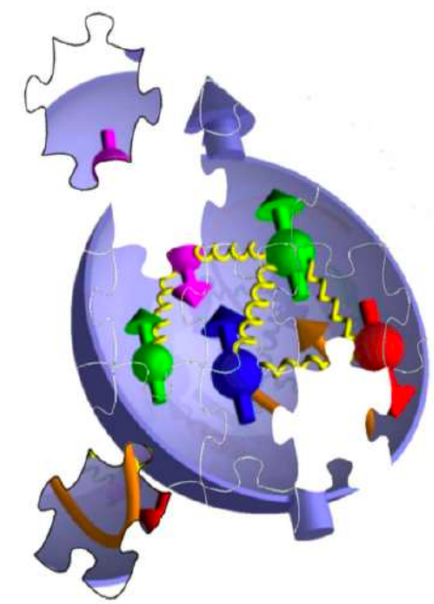

Not really a puzzle:

- Sea quark and gluon contributions
- Parton orbital angular momentum

But there are still open questions:

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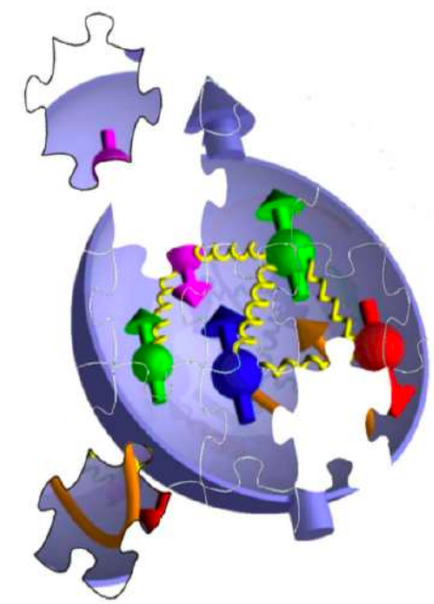

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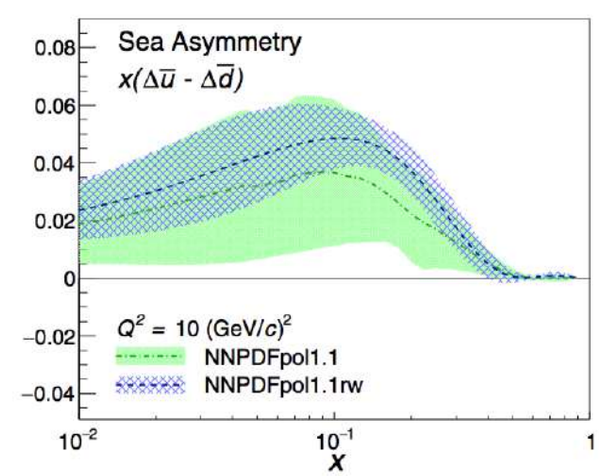
Recent RHIC results on flavor decomposition of antiquarks in spin

J. Adam et al. (STAR Collaboration), Phys. Rev. D 99, 051102(R)



Spin structure from first principles

Lattice QCD can provide important information on the spin

Ji's Spin Decomposition

$$\frac{1}{2} = \sum_q J^q + J^G = \sum_q \left(L^q + \frac{1}{2}\Delta\Sigma^q \right) + J^G$$

L_q: Quark orbital angular momentum

$\Delta\Sigma_q$: Intrinsic spin

J_g: Gluon spin

All these quantities can be computed within Lattice QCD

Extraction from Lattice QCD:

$$J^q = \frac{1}{2}\left(A_{20}^q + B_{20}^q \right)$$

$$L^q = J^q - \Sigma^q$$

$$\Sigma^q = g_A^q$$

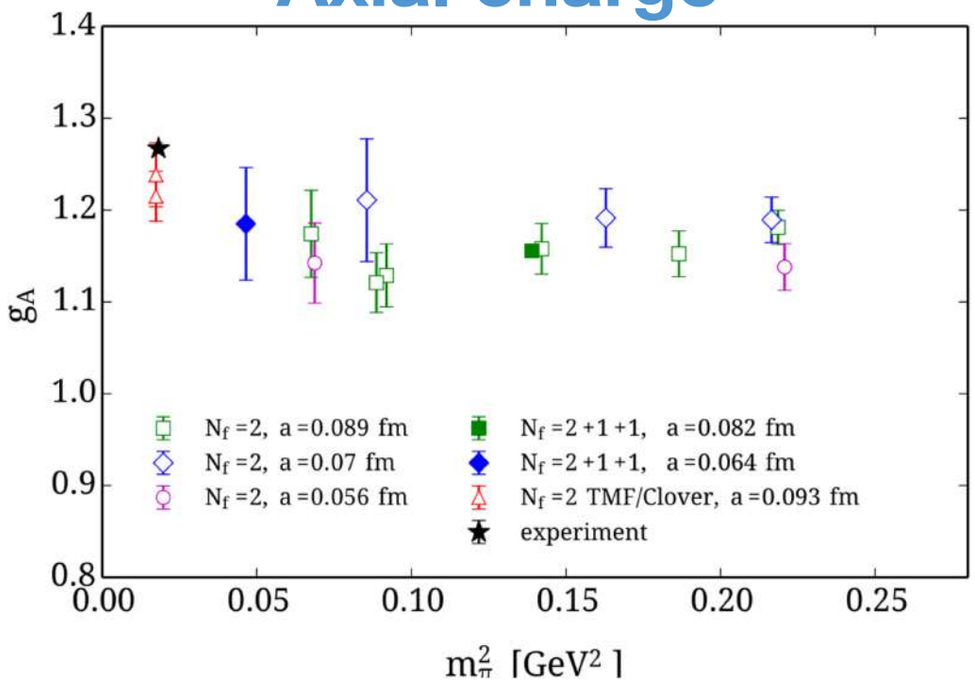
Necessary computations:

- Axial Charge
- Quark momentum fraction
- Gluon momentum fraction

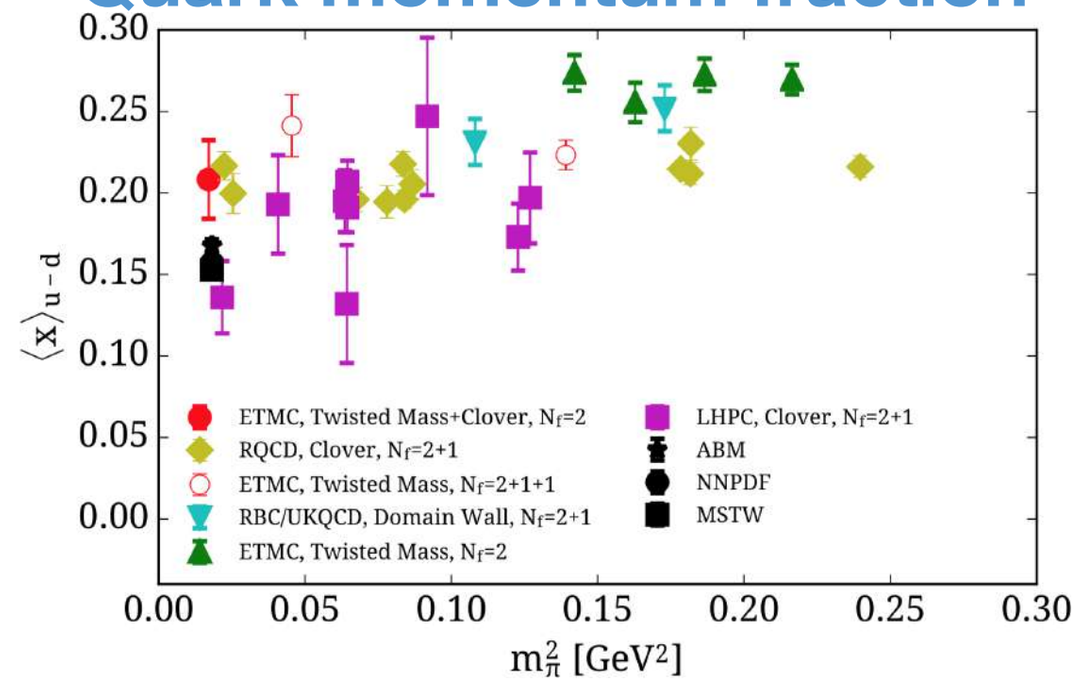
Quark Orbital Angular extracted indirectly

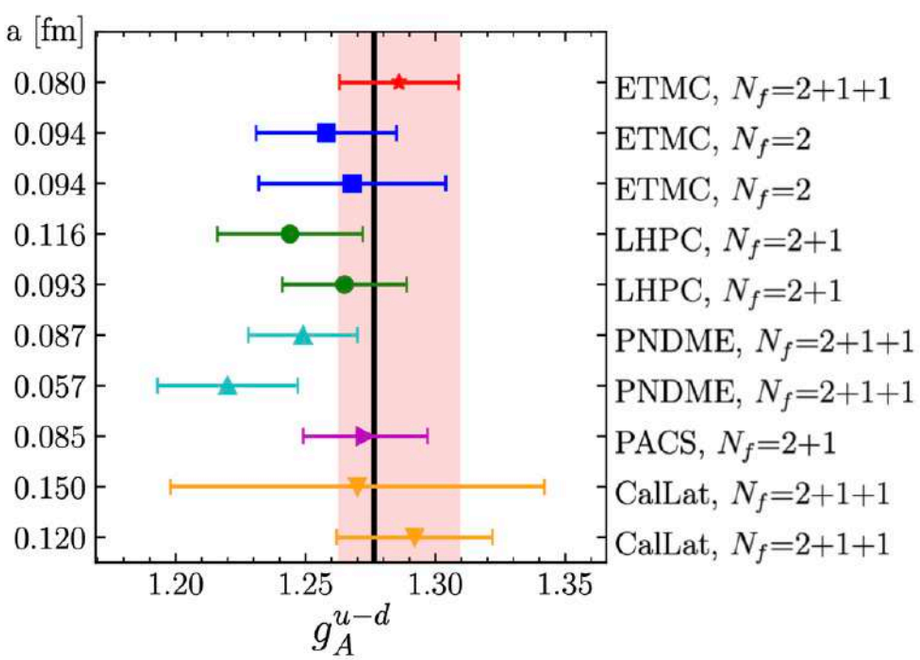
Spin components in Lattice QCD

Axial charge



Quark momentum fraction





Spin components in Lattice QCD

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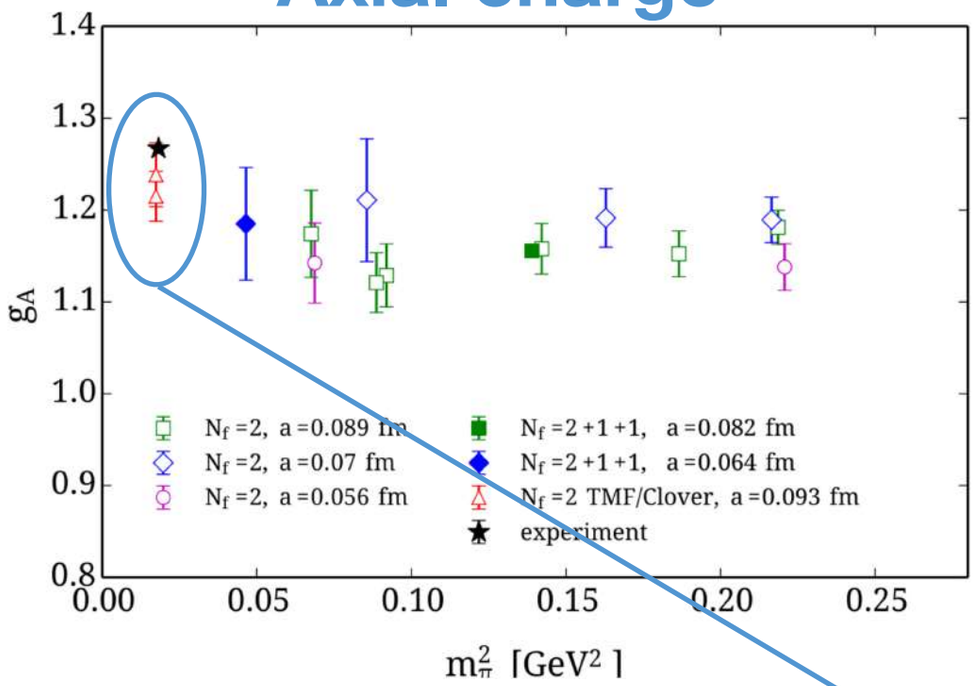

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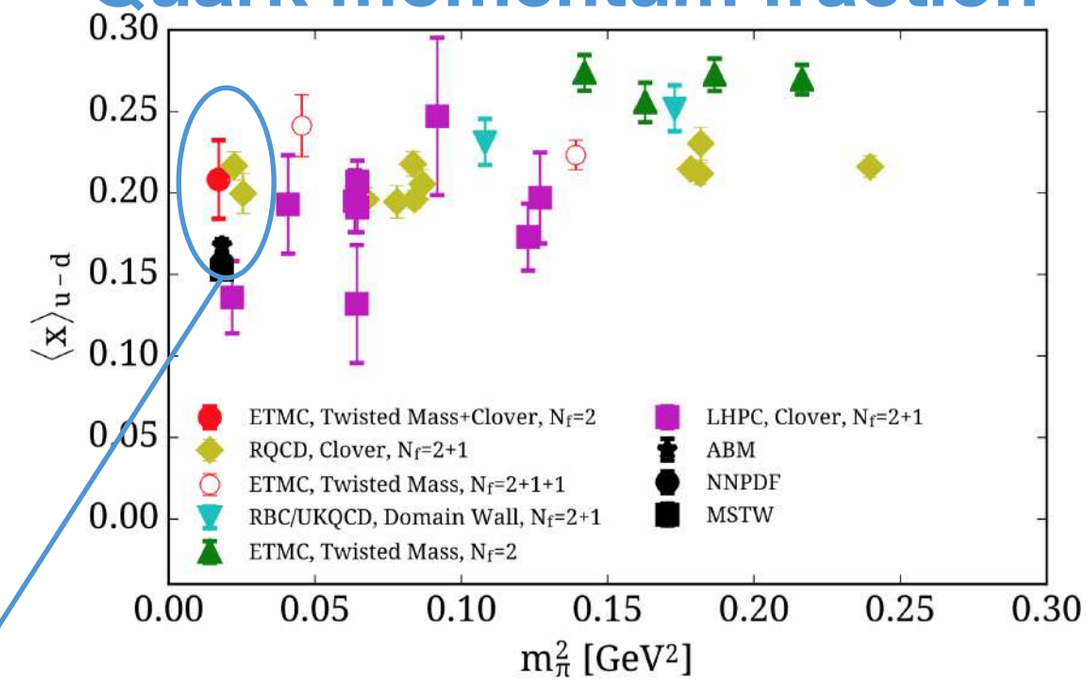
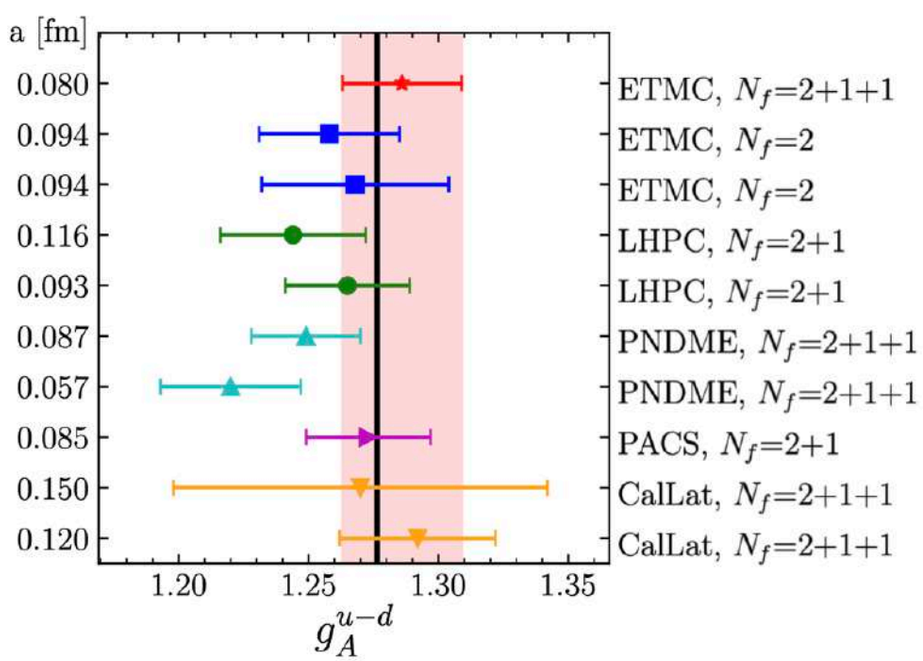


Simulations at the physical point eliminate systematic uncertainties



Spin components in Lattice QCD

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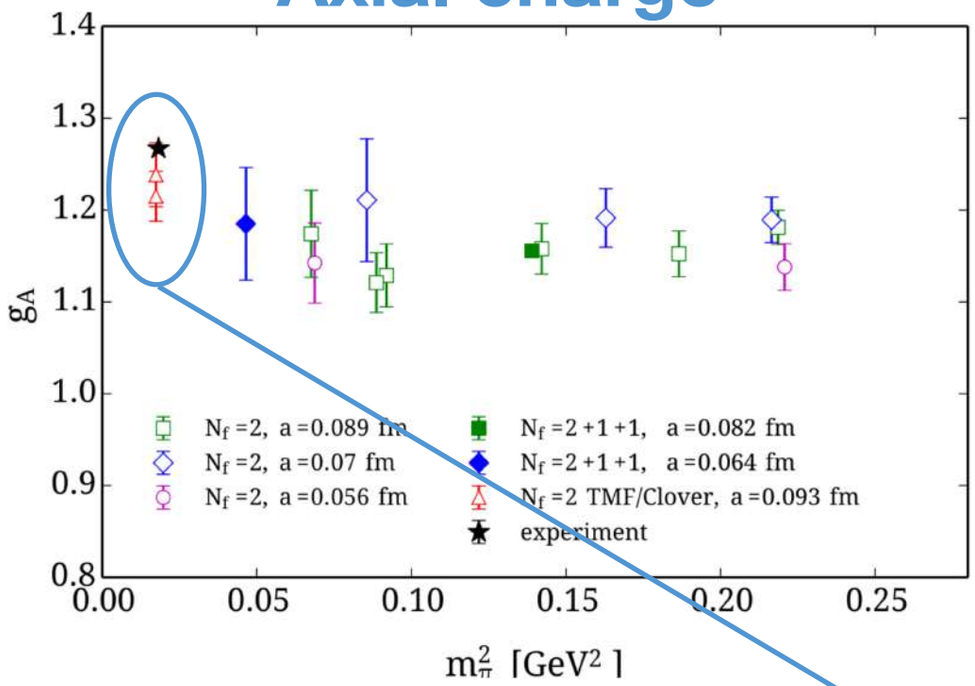
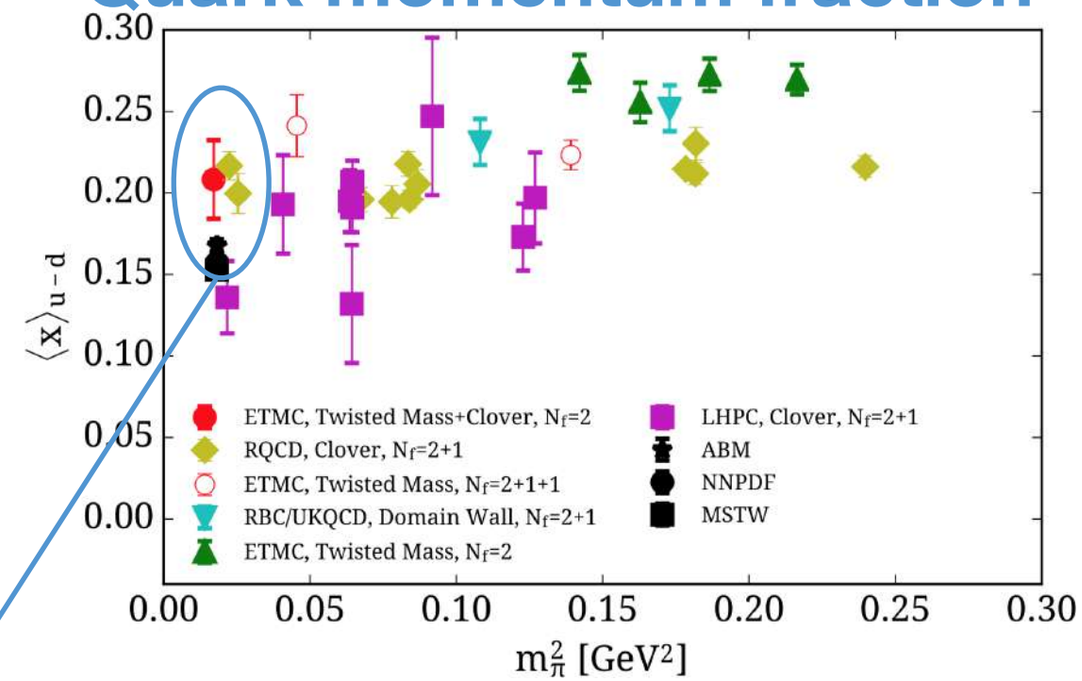
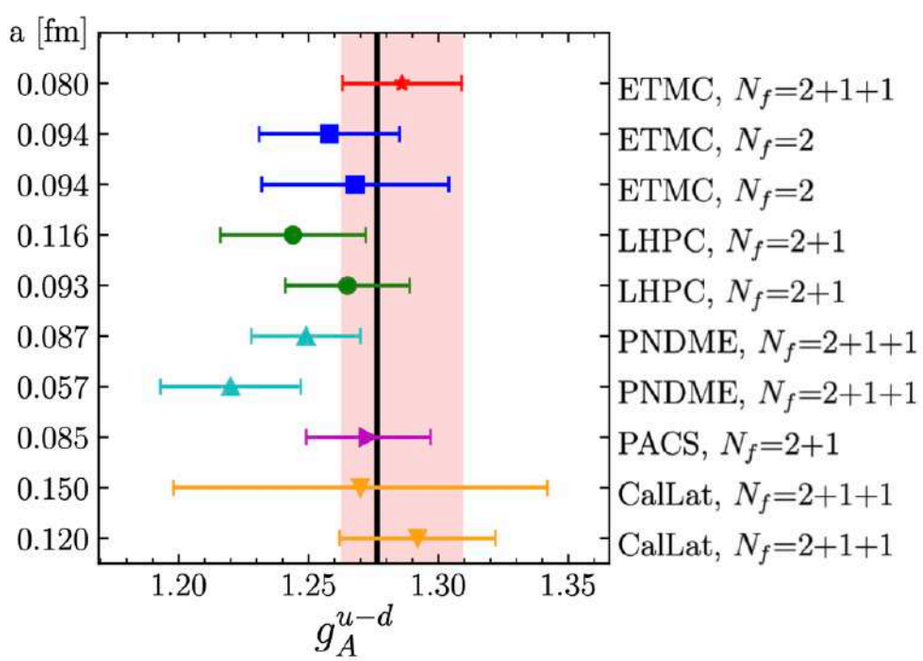


Quark momentum fraction



Simulations at the physical point eliminate systematic uncertainties



	u	d	s	c
g_A	0.862(17)	-0.424(16)	-0.0458(73)	-0.0098(34)

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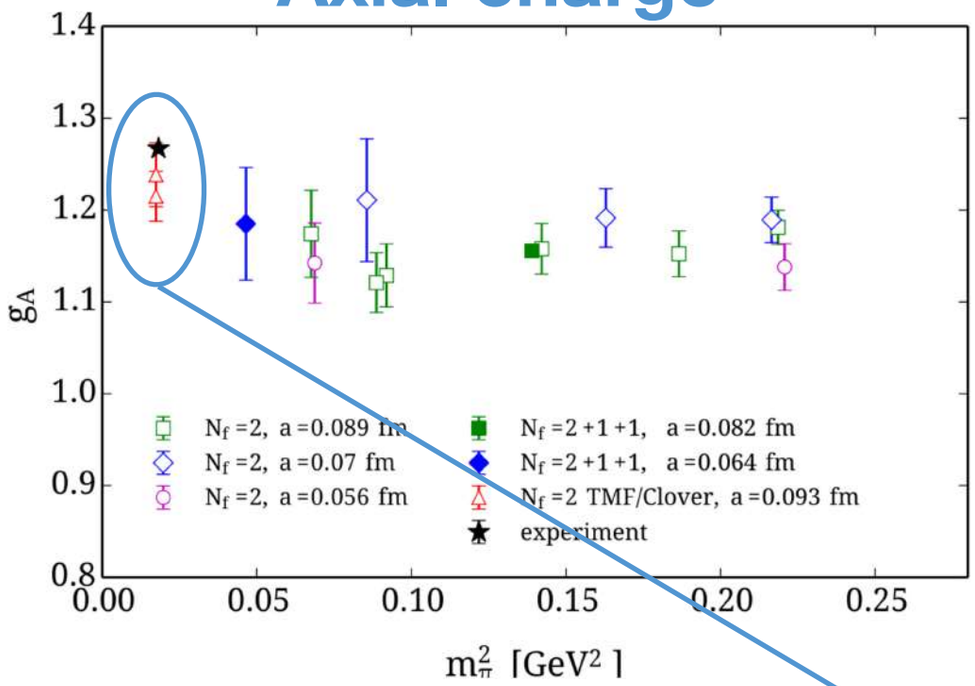

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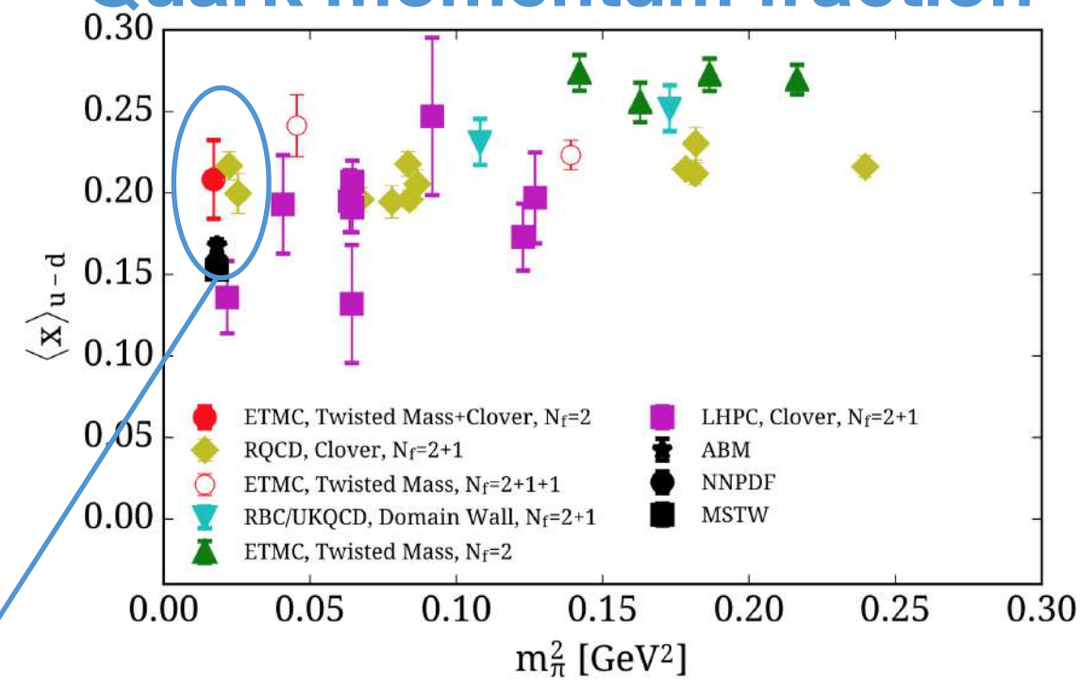

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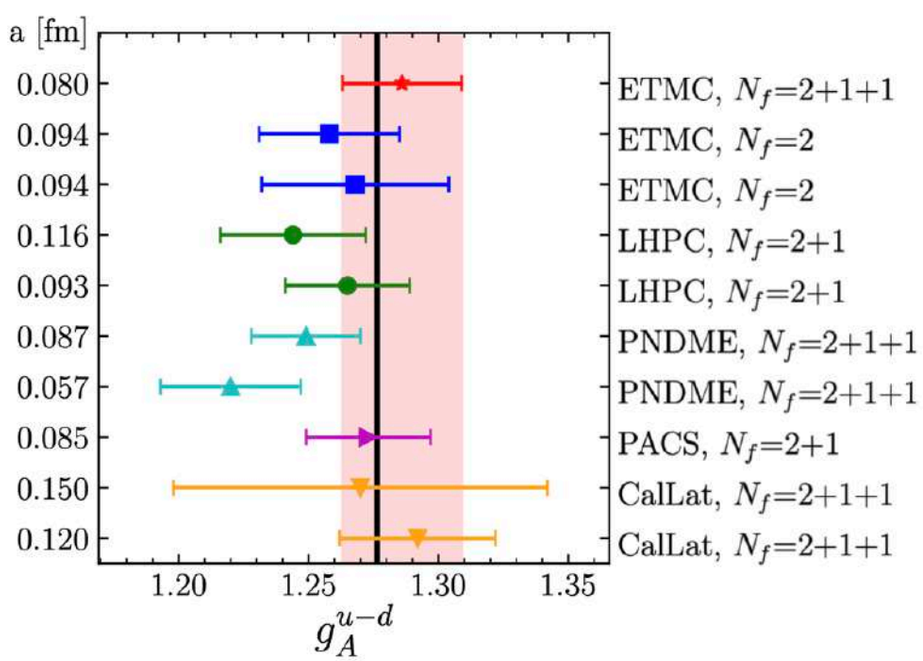

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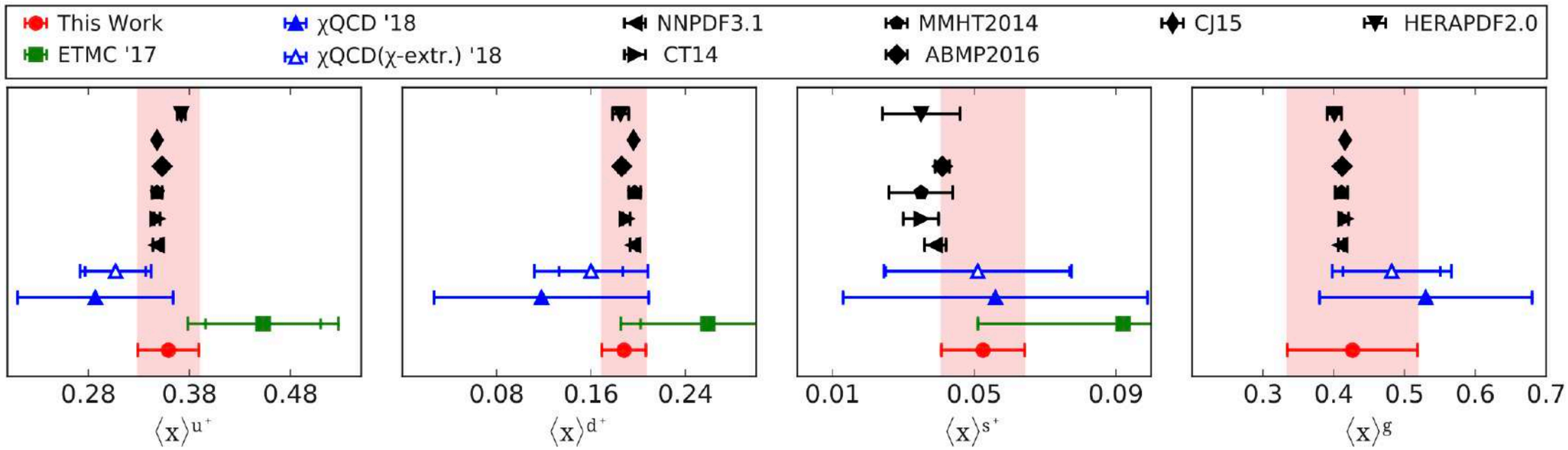
Taking into account the disconnected contributions is crucial for the spin

Momentum fraction

Collection of various results



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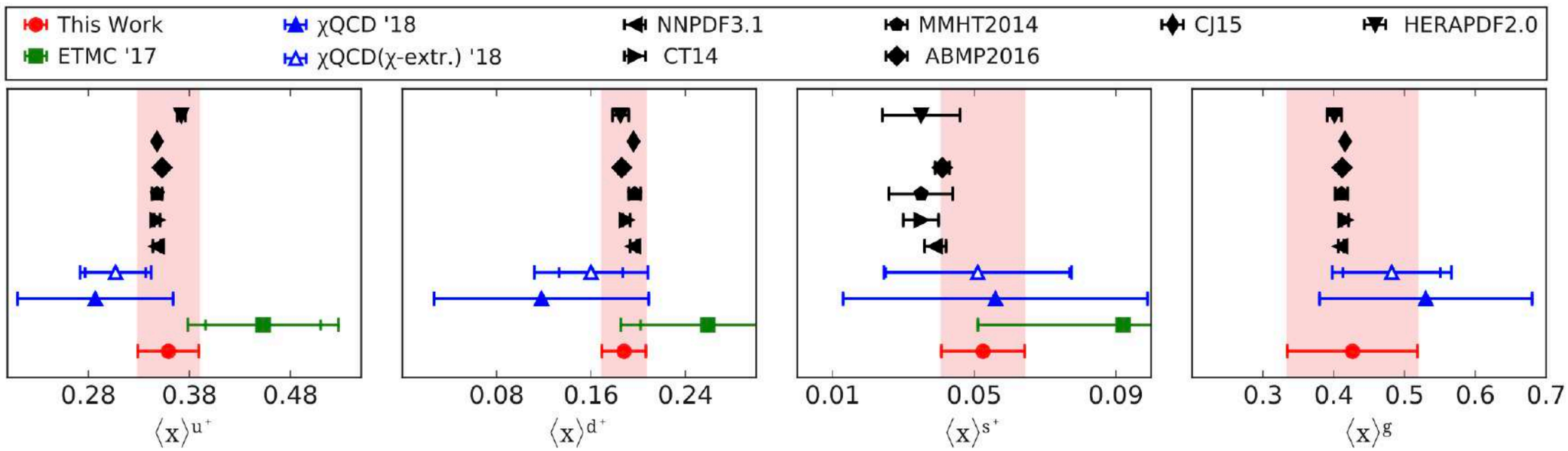
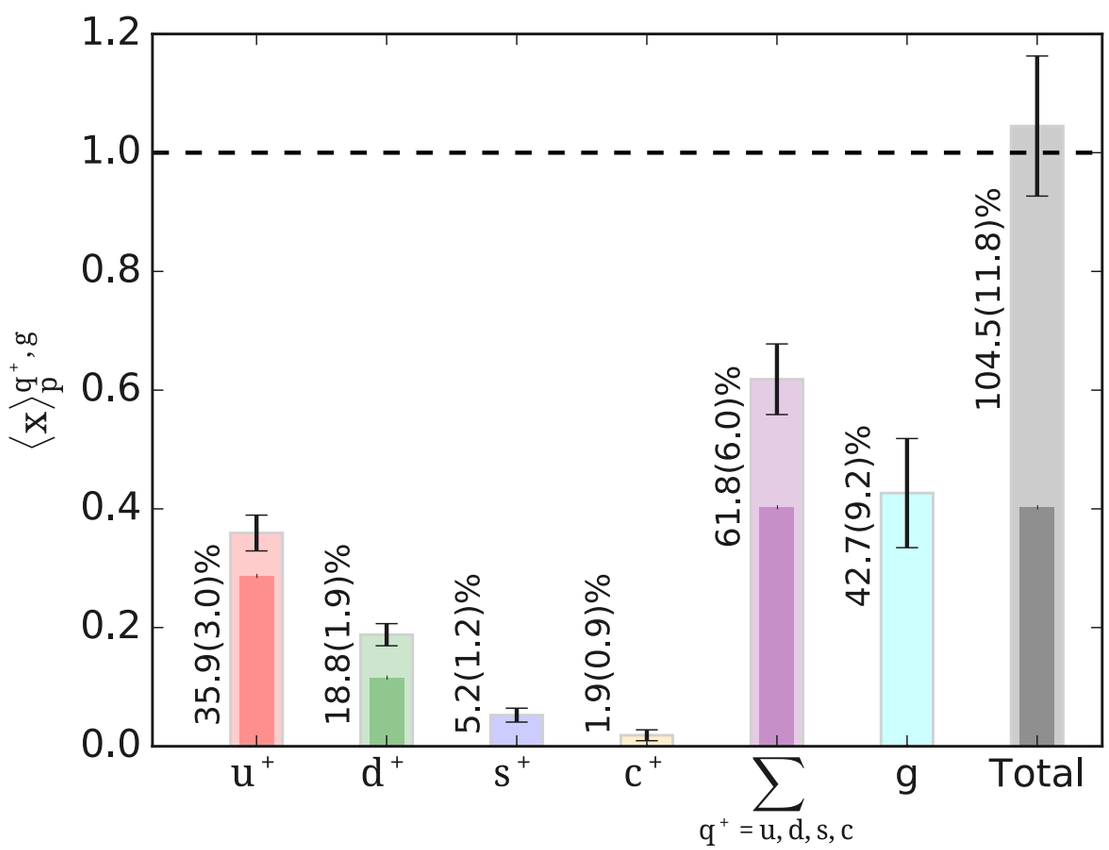
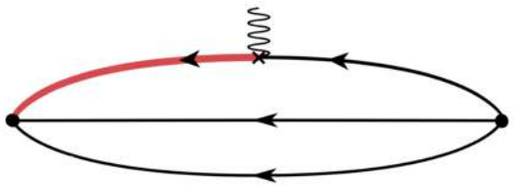


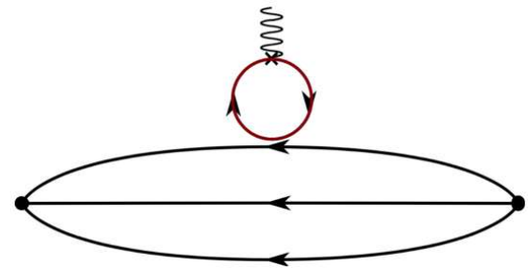


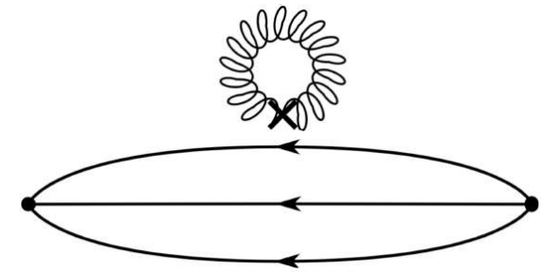
Total momentum satisfied

Results @ physical pion mass

$\overline{MS}(2\mathrm{GeV})$







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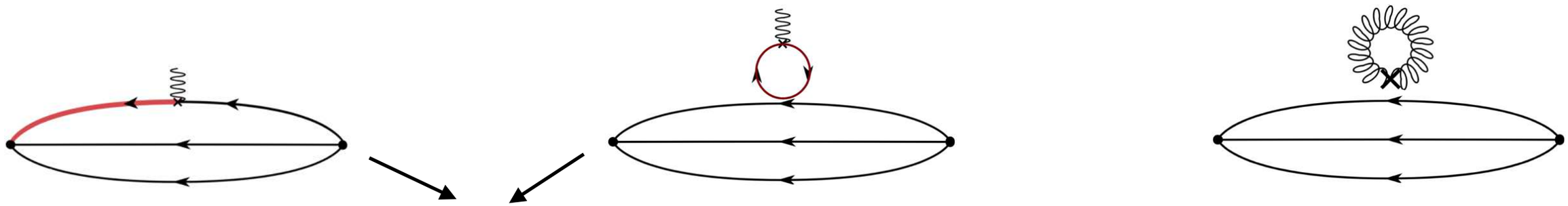

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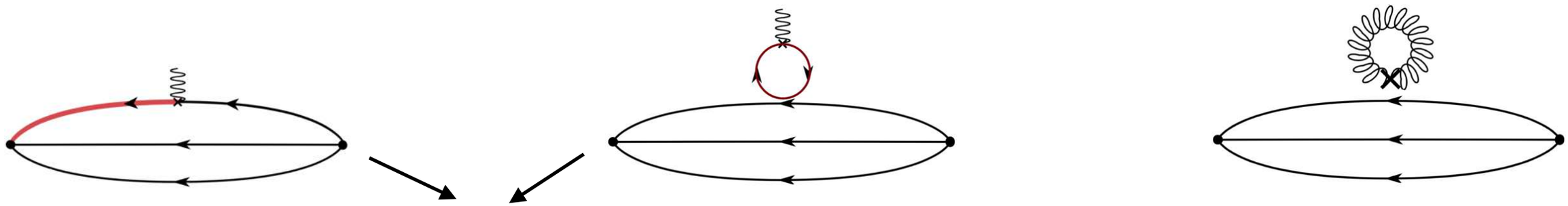

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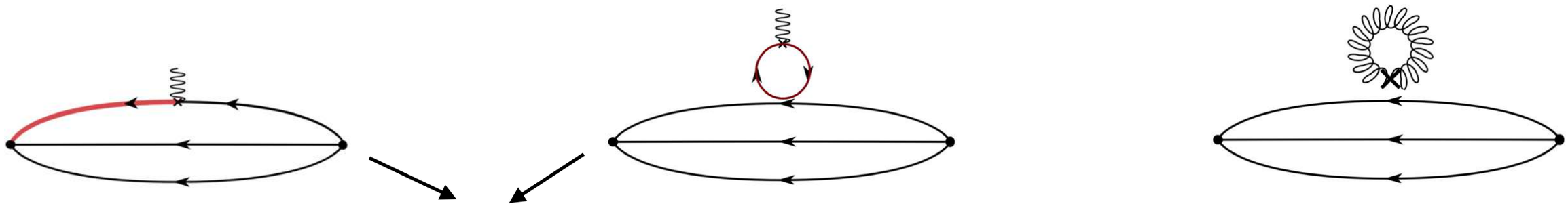

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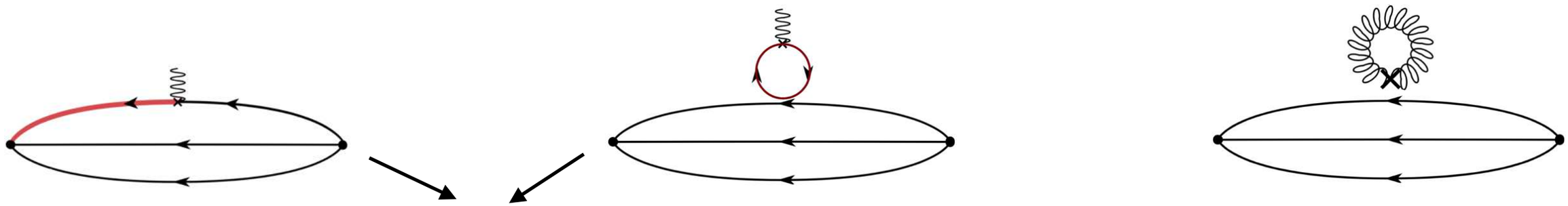

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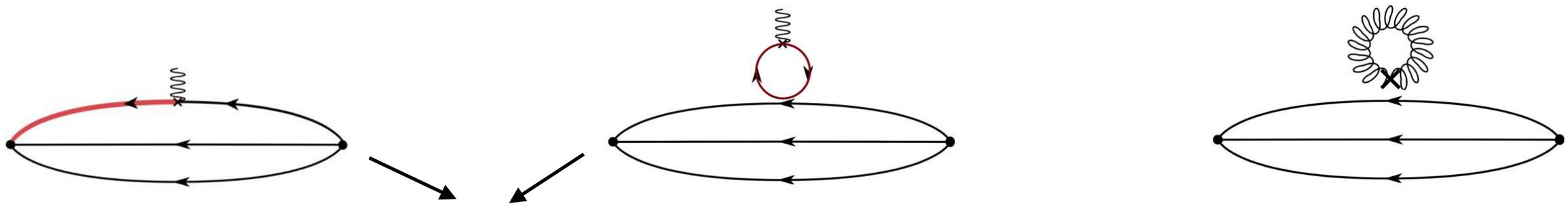

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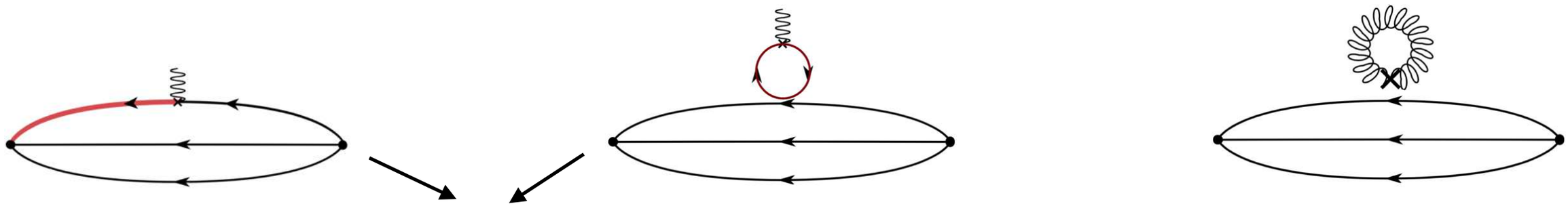

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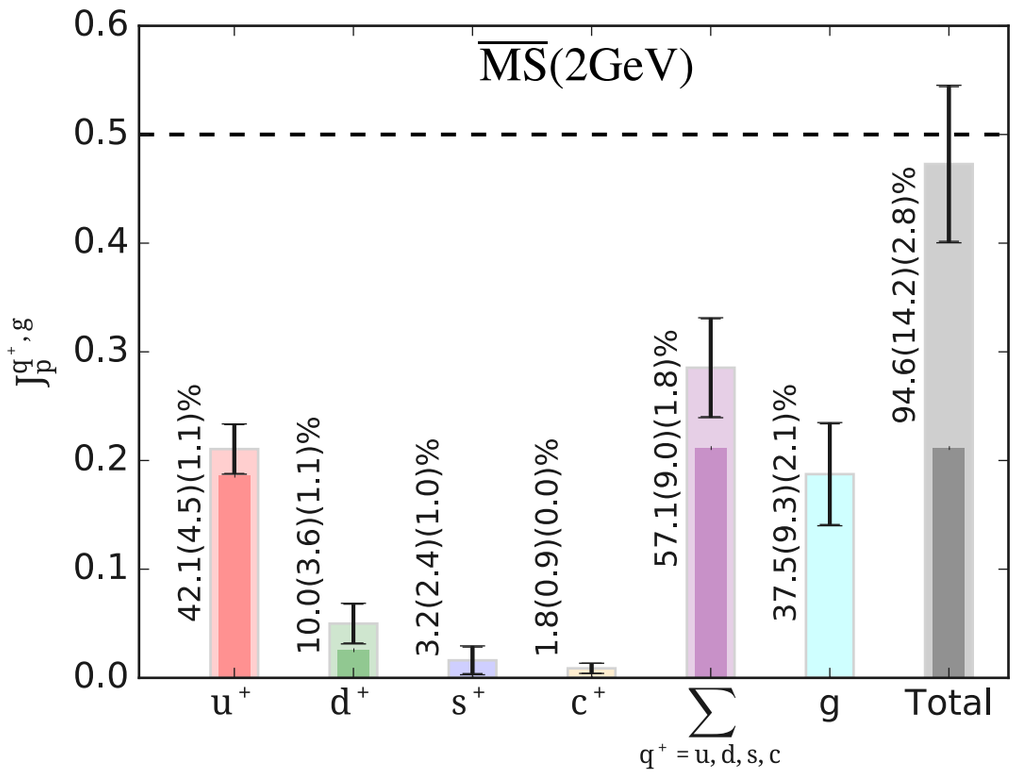
Momentum sum rule satisfied!

Spin decomposition

[C. Alexandrou et al., Phys. Rev. D 101, 094513 (2020), arXiv:2003.08486]



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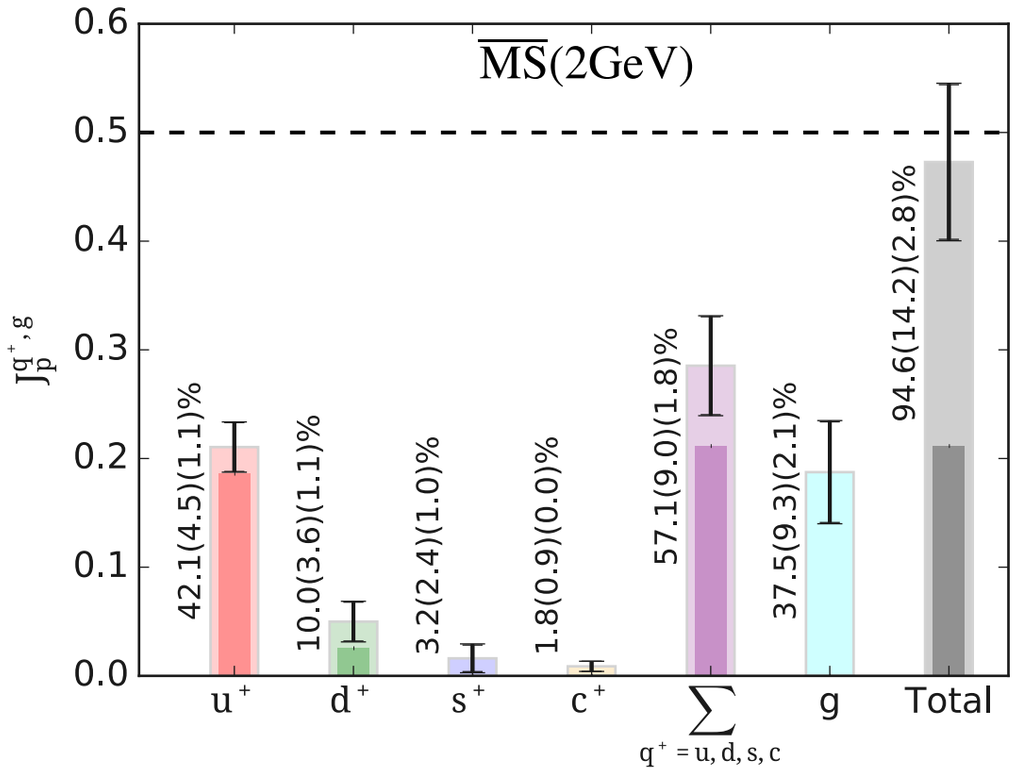

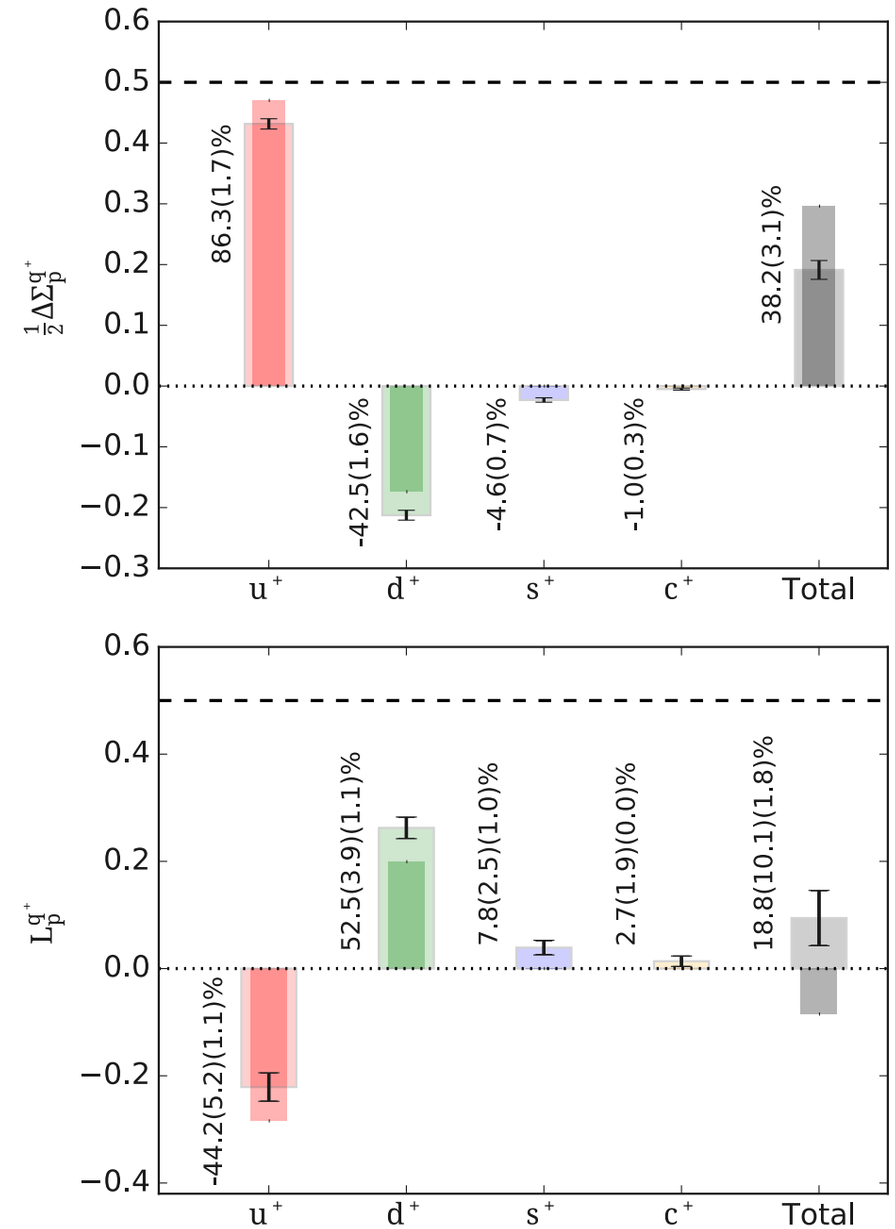

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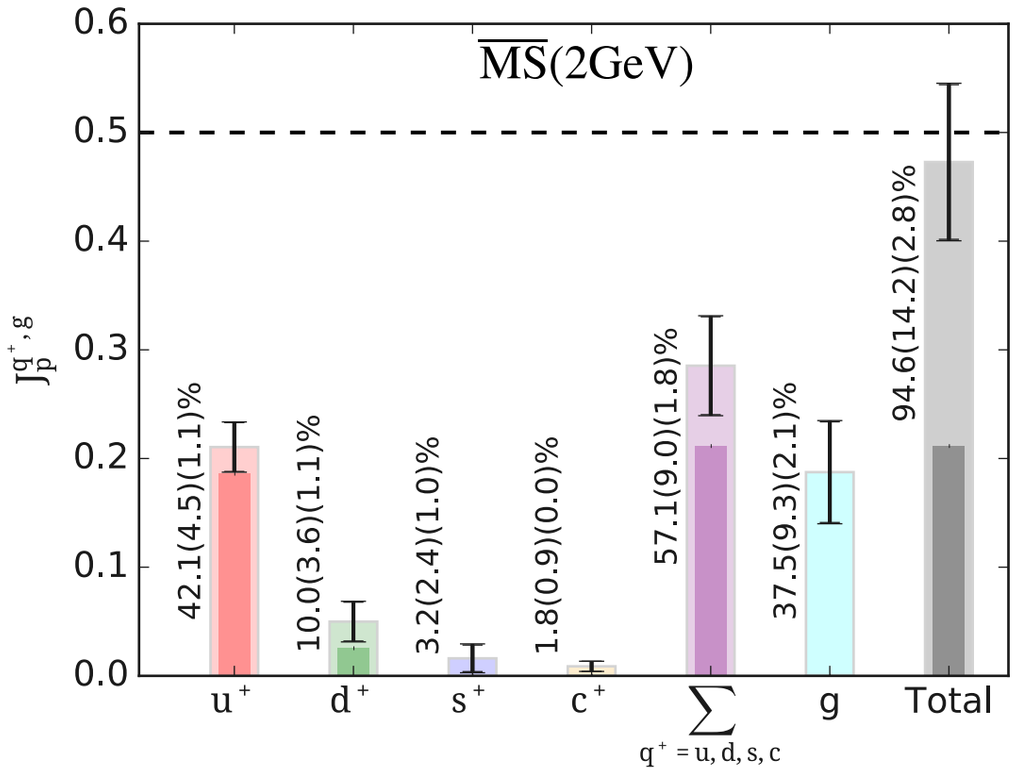

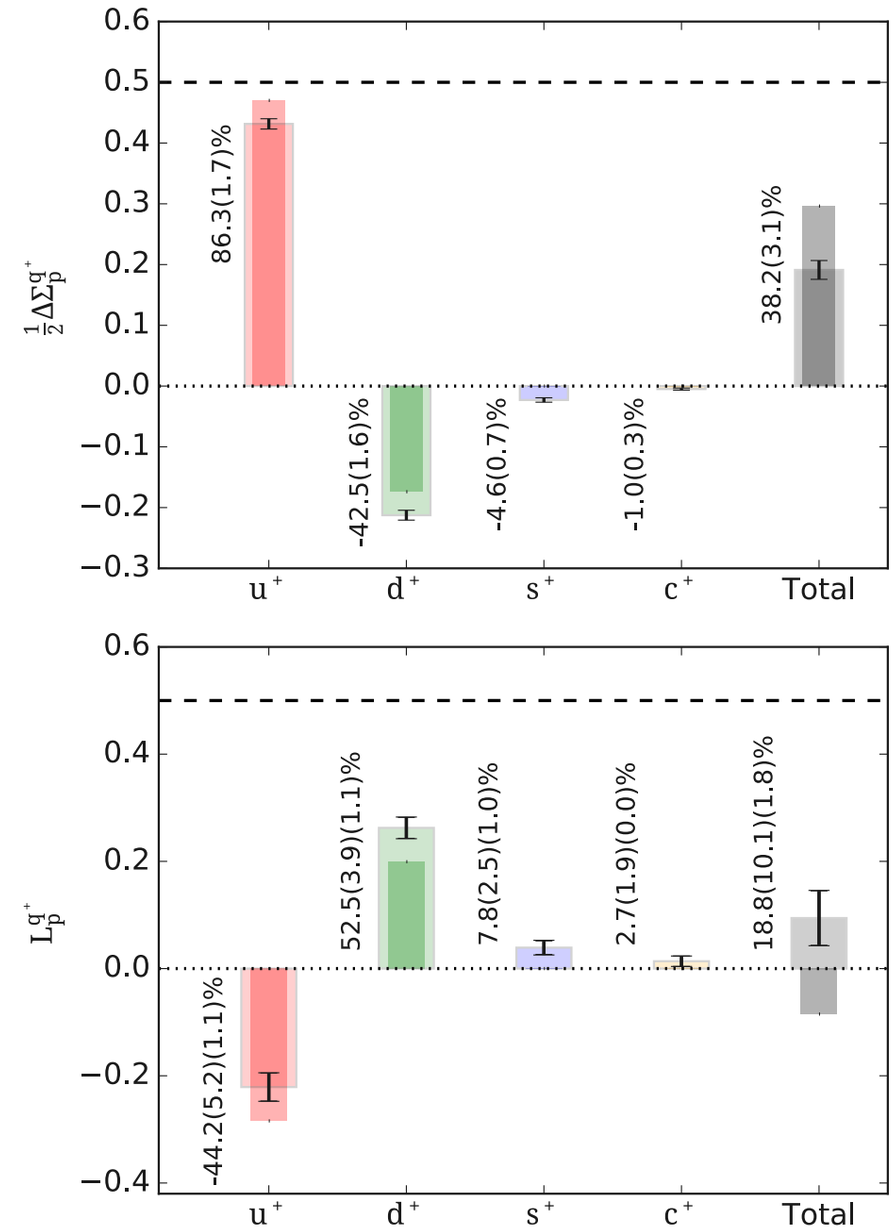

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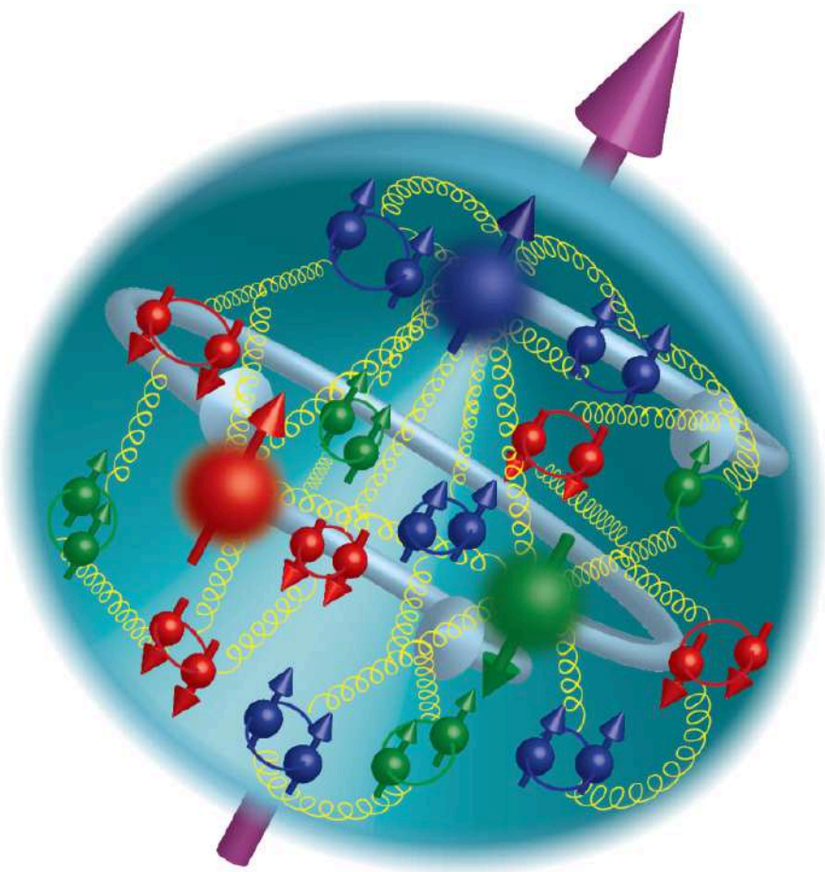
Satisfaction of spin and momentum sum rule is not forced

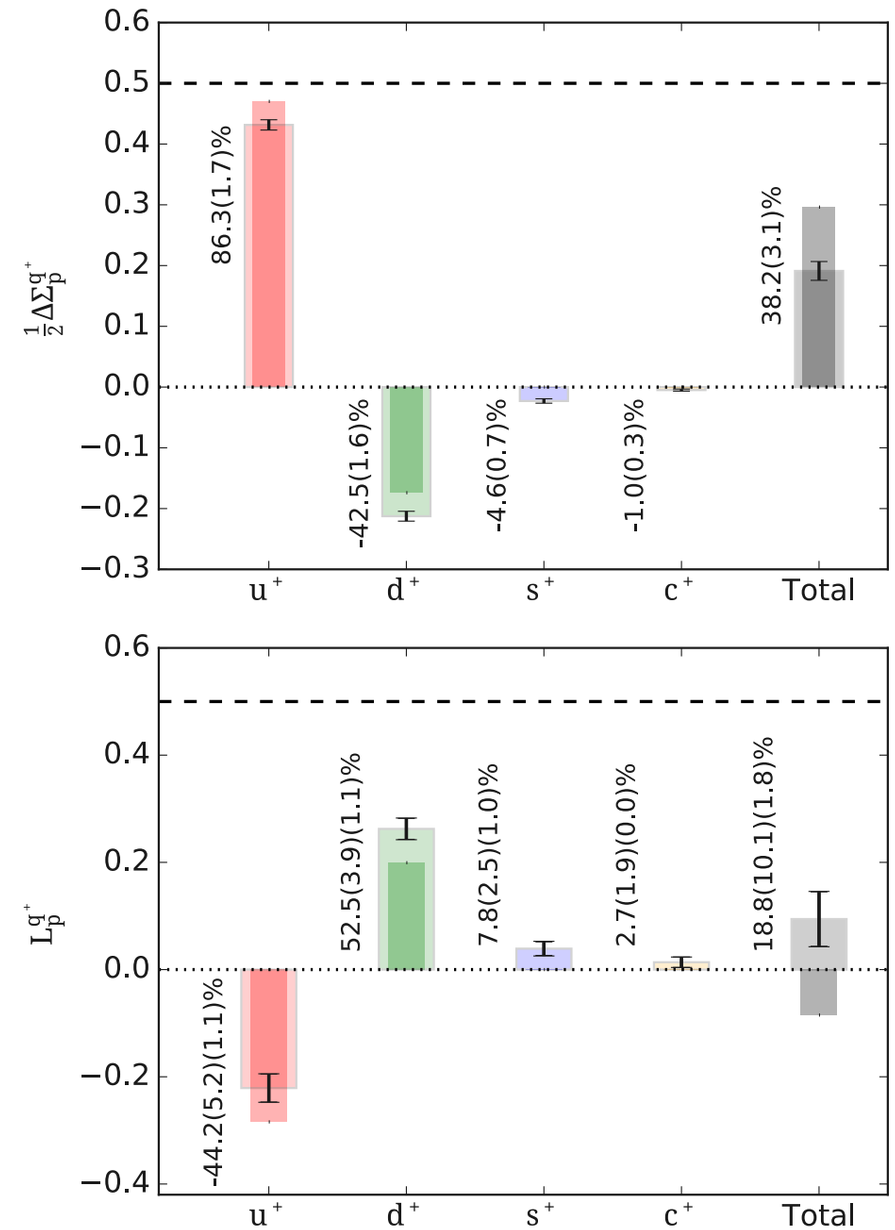
Spin decomposition

[C. Alexandrou et al., Phys. Rev. D 101, 094513 (2020), arXiv:2003.08486]

Better understanding of the spin distribution



Designed by Z.-E. Meziani



Satisfaction of spin and momentum sum rule is not forced

Proton Mass

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Higgs mechanism responsible for a fraction of the proton mass

Despite major advances the mass decomposition is not well-understood

Proton Mass Decomposition

Based on sum rules

(not unique)

$$\frac{\langle T^{\mu}_{\mu}\rangle}{\langle N|N\rangle} = M\,, \qquad \frac{\langle T^{00}\rangle}{\langle N|N\rangle} = M$$

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★ **Trace Decomposition**

see, e.g., [M. Shifman et al., Phys. Lett. 78B (1978); D. Kharzeev, Proc. Int. Sch. Phys. Fermi 130 (1996)]

★ **Decomposition of T^{00} in trace and traceless parts in rest frame**

[X.D. Ji, Phys. Rev. Lett. 74, 1071 (1995); X. D. Ji, Phys. Rev. D 52, 271 (1995)]

★ **Decomposition of T^{00} with pressure effects**

[C. Lorce´, Eur. Phys. J. C78 (2018) 2, arXiv:1706.05853]

★ **Quark/Gluon decomposition of trace T^{μ}_{μ}**

[Y. Hatta, A. Rajan, K. Tanaka, JHEP 12, 008 (2018) arXiv:1810.05116; K. Tanaka, JHEP 01, 120 (2019), arXiv:1811.07879]

Ji’s Decomposition

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$$m = M_m + M_q + M_g + M_a$$

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quark mass

quark energy

gluon energy

trace anomaly

Question:

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Answer:

Components associated with operators calculable in lattice QCD

- ★ **Quark mass** $$M_m = \sum_q \sigma_q$$
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σ_q: sigma-terms

$\langle x\rangle_q$: Quark momentum fraction

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Results at the physical point

[C. Alexandrou et al., PRD 102, 054517 (2020), arXiv:1909.00485]

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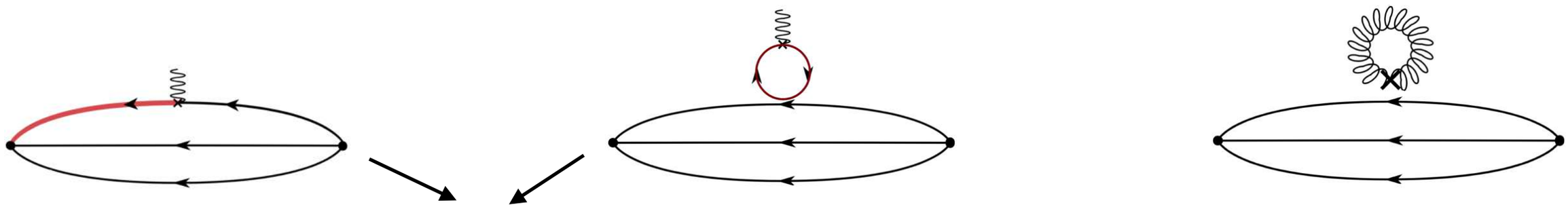

$\sigma_{u+d} = 41.6(3.8)\,MeV$

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Ji's Decomposition

Proton Mass Budget

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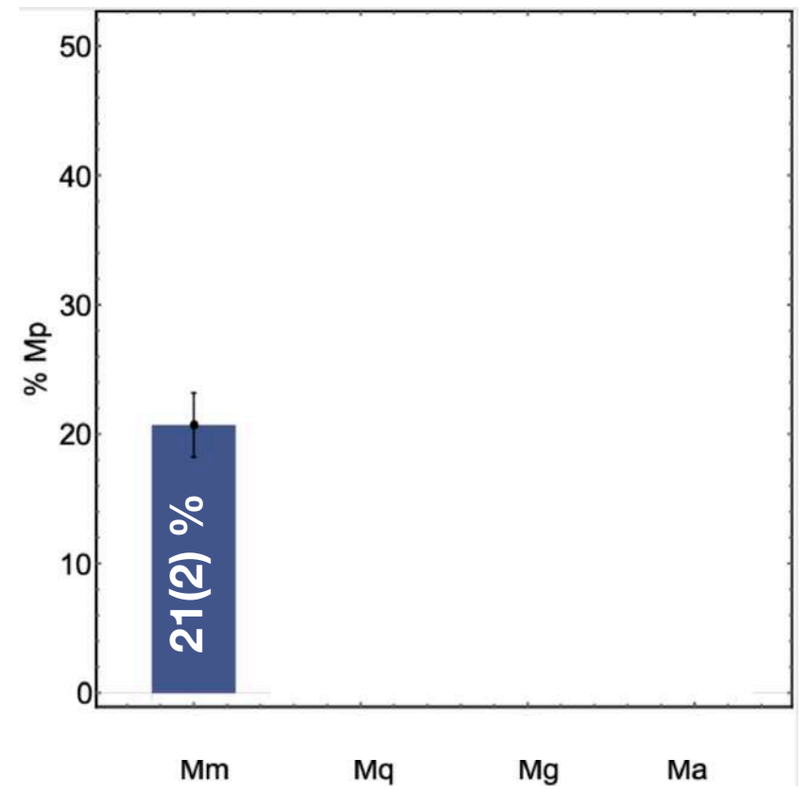

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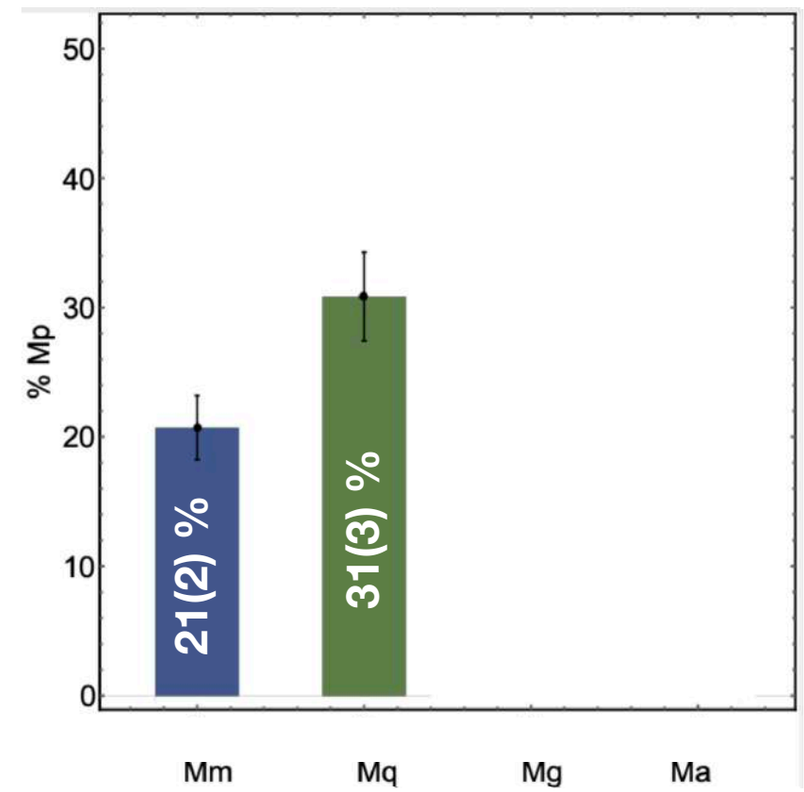

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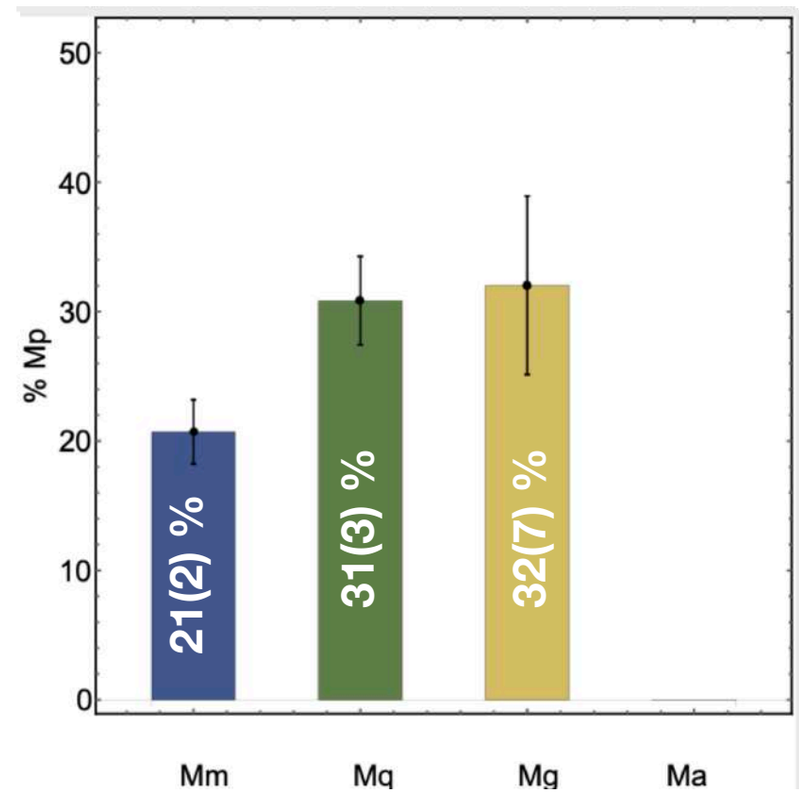

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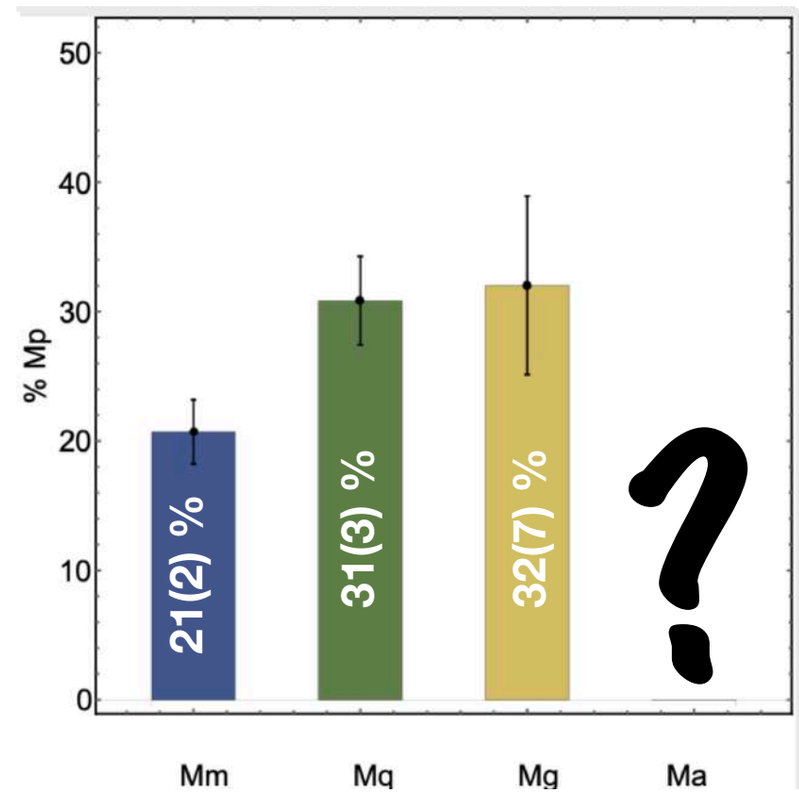

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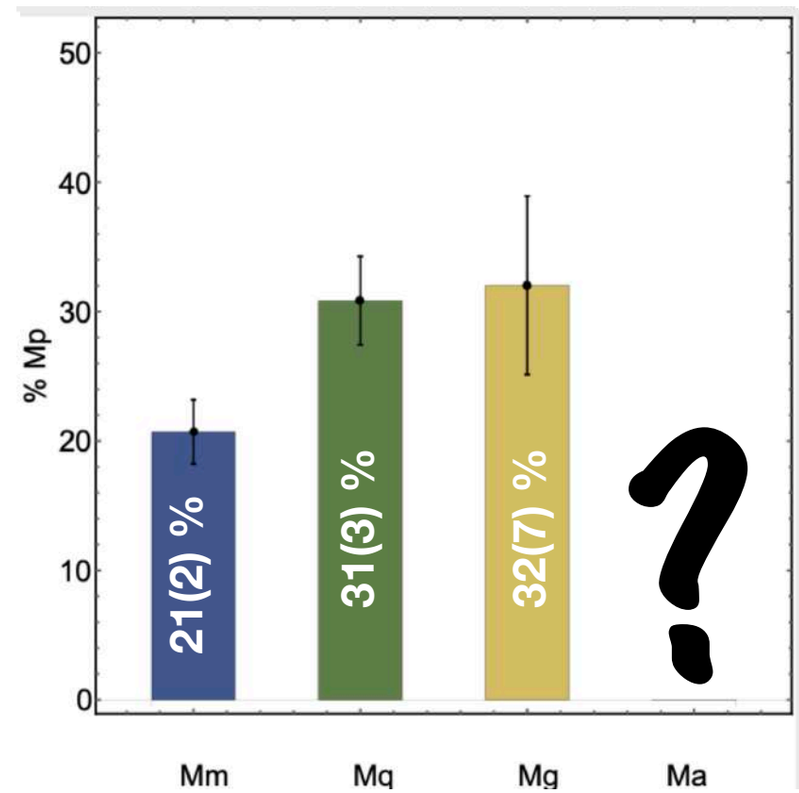

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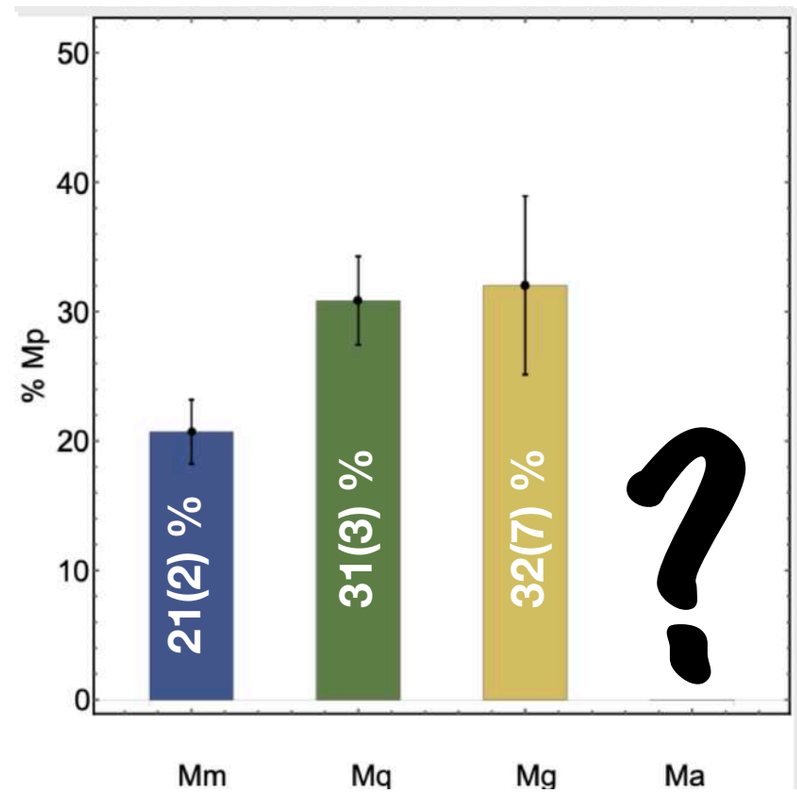


Currently not available

★ **Possibility to access trace anomaly indirectly from sum rules**

$$M_a = \frac{M}{4} - \sum_q \frac{\sigma_q}{4} \qquad M_a = M - \sum_{i=m,q,g} M_i$$

Ji's Decomposition

Proton Mass Budget

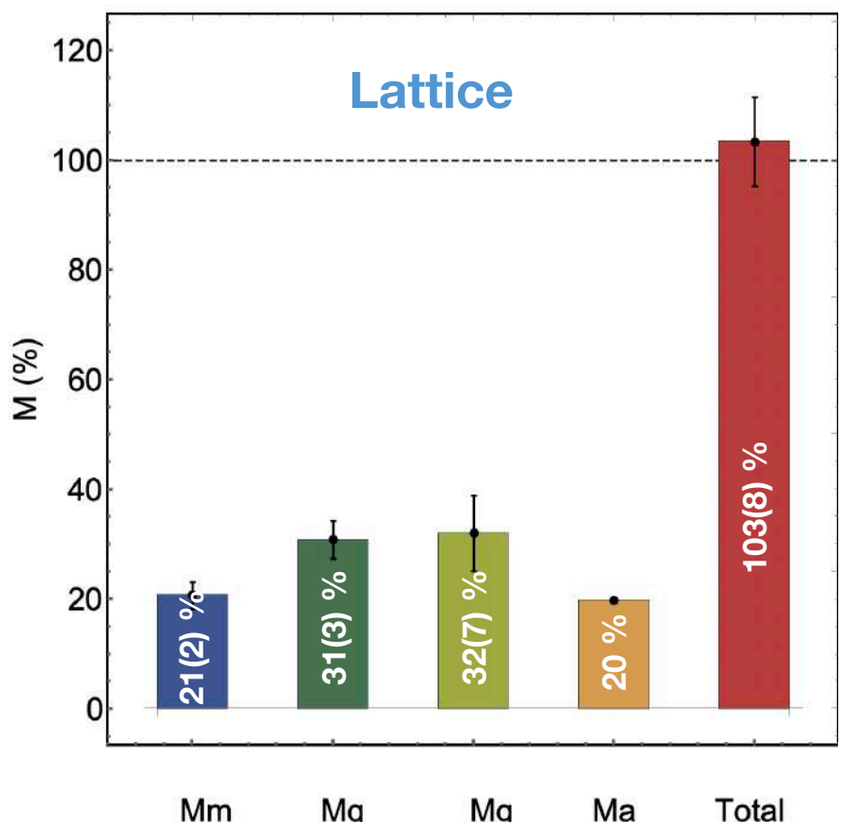
Ji's Decomposition

Proton Mass Budget

Approach A

$$M_a = \frac{M_p}{4} - \sum_q \frac{\sigma_q}{4} \sim 19.83(0.07)\,\%$$

$$M_p = M_m + M_q + M_g + M_a = 103.39(8.09)\,\%$$



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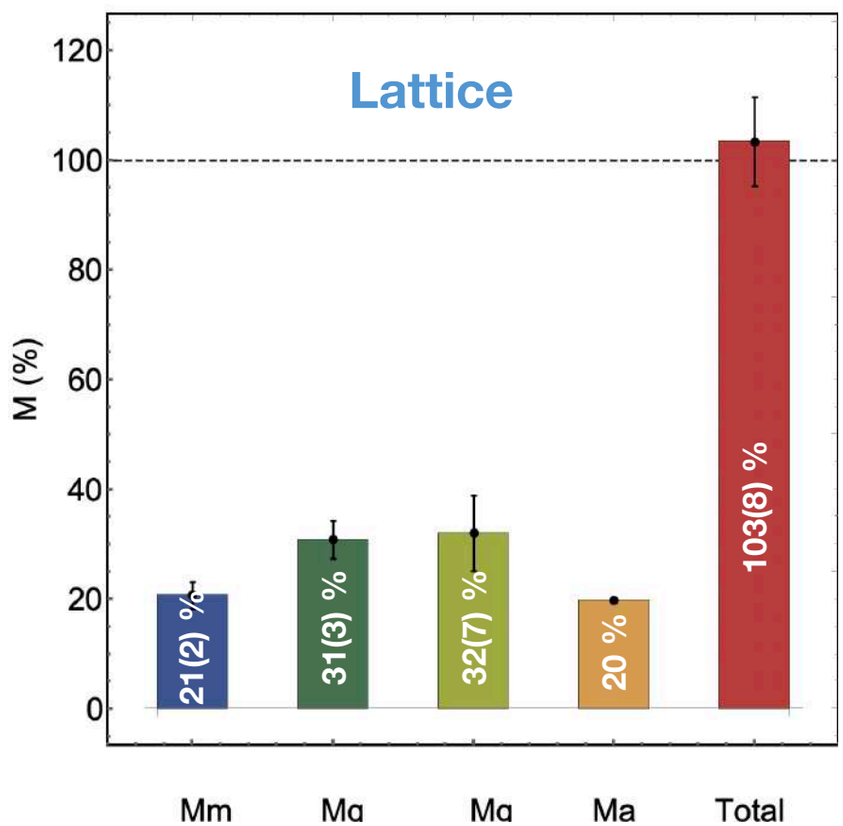
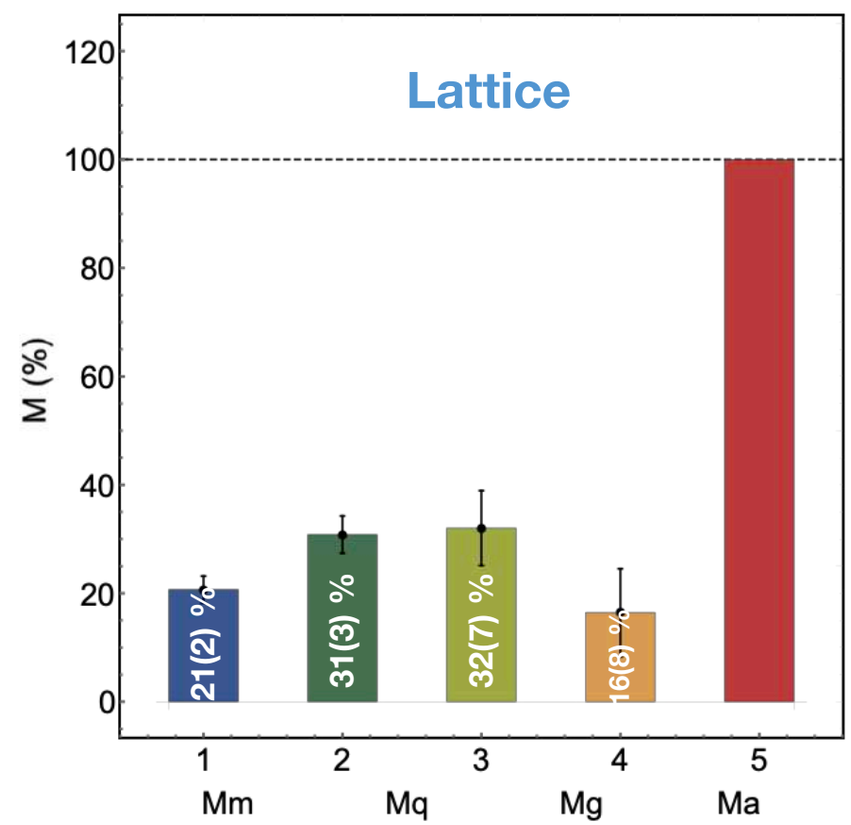


Approach B

$$M_a = M_p - \sum_{i=m,q,g} M_i \sim 16.45(8.09)\,\%$$

M_p : sum rule enforced



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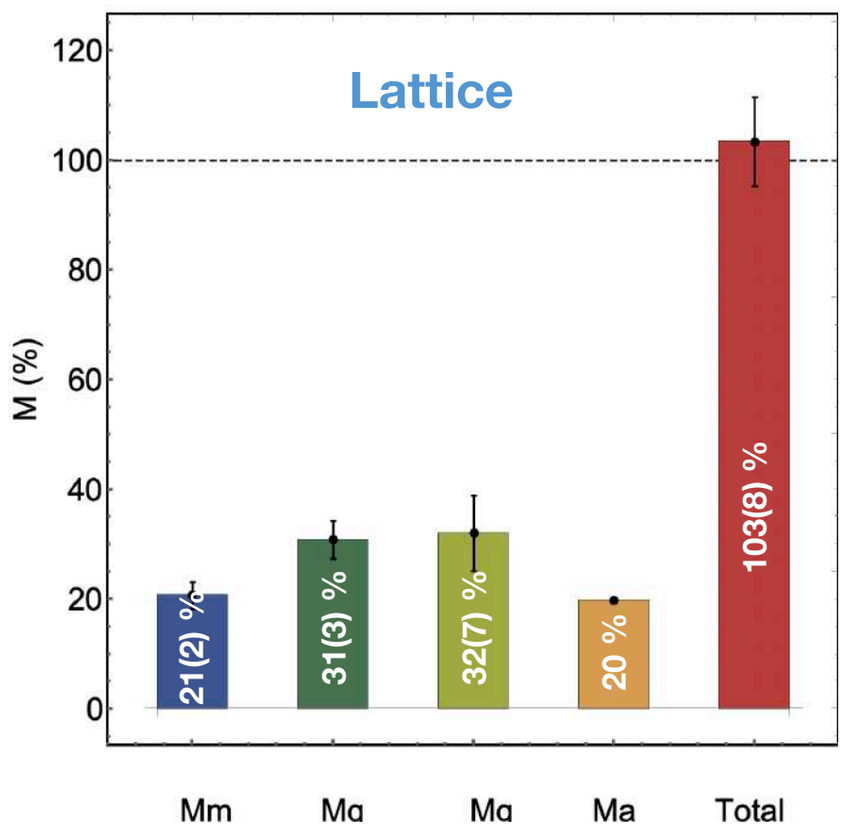

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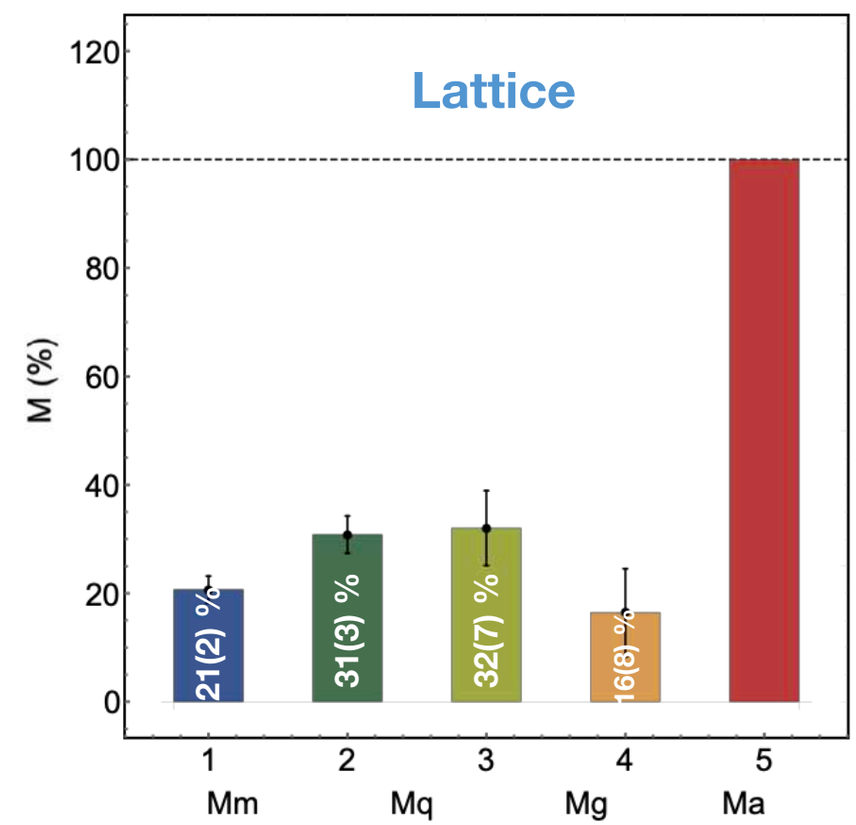
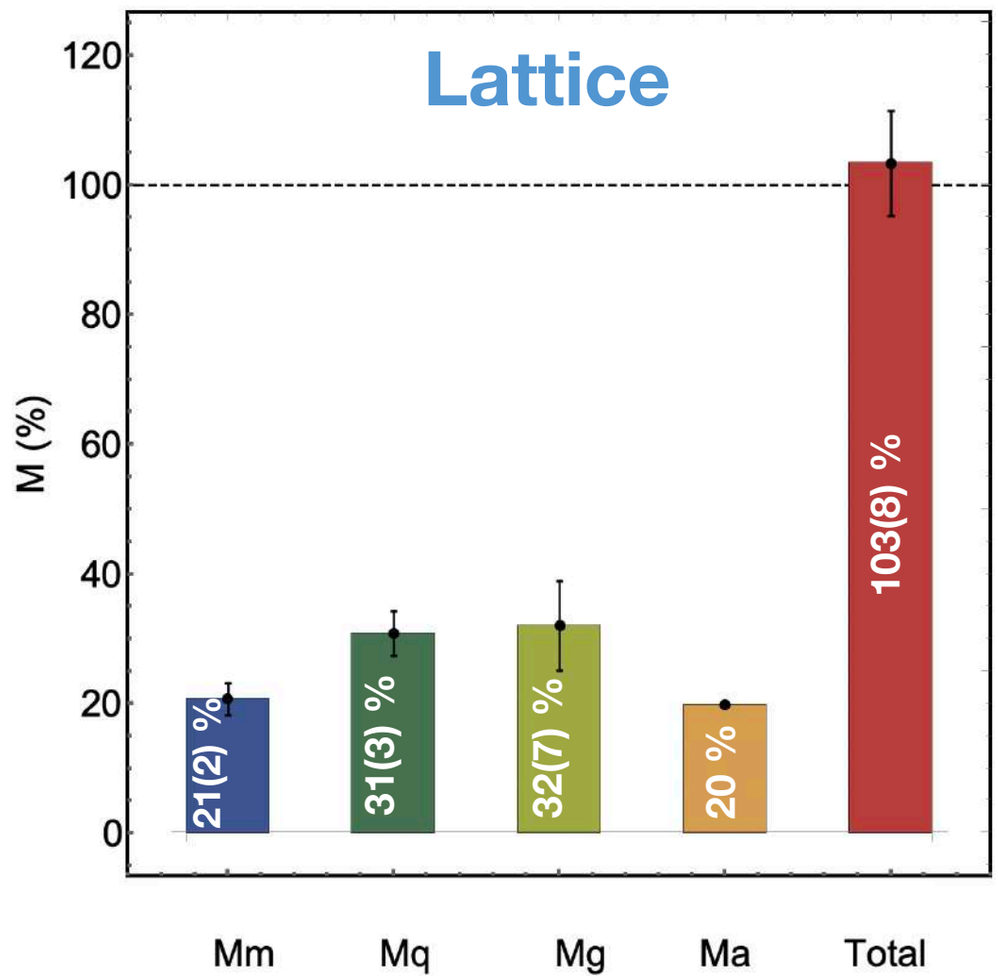
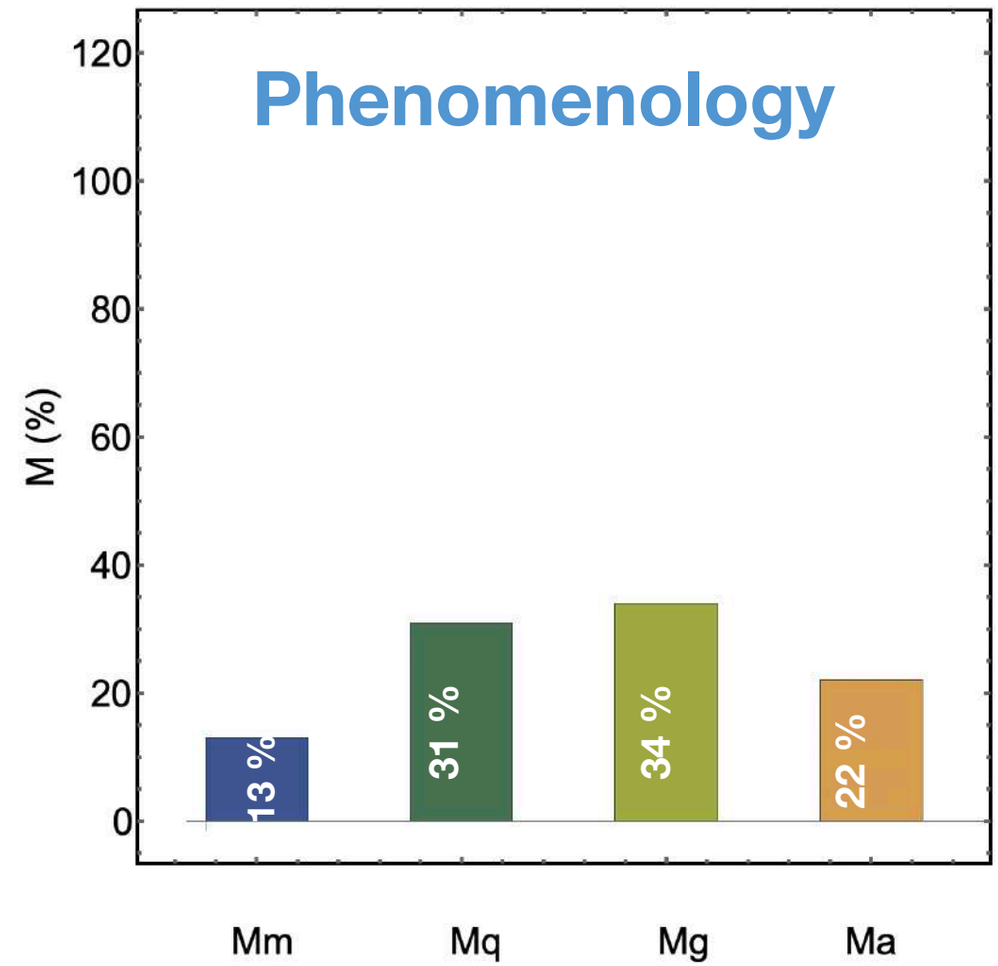


- ★ M_a compatible but different systematic uncertainties
- ★ Uncertainties of trace anomaly term depend on the sum rule

Ji's Decomposition

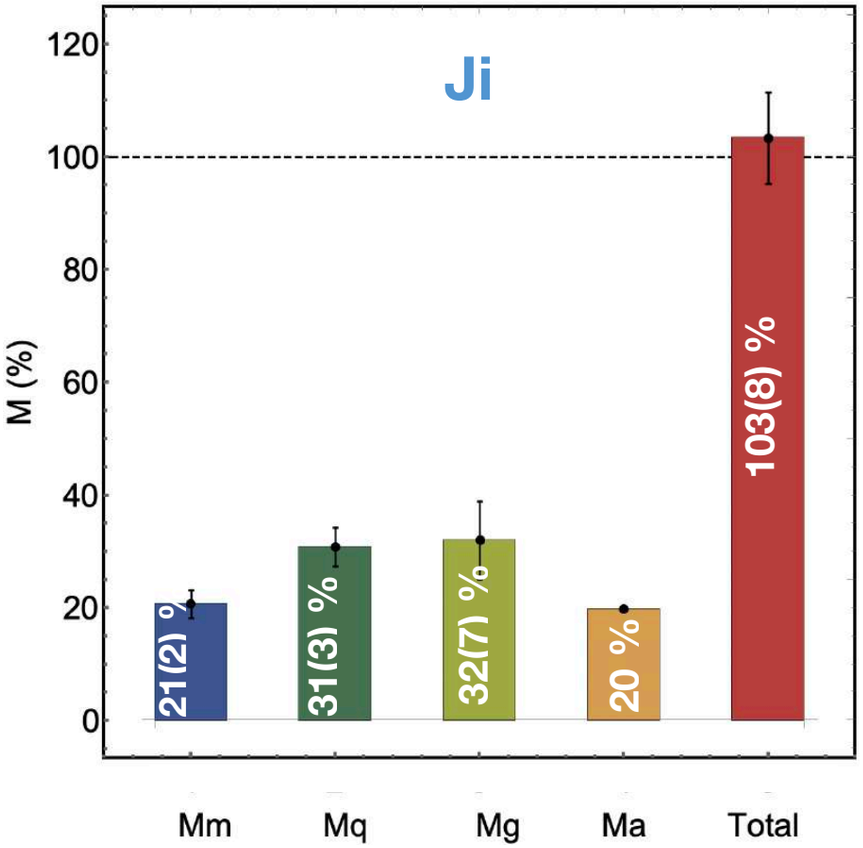


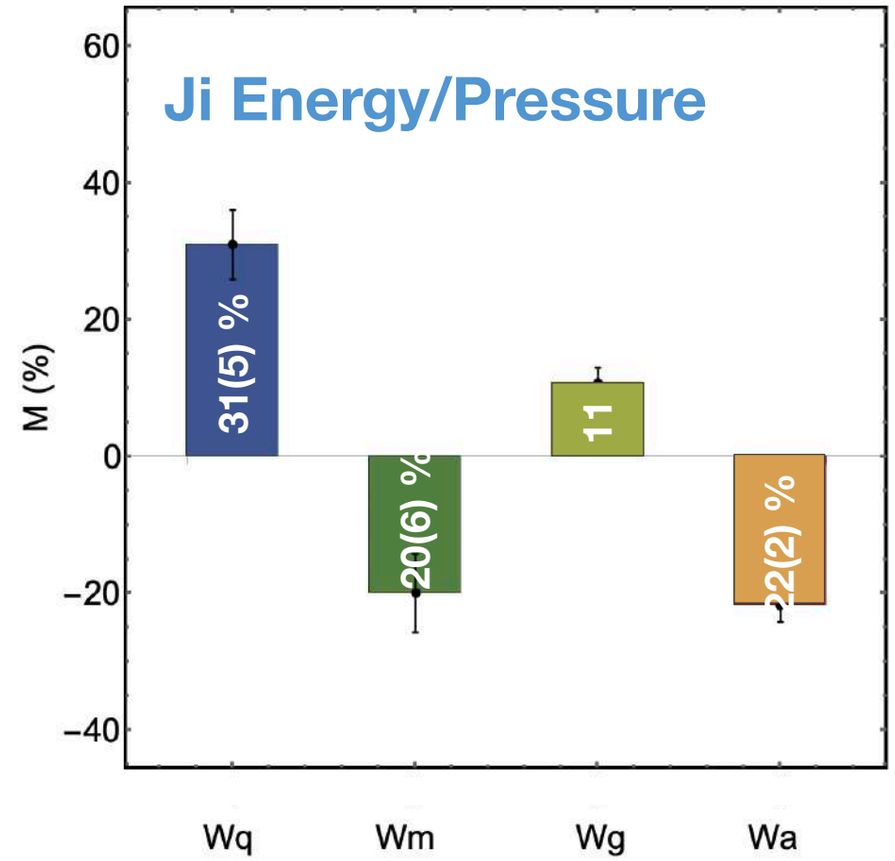


[C. Lorce´, EPJ. C78 (2018) 2]
[L. Harland-Lang et al., EPJ. C 75 (2015)]
[M. Hoferichter et al., PRL 115 (2015)]

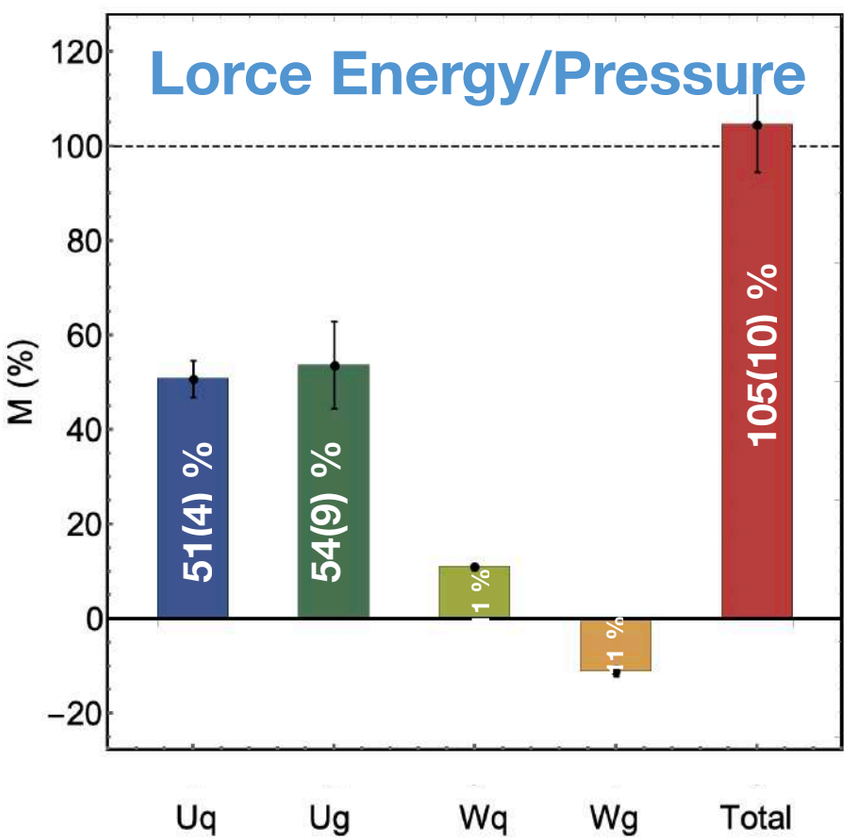
- ★ Lattice and pheno data give similar picture
- ★ The tension in the sigma terms affects M_m
- ★ Contributions are of similar order

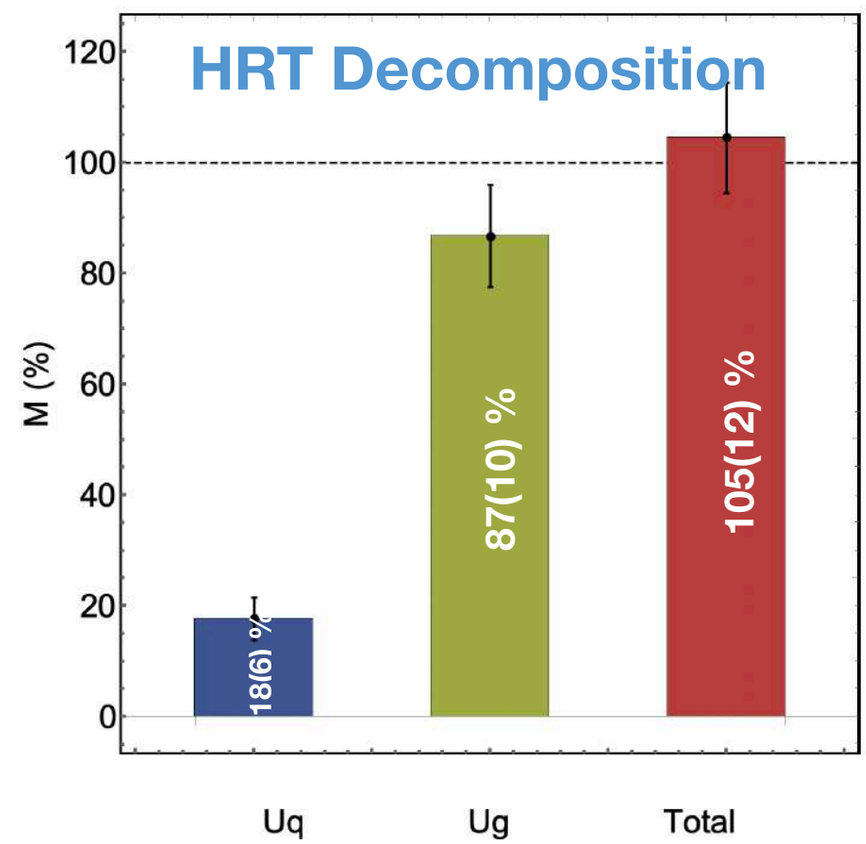
Summary





Such a detailed understanding is not available from experiments





Concluding Remarks

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- ★ **Lattice QCD calculations are finally addressing open scientific questions**

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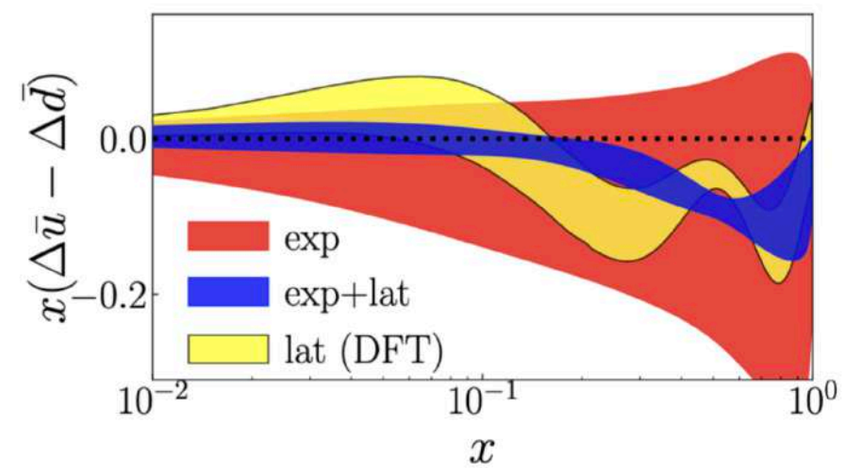
[J. Bringewatt et al, Phys. Rev. D 103, 016003 (2021)



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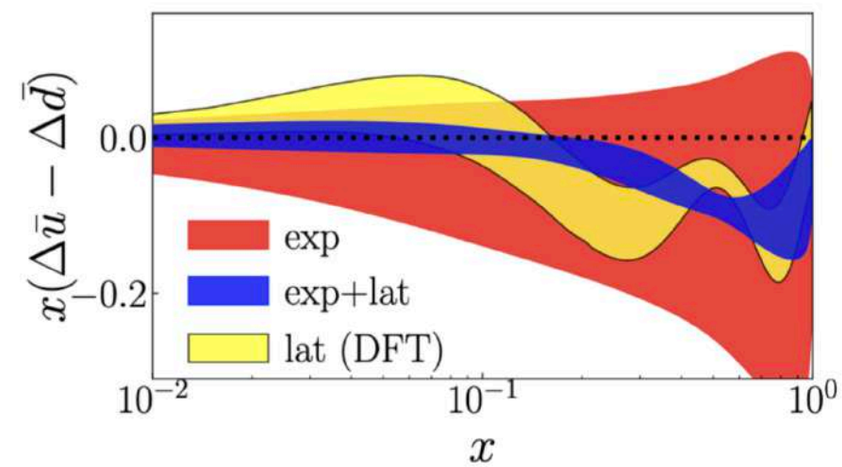
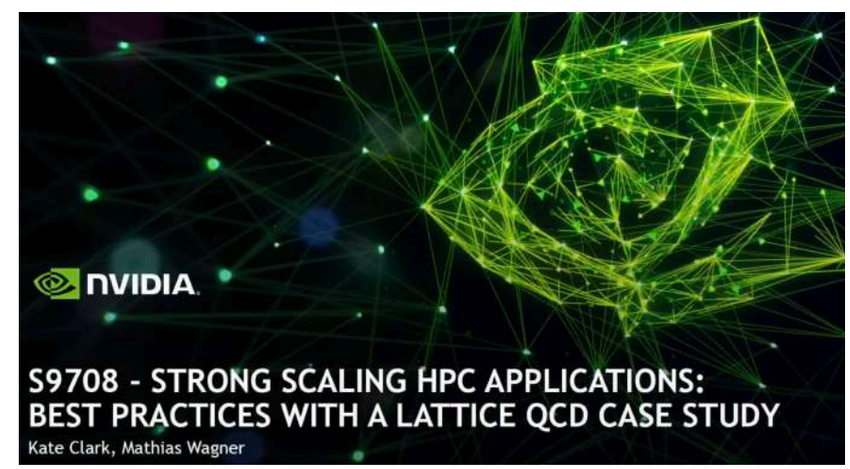


- ★ **Lattice QCD plays an important role in the development of new computer architecture**



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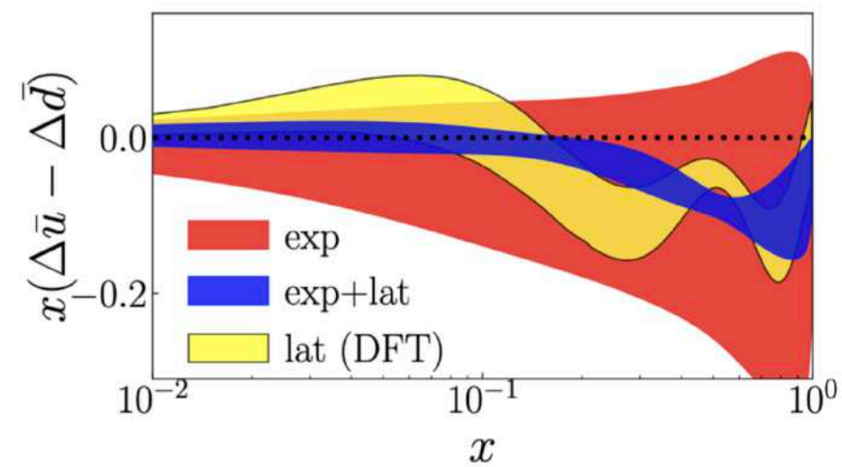

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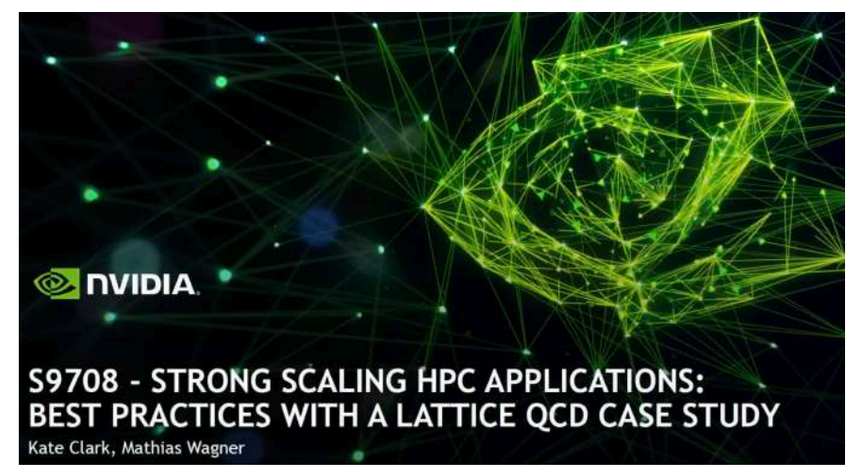

★ **Computational centers seek assistant from lattice QCD practitioners to define the next generation of computers**

Now Open: Call for Leadership-Class Computing Facility Application Partners

Thank you

DOE Early Career Award
Grant No. DE-SC0020405

TMD Topical Collaboration

Grant No. PHY-1714407