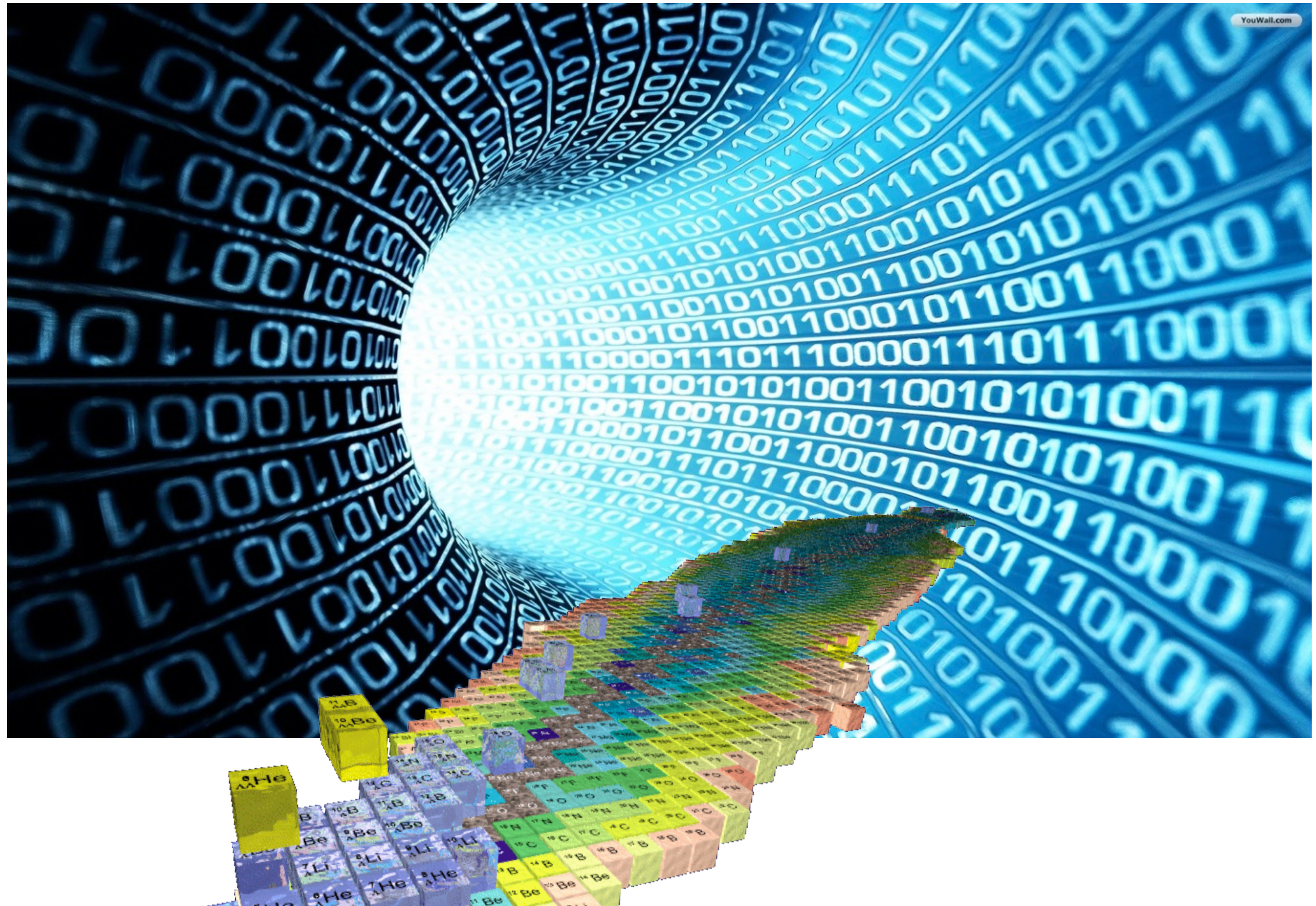
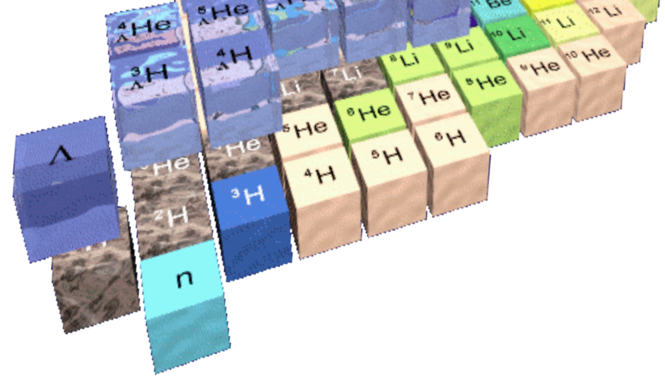

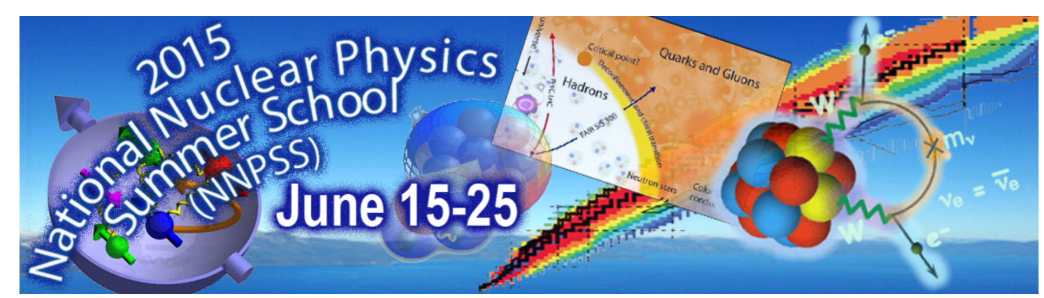

Lattice QCD for Nuclear Physics

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INSTITUTE for NUCLEAR THEORY

2015 National Nuclear Physics Summer School
Lake Tahoe, California, June 15-25, 2015

Topics

- Motivation for solving QCD
- Basic aspects of the structure of the nucleon and of quantum field theory
- An introduction to QCD - gauge symmetry, flavor symmetry, chiral symmetry
- Quantum fluctuations, the path integral and QCD
- Length scales in, and pertinent features of, Nuclear Physics
- Lattice QCD - formulation, gauge and fermion action, doublers, Symanzik action and Improvement, Tadpole-improvement, the clover action, Ginsparg-Wilson fermions and chiral symmetry
- Elements of a LQCD calculation
- Monte-Carlo algorithms for generating ensembles of gauge fields
- Iterative Algorithms for quark propagators
- Contractions of quark propagators
- Setting the lattice spacing - masses, static potential and Wilson flow
- Recovering rotational symmetry from cubic symmetry
- Correlation functions - production, statistics of, noise, the signal-to-noise issue with baryons
- Re-sampling techniques, Robust estimators and fitting, statistical behavior of correlators
- Uncertainty quantification - volume and lattice-spacing extrapolations, the dispersion relations
- Error budgets

Topics

- Status and the future
- USQCD
- Tuning, Hadron masses and light-quark masses
- Nucleon mass, static moments, strange-quark content and form factors, beta-decay matrix elements
- Hyperon form factors
- Scattering, Maiani-Testa theorem, Luscher's method,
- Resonances, exotic meson spectra, I=2 pion-pion scattering phase shift, multi-meson systems
- Coupled channels
- Nucleon-nucleon scattering and the deuteron
- Light nuclei, matching to effective field theory
- Dark matter matrix elements
- Hyperon-nucleon scattering
- Nuclear Magnetic moments, radiative capture cross section, Feshbach resonance in nn
- Exotic nuclei
- Parity violation
- Formal developments - boosted deuteron, i-periodic boundary conditions, FV QED
- Impact of algorithmic developments - AMG, recursive contraction, …
- Resource requirements
- Status and near term outlook
- Conclude

Primary Objective

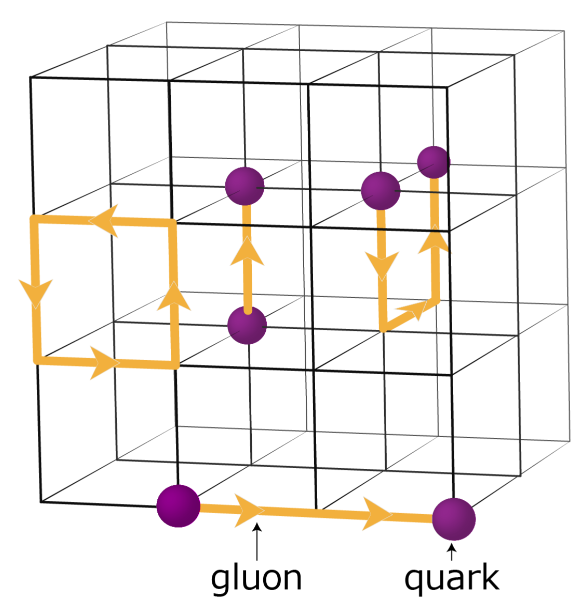
To develop first principles predictive capabilities for nuclear physics.

This will occur either by direct calculation or, more likely,
by providing input into nuclear many-body calculations that cannot be obtained experimentally.

e.g., multi-neutron forces, hyperon-nucleon, hyperon-hyperon interactions

- First step is verification of technology/method by precision comparisons with experiment.
- Second step is to make predictions for quantities that are followed up/verified by experiment
- Third step is predictions for important quantities that cannot be accessed experimentally (on appropriate time-scales).

Lattice QCD is the only known way to rigorously solve QCD without any uncontrolled assumptions. Peta-scale computational resources will soon become available for such calculations.
This will be a turning point for nuclear theory.



2015 National Nuclear Physics Summer School (NNPSS) June 15-25

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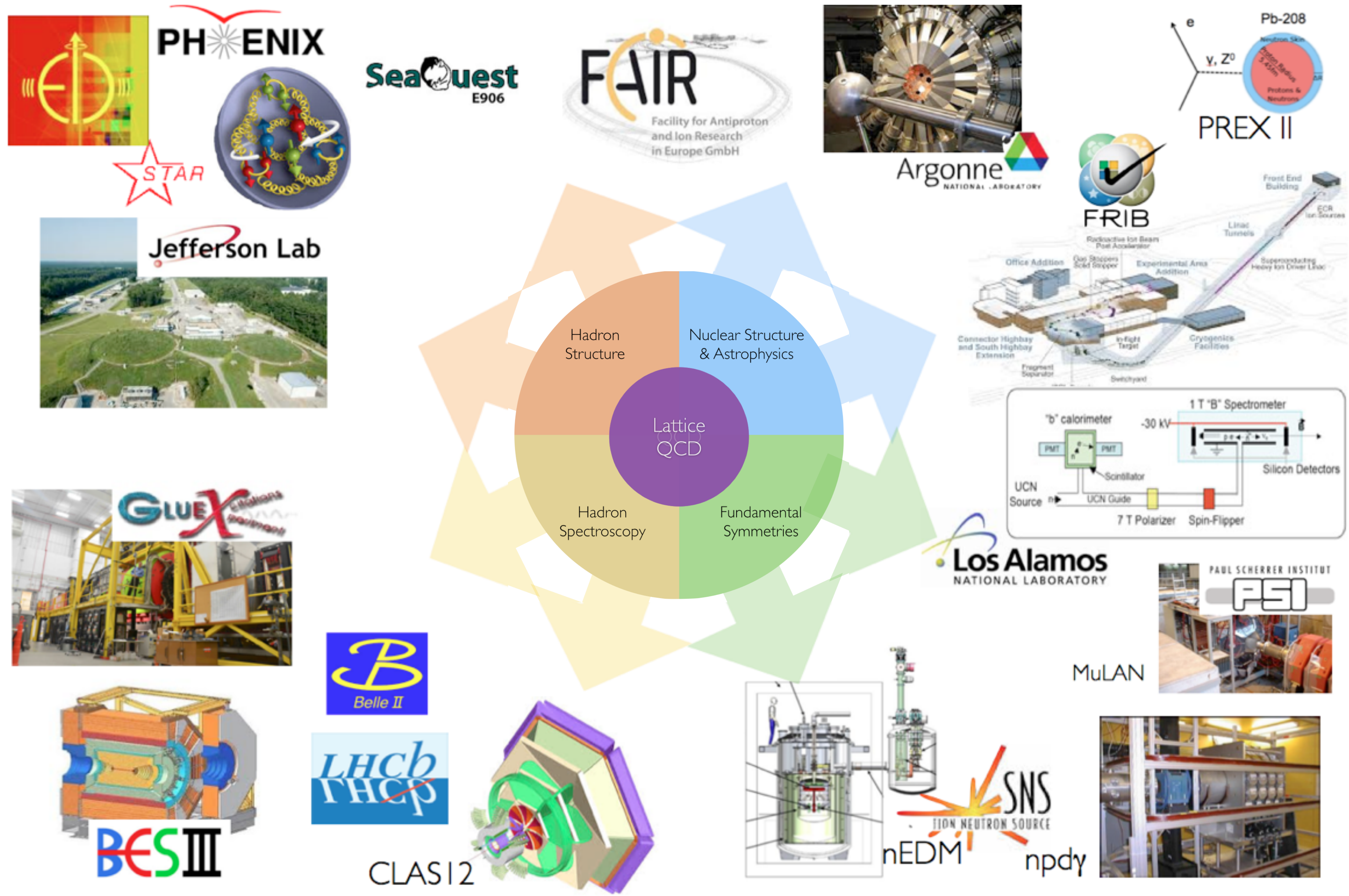
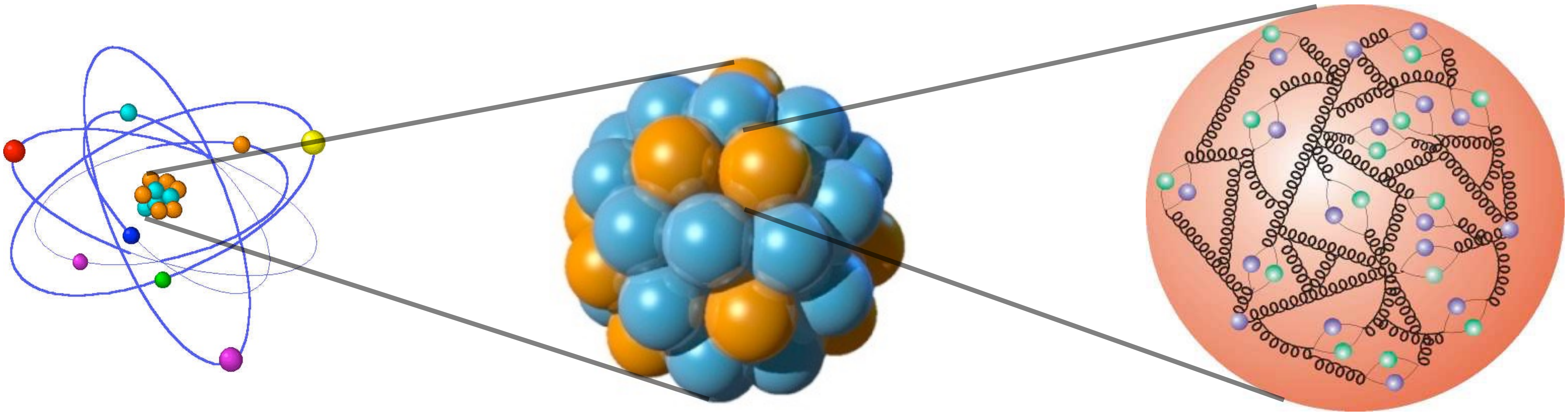
Supports NP Experimental Program



Quantum Chromodynamics

Atom | Nucleus | Proton

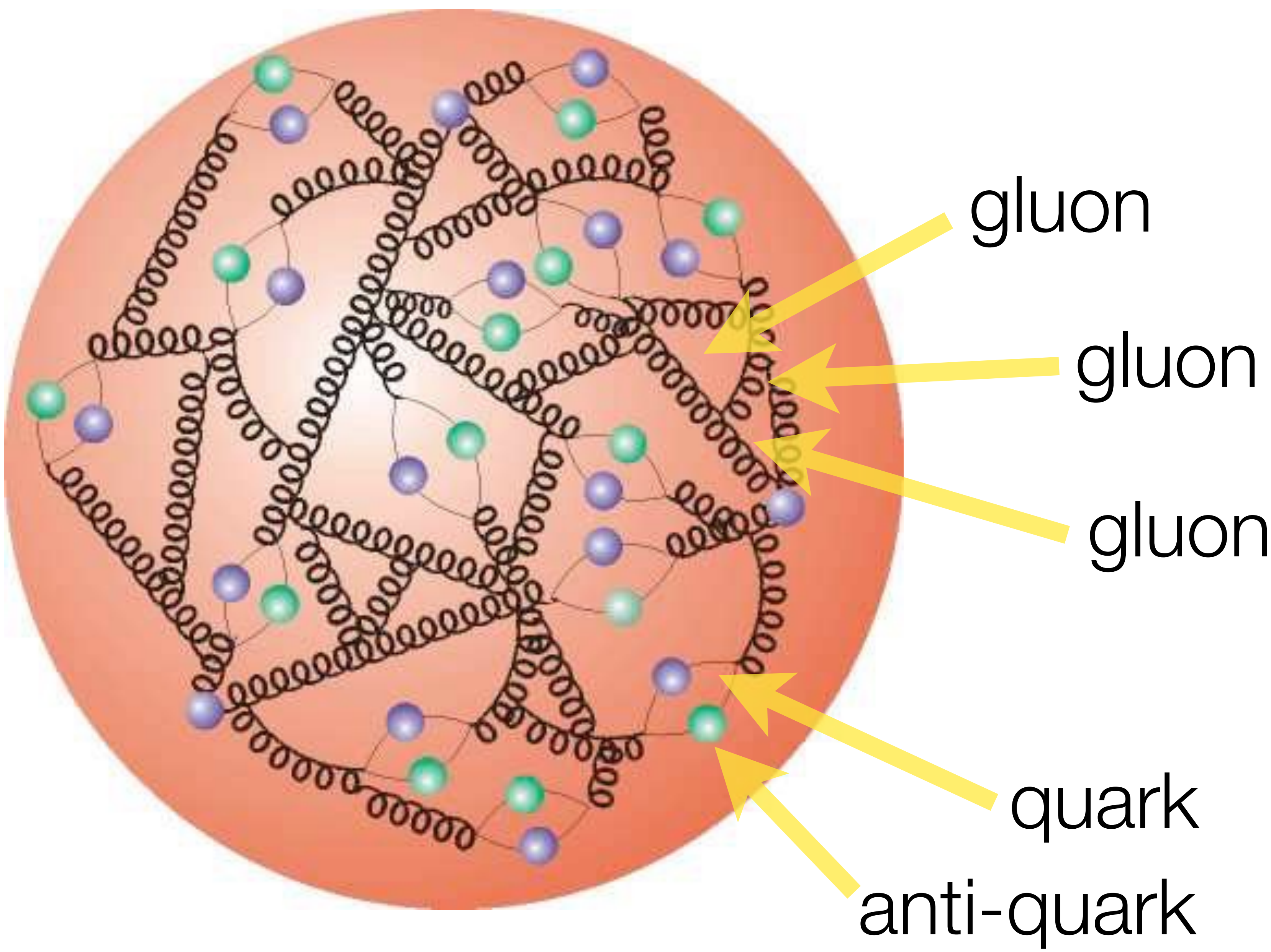


Electrons and Nuclei | Protons and Neutrons | Quarks and Gluons

Quantum Chromodynamics

A quantum field theory describing the dynamics of massless gluons and quarks with a wide range of masses

Quantum Chromodynamics



Nucleon

up-quark mass ~ 3 MeV

down-quark mass ~ 5 MeV

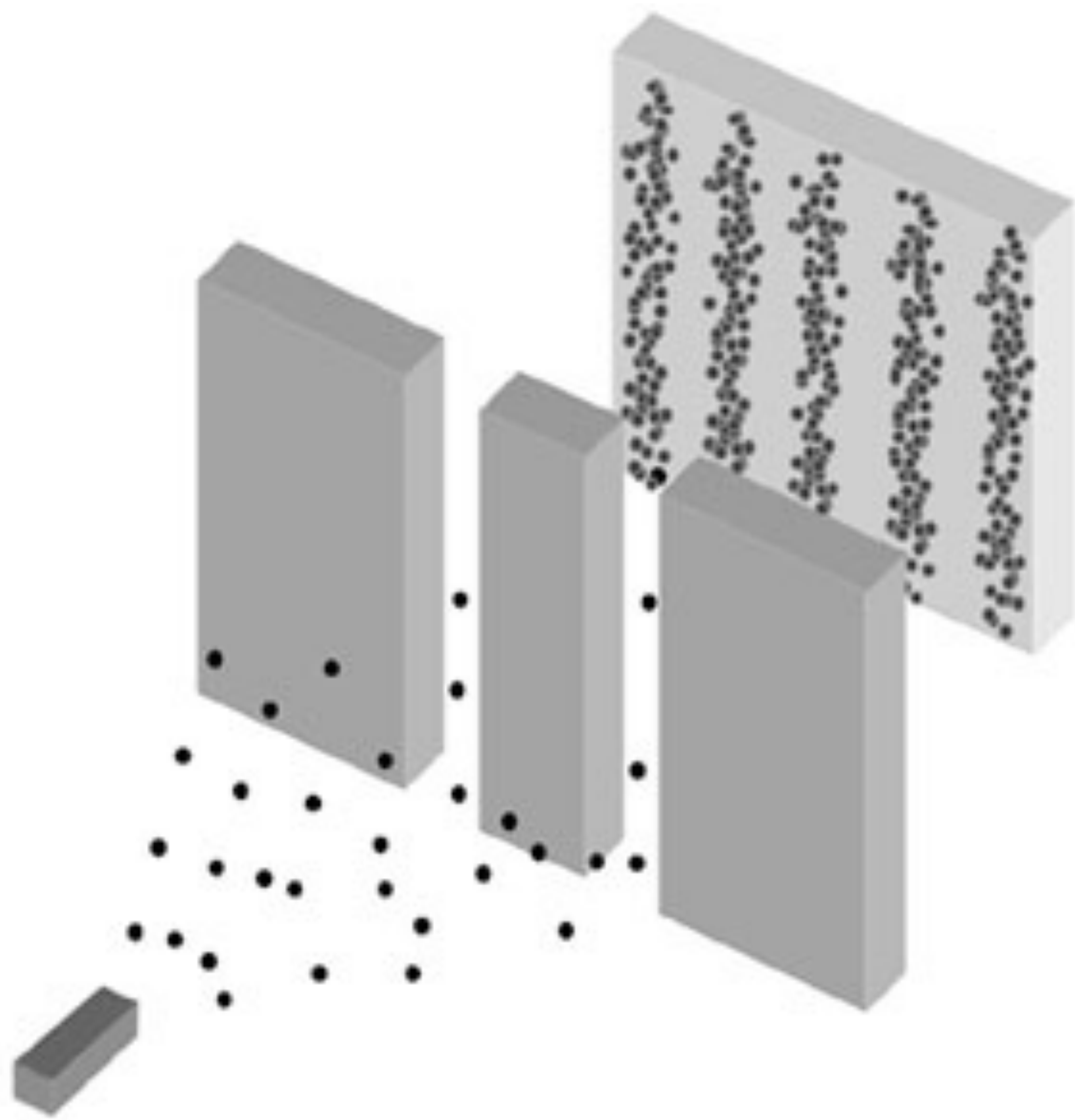
gluon mass = 0 MeV

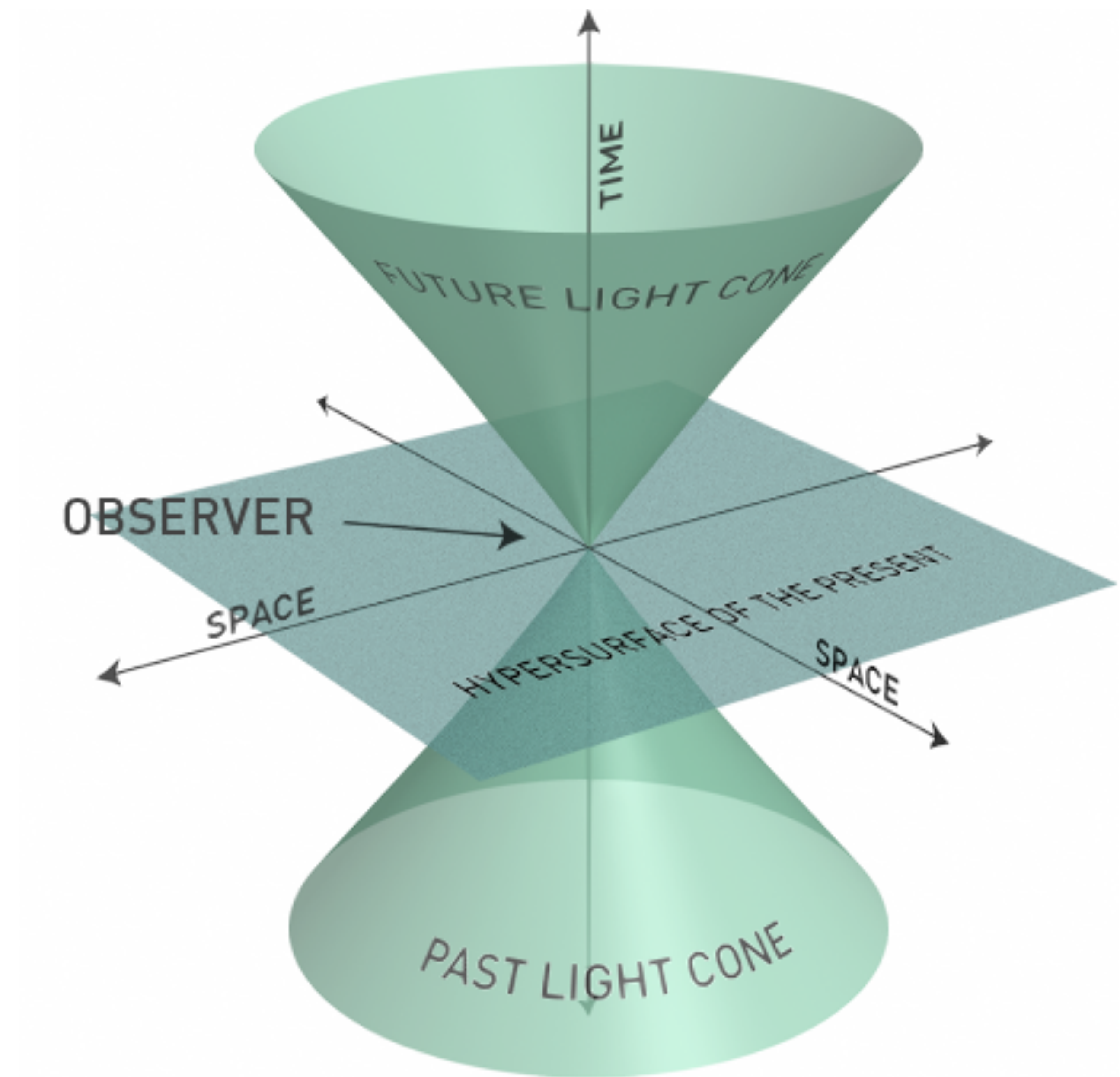
proton ~ 940 MeV

Nucleon is an entangled state of indefinite particle number with spin-1/2

quark masses defined in a scheme at a scale: e.g. Dim. Reg. with MSbar at μ=2 GeV

Quantum Mechanics and Special Relativity





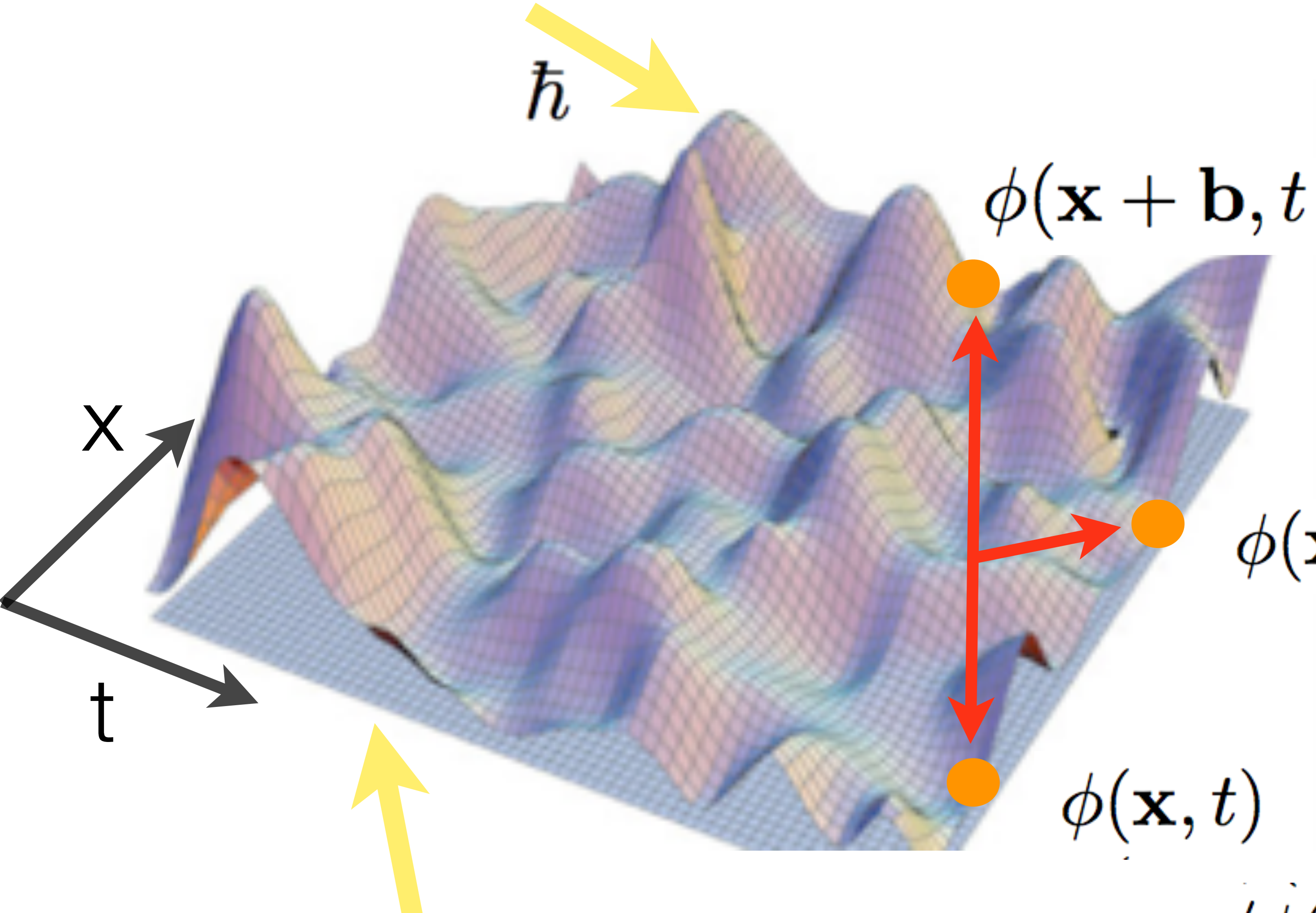
$$\hbar = 1.055 \times 10^{-34}\ \mathrm{Js}$$

$$c = 2.998 \times 10^{8}\ \mathrm{m/s}$$

‘ i ’ $\Psi(\mathbf{x}, t)$

Quantum Field Theory
e.g. a Scalar Field

Quantum Vacuum



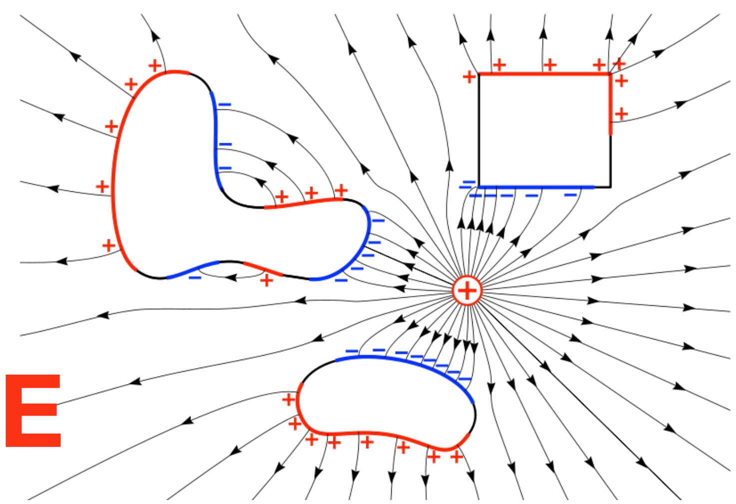
$$e^{\frac{i}{\hbar}S[\phi]}$$

Classical Vacuum

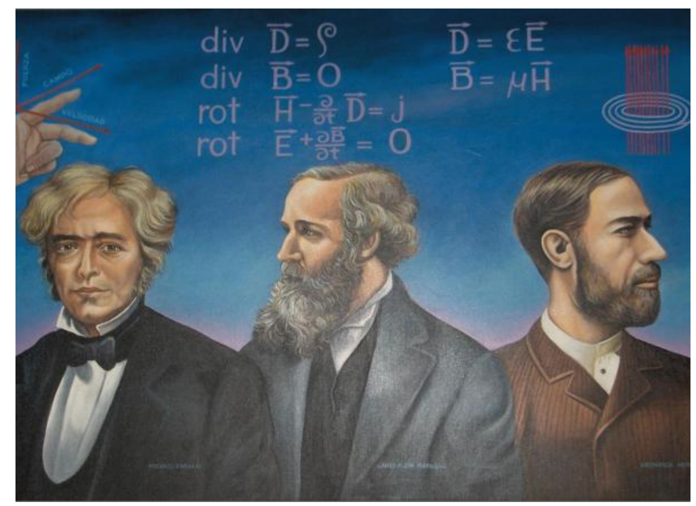
e.g. $\langle\phi(\mathbf{x}, t)\phi(\mathbf{x}+\mathbf{a}, t+s)\phi(\mathbf{x}+\mathbf{b}, t+u)\rangle$

Quantum Fluctuations in the Vacuum Dictate Observables

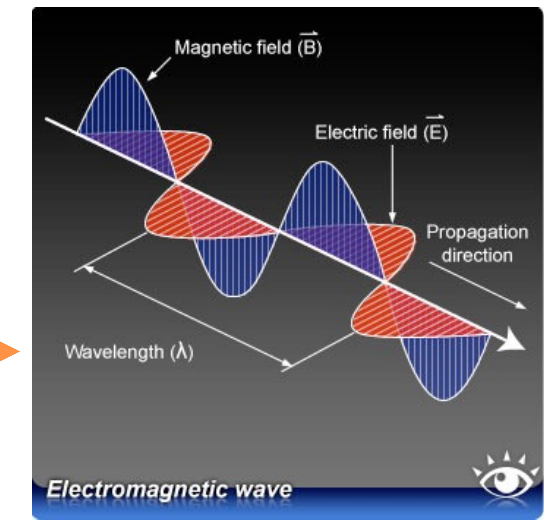
Electromagnetism (1861)



Experiment

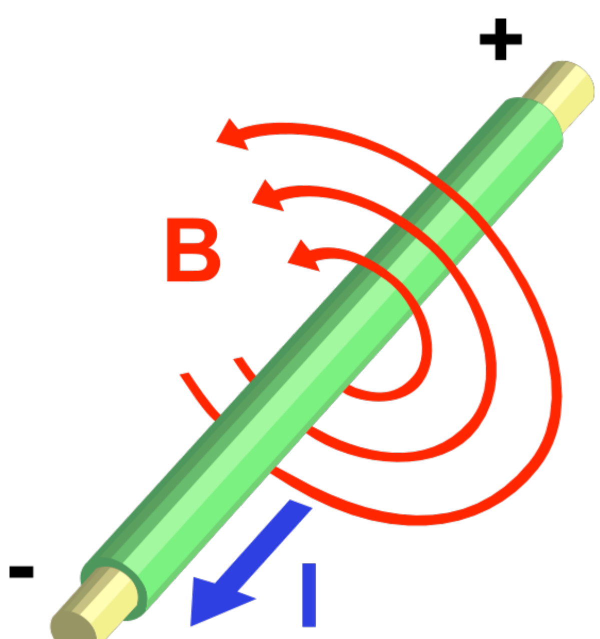


Thinking



Theoretical Prediction
- EM Waves

EM is Linear and essentially Classical

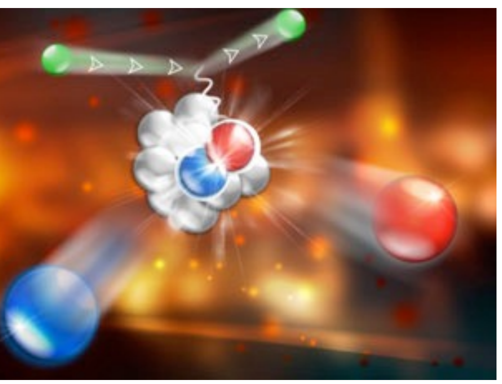


Experiment

Application

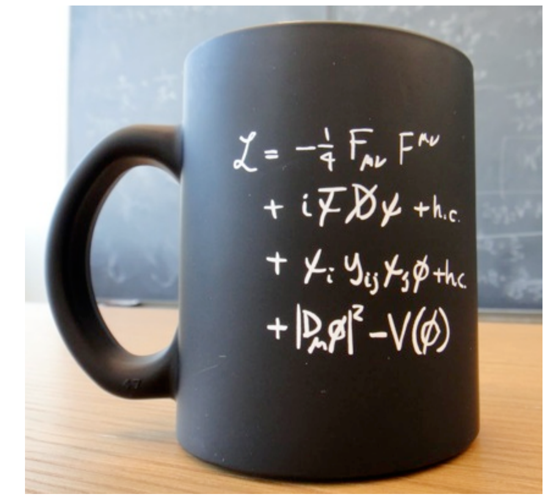
Experiment

Quantum Chromodynamics

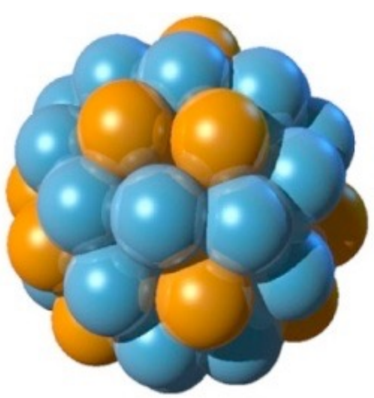


Experiment

Thinking



QCD



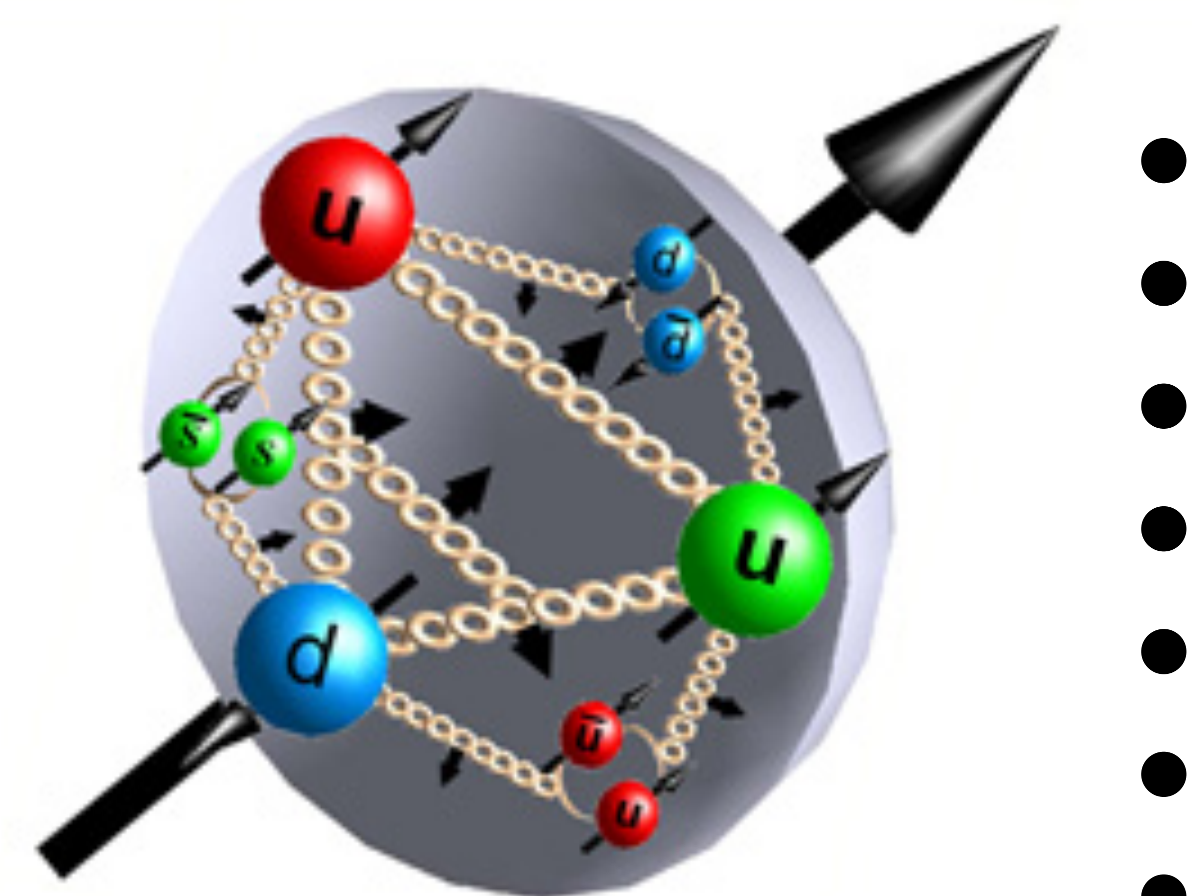
Experiment

electric charges ↔ color charges

EM waves ↔ Excited Glue

QCD is Non-Linear
and essentially Quantum

Important Features of QCD



Nucleon

- Each quark comes in 3 colors
- SU(3) Local Gauge Symmetry
- 8 gluons - ``photon-like”
- Asymptotic Freedom (QM)
- Confinement (QM)
- Chiral Symmetry Breaking (QM)
- 4 well-defined input parameters

QCD Lagrange Density

A Renormalizable Quantum Field Theory

$$\mathcal{L} = \sum_{i=u,d,s,c,b,t} \bar{q}_i \left[\, i \not{D} - m_i \,\right] q_i \; - \; \frac{1}{4} \sum_{a=1,\ldots,8} G^a_{\mu\nu} G^{\mu\nu,a}$$

quark kinetic

quark mass
(Higgs mechanism)

gluon kinetic
Yang-Mills action

$$D_\mu q(x) \; = \; \partial_\mu q(x) + ig \sum_{a=1,\ldots,8} A^a_\mu(x) T^a q(x)$$

covariant
derivative

$$G_{\mu\nu}(x) \; = \; \frac{1}{ig} \left[\, D_\mu, D_\nu \,\right] \; = \; \sum_{a=1,\ldots,8} T^a G^a_{\mu\nu}(x)$$

gluon field
strength

QCD Lagrange Density

Gauge Symmetry - local

$$\mathcal{L} = \sum_{i=u,d,s,c,b,t} \bar{q}_i \left[\, i\not{D} - m_i \,\right] q_i - \frac{1}{4} \sum_{a=1,\ldots,8} G^a_{\mu\nu} G^{\mu\nu,a}$$

$$d(x) = \begin{pmatrix} d^1(x) \\ d^2(x) \\ d^3(x) \end{pmatrix}$$

$$q(x) \rightarrow q'(x) = \Omega(x) q(x)$$

$$\overline{q'} \not{D}' q' = \bar{q}\, \Omega^{-1} \not{D}'\, \Omega\, q = \bar{q} \not{D} q$$

$$D'_\mu = \Omega D_\mu \Omega^{-1}$$

$$A'_\mu = \Omega A_\mu \Omega^{-1} + \frac{1}{ig} \Omega \partial_\mu \Omega^{-1}$$

QCD Lagrange Density

Gauge Symmetry - local

$$\mathcal{L} = \sum_{i=u,d,s,c,b,t} \bar{q}_i \left[\, i\not{D} - m_i \, \right] q_i \; - \; \frac{1}{4} \sum_{a=1,\ldots,8} G^a_{\mu\nu} G^{\mu\nu,a}$$

$$d(x) = \begin{pmatrix} d^1(x) \\ d^2(x) \\ d^3(x) \end{pmatrix}$$

$$q(x) \;\to\; q'(x) \;=\; \Omega(x) q(x)$$

$$\overline{q'} \; \not{D}' \; q' \;=\; \bar{q} \, \Omega^{-1} \not{D}' \, \Omega \; q \;=\; \bar{q} \; \not{D} \, q$$

$$D'_\mu \;=\; \Omega D_\mu \Omega^{-1}$$

$$A_\mu \;\to\; A'_\mu \;=\; \Omega A_\mu \Omega^{-1} + \frac{1}{ig} \Omega \partial_\mu \Omega^{-1}$$

QCD Lagrange Density

Gauge Symmetry - local

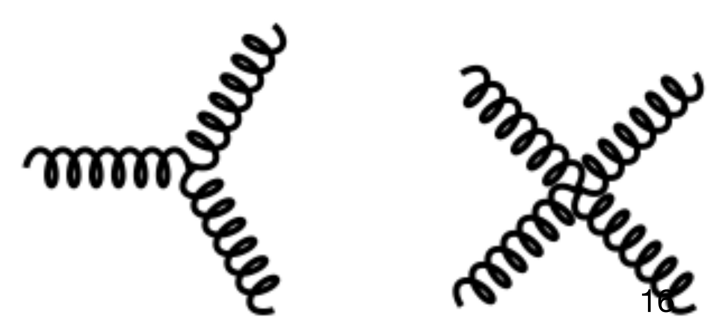
$$\mathcal{L} = \sum_{i=u,d,s,c,b,t} \bar{q}_i \, [\, i \not{D} - m_i \,] \, q_i \; - \; \frac{1}{4} \sum_{a=1,\ldots,8} G^a_{\mu\nu} G^{\mu\nu,a}$$

$$q(x) \;\rightarrow\; q'(x) \;=\; \Omega(x) q(x)$$

$$A_\mu \;\rightarrow\; A'_\mu \;=\; \Omega A_\mu \Omega^{-1} + \frac{1}{ig} \Omega \partial_\mu \Omega^{-1}$$

Gauge transformation

- SU(3) (special unitary) local color gauge symmetry is an exact symmetry of nature, i.e., it holds at each point in spacetime



QCD Lagrange Density

Flavor Symmetries - global

$$\mathcal{L} = \overline{Q}\,[\, i \not{D} - M_Q \,]\, Q - \frac{1}{4} G^2$$

$$Q(x) = \begin{pmatrix} u(x) \\ d(x) \end{pmatrix} \qquad M_Q = \begin{pmatrix} m_u & 0 \\ 0 & m_d \end{pmatrix}$$

When $m_u = m_d$

$$Q(x) \rightarrow V Q(x)$$

SU(2) (vector) flavor symmetry
of QCD Lagrange density.
V is a spacetime independent SU(2) matrix

Spectrum of the Hamiltonian classified into irreps. of flavor SU(2)
e.g., the neutron and proton are degenerate - the nucleon is a doublet of SU(2)

QCD Lagrange Density

Chiral Symmetry - global

$$\mathcal{L} = \overline{Q}\,[\, i\not{D} - M_Q \,]\,Q - \frac{1}{4}G^2$$

$$\overline{Q}\,[\, i\not{D} - M_Q \,]\,Q = \overline{Q}_L i\not{D}\, Q_L + \overline{Q}_R i\not{D}\, Q_R - \overline{Q}_L M_Q Q_R - \overline{Q}_R M_Q^\dagger Q_L$$

Invariant

NOT Invariant

$$Q_L \to L\, Q_L$$
$$Q_R \to R\, Q_R$$

Condensate spontaneously break chiral symmetry $\langle \overline{Q}_R Q_L \rangle_i^j = v\delta_i^j$

Goldstone's theorem : massless particle for each broken generator : 3 massless pions

Explicit chiral symmetry breaking by quark masses : small pion masses

QCD Lagrange Density

Quantum Effects - Path Integral

So far only classical Lagrange density !
Quantum effects included via the path integral (as usual)

$$Z \ \propto \int \mathcal{D}A_\mu^a \mathcal{D}\overline{q}_i \mathcal{D}q_i \ e^{\frac{i}{\hbar}\int d^4x \ \mathcal{L}+\mathcal{L}_{g.f.}+\mathcal{L}_{\mathrm{ghosts}}}$$

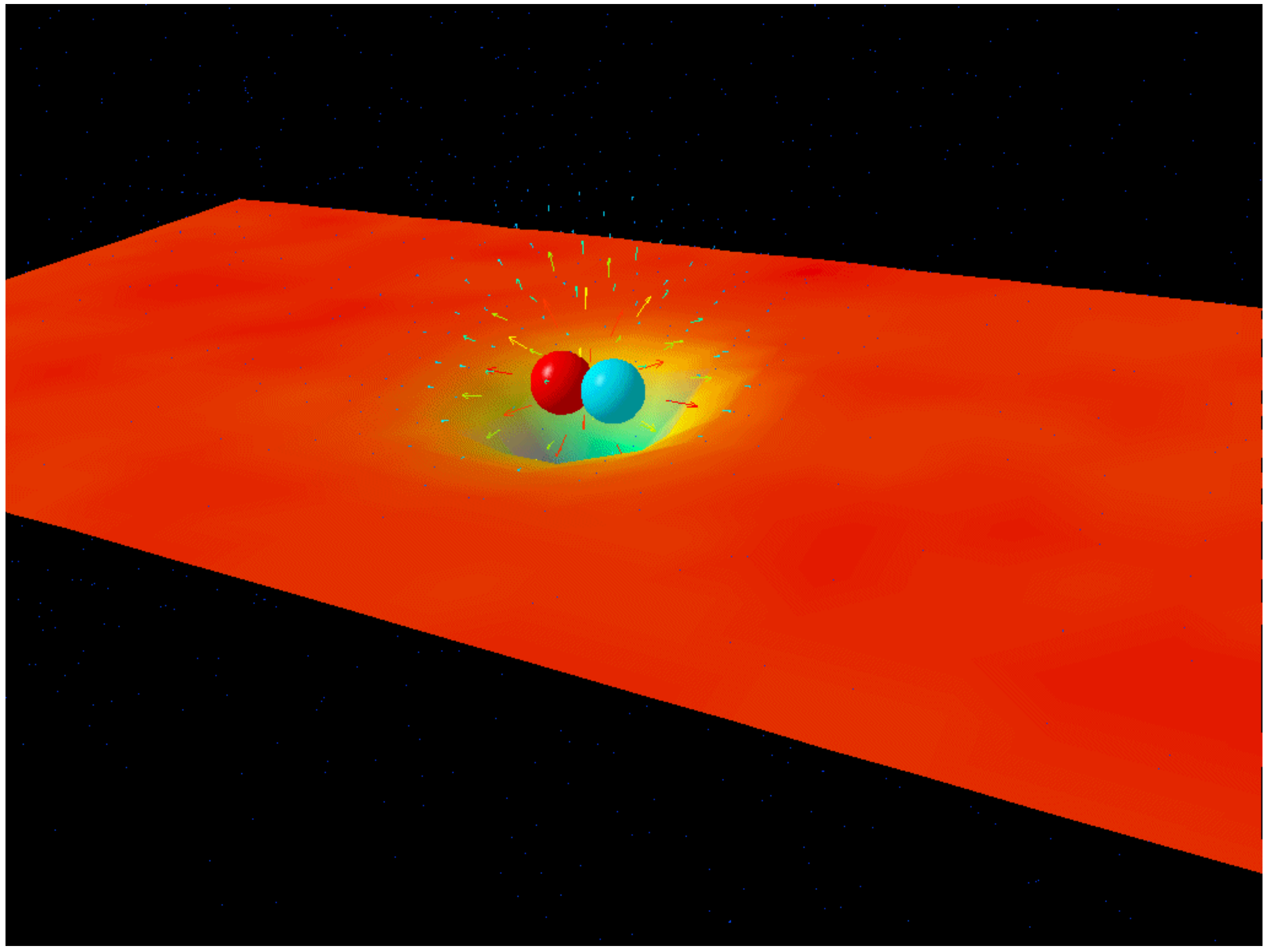
Planck's constant dictates fluctuations away from classical field configuration(s).

Integrate over all possible values of every field at each point in spacetime
Observables dictated by expectation values over these fluctuations

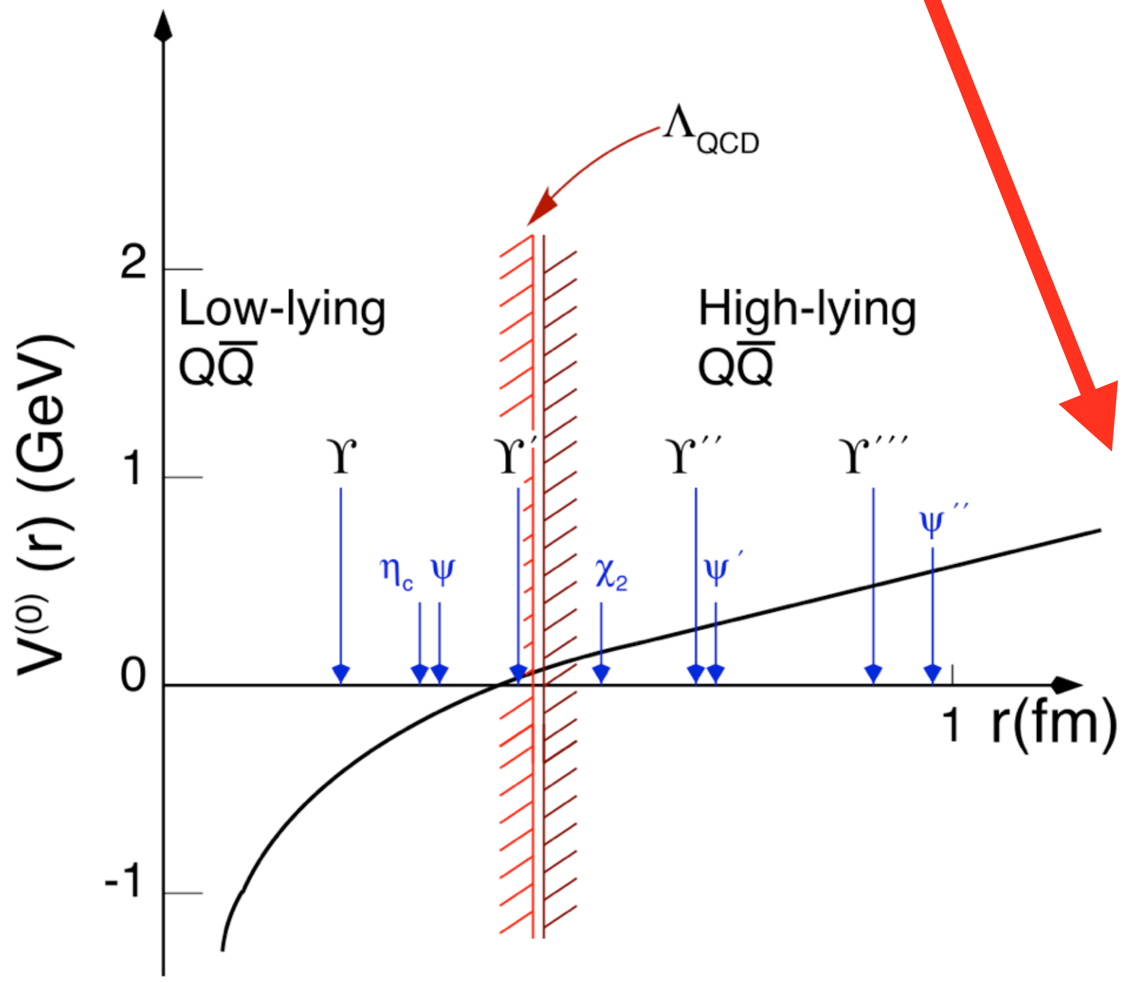
QCD Lagrange Density

Quarks and Gluons are confined

F ~ 2 x 10^5 N



Gluon Energy Density (Derek Leinweber)



Flux-Tubes between color charges

QCD Lagrange Density

Quantum Effects - Renormalization group

RG is used to sum the contributions from quantum fluctuations with wavelengths smaller than the scale of physics of interest

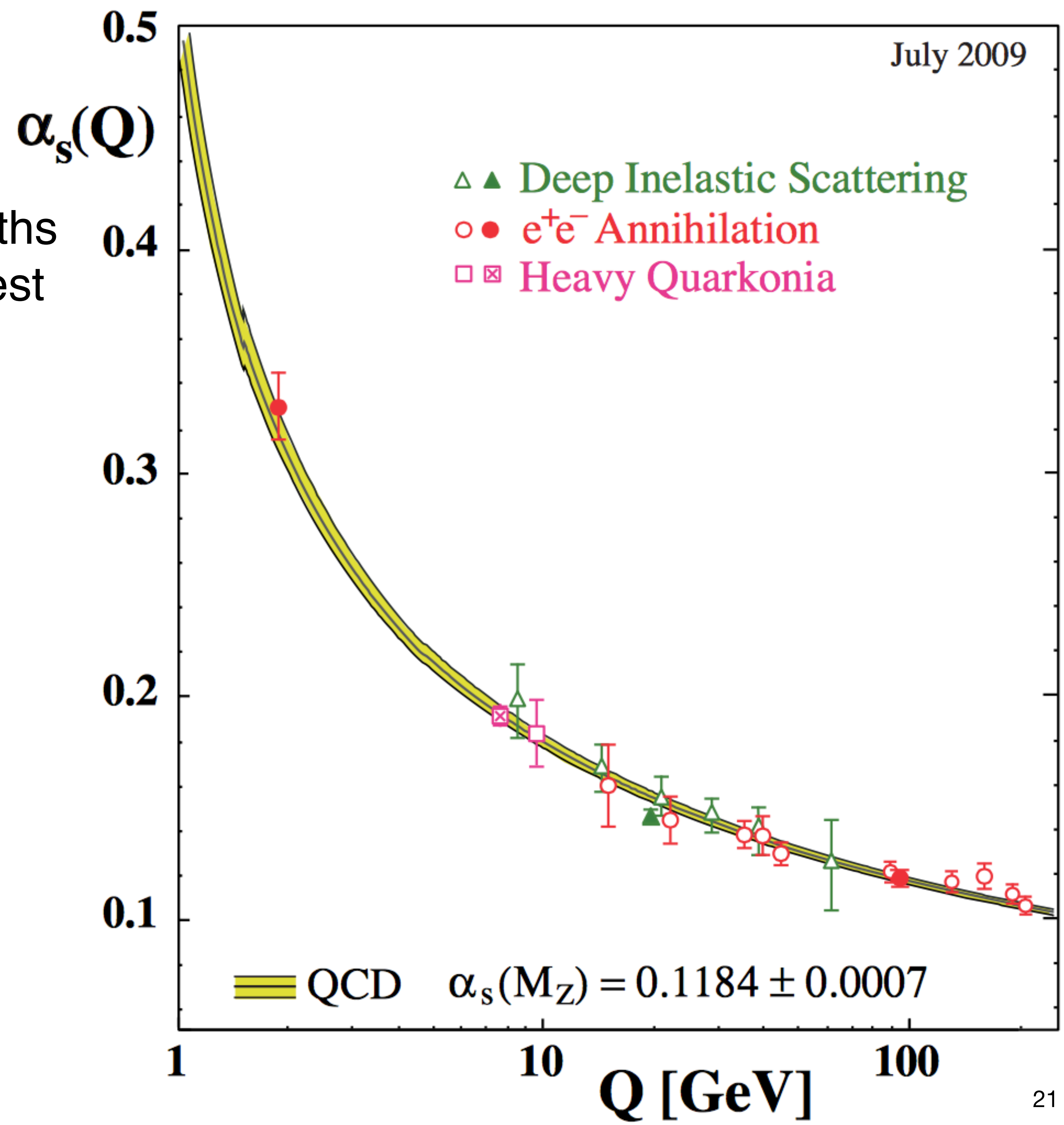
As there is no intrinsic length scale,

~ Log(Q/μ), which can become large.

e.g., g(μ) , m(μ) to describe quantities involving momenta Q ~ μ

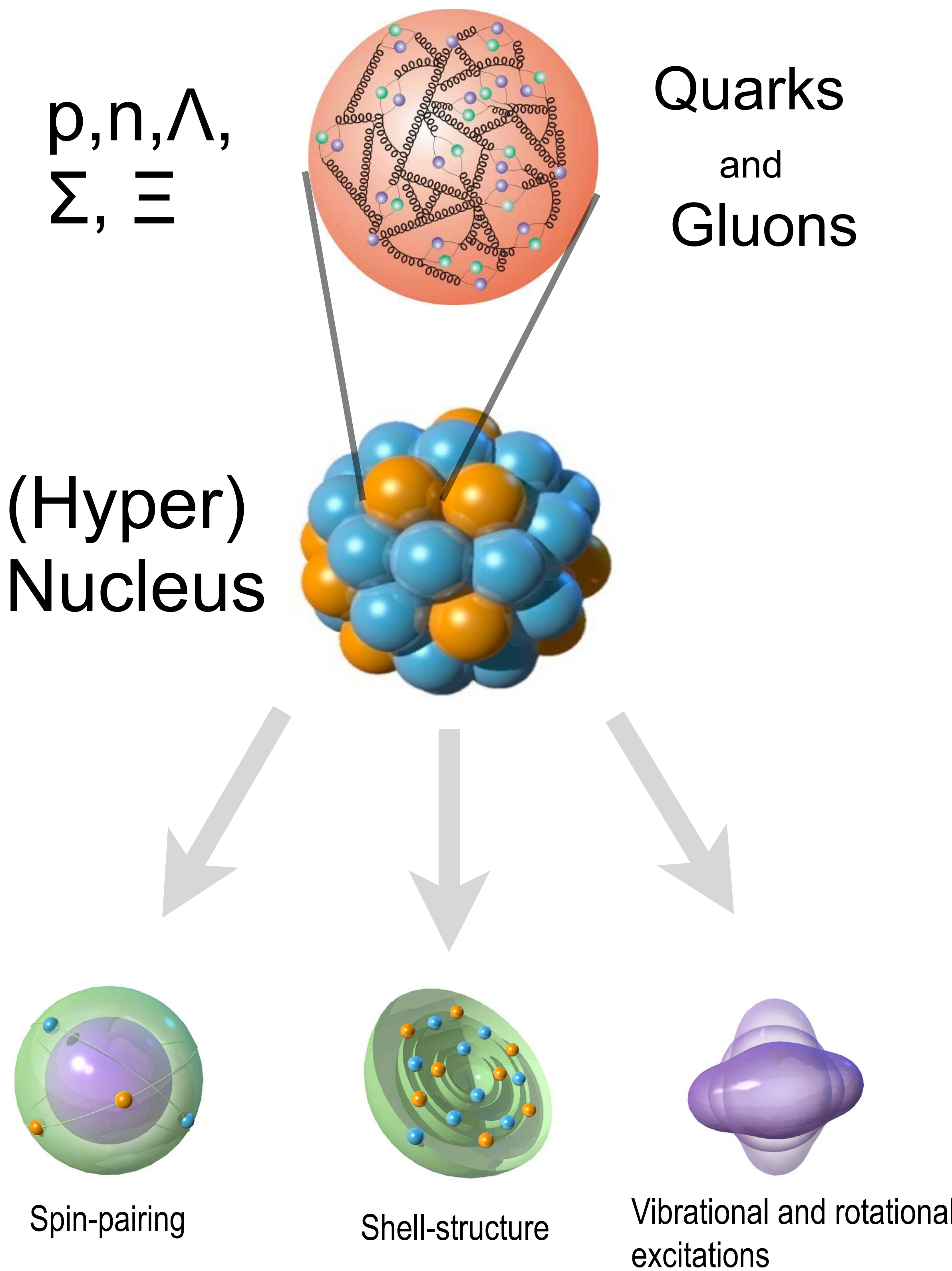
Observables are independent of YOUR choice of RG scale, μ

Dimensional transmutation relates dimensionless coupling constant to quantum-induced scale, Λ_{QCD}



QCD Lagrange Density

Low-energy QCD



$$\Lambda_{\mathrm{QCD}}$$

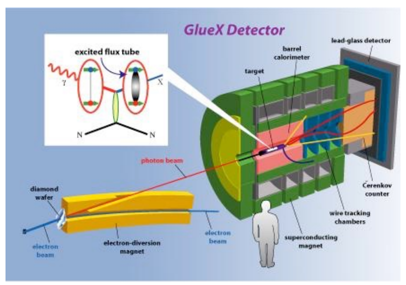
$$\frac{m_u}{\Lambda_{\mathrm{QCD}}} \quad \frac{m_d}{\Lambda_{\mathrm{QCD}}} \quad \frac{m_s}{\Lambda_{\mathrm{QCD}}}$$

$$\alpha_e$$

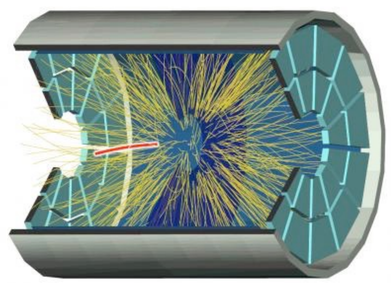
Small number of input parameters responsible for all of strongly interacting matter

Refine predictive capabilities for low-energy nuclear physics with complete uncertainty quantification

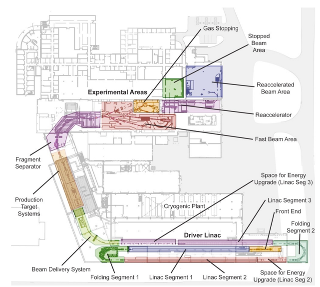
The Roadmap from QCD to Nuclear Physics



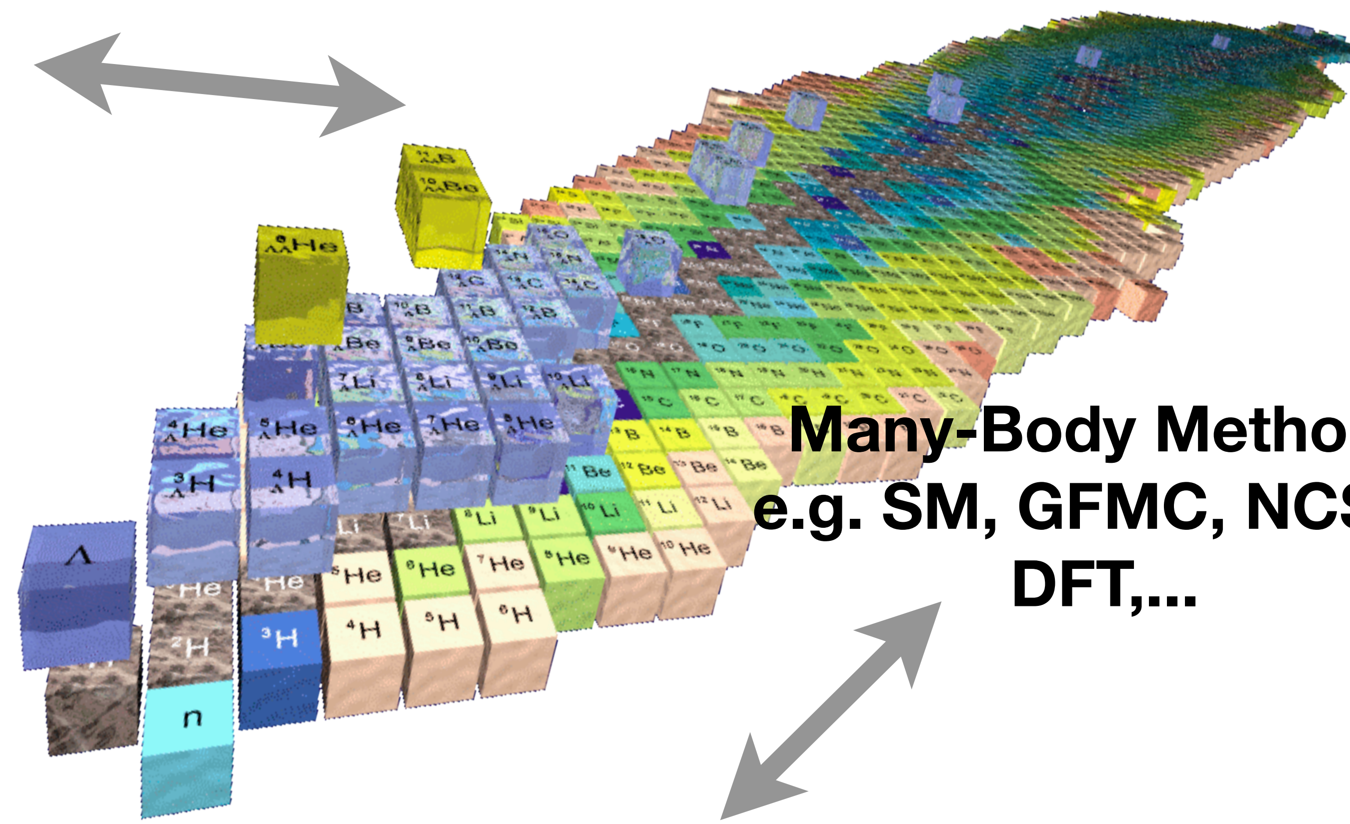
JLab



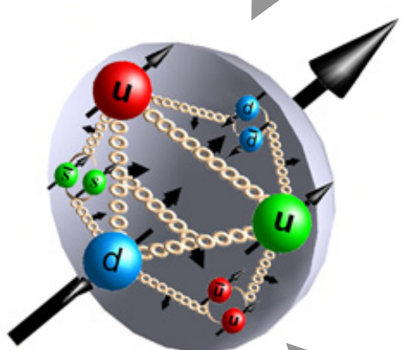
RHIC

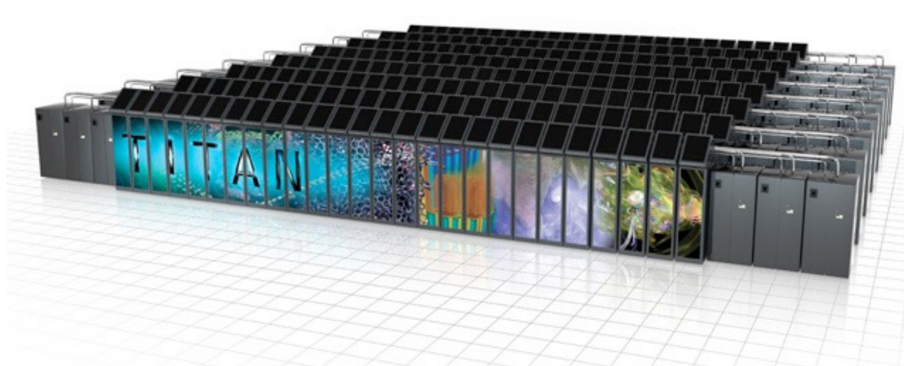


FRIB

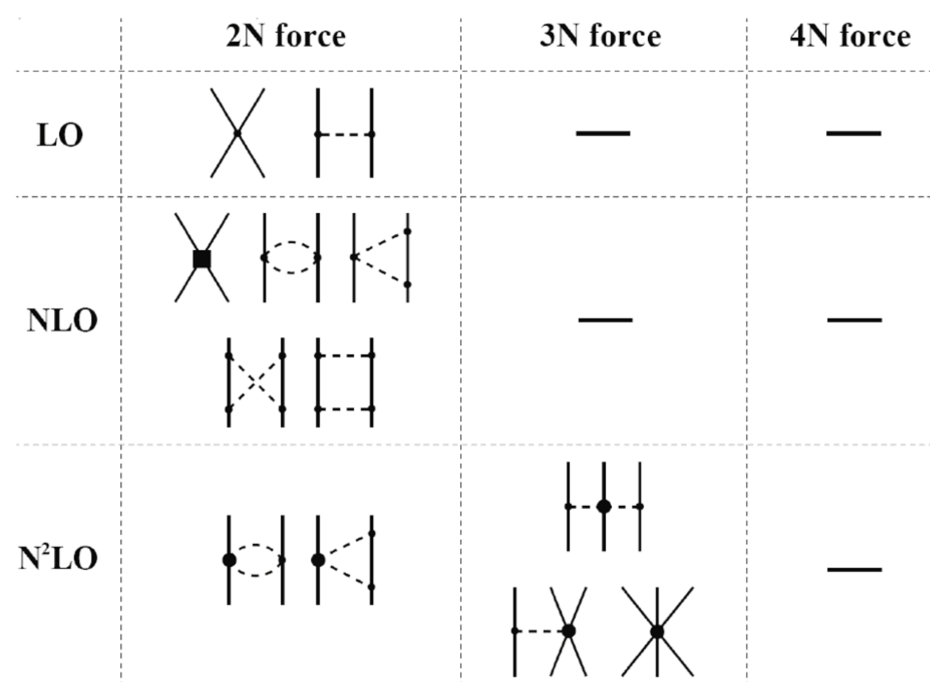


Many-Body Methods e.g. SM, GFMC, NCSM, DFT,...

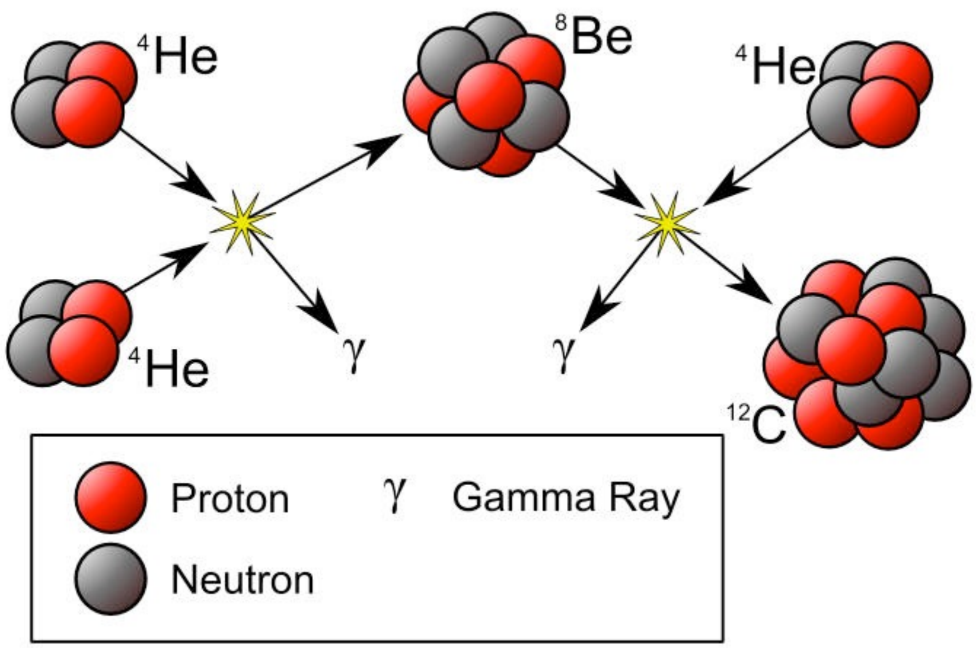


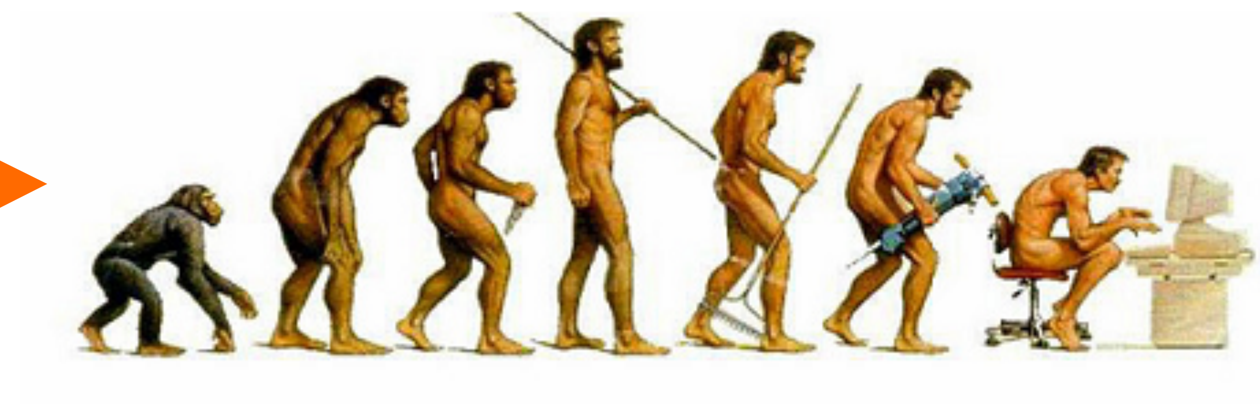


Solve QCD



Fine-Tunings Define Our Universe

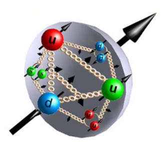


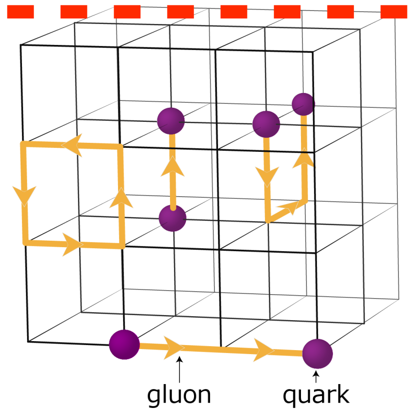


- Nuclear physics exhibits fine-tunings
  - *Why ??*
  - *Range of parameters to produce sufficient carbon ?*
  - *Large cancellation in NN interactions - weakly bound deuteron*

Energy Scales

Dynamical Degrees of Freedom





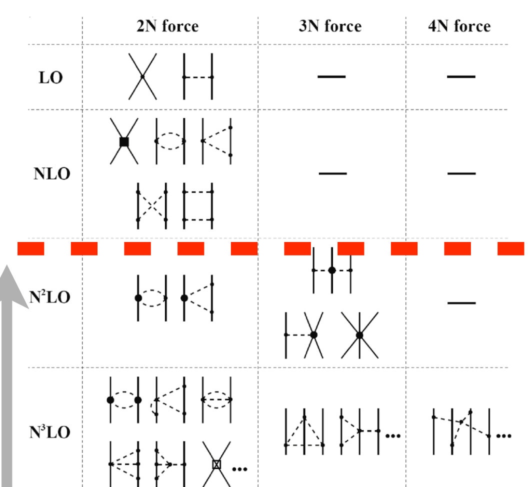
Lattice QCD

≳ 2 GeV

Nucleon

~ 1 GeV

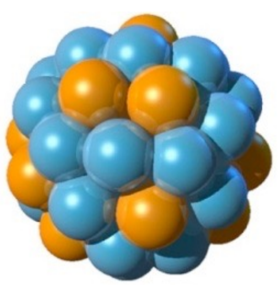
size set by pion



pionful EFT

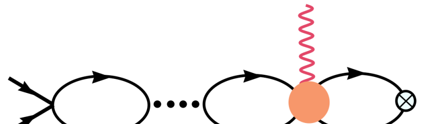
ρ mass/2

~ 390 MeV



Nucleus

~ 250 MeV

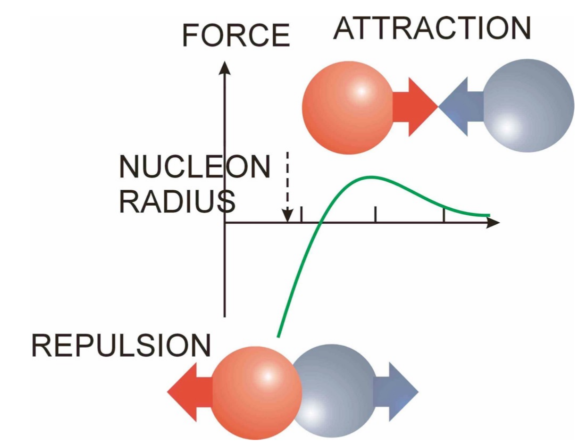


pionless EFT

~ 70 MeV

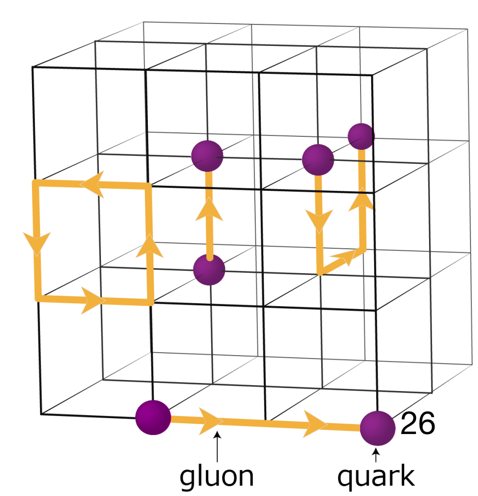
Why Lattice QCD

- Nuclear Models provide a QM ***interpolation*** of experimental data

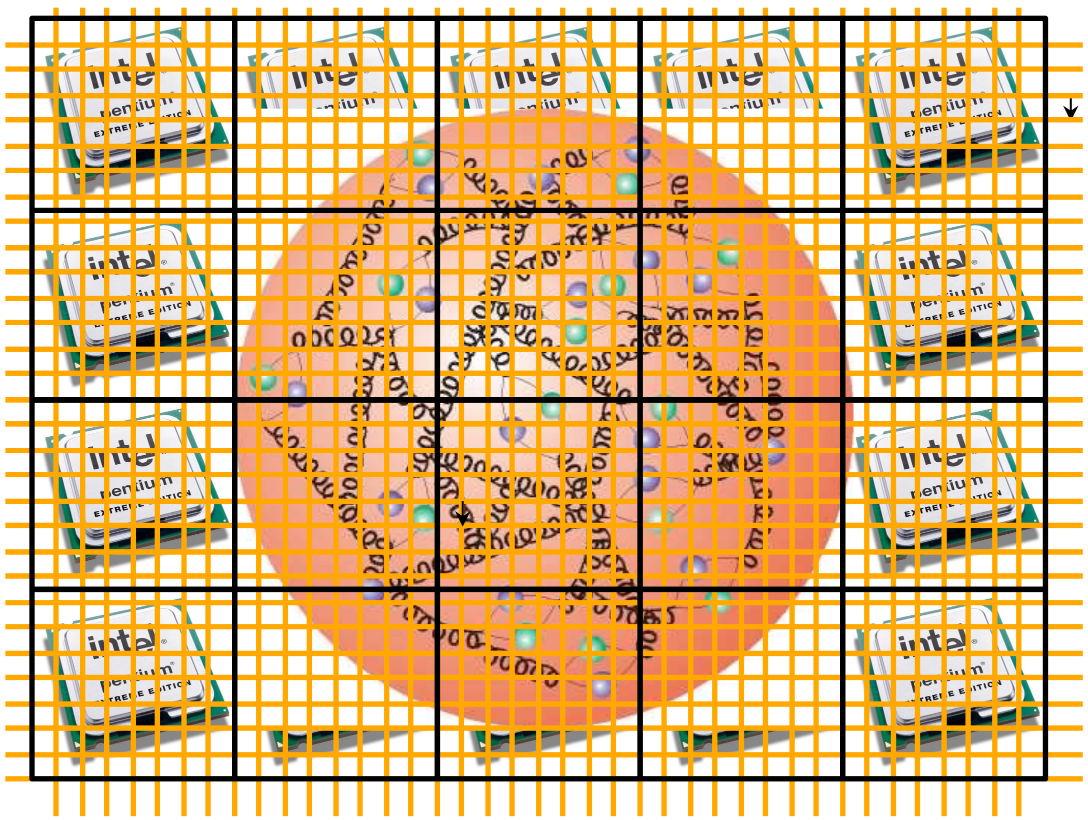


- EFTs for Nuclei
  - model dependence largely pushed to higher orders - truncation
  - proliferation of counterterms for higher precision - run out of constraints
  - momentum and quark-mass expansions below p~1 GeV (350 MeV)
    - pionful - chiral symmetries of QCD
    - required to rigorously describe nuclei at physical light-quark masses
  - momentum expansion below p~70 MeV
    - pionless - ERE (Bethe 1930's), EFT generalization in 1990's (SNO analysis, etc)
    - not rigorously applicable to nuclei, but numerically seems to not be too bad (why?)

- Lattice QCD
  - valid below p~π/a - corrections to QCD $\sim(a\ p)^n$ - no truncation
    - $a \sim 0.1$ fm $\sim (2\ \text{GeV})^{-1}$
    - systematically remove by extrapolating calcs with different a's



Lattice QCD:
A Discretized Euclidean Spacetime

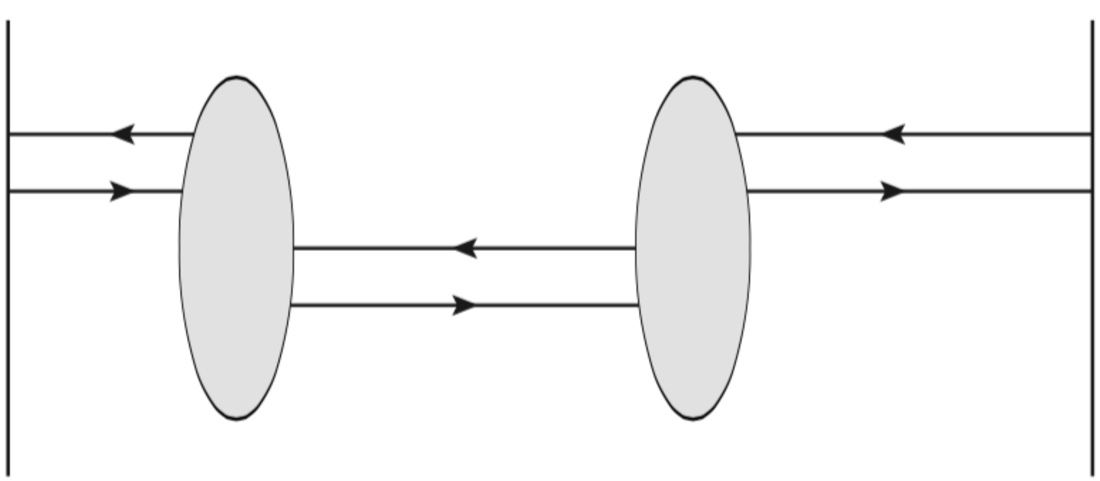


Lattice Spacing : $a << 1/\Lambda\chi$ (Nearly Continuum)

Lattice Volume : $m_\pi L >> 2\pi$ (Nearly Infinite Volume)

Extrapolation to $a = 0$ and $L = \infty$

Systematically remove non-QCD parts of calculation through the Symanzik action and p-regime effective field theories

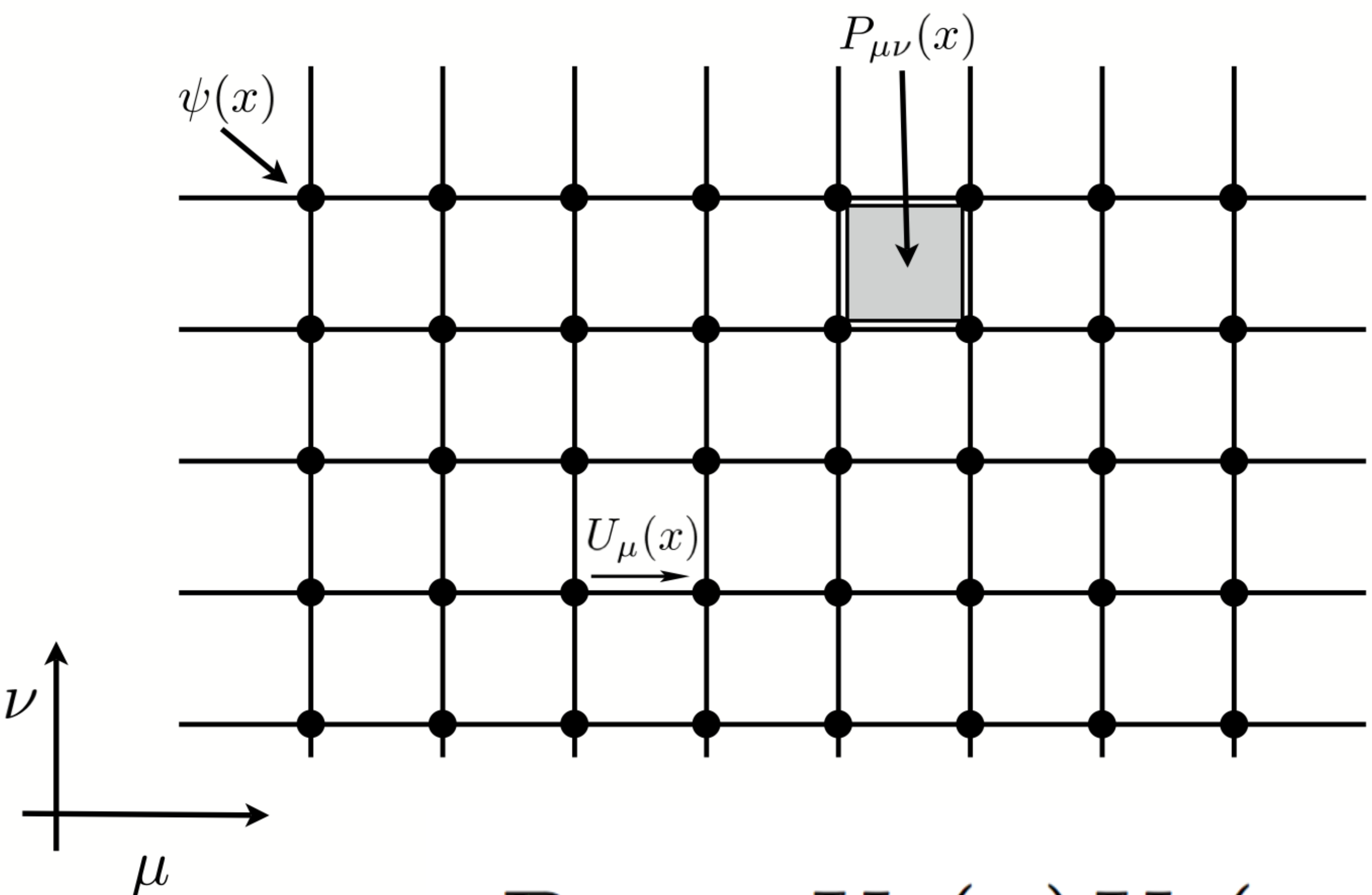


Thermal effects can be problematic, requires

$$m_\pi T \gg 10$$

Lattice QCD:

Simplest Discretization : Gauge Fields



$$U_\mu(x) = \exp\left(i \int_x^{x+\hat{\mu}} dx' A_\mu(x')\right)$$

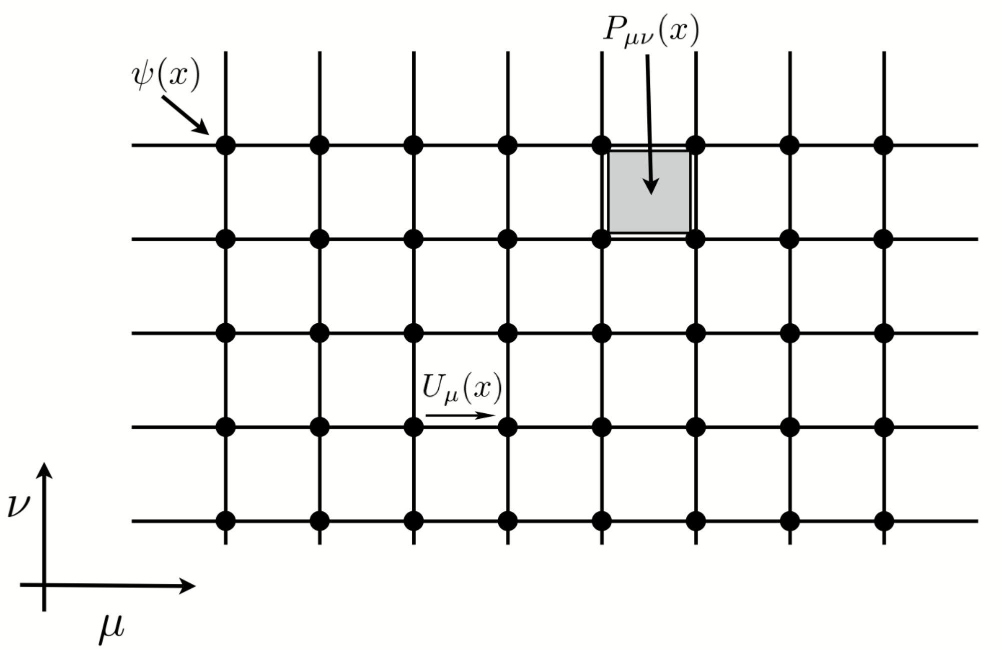
$$U_\mu(x) \;\rightarrow\; U'_\mu(x) \;=\; \Omega(x) U_\mu(x) \Omega^{-1}(x+\hat{\mu})$$

$$P_{\mu\nu} = U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x)$$

$$P_{\mu\nu} \;=\; 1 - i a^2 G_{\mu\nu} - \frac{a^4}{2} G_{\mu\nu} G_{\mu\nu} + \ldots$$

HMWK: find the a^6 contribution, and find a set of other loops to add to exactly cancel this term. This is called ``improvement''.

Lattice QCD:
Simplest Discretization : Gauge Fields



$$\sum_{x,\mu>\nu} \left[N_c - \mathrm{Tr}\left[P_{\mu\nu}\right]\right] = \int d^4x \, \frac{1}{8} G_{\mu\nu} G_{\mu\nu} + \ldots$$

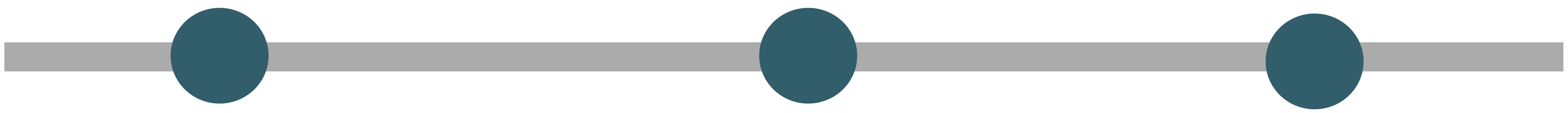
$$S = \frac{\beta}{N_c} \sum_{x,\mu>\nu} \left[N_c - \mathrm{Tr}\left[P_{\mu\nu}\right]\right] \qquad \beta = \frac{2N_c}{g^2}$$

N_c is the number of colors - shows how to generalize to possible BSM physics or to explore hadronic and nuclear physics on the large-N_c limit of QCD.

β=6.1 corresponds to a lattice spacing of a~0.11, and
β=6.3 corresponds to a lattice spacing of a~0.09 for N_c=3

Lattice QCD:

Simplest Discretization : Scalar Fields



$\phi(x-a) \sim e^{ikx} e^{-ika}$ $\qquad \phi(x) \sim e^{ikx}$ $\qquad \phi(x+a) \sim e^{ikx} e^{ika}$ $\qquad -\frac{\pi}{a} \leq k_\mu \leq \frac{\pi}{a}$

$$-\phi^*(x)\partial_\mu^2\phi(x) \;\rightarrow\; -\frac{1}{a^2}\phi^*(x)\left(\phi(x+a\hat{\mu}) + \phi(x-a\hat{\mu}) - 2\phi(x)\right)$$
$$= \frac{4}{a^2}\sin^2\left(\frac{ak_\mu}{2}\right)$$

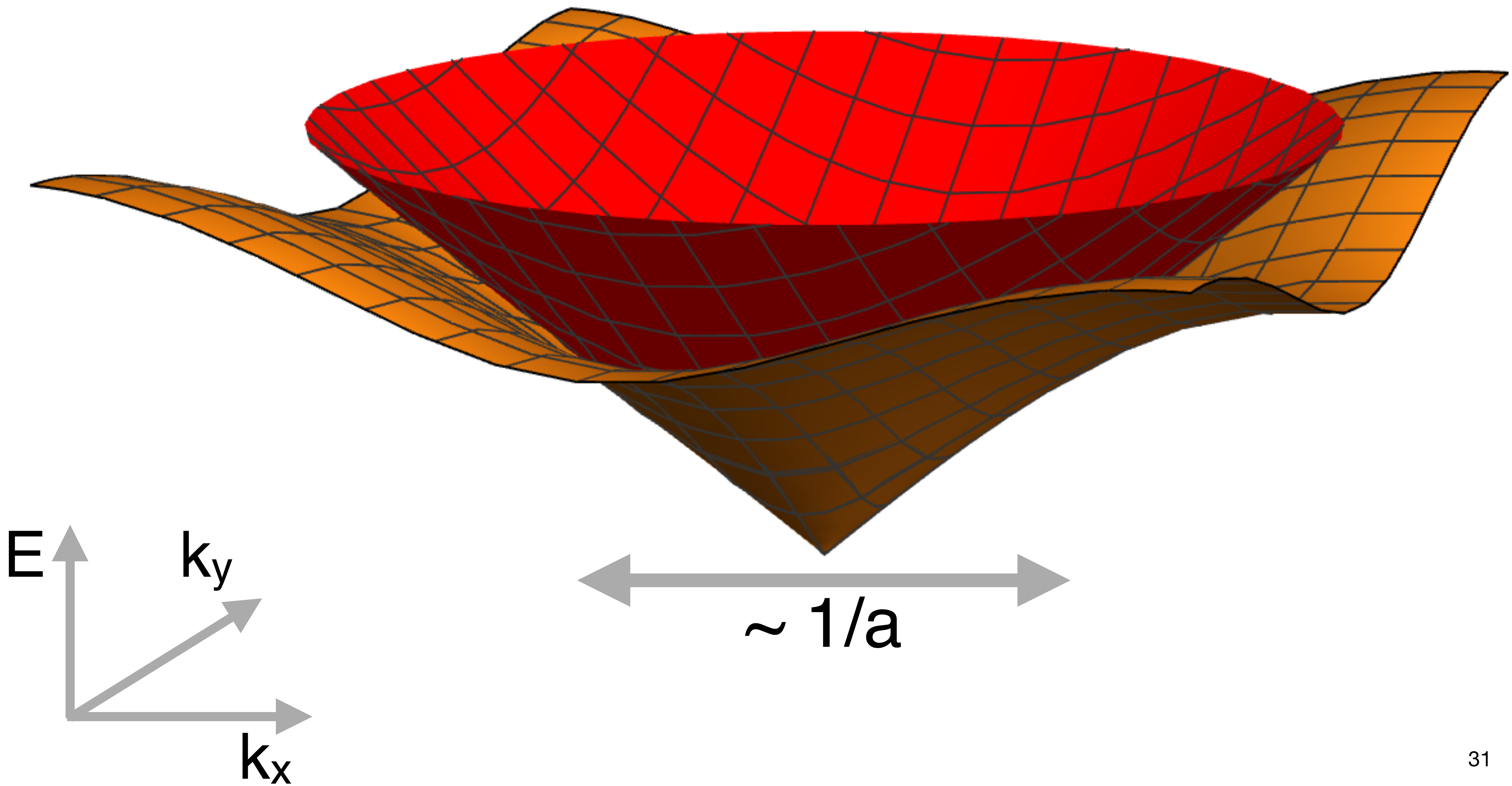
$$-\sum_\mu \phi^*(x)\partial_\mu^2\phi(x) \;=\; \frac{4}{a^2}\sum_\mu \sin^2\left(\frac{ak_\mu}{2}\right) \;\rightarrow\; k^2 \;-\; \frac{a^2}{6}\sum_\mu k_\mu^4 \;+\; \ldots$$

Lorentz violating

Lattice QCD:

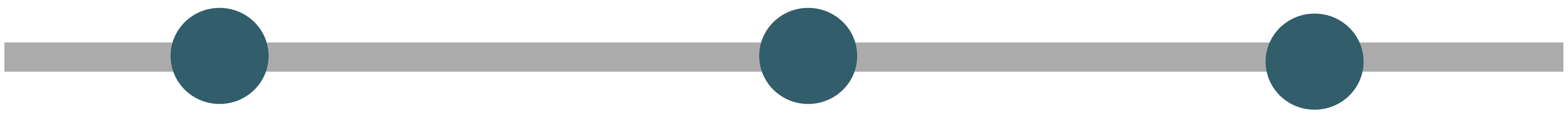
Simplest Discretization : Scalar Fields

Dispersion Relation



Lattice QCD:

Simplest Discretization : Fermions



$\phi(x-a) \sim e^{ikx}e^{-ika}$ $\quad\phi(x) \sim e^{ikx}$ $\quad\phi(x+a) \sim e^{ikx}e^{ika}$

$$-\frac{\pi}{a} \leq k_\mu \leq \frac{\pi}{a}$$

$$\overline{\psi}(x)\gamma_\mu\partial_\mu\psi(x) \;\rightarrow\; \frac{1}{2a}\overline{\psi}(x)\gamma_\mu\left(\psi(x-a\hat{\mu})-\psi(x+a\hat{\mu})\right)$$

$$\sim\; \frac{1}{a}\sin\left(k_\mu a\right)\gamma_\mu$$

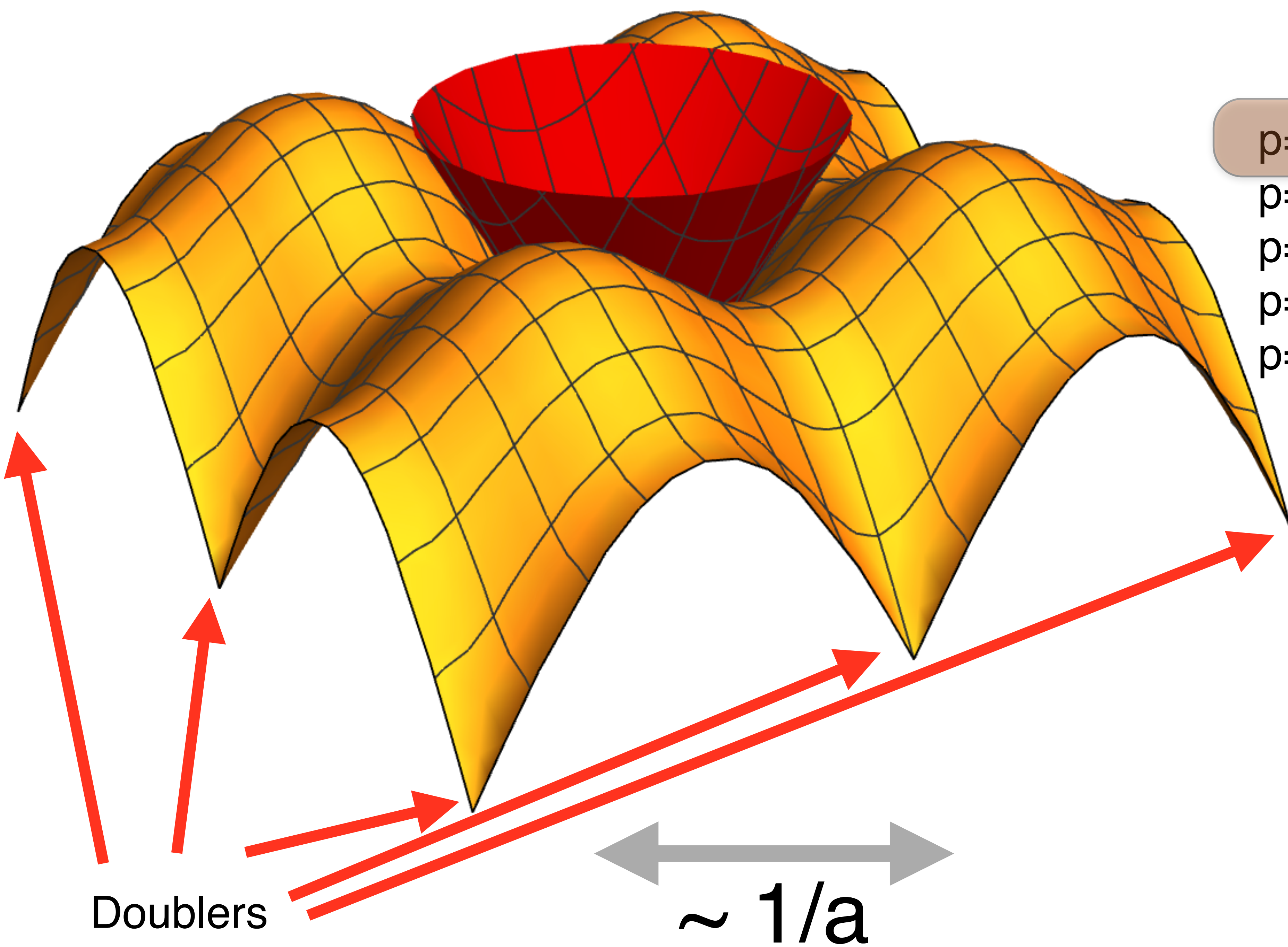
$$\frac{1}{a}\sum_\mu \gamma_\mu \sin\left(k_\mu a\right) \;\rightarrow\; \not{k} - \frac{a^2}{6}\sum_\mu \gamma_\mu k_\mu^3 \;+\; \ldots$$

Lorentz violating

Lattice QCD:

Simplest Discretization : Doublers

Tried to describe 1 massless particle, but actually got 16.
The 15 at the edges of the Brillouin zone are called doublers



p=(0,0,0,0)	: deg =1
p=(π/a,0,0,0)	: deg=4
p=(π/a,π/a,0,0)	: deg=6
p=(π/a,π/a,π/a,0)	: deg=4
p=(π/a,π/a,π/a,π/a)	: deg=1

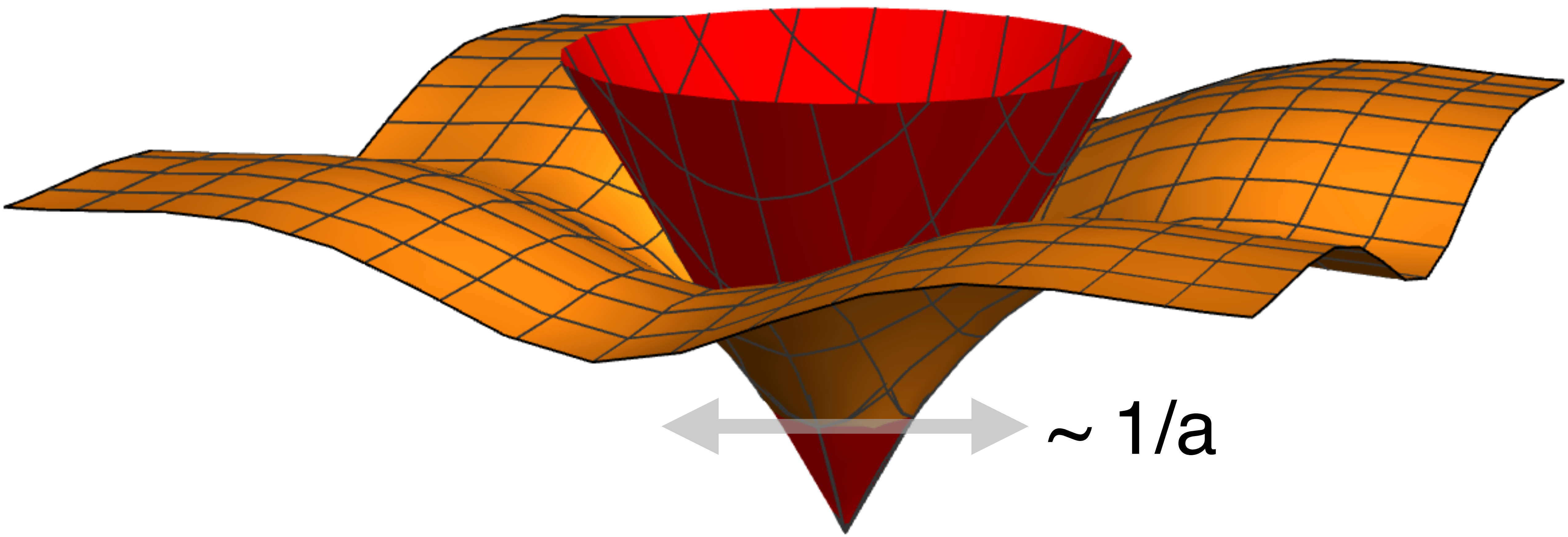
Lattice QCD:

Less Simple Discretization : Wilson Term

Simplest way to eliminate doublers is to include the Wilson Term:

$$\frac{r}{2a}\overline{\psi}(x)\left(\psi(x-a\hat{\mu})+\psi(x+a\hat{\mu})-2\psi(x)\right) \rightarrow \frac{2r}{a}\sin^2\left(\frac{ak_\mu}{2}\right)$$

$$\rightarrow ark_\mu^2 + \ ....$$

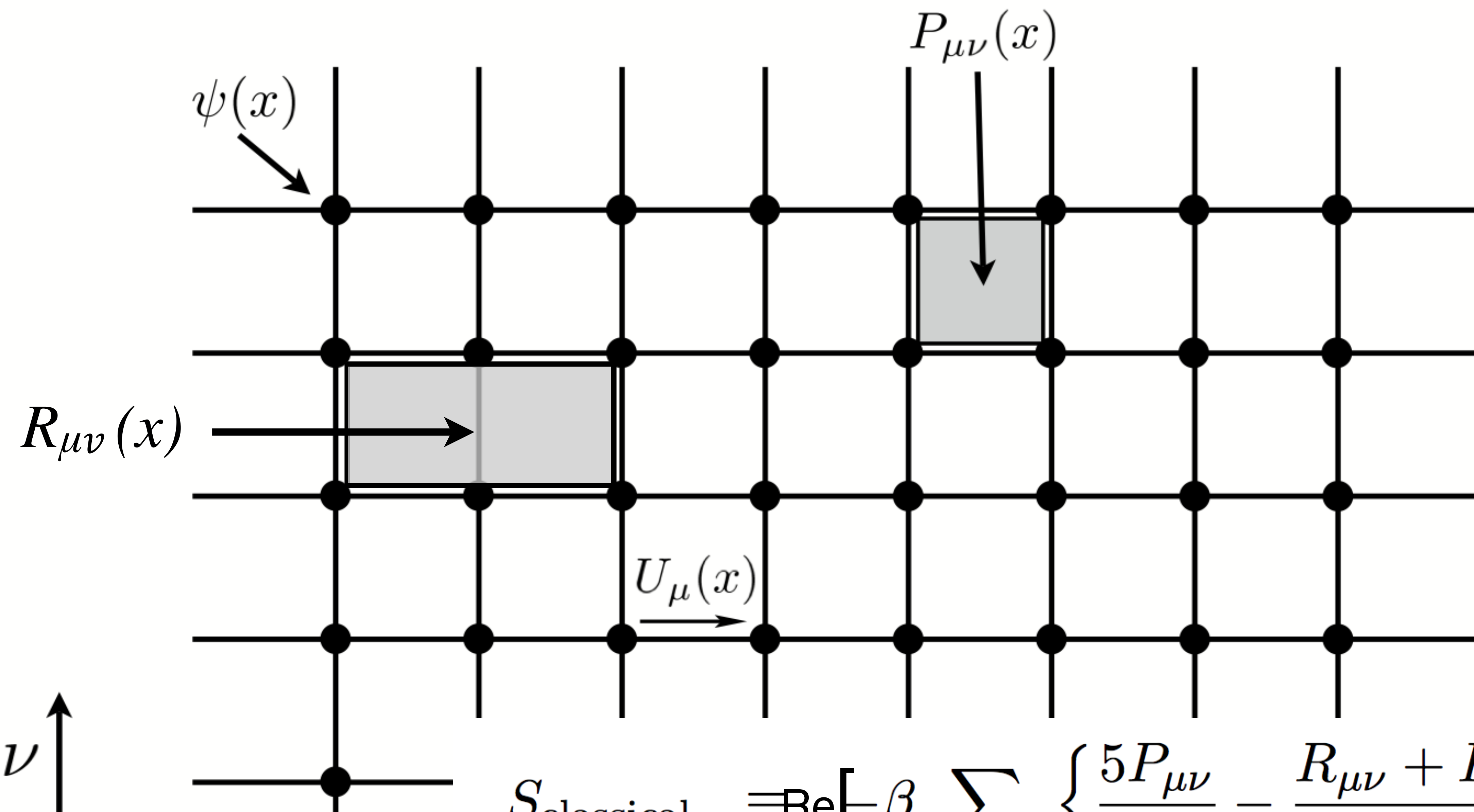


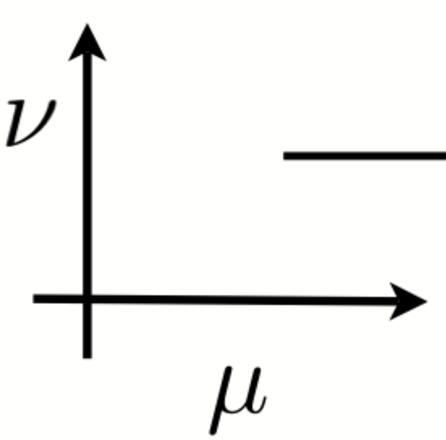
Breaks chiral symmetry - no gamma matrix

introduces a bare mass term for quarks, chiral symmetry breaking higher dim. operators

Lattice QCD:

Symanzik Action and Improved Discretizations



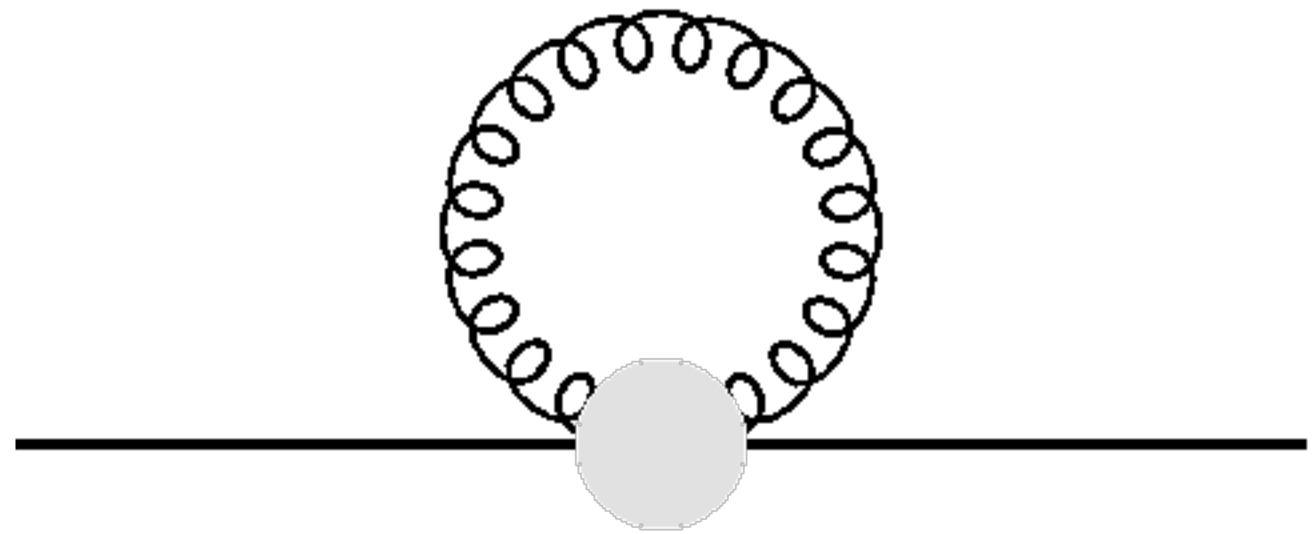


$$S_{\text{classical}} \equiv \text{Re}\Big[-\beta \sum_{x,\mu>\nu} \left\{ \frac{5P_{\mu\nu}}{3} - \frac{R_{\mu\nu}+R_{\nu\mu}}{12} \right\} + \text{const}\Big]$$

$$= \int d^4x \sum_{\mu,\nu} \tfrac{1}{2}\,\text{Tr}\, F_{\mu\nu}^2 + \mathcal{O}(a^4).$$

Lattice QCD:
Tadpoles and Improved Discretizations

$U_\mu(x)$ contains
(at quantum level)



$$\text{tadpole} \sim \int \frac{d^4 q}{(2\pi)^4} \frac{1}{q^2} = 0 \text{ (DR)} \sim \frac{\pi^2}{a^2} \text{ (Lattice)}$$

$$u_0 = \langle 0 | P_{\mu\nu} | 0 \rangle^{1/4}$$

Quantum gauge action
tadpole improved

$$S = \mathrm{Re}\left[-\beta \sum_{x,\mu>\nu} \left\{ \frac{5}{3} \frac{P_{\mu\nu}}{u_0^4} - \frac{R_{\mu\nu} + R_{\nu\mu}}{12\, u_0^6} \right\}\right]$$

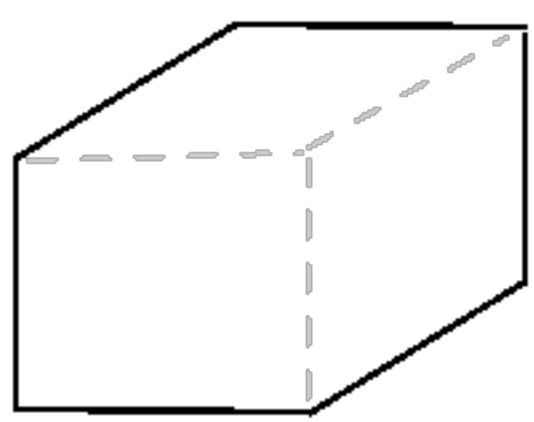
Lattice QCD:

Improved Discretizations : Improved Gauge Action

$$
\begin{aligned}
\delta\mathcal{L} &= \alpha_s\, r_1\, a^2 \sum_{\mu,\nu} \mathrm{Tr}(F_{\mu\nu} \mathrm{D}_\mu^2 F_{\mu\nu}) \\
&+ \alpha_s\, r_2\, a^2 \sum_{\mu,\nu} \mathrm{Tr}(\mathrm{D}_\mu F_{\nu\sigma} \mathrm{D}_\mu F_{\nu\sigma}) \\
&+ \alpha_s\, r_3\, a^2 \sum_{\mu,\nu} \mathrm{Tr}(\mathrm{D}_\mu F_{\mu\sigma} \mathrm{D}_\nu F_{\nu\sigma}) \\
&+ \cdots,
\end{aligned}
$$

From momentum scales above π/a

Can add these terms directly to LQCD action and tune coefficients
OR remove by adding more loops to discretization to improve action to order $\alpha^2 a^2$, a4



Lattice QCD:

Improved Discretizations : e.g. the Clover Action

Broken chiral symmetry means that :

- the quark mass suffers arbitrary shift
- UV physics induces low-energy chiral symmetry breaking operators into action

Sheikholeslami-Wohlert term

$$\delta\mathcal{L} \;=\; a\ c_1\ \overline{\psi}\sigma_{\mu\nu}G^{\mu\nu}\psi$$

Add this to action and tune c_1 to eliminate order-a effects (remain in operator).
This is called the clover action

Lattice QCD:
Chiral Symmetry : Ginsparg-Wilson fermions

$$S_F = a^4 \sum_{x,y} \overline{\psi}(x) D(x-y) \psi(y)$$

1. Require a local action $\qquad |D(x)| \leq c e^{-\gamma x}$
2. Require the correct continuum limit $\qquad D(p) = \not{p} + \mathcal{O}(a^2 p^2)$
3. Require D to be invertible, i.e. no doublers
4. Require chiral symmetry $\qquad \gamma_5 D + D \gamma_5 = 0$

Nielson-Ninomiya Theorem (1981) : Cannot satisfy all of these !!!!

Wilson term violates 4
Staggered fermions (Kogut-Susskind) violates 3

Lattice QCD:

Chiral Symmetry : Ginsparg-Wilson fermions (1982)

$$S_F \;=\; a^4 \sum_{x,y} \overline{\psi}(x) D(x-y) \psi(y)$$

4. Require chiral symmetry

$$\gamma_5 D + D\gamma_5 \;=\; 0 \quad \longrightarrow \quad \gamma_5 D + D\gamma_5 \;=\; a\ 2R\ D\gamma_5 D$$

vanishes for eigenstates

$$\gamma_5 D^{-1}(p) + D^{-1}(p)\gamma_5 \;=\; a\ 2R\ \gamma_5$$

$$\gamma_5 D^{-1}(x) + D^{-1}(x)\gamma_5 \;=\; a\ 2R\ \gamma_5\ \delta^{(n)}(x)$$

chiral symmetry preserved for any non-zero separation

$$\psi \;\rightarrow\; \psi \;+\; \epsilon\ \gamma_5\ (1 - aD)\psi$$

$$\overline{\psi} \;\rightarrow\; \overline{\psi} \;+\; \epsilon\ \overline{\psi}\ (1 - aD)\ \gamma_5$$

lattice chiral transformations

Domain-Wall fermions : Kaplan
Overlap fermions : Neuberger

Lattice QCD:
The Mechanics

Simply do the integration over quark fields analytically

$$\int \mathcal{D}\psi\, \mathcal{D}\overline{\psi}\; e^{-\int d^4x\; \overline{\psi} K \psi} = \det\left(K\right)$$

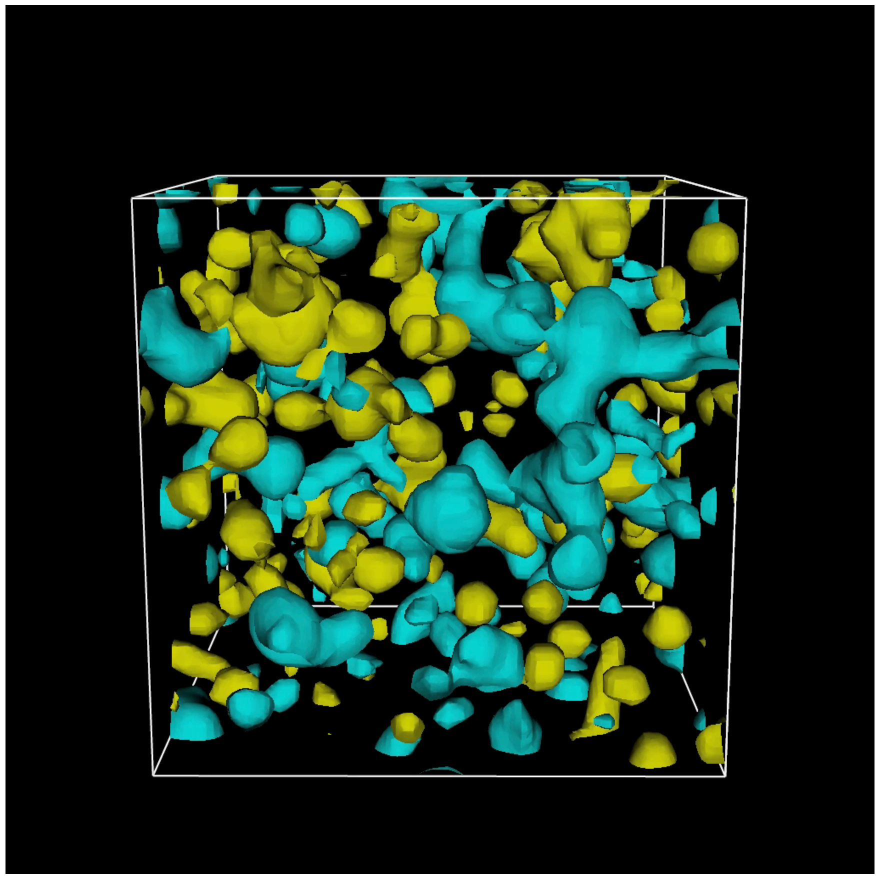
In perfect world - would just do the integrals, but instead we sample over snapshots of the gluon fields:

$$\langle \hat{\theta} \rangle \sim \int \mathcal{D}\mathcal{U}_\mu\; \hat{\theta}[\mathcal{U}_\mu]\; \det[\kappa[\mathcal{U}_\mu]]\; e^{-S_{YM}}$$

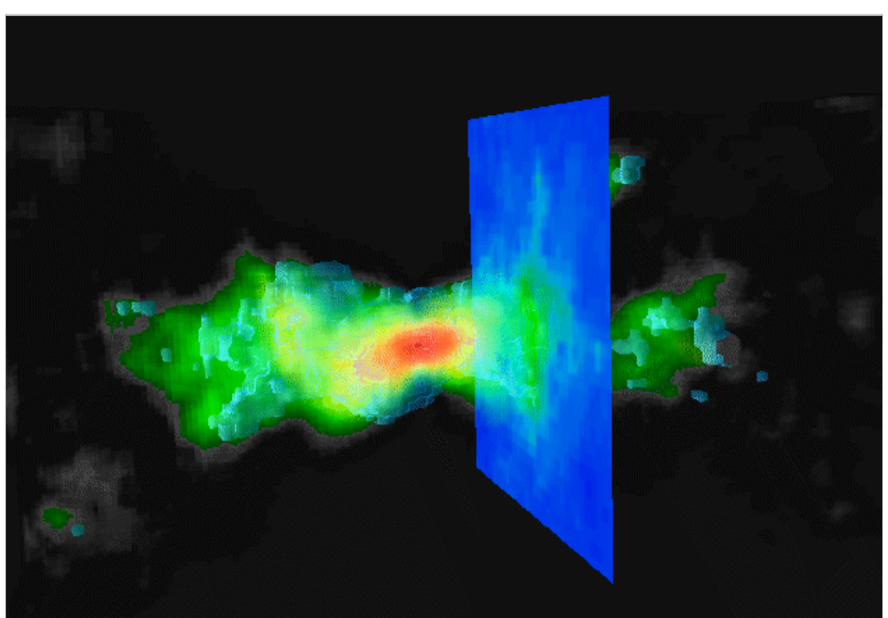
$$\rightarrow \frac{1}{N} \sum_{\text{gluon cfgs}}^{N} \hat{\theta}\left[\mathcal{U}_\mu\right]$$

Large computing resources are required to calculate a statistically decorrelated ensemble of gauge-field configurations - snapshots of the quantum vacuum. Capability compute platforms (Leadership-class) are required for this purpose

Lattice QCD:
Current sizes



Configuration : e.g.,
Vol = 32 x 32 x 32 x 256 lattice sites
Vol x 4 x 8 = 268 Million independent real numbers
to define $U_\mu(x)$ (generally double precision)



Propagator : e.g.,
32 x 32 x 32 x 256 lattice sites
~ 100 Million x 100 Million complex sparse matrix
(to invert and take determinant)

Lattice QCD:
Configurations : Metropolis and Sampling

Metropolis Algorithm:

Start with a set of links $\{U\}$

- Select U_i
- Pick U'_i
- Evaluate $S(U_i)$ and $S(U'_i)$
- Accept U'_i with probability $\min[\, 1\ ,\ \exp(-S(U'_i)\,)/\exp(-S(U_i)\,)\,]$
- (if action is smaller - always accept)
- Repeat over all links and many times

After a long period of time the $\{U\}$ with have a distribution $\exp(-S(U)\,)$

Downside - it is very slow as this has to be repeated on each link sequentially and there are a large number of links

Not practical for Lattice QCD

Lattice QCD:
Configurations : HMC and Sampling

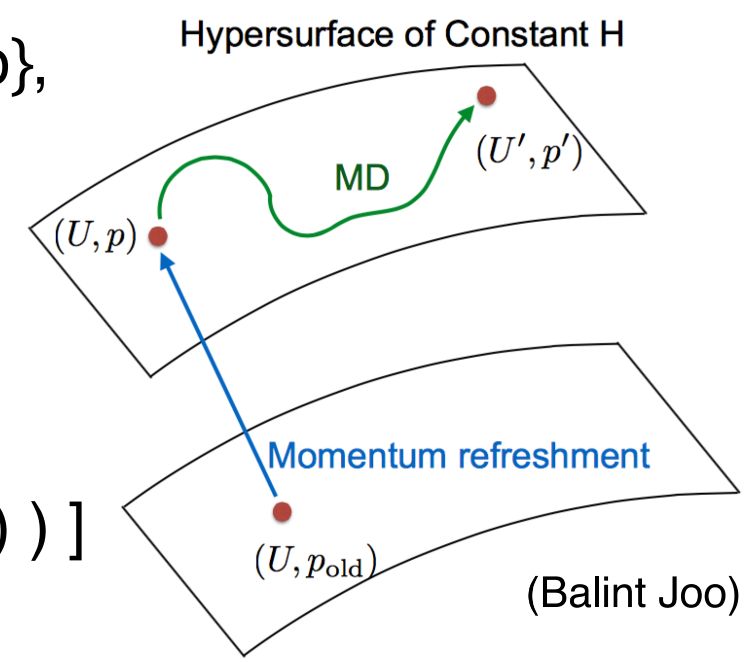
Figure from: "Improving dynamical lattice QCD simulations through integrator tuning, using Poisson Brackets and a force-gradient Integrator", M. A. Clark, B. Joo, A.D. Kennedy, P.J. Silva Phys Rev.D84,071502

HMC Algorithm:

Start with a set of links {U}

To generate one HMC trajectory:

- Assign to each link a Gaussian distributed canonical momentum {p}, hence the variable {U,p}
- Compute Hamiltonian of this system, $H= p^2/(2) + S(U)$
- Perform Molecular Dynamics evolution of the variables using Hamilton's equations to give {U',p'} (need reversible and area preserving integrators to evolve)
- Accept {U',p'} with probability min[1 , exp(-H(U',p'))/ exp(-H(U,p))] (if Hamiltonian is smaller - always accept)
- If rejected, new state is {U,p}



(Balint Joo)

Repeat to produce another trajectory

Advantage - all links updated at once through Hamiltonian evolution in fictitious time

Tuning of evolution is essential to optimize productivity

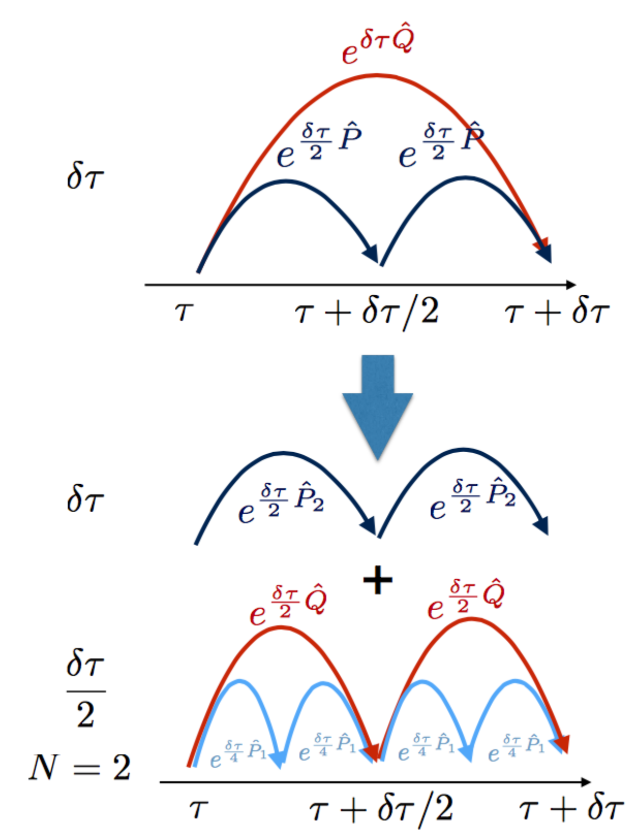
Lattice QCD:
Configurations : HMC and Quarks

$$\int \mathcal{D}\psi\, \mathcal{D}\overline{\psi}\; e^{-\int d^4x\ \overline{\psi} K \psi} \;=\; \det\left(K\right)$$

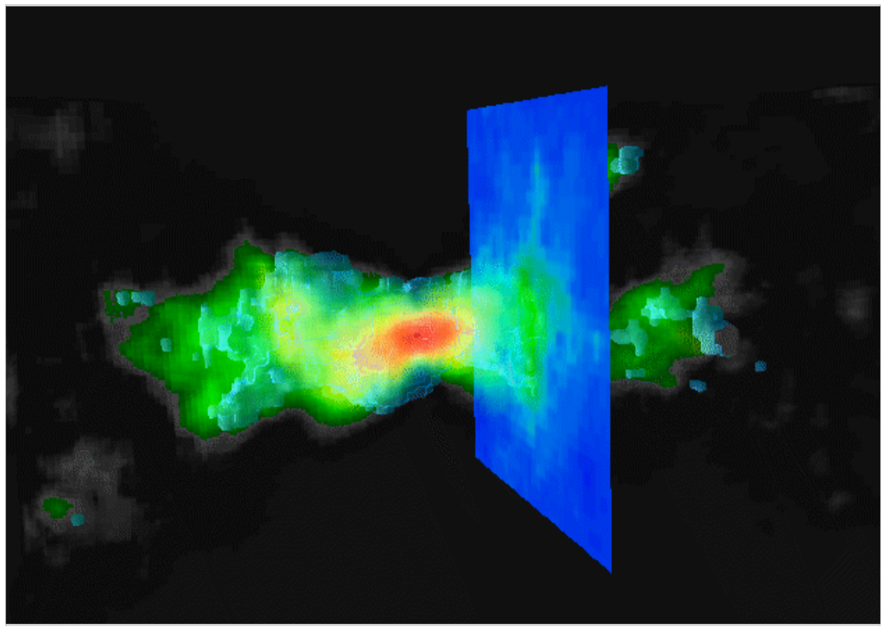
$$\int \mathcal{D}\phi\, \mathcal{D}\phi^\dagger\; e^{-\int d^4x\ \phi^\dagger K^{-1} \phi} \;=\; \det\left(K\right)$$

Pseudo-fermions typically are fixed along a given HMC trajectory, but re-sampled at the beginning of each.

Multiple MD time scales due to different forces (different sectors of the action)



Lattice QCD:
Solvers and Quark Propagators



$$[D(U)]_{X,Y}[S(U)]_{Y,X_0} = G_{X,X_0}$$

light-quark propagator   Source

Iterative using Krylov-subspace solvers
CG, BiCGstab

Condition number of D gets larger as quark mass is reduced toward physical
- critical slowing down in convergence

Preconditioning used to improve condition number

Lattice QCD:
Solvers and Deflation

COMPUTING AND DEFLATING EIGENVALUES WHILE SOLVING MULTIPLE RIGHT HAND SIDE LINEAR SYSTEMS WITH AN APPLICATION TO QUANTUM CHROMODYNAMICS

ANDREAS STATHOPOULOS AND KONSTANTINOS ORGINOS arXiv preprint arXiv:0707.0131, 2007
SIAM J. Sci. Comput. Vol. 32, No. 1, 439--462, 2010

$$A.x = b$$

- Iteratively solve for each source location to a given tolerance. e.g. CG, BiCGstab,
- Heavy on CPU, light on memory

$$U.A.U^{-1} = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_N \end{pmatrix}$$

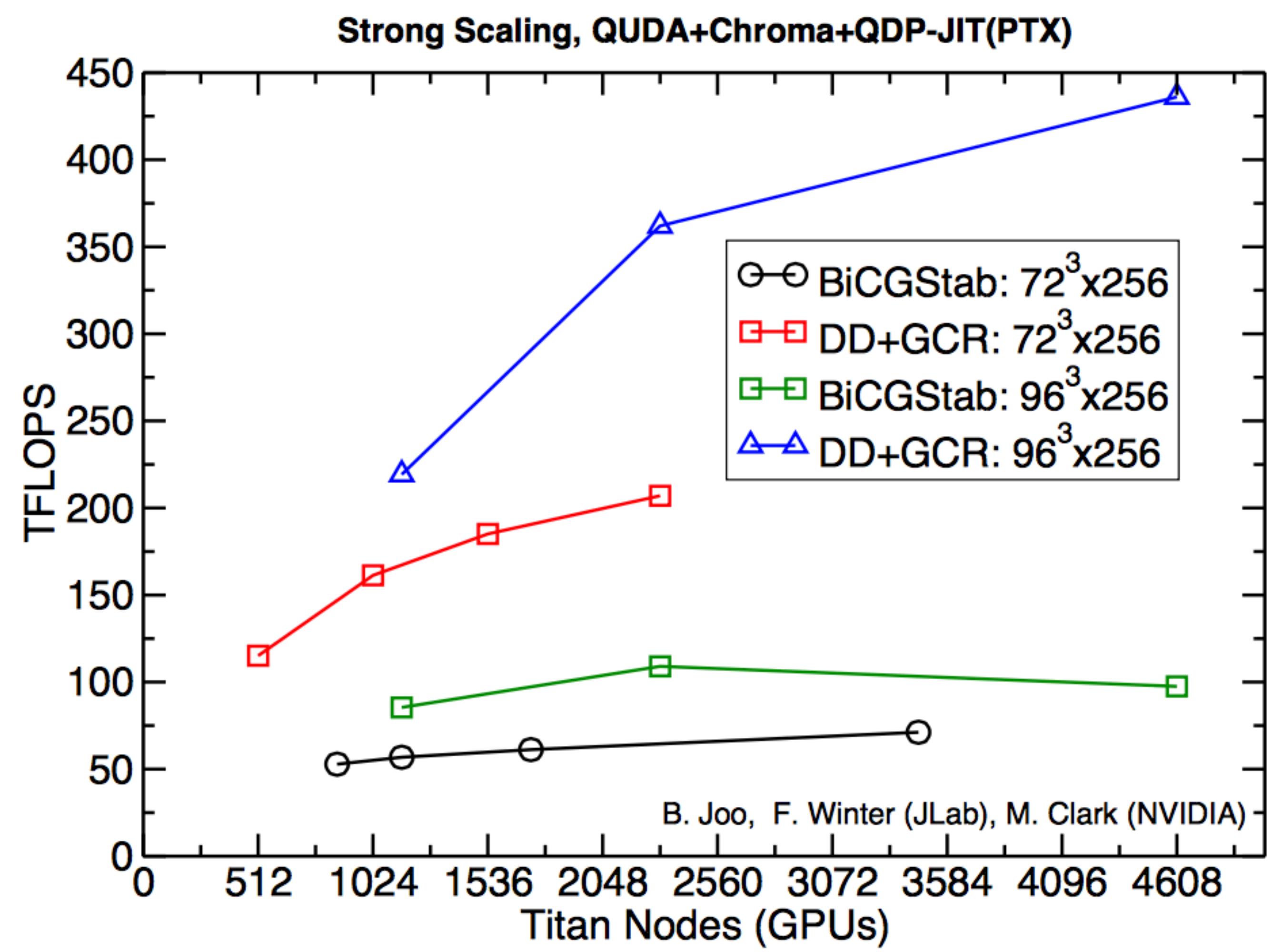
- Inversion solved exactly for all source locations
- Computationally prohibitive - cpu and memory

$$\tilde{U}.A.\tilde{U}^{-1} = \begin{pmatrix} \lambda_1 & & & \\ & \ddots & & \\ & & \lambda_p & \\ & & & \overline{A} \end{pmatrix}$$

- Determine the lowest p eigenvalues and eigenvectors - tune the number p
- Re-use for all sources.
- Memory heavy - depends on p.
- Iteratively solve in reduced space.
- Better condition number.
- Set-up ``costs'' recovered with large number of sources

Lattice QCD:
Solvers and Quark Propagators

- QUDA Solver performance on Titan
  - Cray XK7 system
  - 1 NVIDIA K20X GPU per node
  - Gemini Interconnect
- The DD+GCR solver does considerably better than the standard BiCGStab
- But even DD+GCR is affected by strong scaling effects



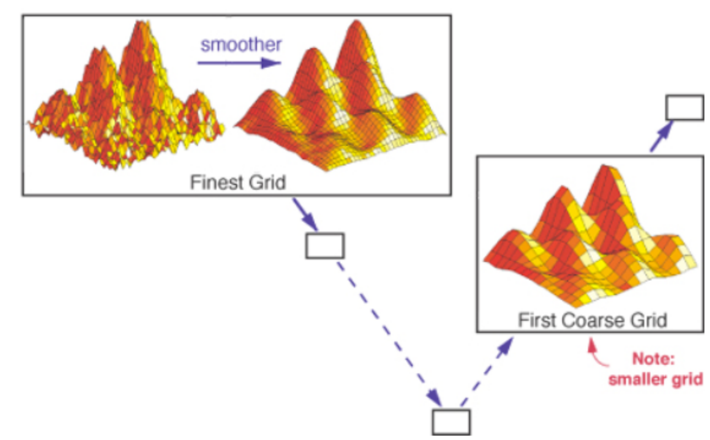
DD = Domain Decomposition Preconditioner
GCR = Generalized Conjugate Residual
multigrid not yet ported to GPUs

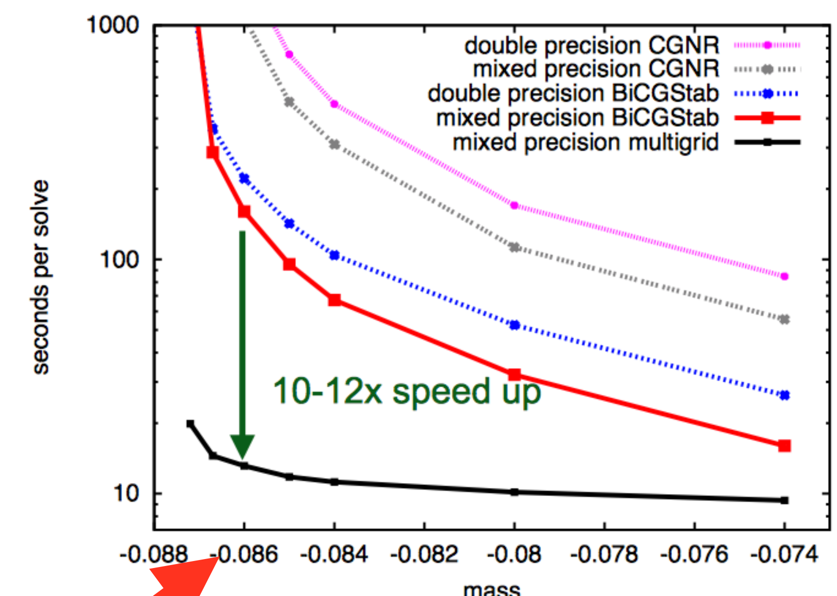
Balint Joo (2014)

Lattice QCD:
Algebraic Multigrid and Quark Propagators

- Critical Slowing down is caused by ‘near zero’ modes
- Multi-Grid method
  - separate (project) low lying and high lying modes
  - solve for high lying modes with “smoother”
  - solve for low modes on coarse grid with reduced dimensional operator
  - Gauge field is ‘stochastic’, so no geometric smoothness on low modes => algebraic multigrid
  - Setting up restriction/prolongation operators is costly
  - Easily amortized in Analysis with O(100,000) solves

Image From: http://computation.llnl.gov/casc/sc2001_fliers/SLS/SLS01.html
Credit: LLNL, CASC





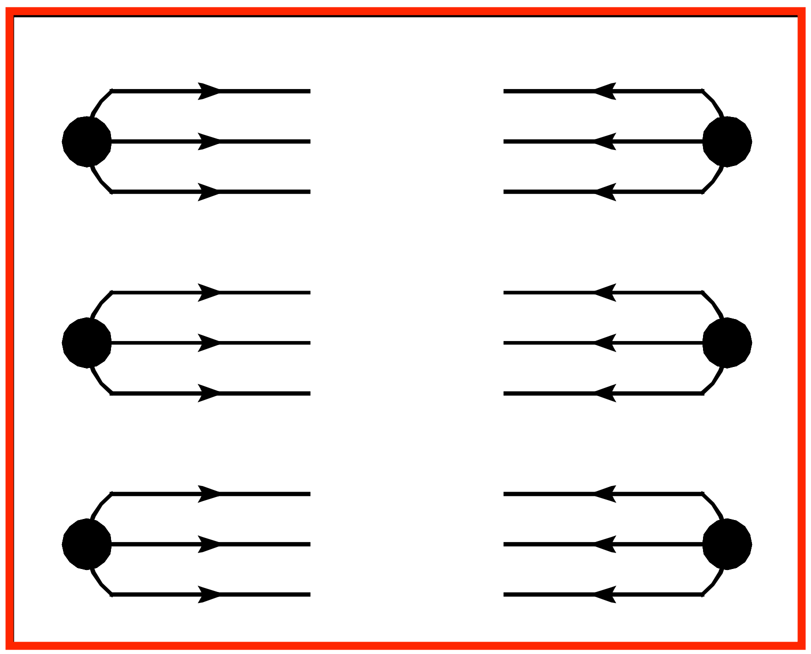
Multi-Grid. figure from J. C. Osborn et. al. PoS Lattice 2010:037,2010, R. Babich et. al. Phys. Rev. Lett, 105:201602,2010

physical point

Balint Joo (2014)

Lattice QCD:
Contractions of Quark Propagators

Large number of Wick contractions



Proton : $N^{\text{cont}} = 2$

^{235}U : $N^{\text{cont}} = 10^{1494}$

$$N_{\text{cont.}} = u!d!s! \quad (\text{Naive})$$
$$= (A+Z)!(2A-Z)!s!$$

Symmetries provide significant reduction

$$^{3}\text{He} \ : \ 2880 \rightarrow 93$$

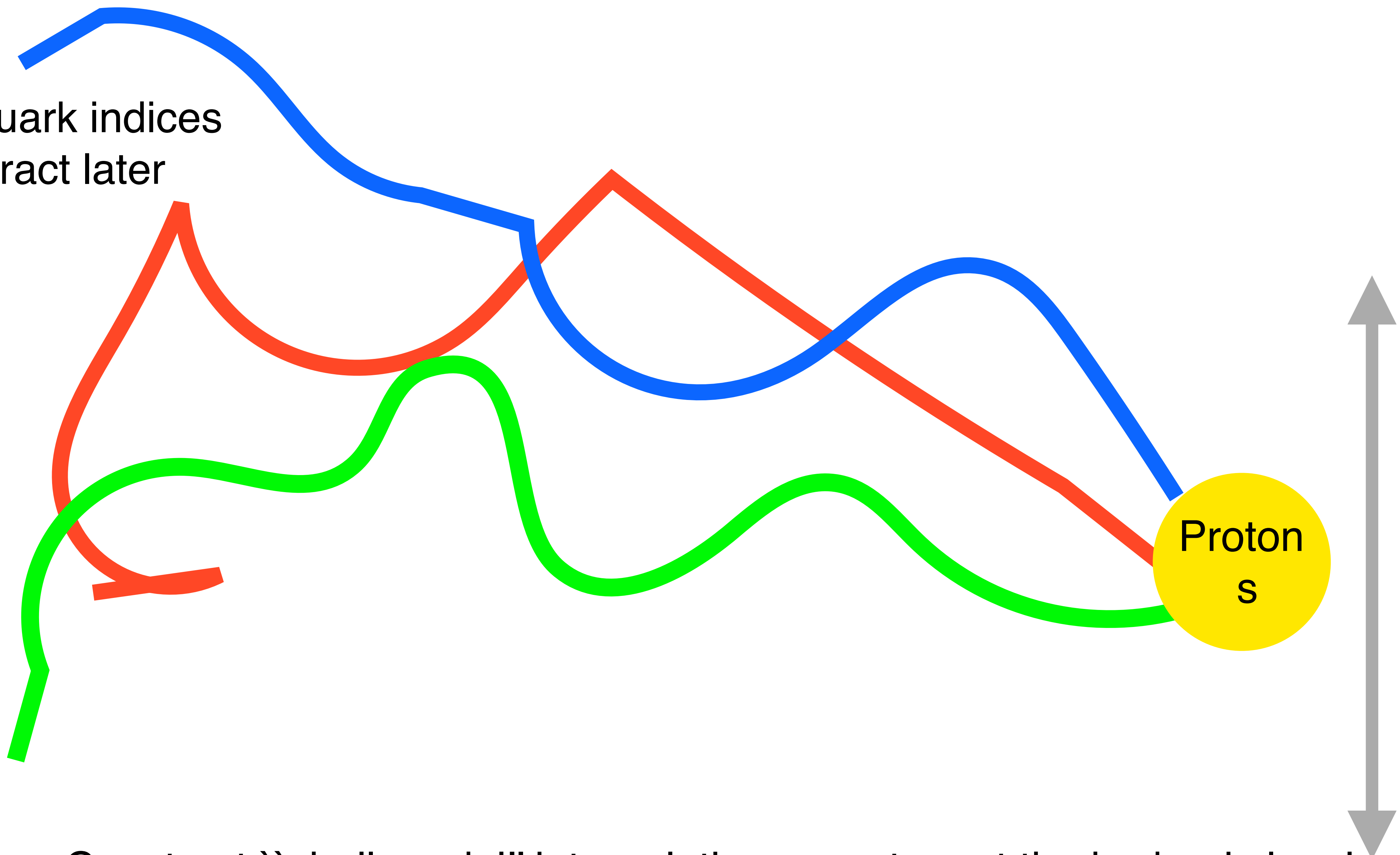
Recursion Relations are crucial

Lattice QCD:

Contractions : Hadronic Building Blocks

e.g.,

Free quark indices
to contract later



Fourier
Transform

Construct ``shell-model'' interpolating operators at the hadronic level
to overlap onto nuclei (?)

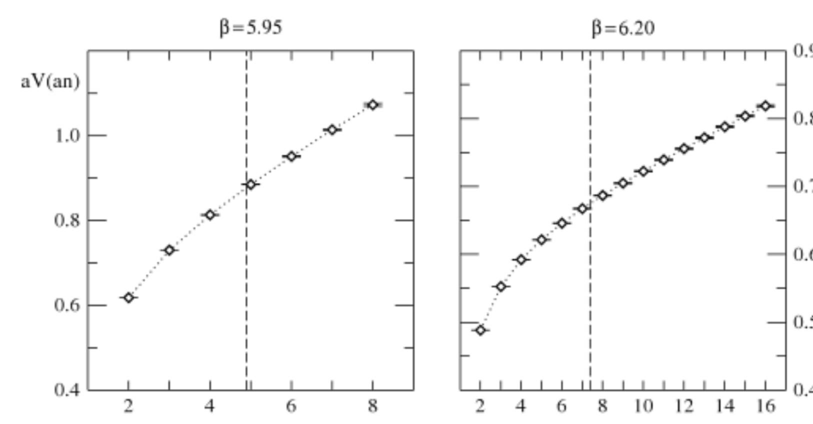
Lattice QCD:
Setting the Scale

Everything that is computed with lattice QCD is in terms of lattice units.
Without EM and isospin breaking, need to tune mu=md , ms , Λ_{QCD}

Of course, there is a need to convert to physical units to make predictions for quantities with dimensions, such as masses and radii.

1) M_Ω , m_π , m_K : M_Ω is quite insensitive to up,down masses

2) Force between static quarks



$$V(r) = A + \frac{B}{r} + \sigma r \qquad F(r) = -\frac{B}{r^2} + \sigma$$

$$r_0^2 \, F(r_0) = 1.65$$

$r_0 \sim 0.5$ fm from expt/phen charmonium, bottomonium

Lattice QCD:
Setting the Scale

$$\partial_t \phi = -\frac{\partial S}{\partial \phi}$$

3) Wilson Flow

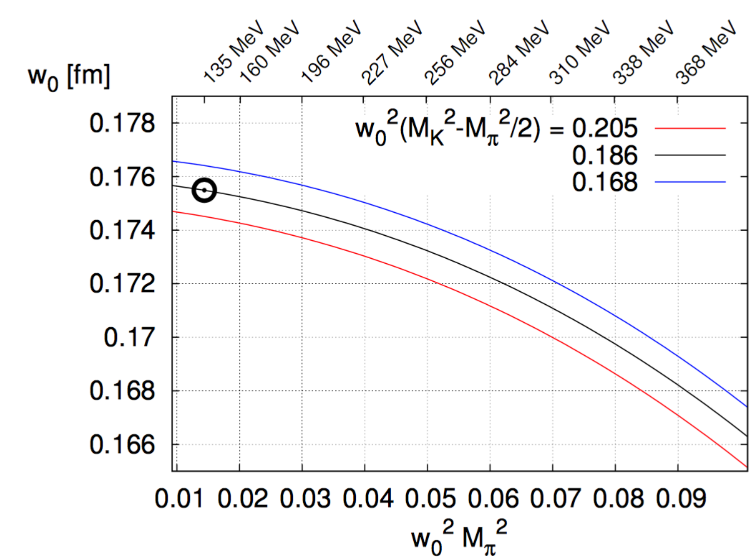
$$\dot{B}_\mu = D_\nu G_{\nu\mu}, \qquad B_\mu|_{t=0} = A_\mu,$$

$$G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu], \qquad D_\mu = \partial_\mu + [B_\mu, \cdot\,],$$

$$W(t) = t\frac{d}{dt}\left[\, t^2 \, \langle \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu} \rangle \right]$$

$$W(t)\big|_{t=w_0^2} = 0.3 \quad , \quad w_0 = 0.1755(18)(04) \text{ fm}$$

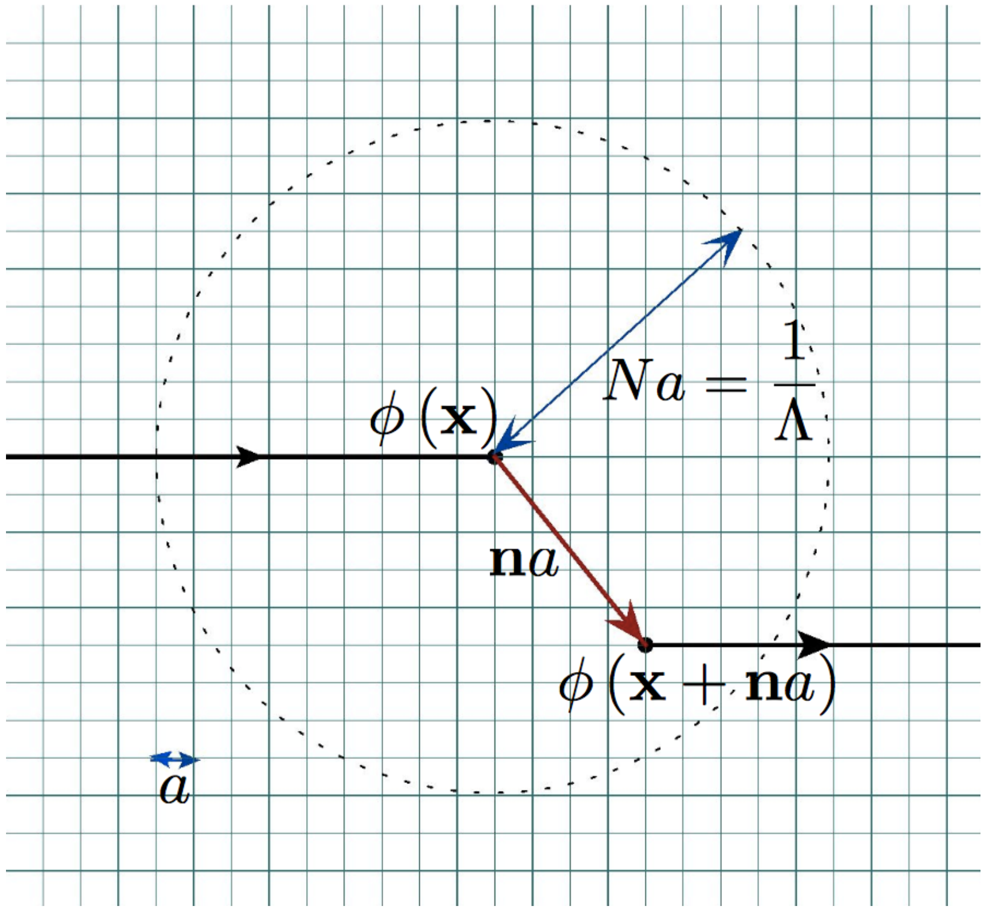
Gaussian smearing parameter - simple to calculate

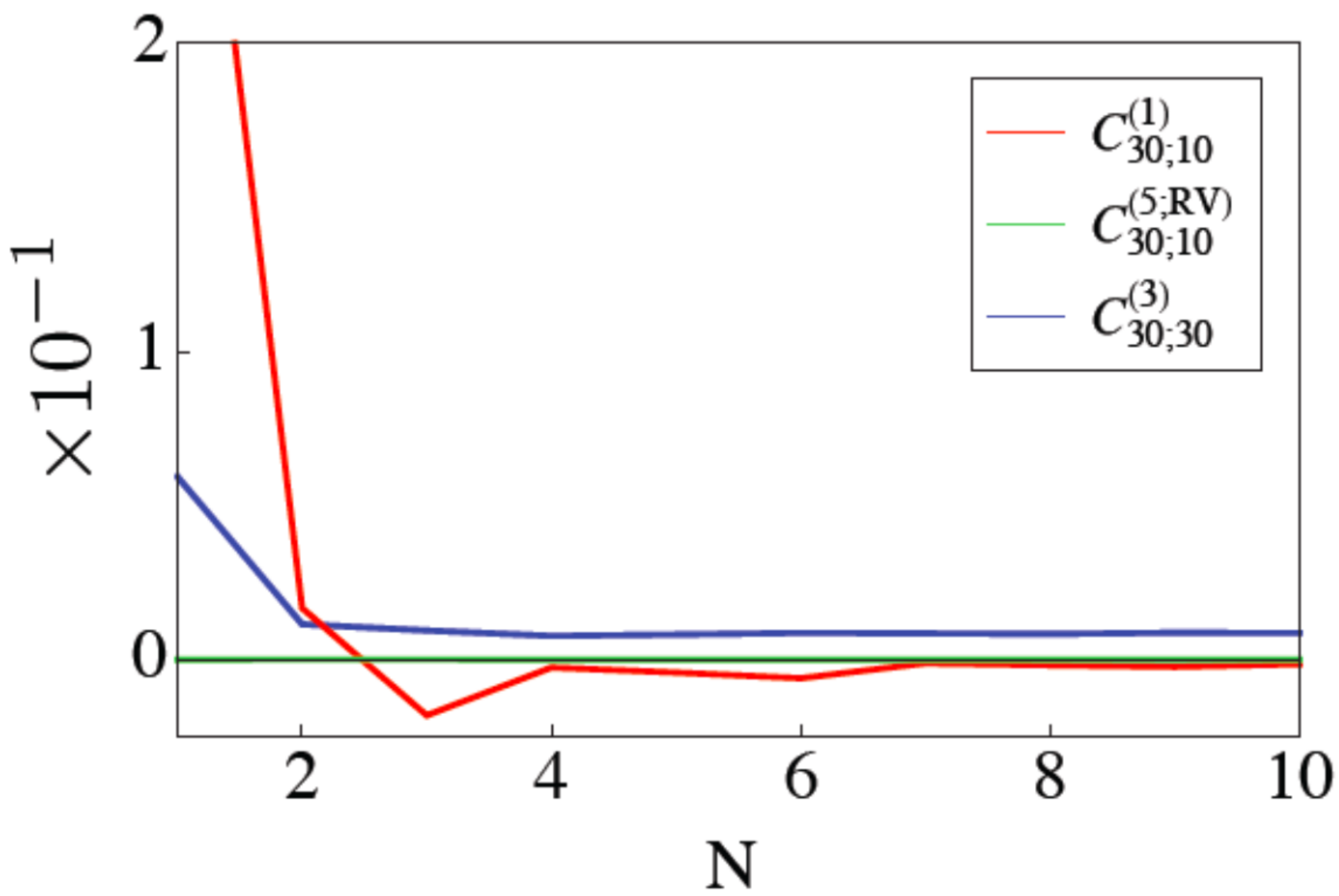


$$\mu^2 = \frac{1}{8\pi t}$$

MSbar renorm. scale related to smearing scale

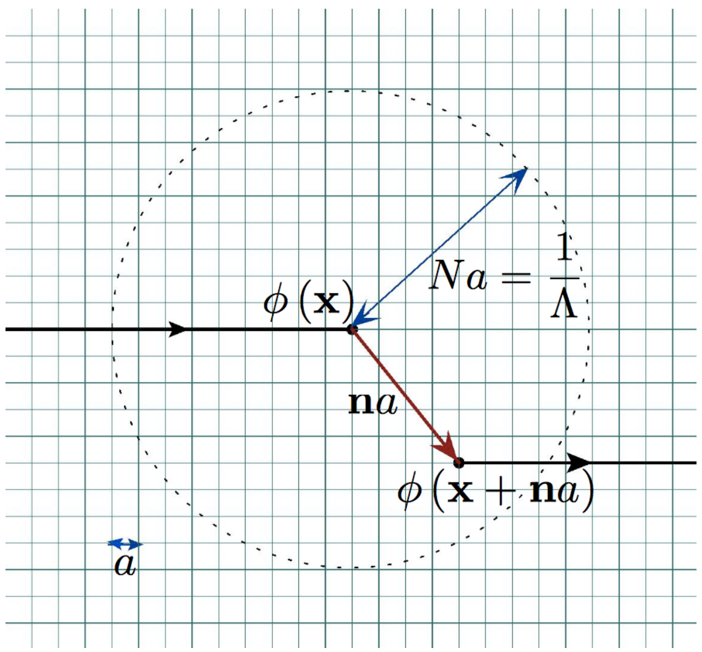
Lattice QCD:
Recovering SO(3) from H(3)





$$\hat{\theta}_{L,M}(\mathbf{x}; a, N) = \frac{3}{4\pi N^3} \sum_{\mathbf{n}}^{|\mathbf{n}|\leq N} \phi(\mathbf{x})\,\phi(\mathbf{x}+\mathbf{n}a)\; Y_{L,M}(\hat{\mathbf{n}})$$

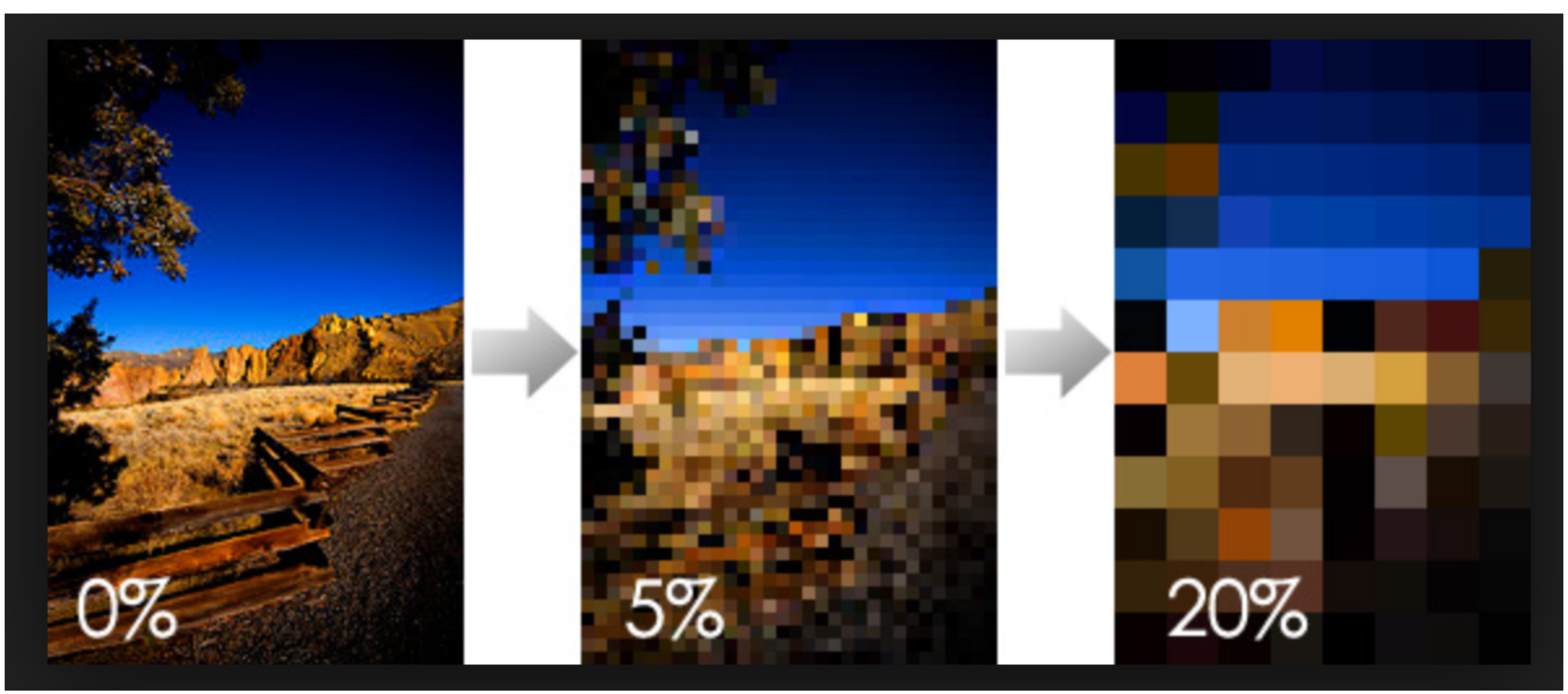
Lattice QCD:
Recovering SO(3) from H(3)



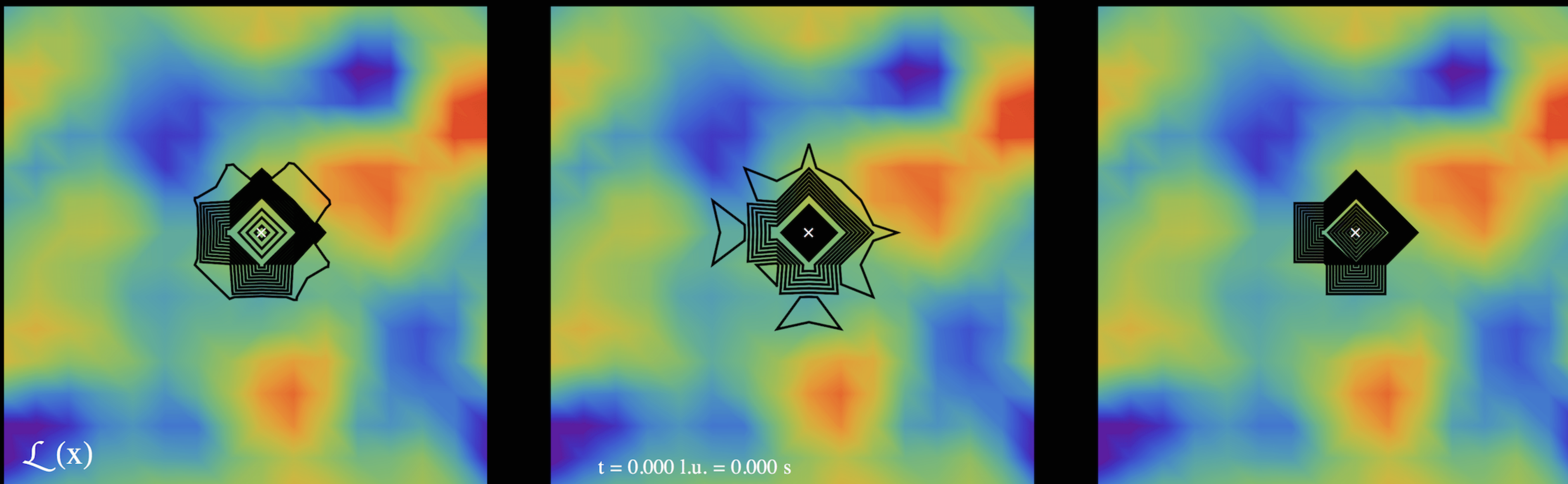
Hold all physical scales, and the renormalization scale fixed when taking lattice spacing to zero

Survives at quantum level in QCD - smearing is critical so as not to ``see'' the UV cubic structure

Multiplicity of irreps of H(3) allow for combinations to approach SO(3) states - both in position space (a) and momentum space (L)



Lattice QCD:
Statistics of Correlation Functions

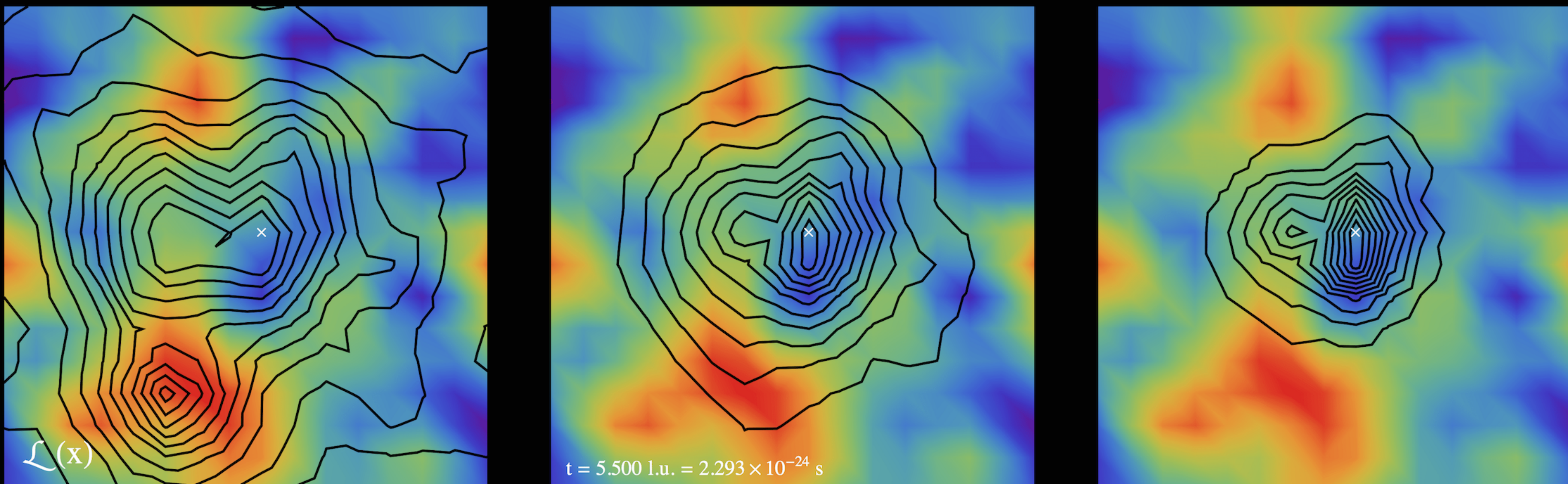


π Propagator | Λ Propagator | H−dibaryon Propagator

The results of a quenched Lattice QCD calculation of the π , Λ , and H−dibaryon correlation functions. The gauge−field configuration was generated with the DBW2 gauge action on a lattice with 16 sites in each spatial direction, 32 sites in the temporal direction and a lattice spacing of approximately 0.12 fermis. The masses of the light quarks were chosen to produce a pion mass of $m_\pi \sim$ 350 MeV and a kaon mass of $m_K \sim$ 490 MeV.
The colors of the background show the (Gaussian−smeared) local action density, while the black contours are a topographical map of the given correlation function.

Lattice QCD:

Statistics of Correlation Functions



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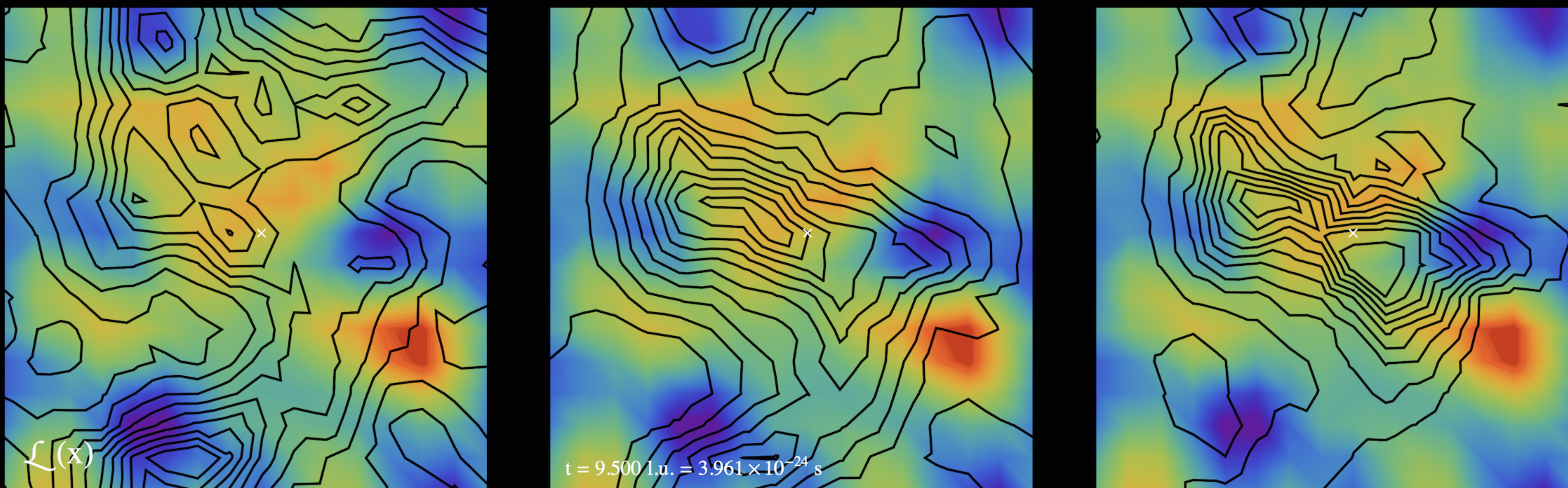
Lattice QCD:
Statistics of Correlation Functions



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The colors of the background show the (Gaussian−smeared) local action density, while the black contours are a topographical map of the given correlation function.

NPLQCD

Lattice QCD:
Analysis of Correlation Functions

e.g., the pion $\overline{u}(\mathbf{x},t)\gamma_5 d(\mathbf{x},t)$

$$C_{\pi^+}(t) = \sum_{\mathbf{x}} \langle 0|\ \pi^-(\mathbf{x},t)\ \pi^+(\mathbf{0},0)\ |0\rangle$$

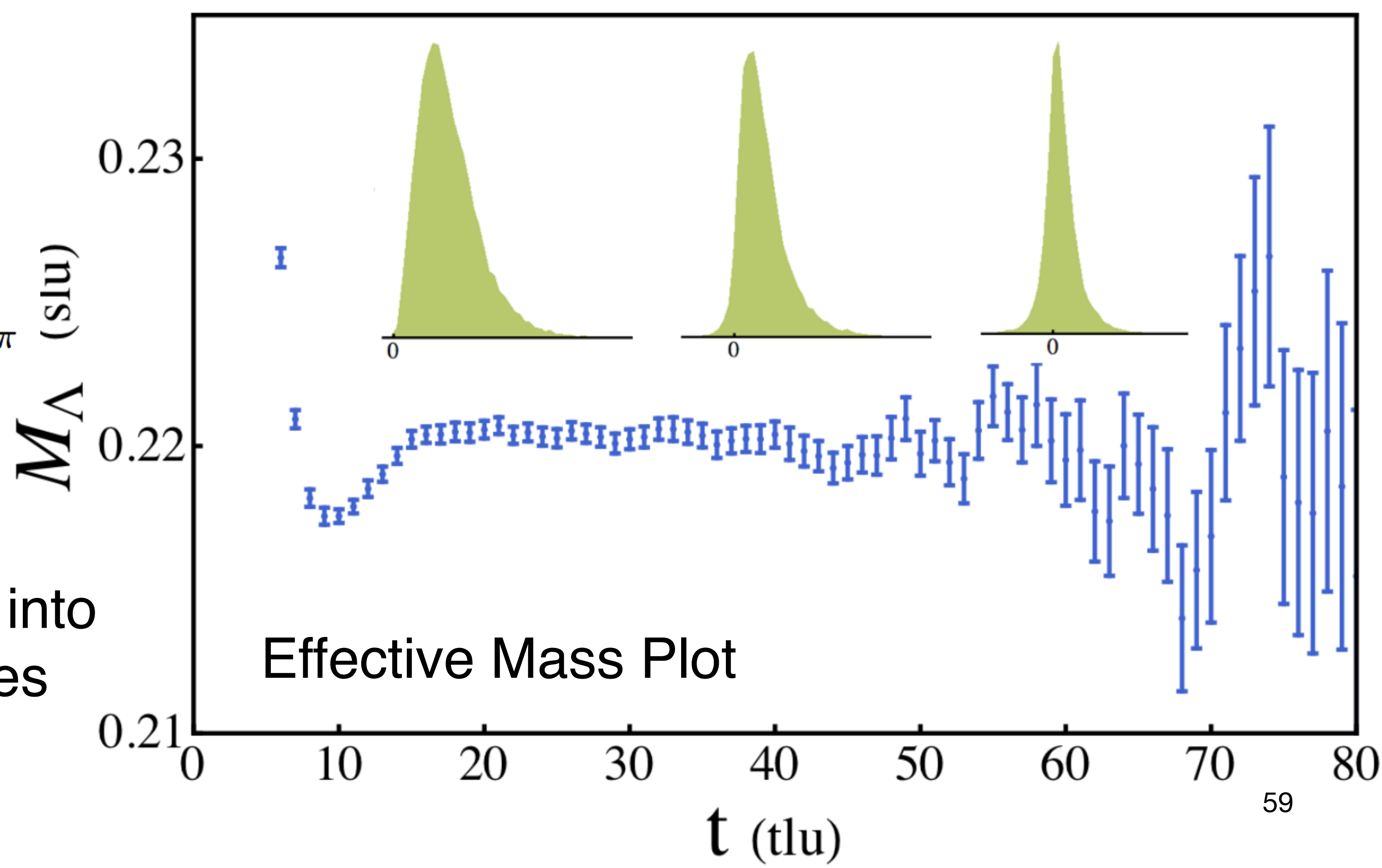
$$= \sum_n \frac{e^{-E_n t}}{2E_n} \sum_{\mathbf{x}} \langle 0|\ \pi^-(\mathbf{x},0)|n\rangle\langle n|\pi^+(\mathbf{0},0)|0\rangle \ \rightarrow\ |Z_0|^2\ \frac{e^{-E_0 t}}{2E_0}$$

(the mean value of measurements from different sources throughout the ensemble)

e.g., the effective mass

$$M_{\text{eff.}}(t;t_J) = \frac{1}{t_J}\ \log\left(\frac{C_{\pi^+}(t)}{C_{\pi^+}(t+t_J)}\right) \ \rightarrow\ m_\pi$$

Non-Gaussian (interacting field theory)
~ Log Normal in plateau region evolves into symmetric but non-Gaussian at late times



Lattice QCD:
Noise is Worth Listening to

e.g., Nucleon Correlation function

$$\langle \theta_N(t) \rangle = \sum_{\mathbf{x}} \Gamma_+^{\beta\alpha} \ \langle 0 | \ N^\alpha(\mathbf{x}, t) \overline{N}^\beta(\mathbf{0}, 0) \ | 0 \rangle \ \rightarrow \ Z_N \ e^{-M_N t}$$

At long times - non-Gaussian symmetric distribution - signal-to-noise problem

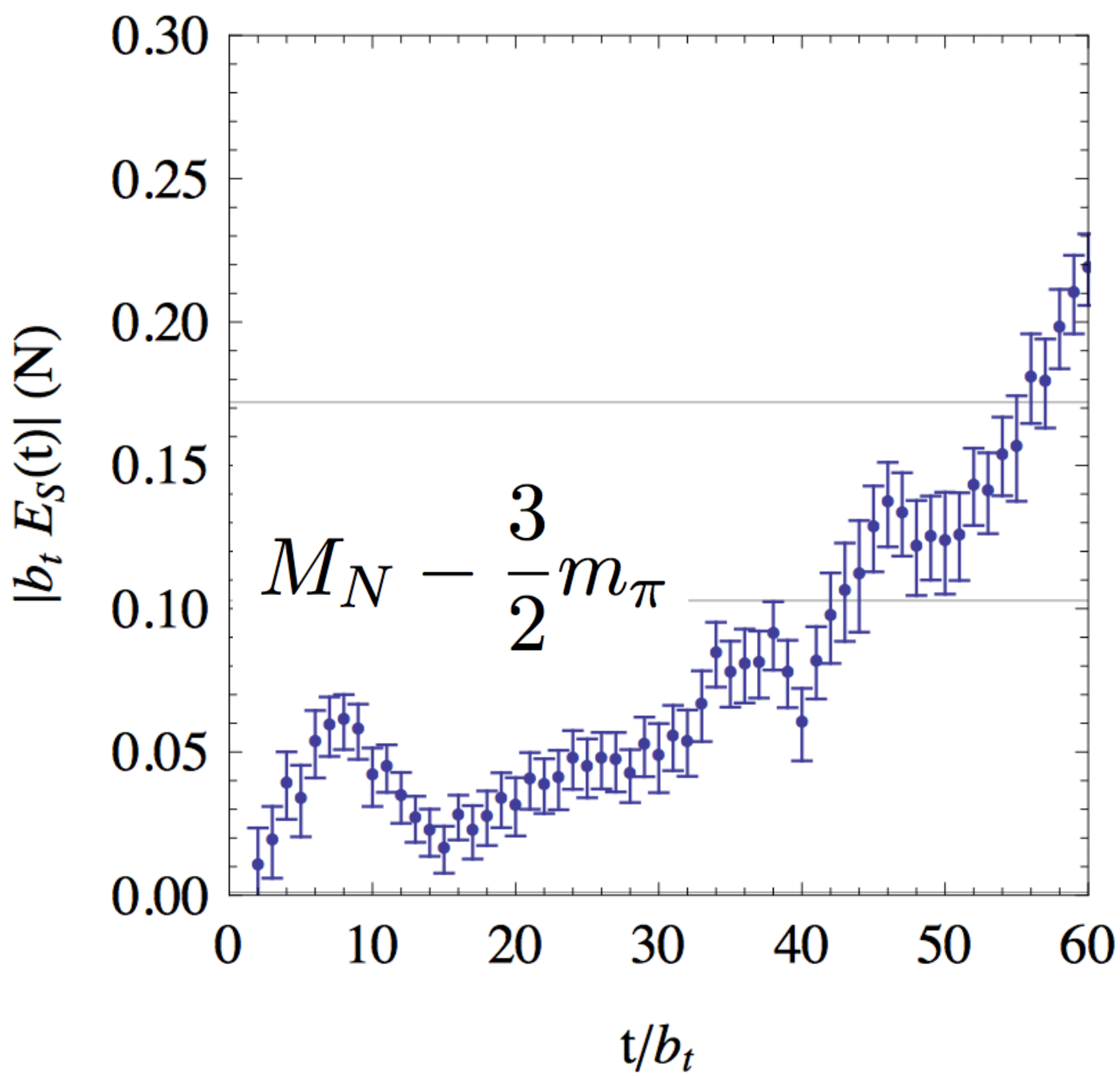
$$\langle \left(\theta_N^\dagger \theta_N \right)^{2n} \rangle \sim e^{-3n m_\pi t} \quad , \quad \langle \left(\theta_N^\dagger \theta_N \right)^{2n+1} \rangle \ \sim \ e^{-M_N t} e^{-3n m_\pi t}$$

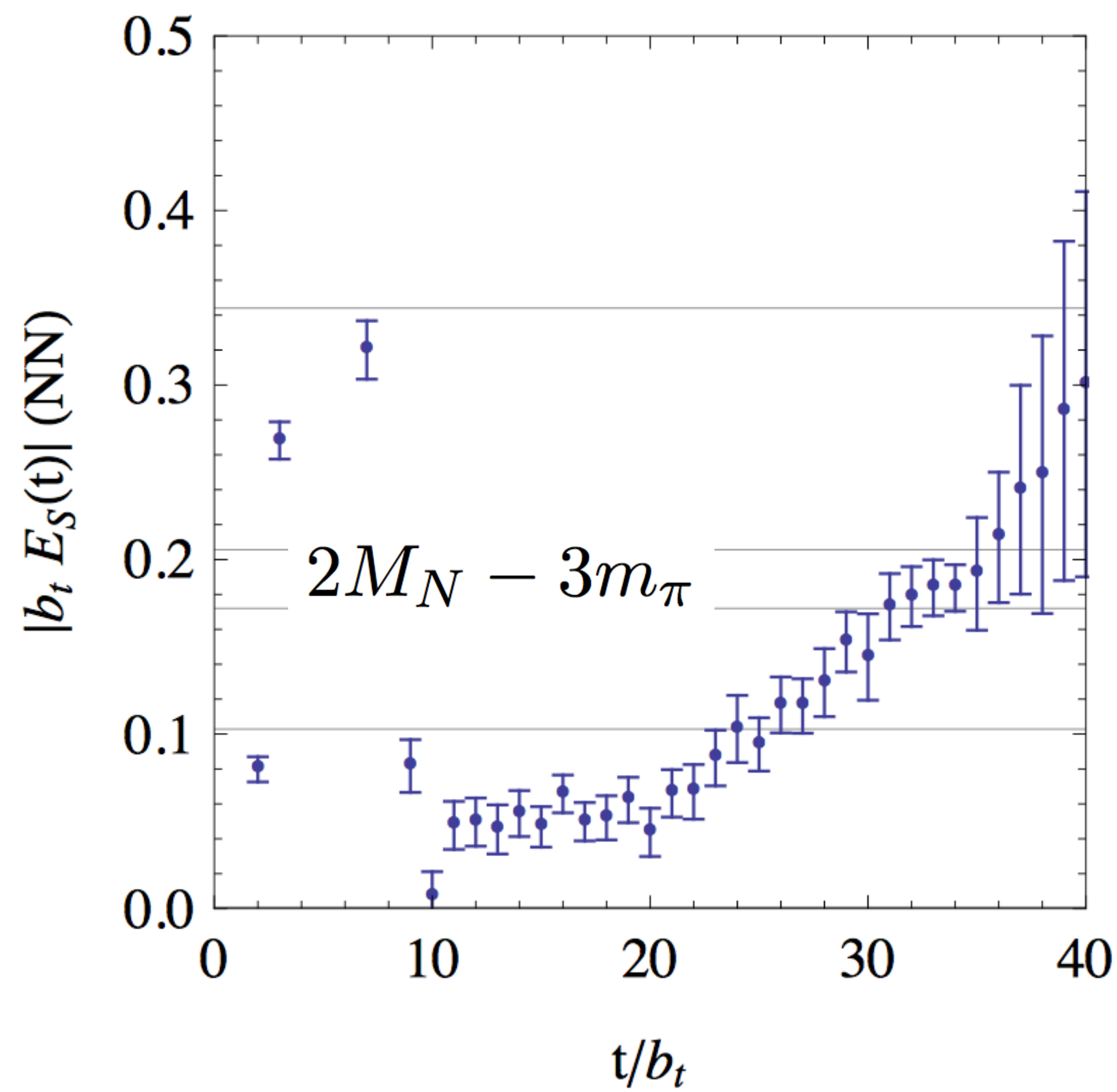
At short times - asymmetric distribution - no signal to noise problem

$$\langle \left(\theta_N^\dagger \theta_N \right)^{n} \rangle \sim e^{-n M_N t}$$

Lattice QCD:
Noise is Worth Listening to

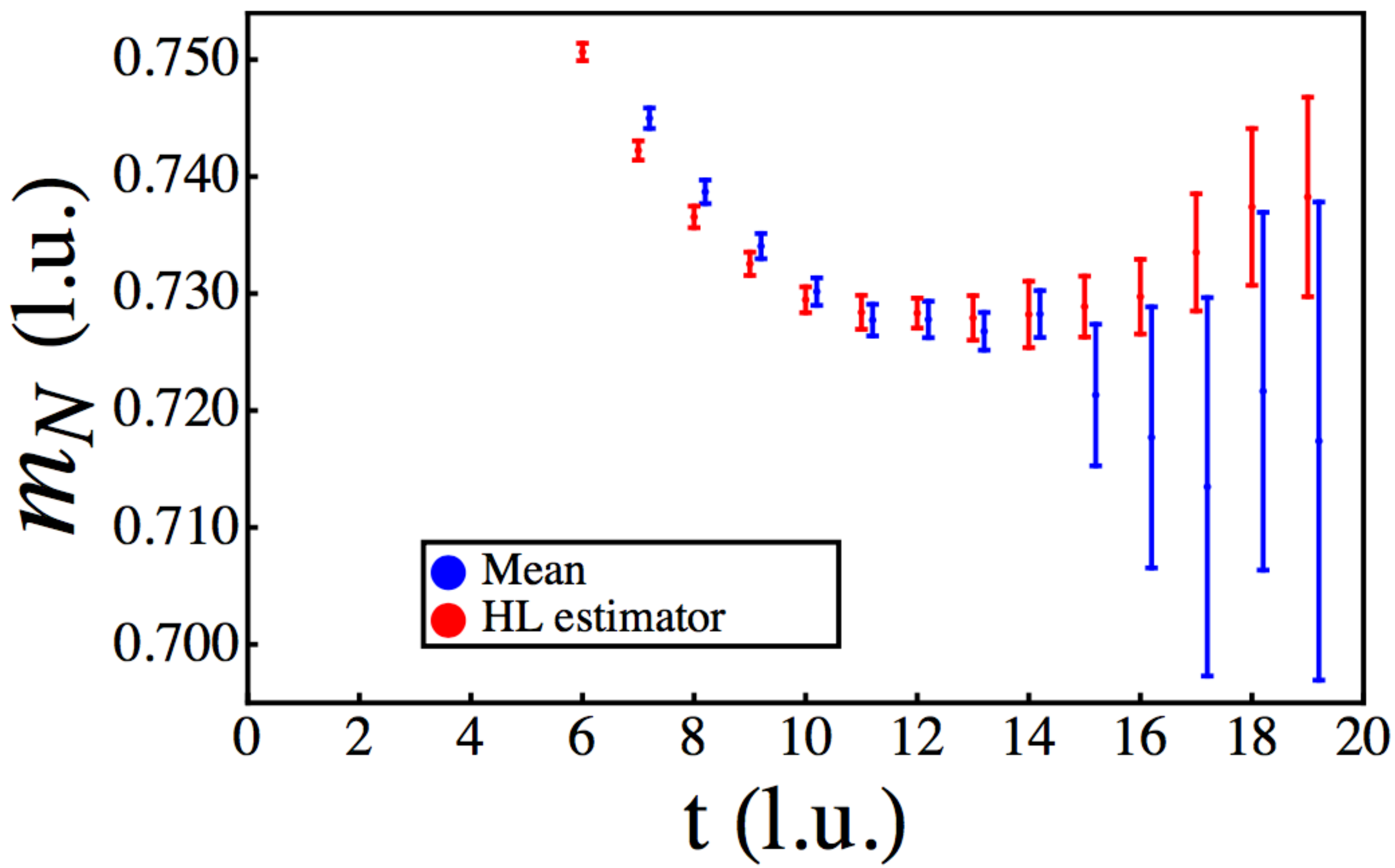
Energy scale of the signal-to-noise ratio





Lattice QCD:
Analysis of Correlation Functions

- One averaged correlator per configuration per species
- Block multiple configurations down to ~ 100 decorrelated correlation functions
- Central Limit Theorem has distribution becoming Gaussian - mean equals median
- Jackknife and Bootstrap resampling techniques commonly used as samples typically have residual correlations
- Outliers present from initial non-Gaussianity - disturbs mean but not median
- Robust estimators (Hodges-Lehmann etc).

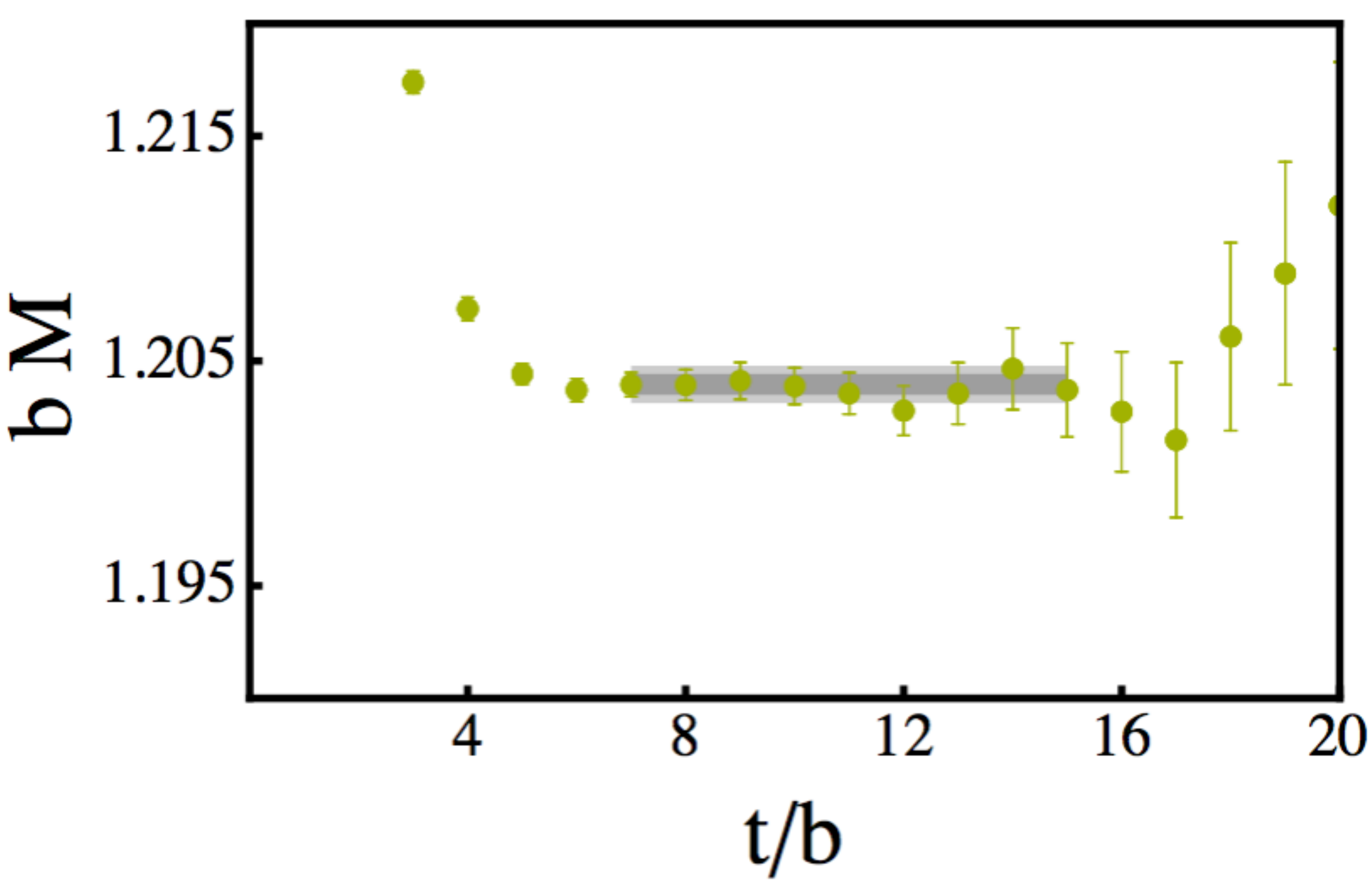


Lattice QCD:

Effective Mass Plots and Plateau Fitting

$$\chi^2(A) = \sum_{i,j>i_{\min}}^{i_{\max}} \left[\bar{G}(t_i) - F(t_i, A)\right] \left[C^{-1}\right]_{ij} \left[\bar{G}(t_j) - F(t_j, A)\right]$$

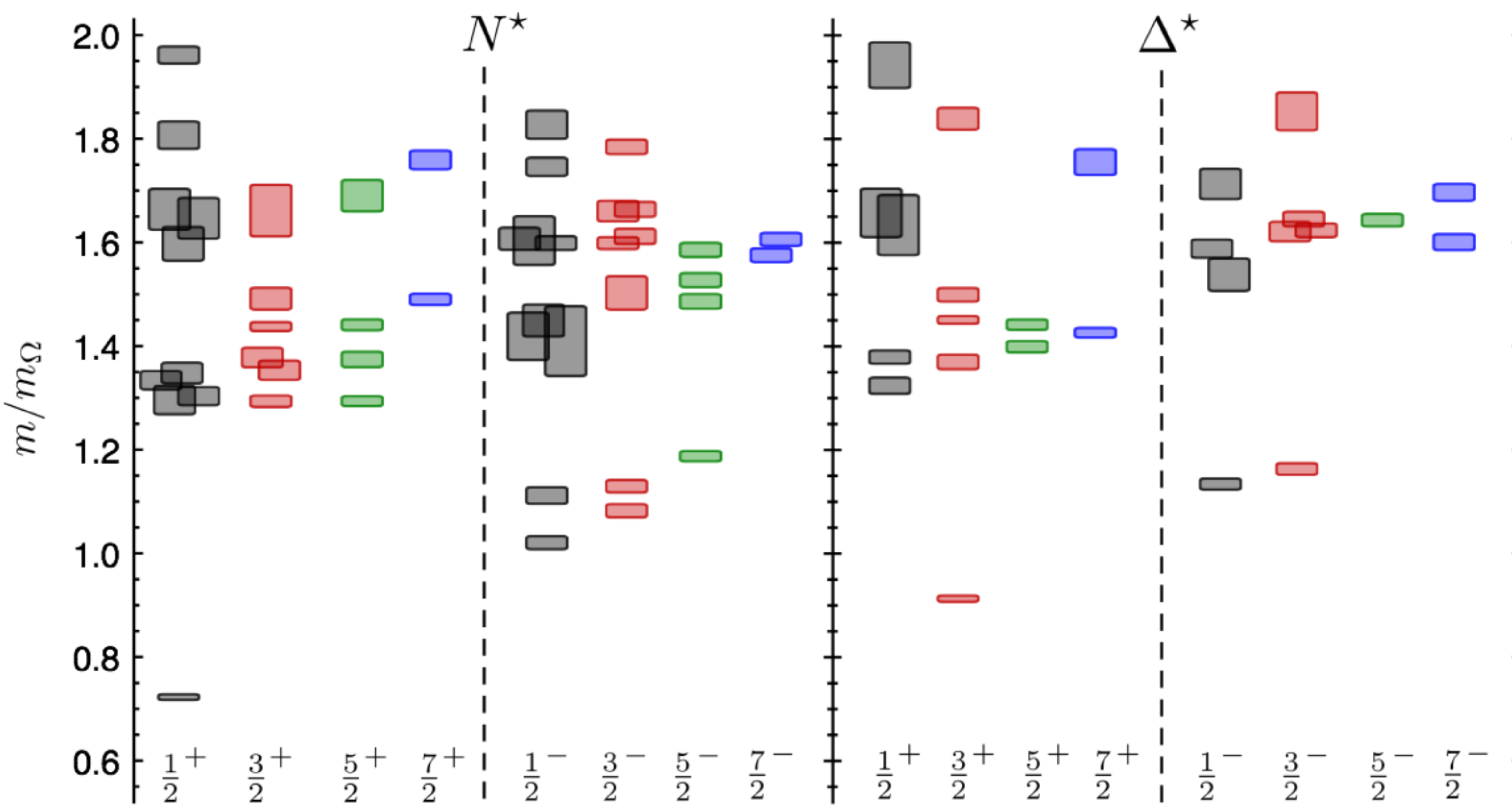
$$\bar{G}(t) = \frac{1}{N}\sum_{k=1}^{N} G_k(t) \ , \ C_{ij} = \frac{1}{N(N-1)}\sum_{k=1}^{N} \left[G_k(t_i) - \bar{G}(t_i)\right] \left[G_k(t_j) - \bar{G}(t_j)\right]$$



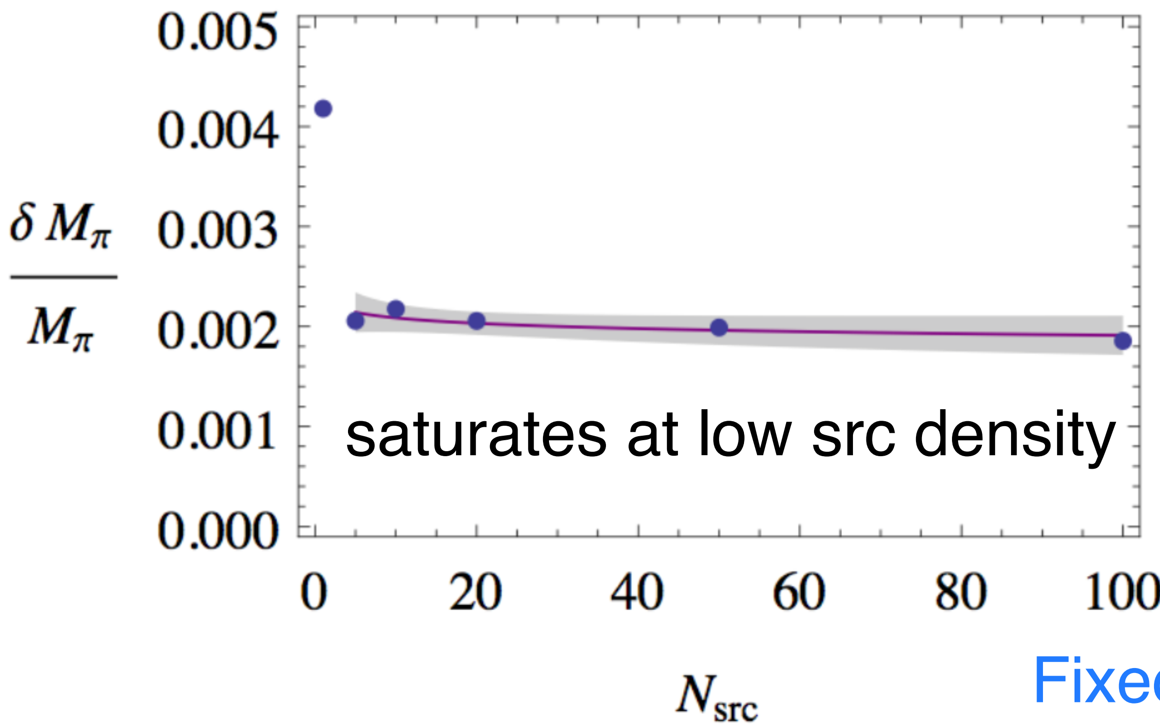
- Statistical uncertainty from χ^2
- Systematic uncertainty from baryon fit region

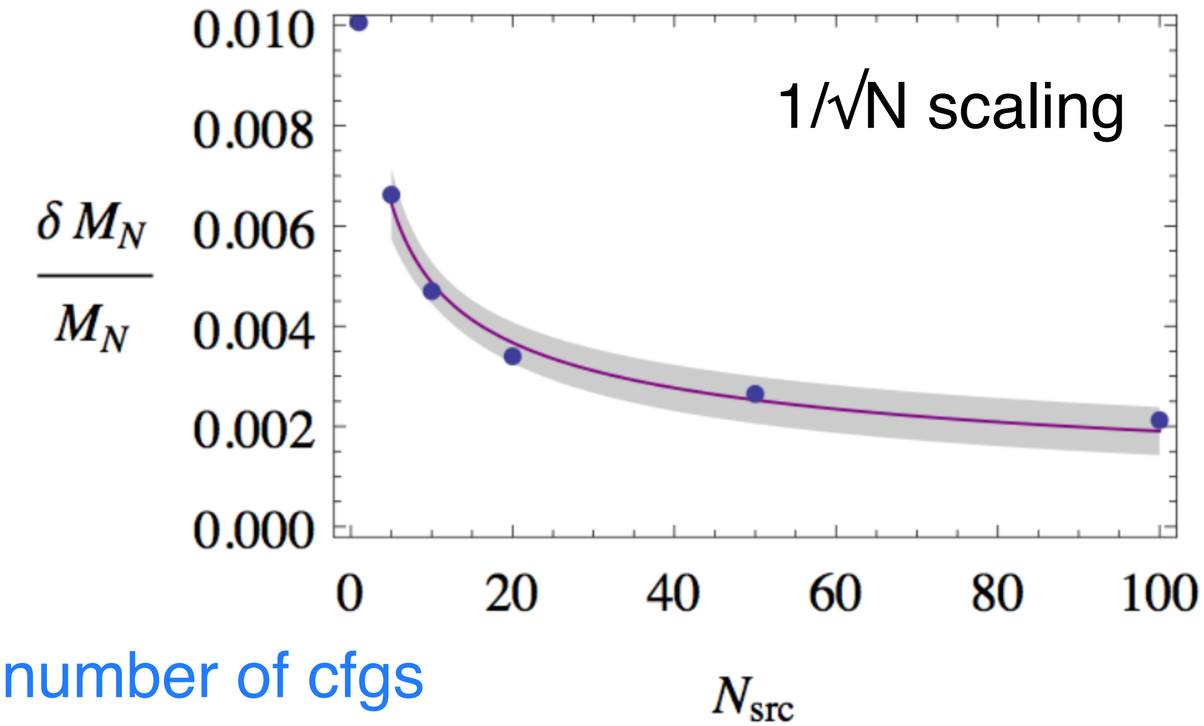
Lattice QCD:
Effective Mass Plots and Plateau Fitting

- Excited states require correlation functions with the same quantum numbers but different spacetime structure at the source and sink (with different overlaps onto the lowest-lying states)
- Also requires good temporal resolution to distinguish/identify multiple exponentials

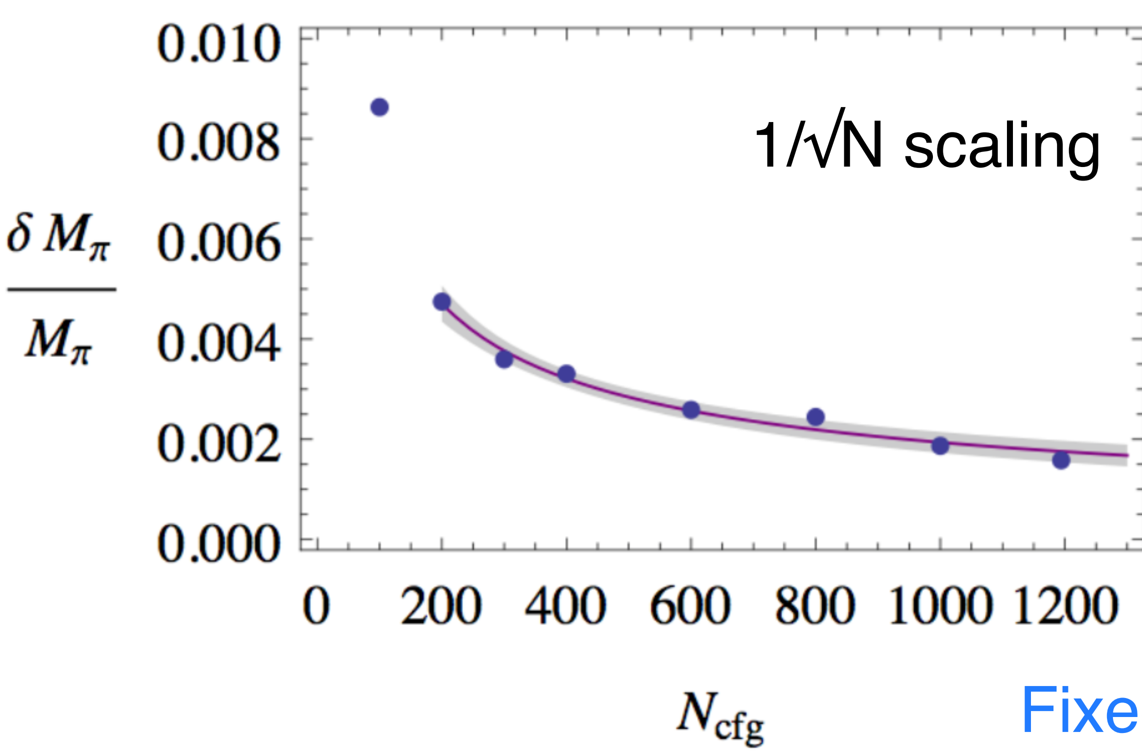


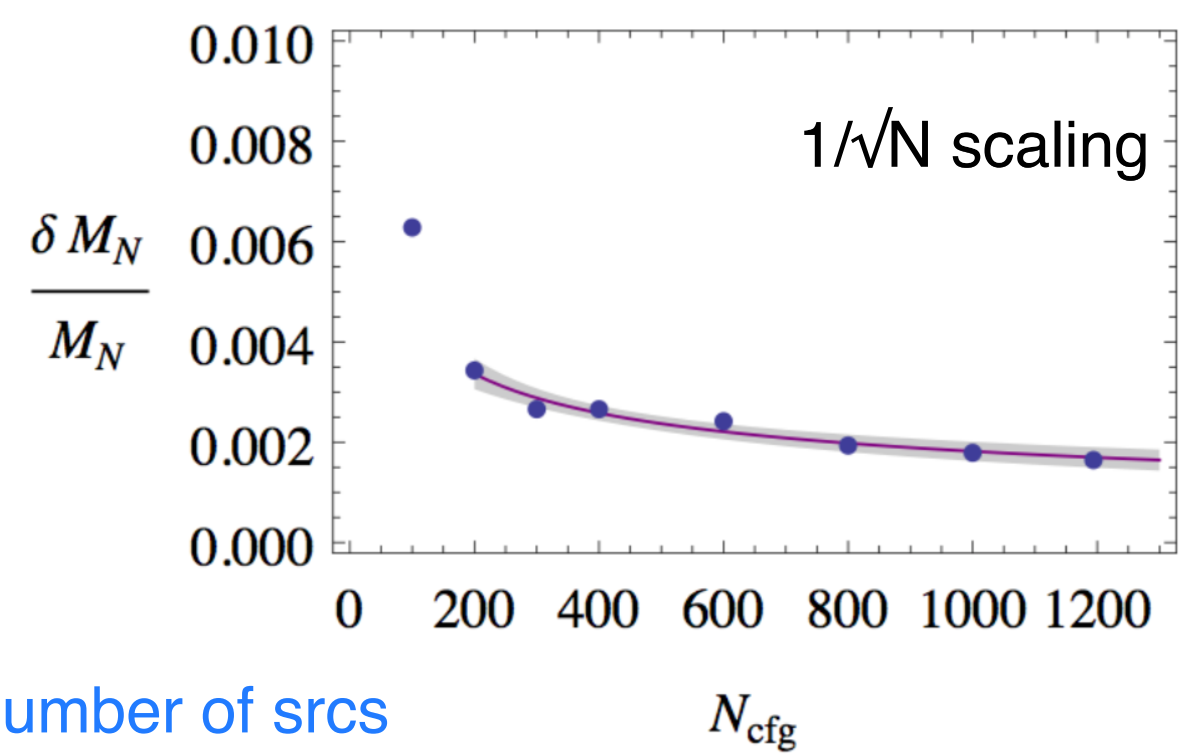
Lattice QCD:
Statistics of Correlation Functions





Fixed number of cfgs

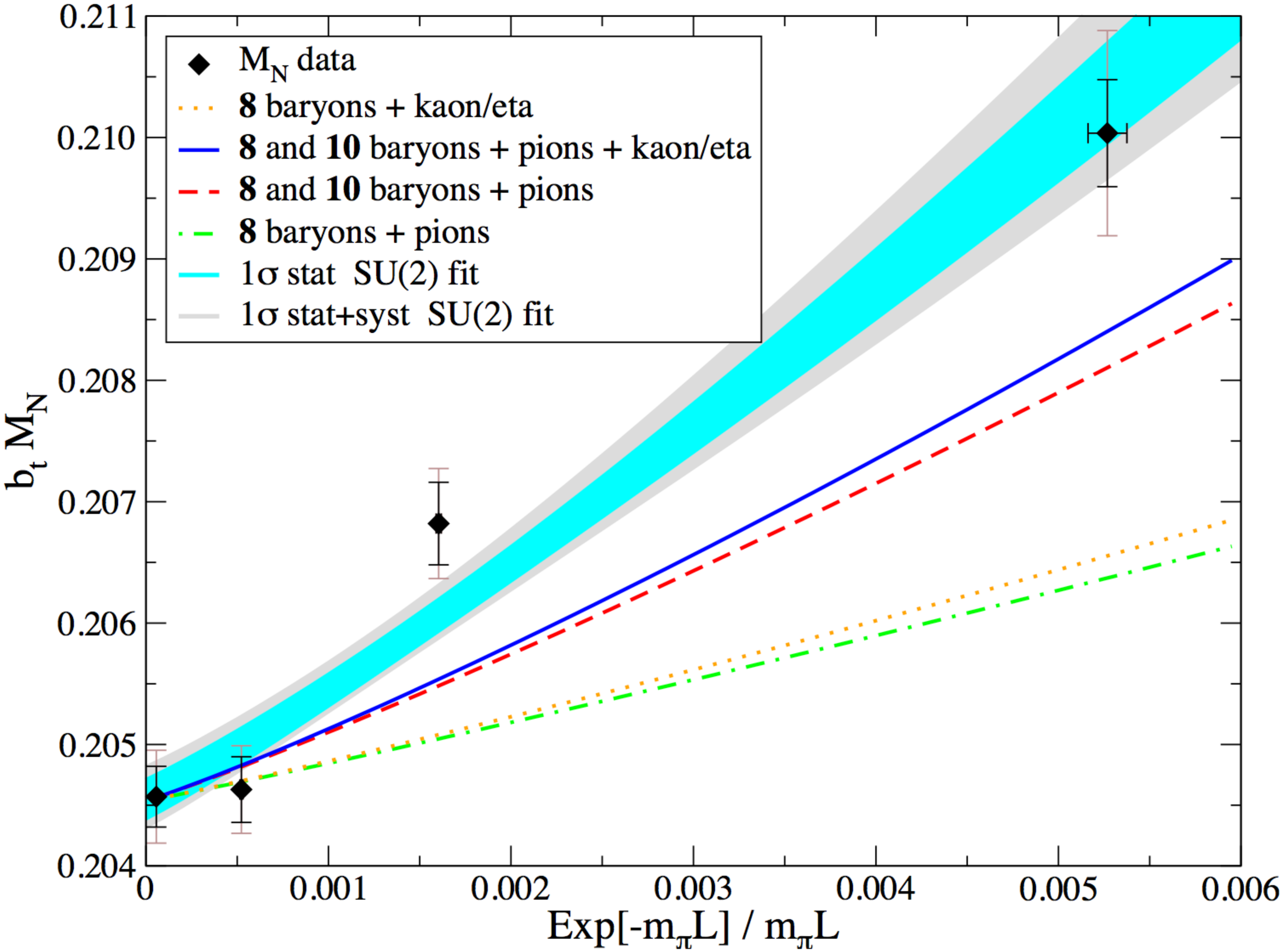




Fixed number of srcs

Lattice QCD:

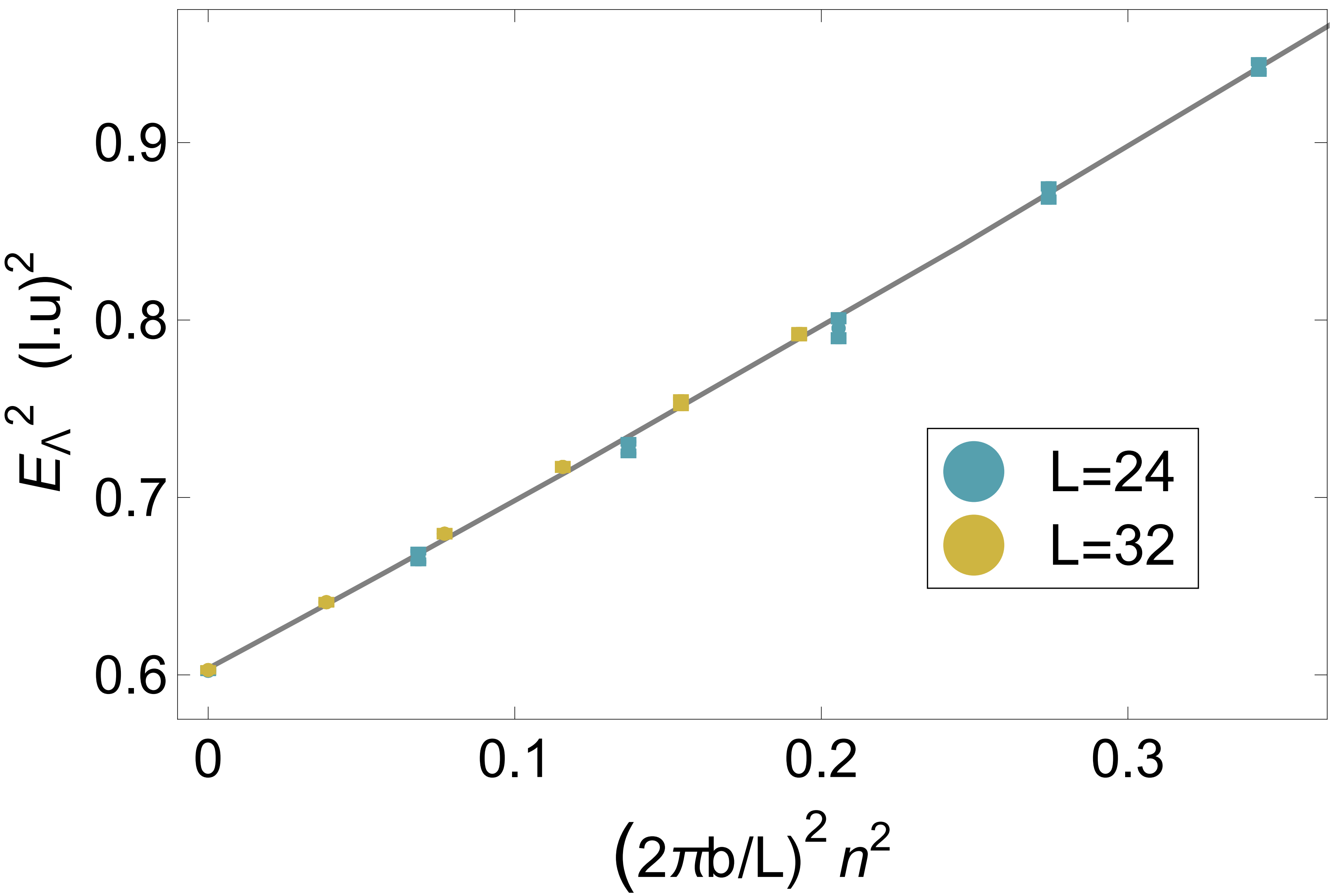
FV Effects - Uncertainty Quantification



Low-energy EFT dictates form of the volume extrapolation

Lattice QCD:

Dispersion Relations - Uncertainty Quantification

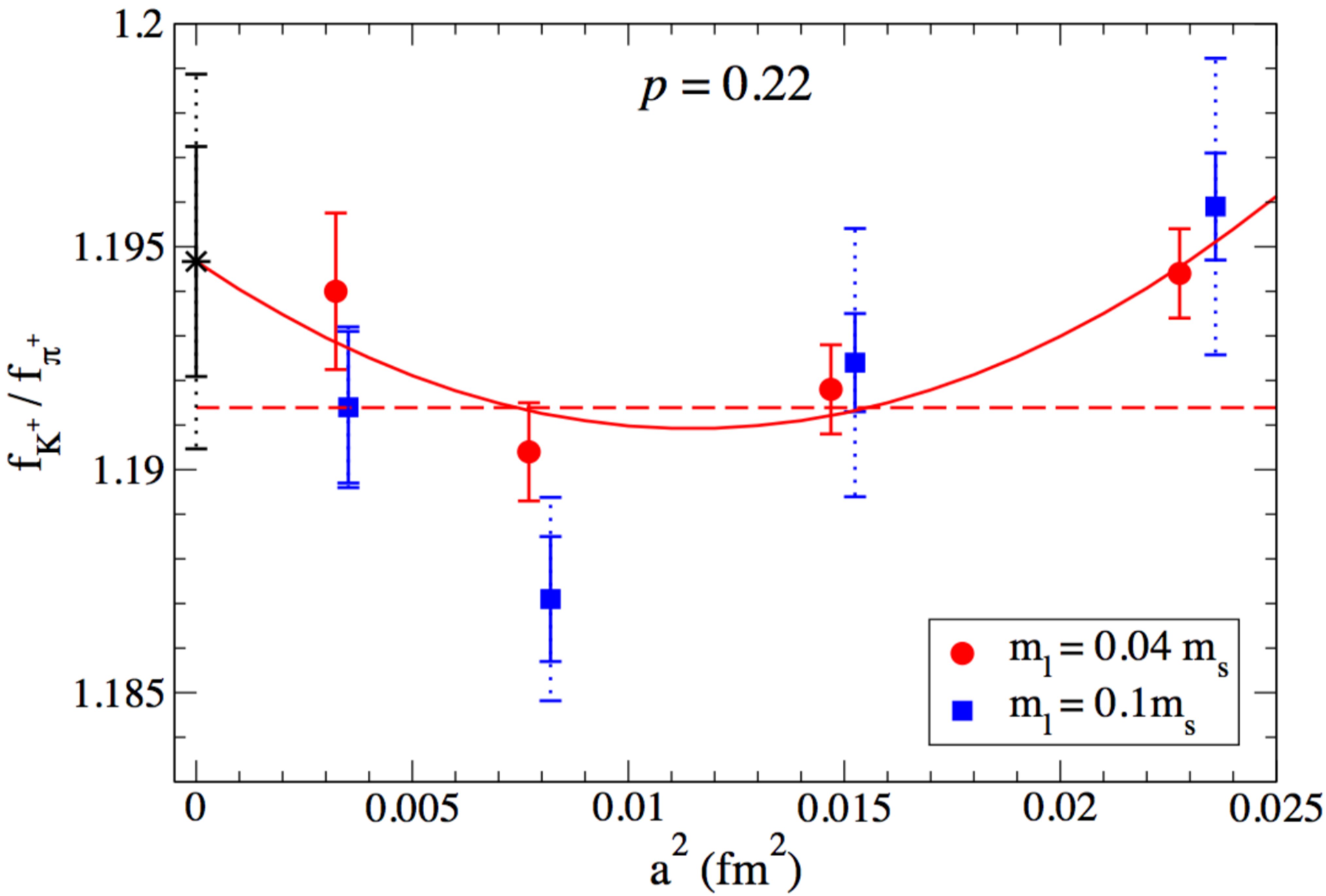


v = 1.016 +-0.019 +- 0.001

Do not expect them to be ``as bad'' as the quark and gluon dispersion relations as the typical momenta of the q's and g's is much smaller.

Lattice QCD:

Lattice-Spacing Extrapolation - Uncertainty Quantification



Symanzik action and low-energy EFT dictates form of lattice-spacing extrapolation

Lattice QCD:
Uncertainty Quantification - Error Budgets

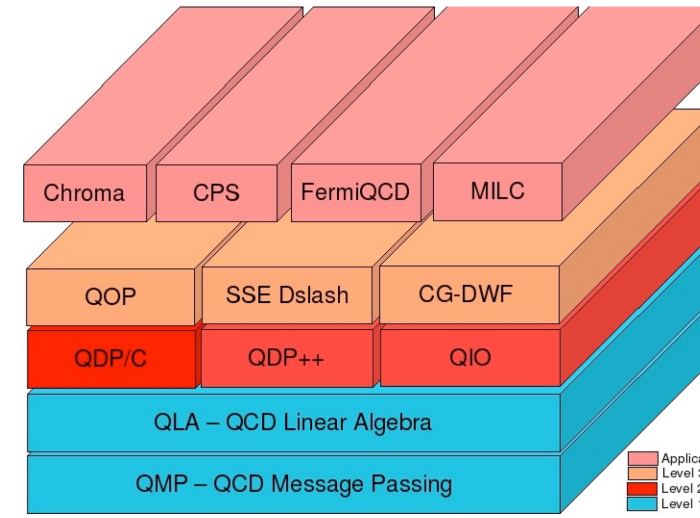
Error	$f_\Upsilon\sqrt{M_\Upsilon}$	$\overline{m}_b(10\text{GeV})$
Statistics	0.3	0.0
Z_V/k_1	2.5	0.3
perturbation theory/α_s	-	0.3
uncertainty in a	1.6	0.0
lattice spacing dependence	3.4	0.4
sea-quark mass dependence	1.0	0.0
b-quark mass tuning	1.0	0.0
NRQCD systematics	1.0	0.3
electromagnetism η_b annihilation	0.0	0.0
total	4.8	0.7

Error (Uncertainty) Budgets are standard in Lattice QCD - to provide a breakdown of the fully-quantified uncertainties of the calculation(s).

Status and Future

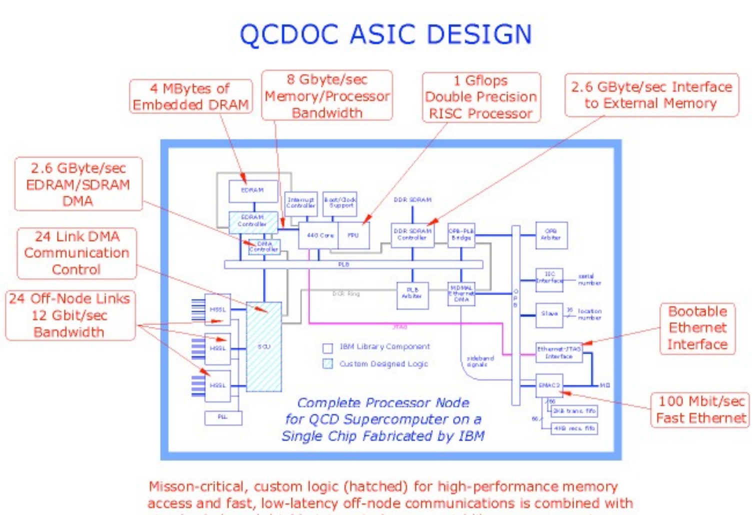
Lattice QCD

USQCD Collaboration

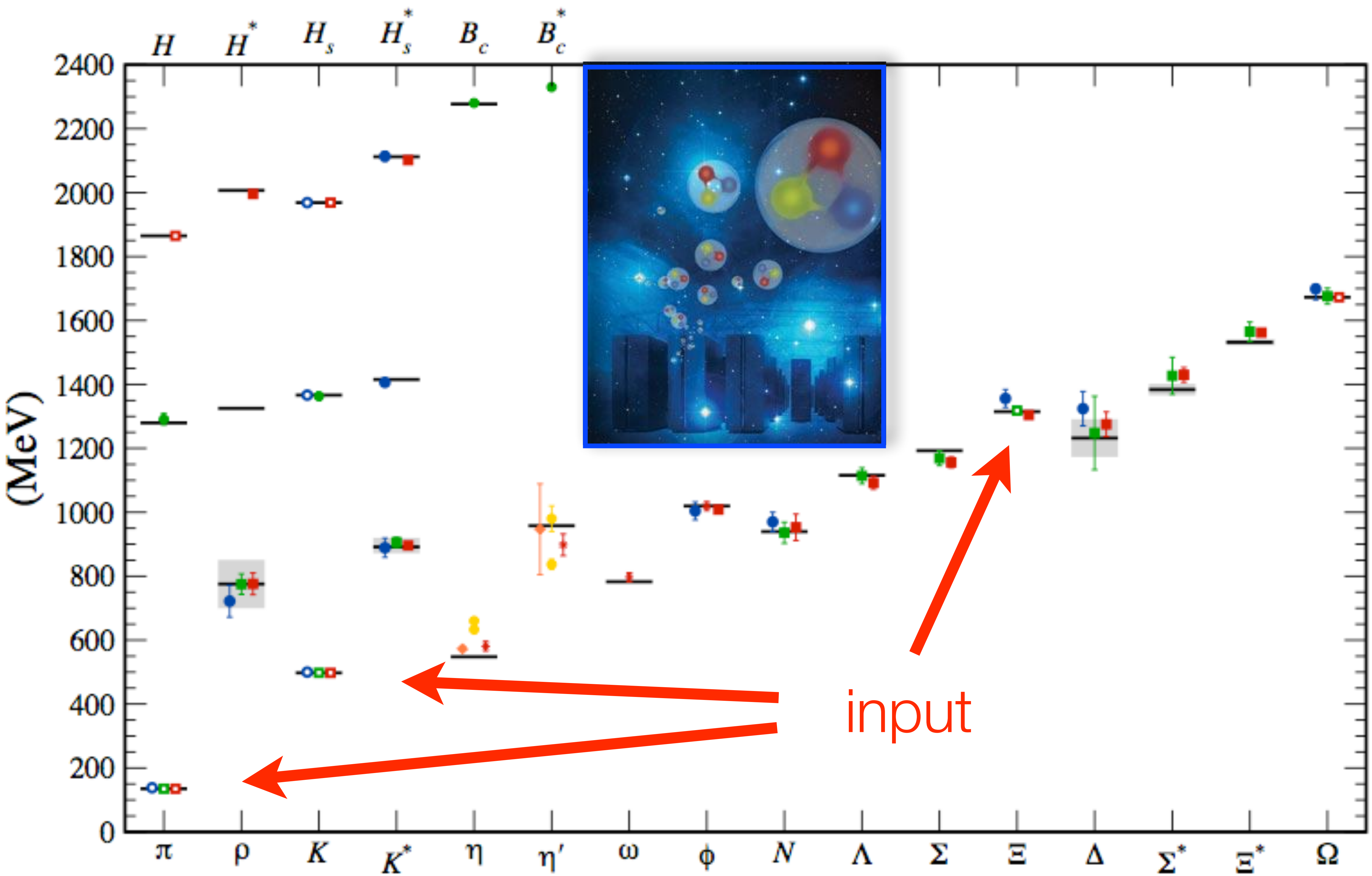


Ancient History -

QCDSP : 1998 Gordon Bell Prize



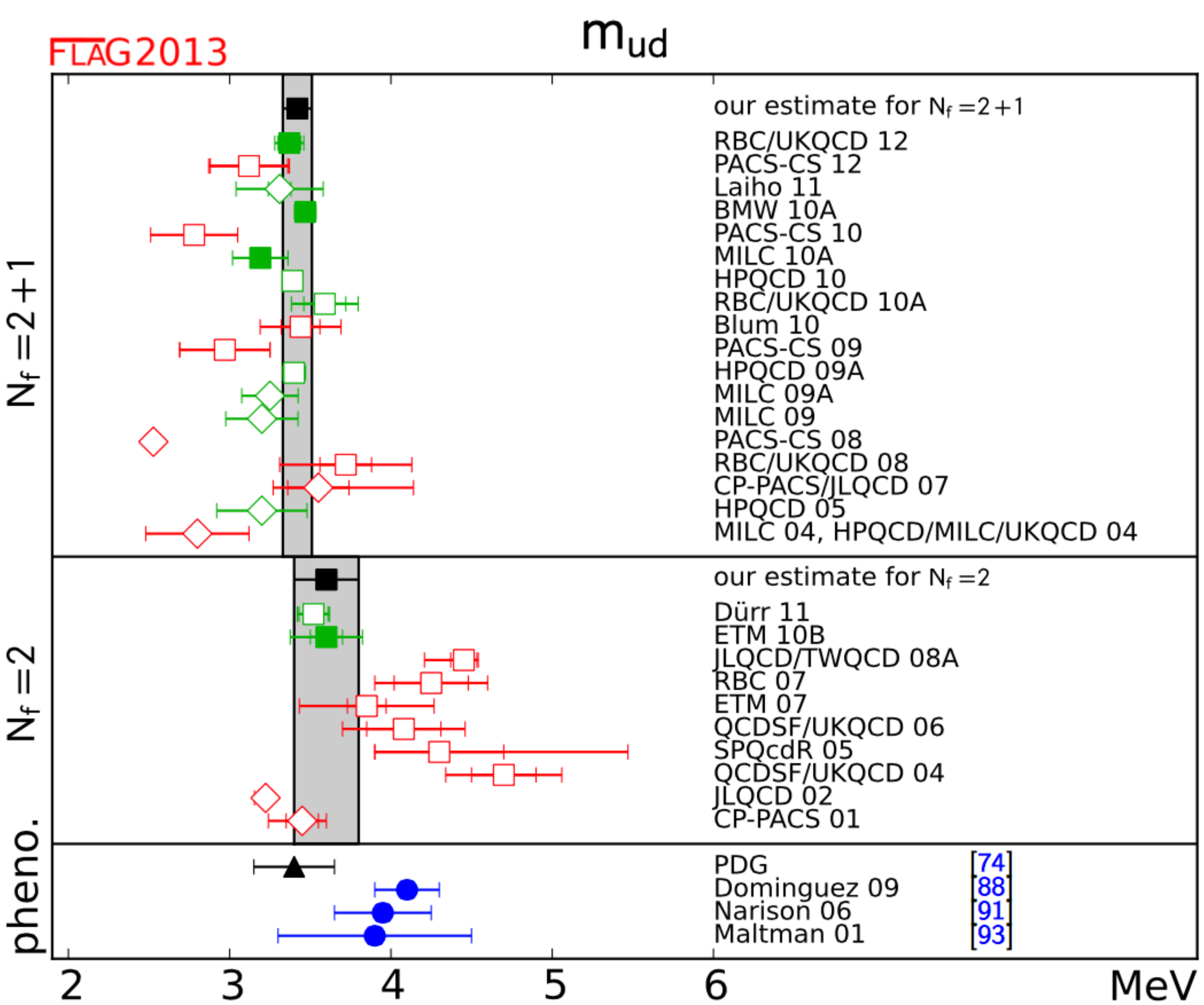
Hadron Masses

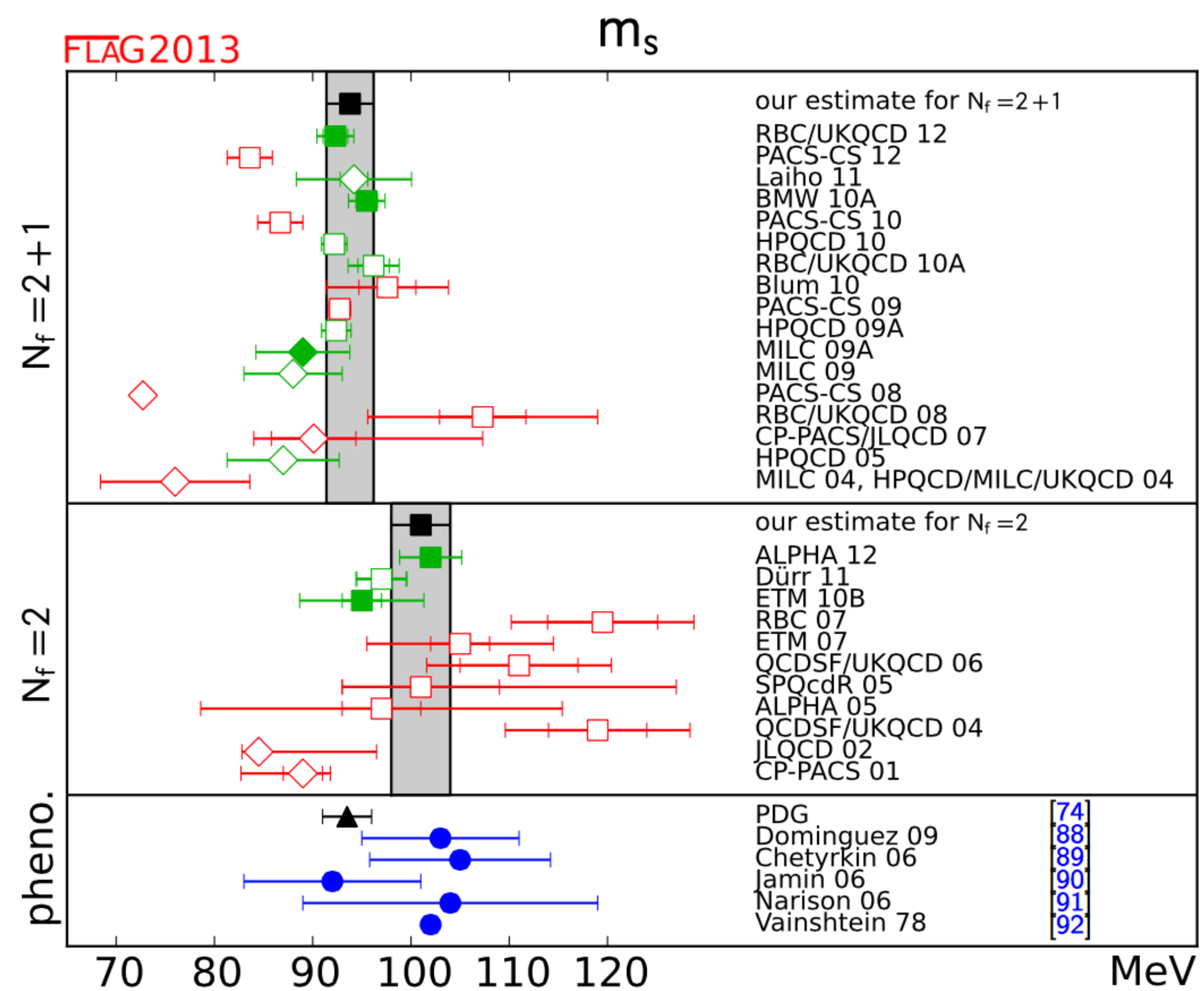


(Kronfeld)

Lattice QCD:

Results - quark masses

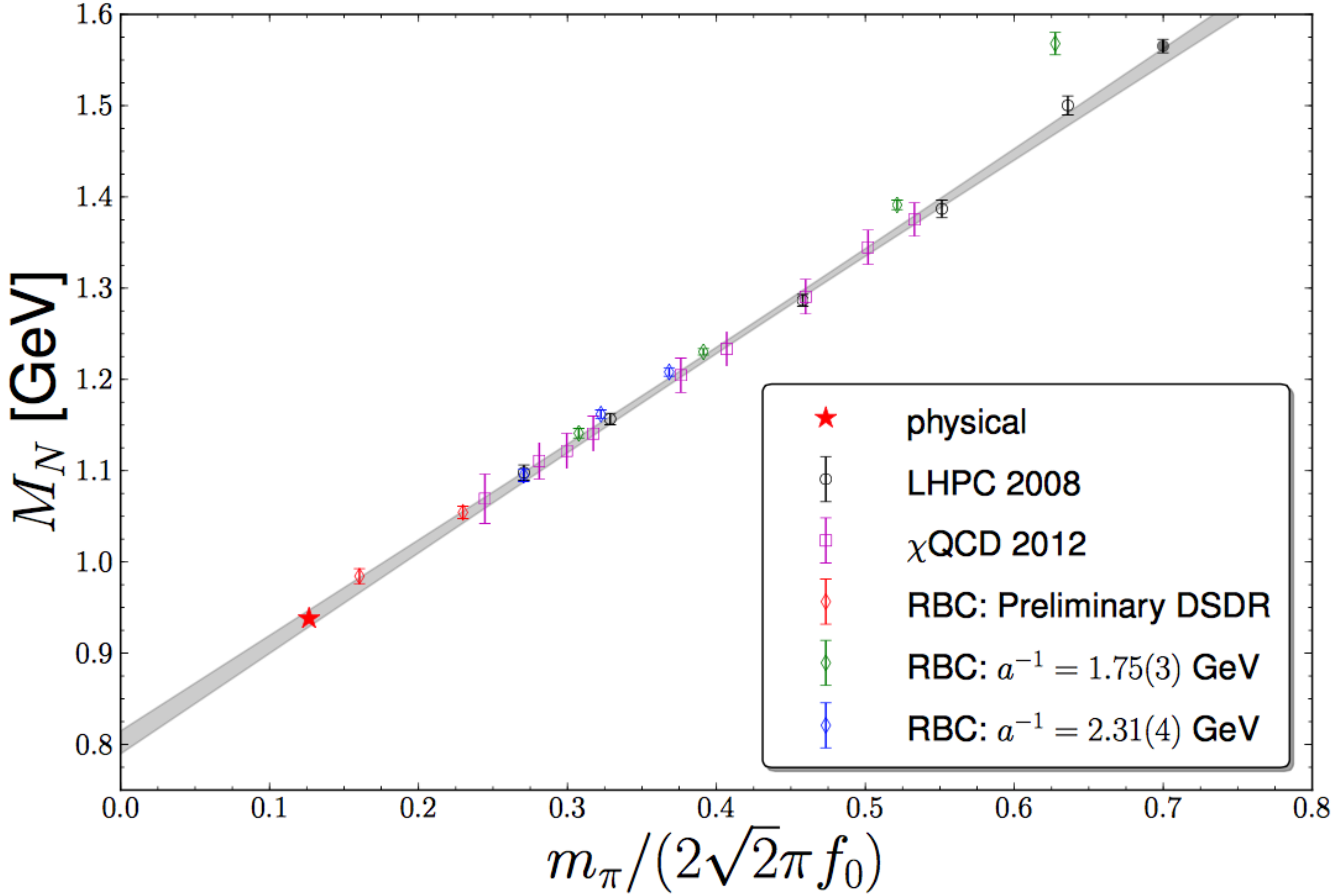




N_f	m_u	m_d	m_u/m_d
2+1	2.16(9)(7)	4.68(14)(7)	0.46(2)(2)
2	2.40(23)	4.80(23)	0.50(4)

$$\overline{\mathrm{MS}}\ ,\ \mu = 2\ \mathrm{GeV}$$

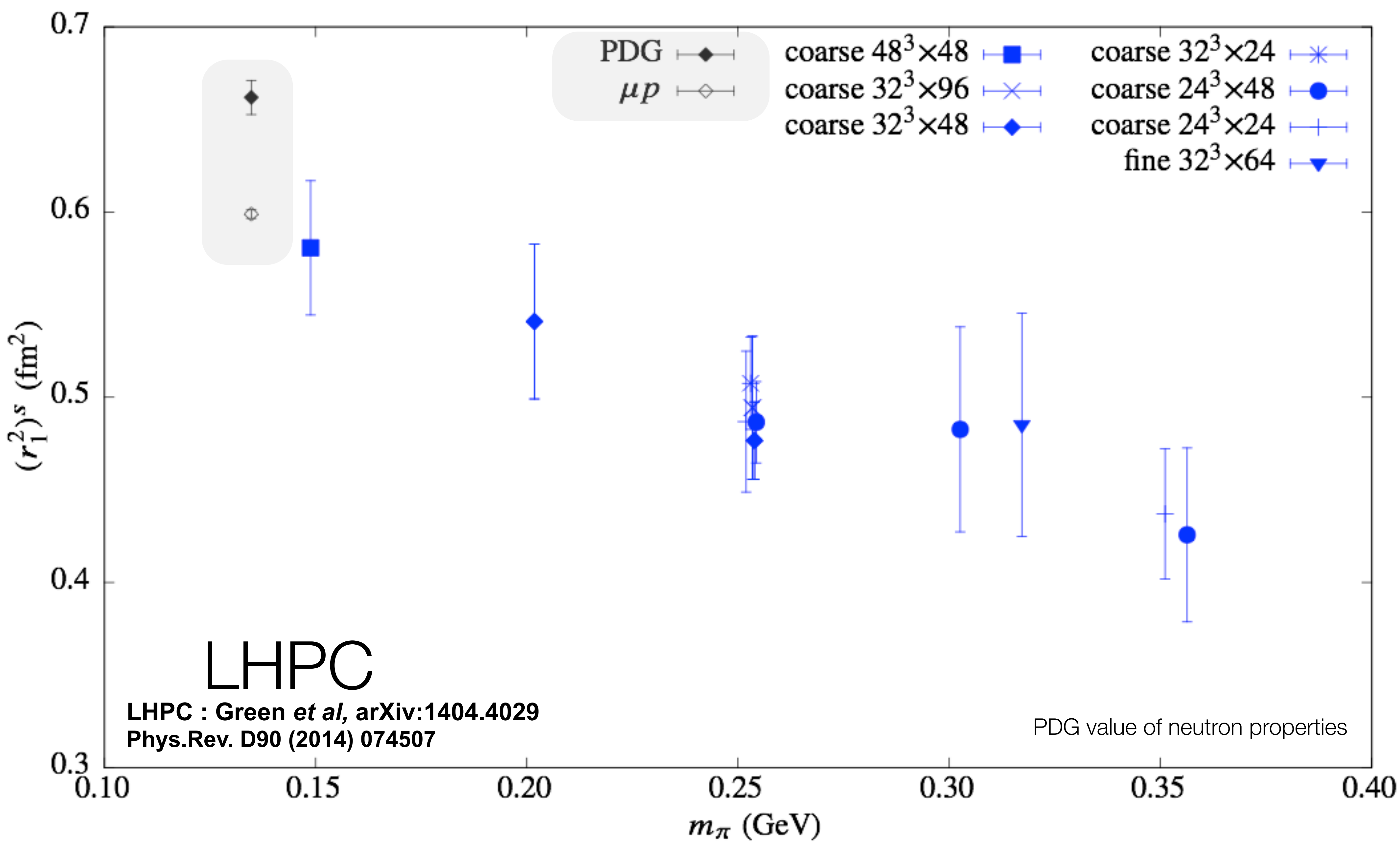
Lattice QCD:
Results - Nucleon



$$M_N = 800 \text{ MeV} + m_\pi$$

Unexpected behavior !!

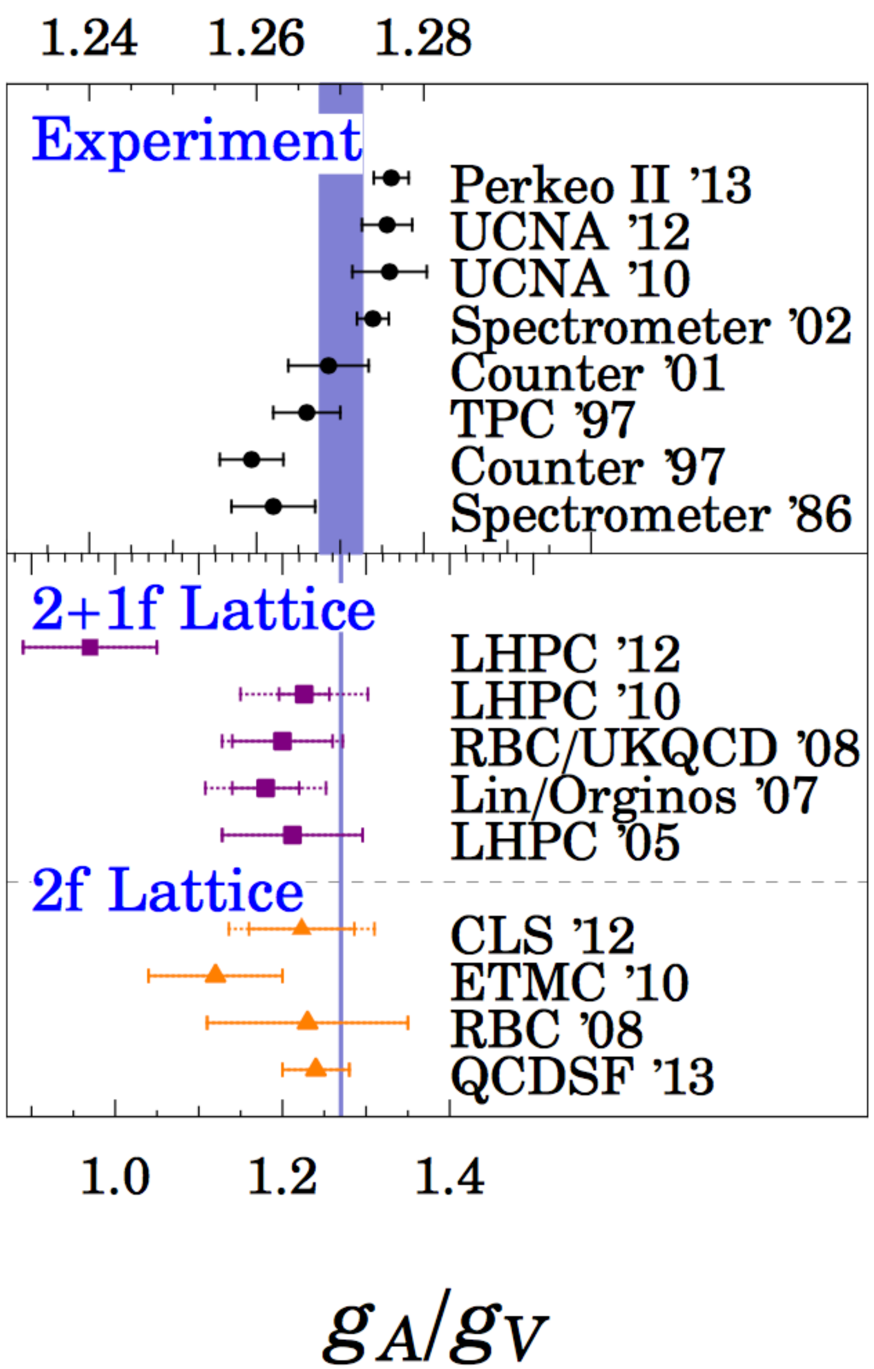
Lattice QCD:
Results - Nucleon Size

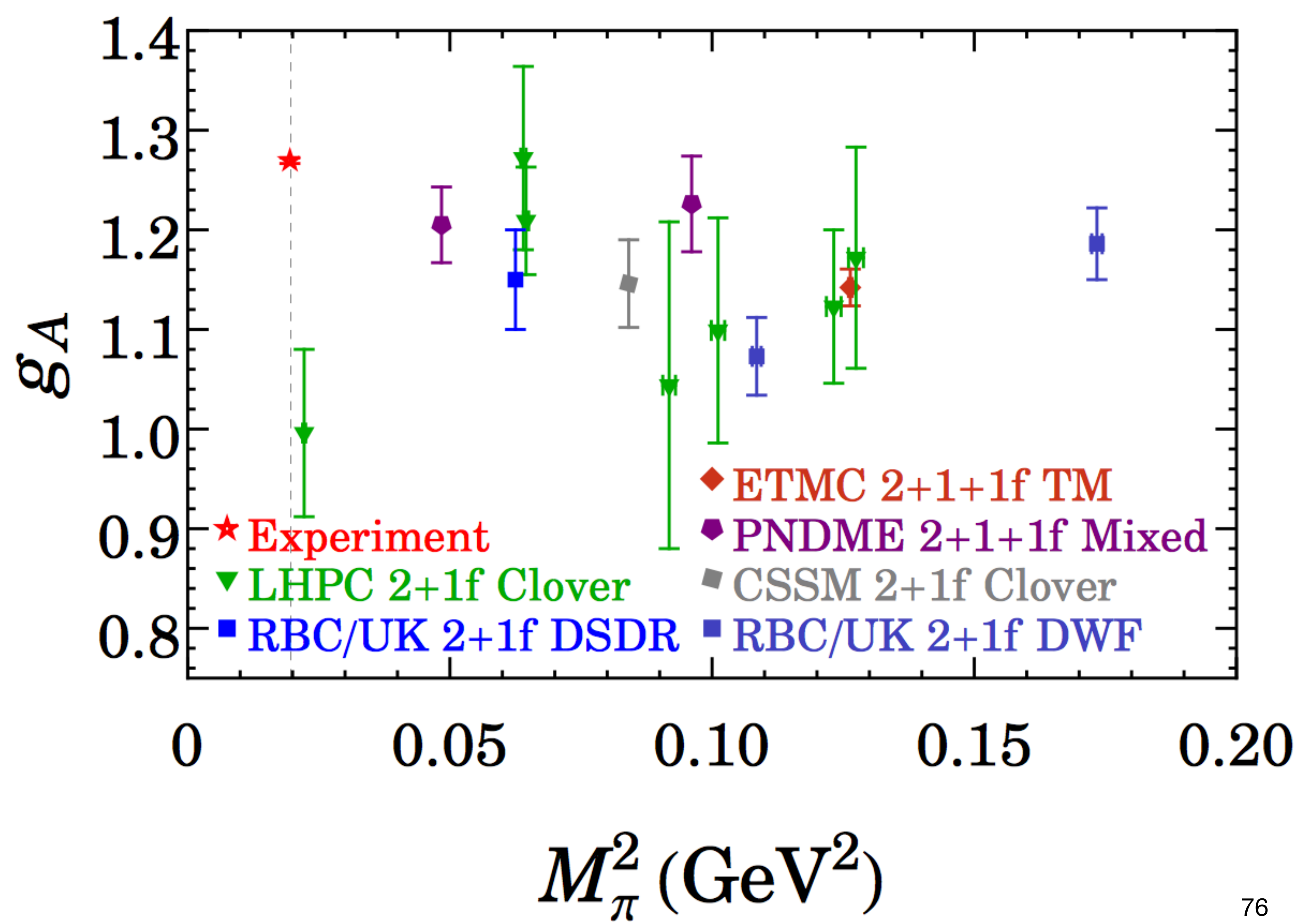


First LQCD calculations at physical pion mass during 2012

Lattice QCD:

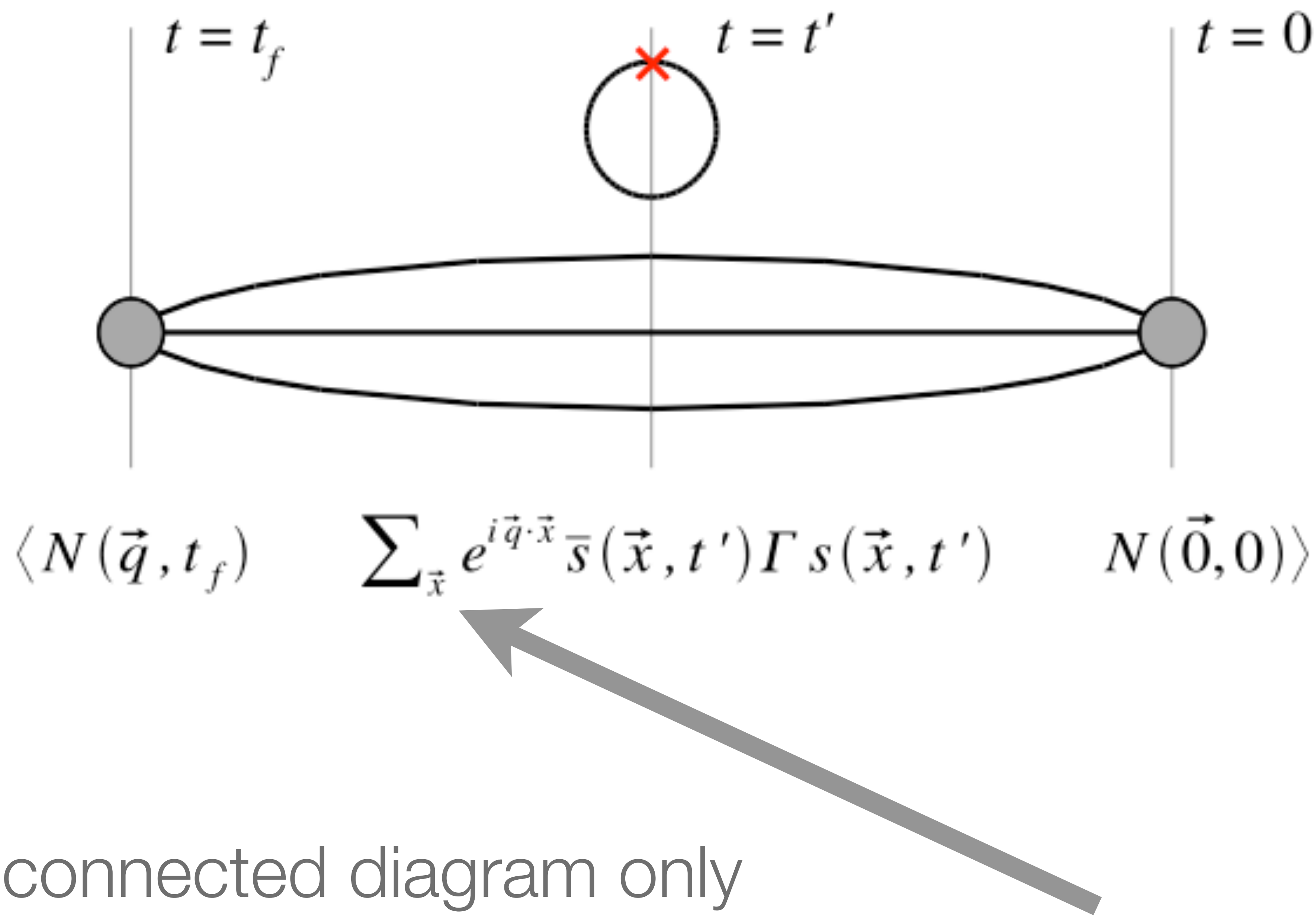
Results - Nucleon Axial Charge





Lattice QCD:

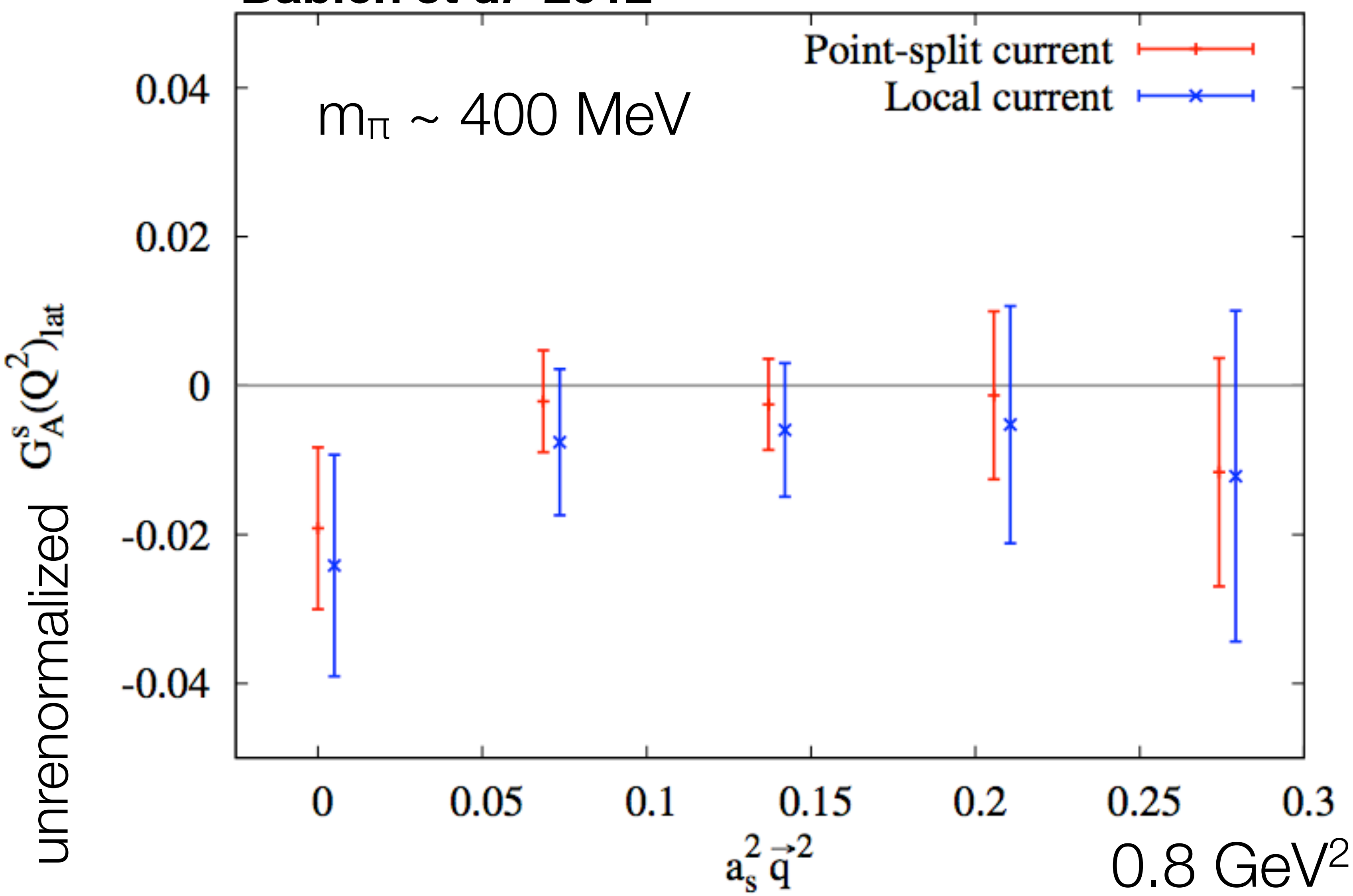
Results - Nucleon Strangeness



- Disconnected diagram only
- Need propagator at each point in the lattice volume
- GPU's have allowed for major progress

Lattice QCD:
Results - Nucleon Strangeness

Babich *et al* 2012



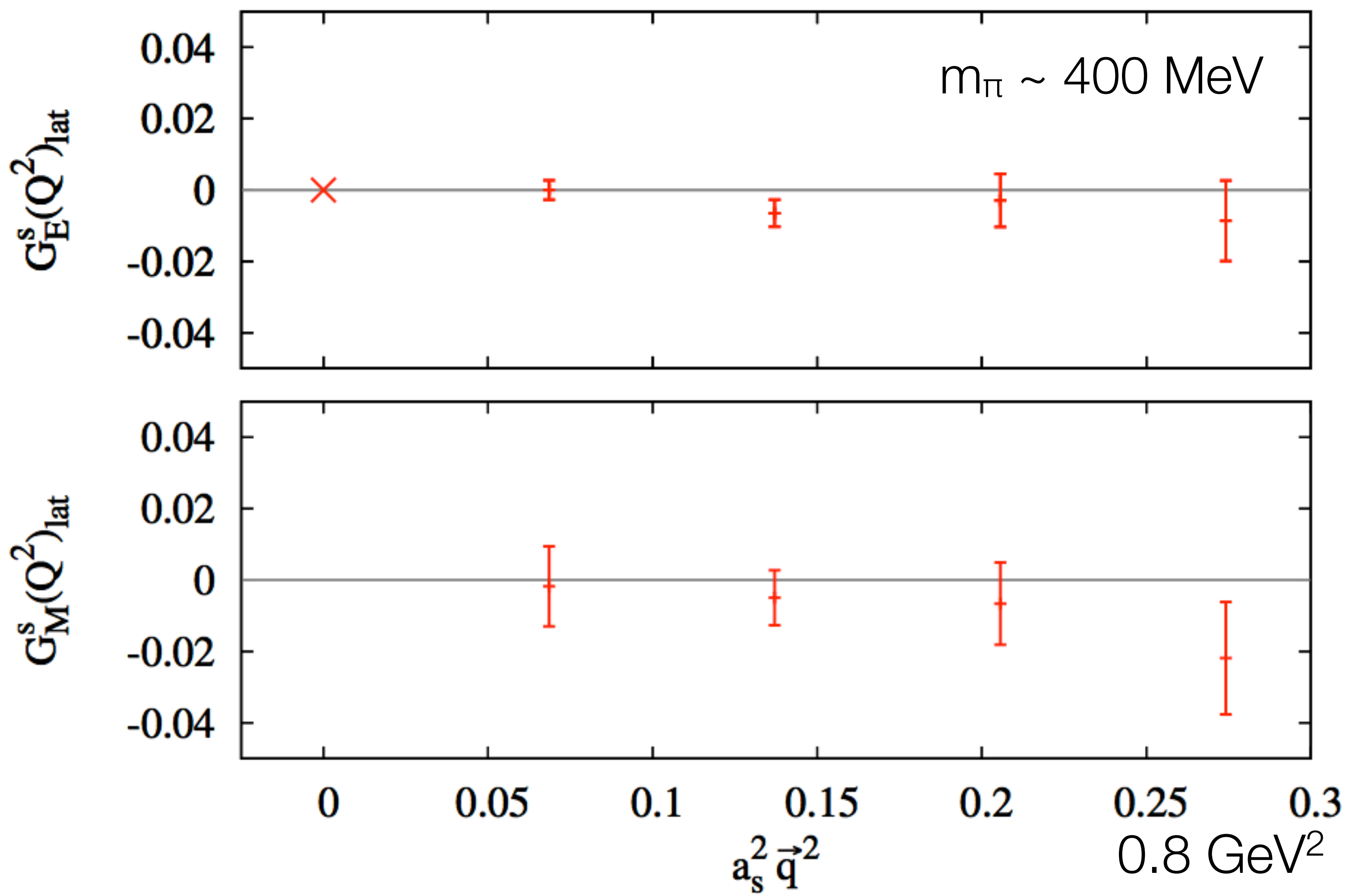
Engelhardt (2012)

$$\Delta s = -0.031(16)(^{+3}_{-1})(1)(4)(3)(4)$$

m_π ~ 140 MeV

Lattice QCD:
Results - Nucleon Strangeness

Babich *et al* 2012

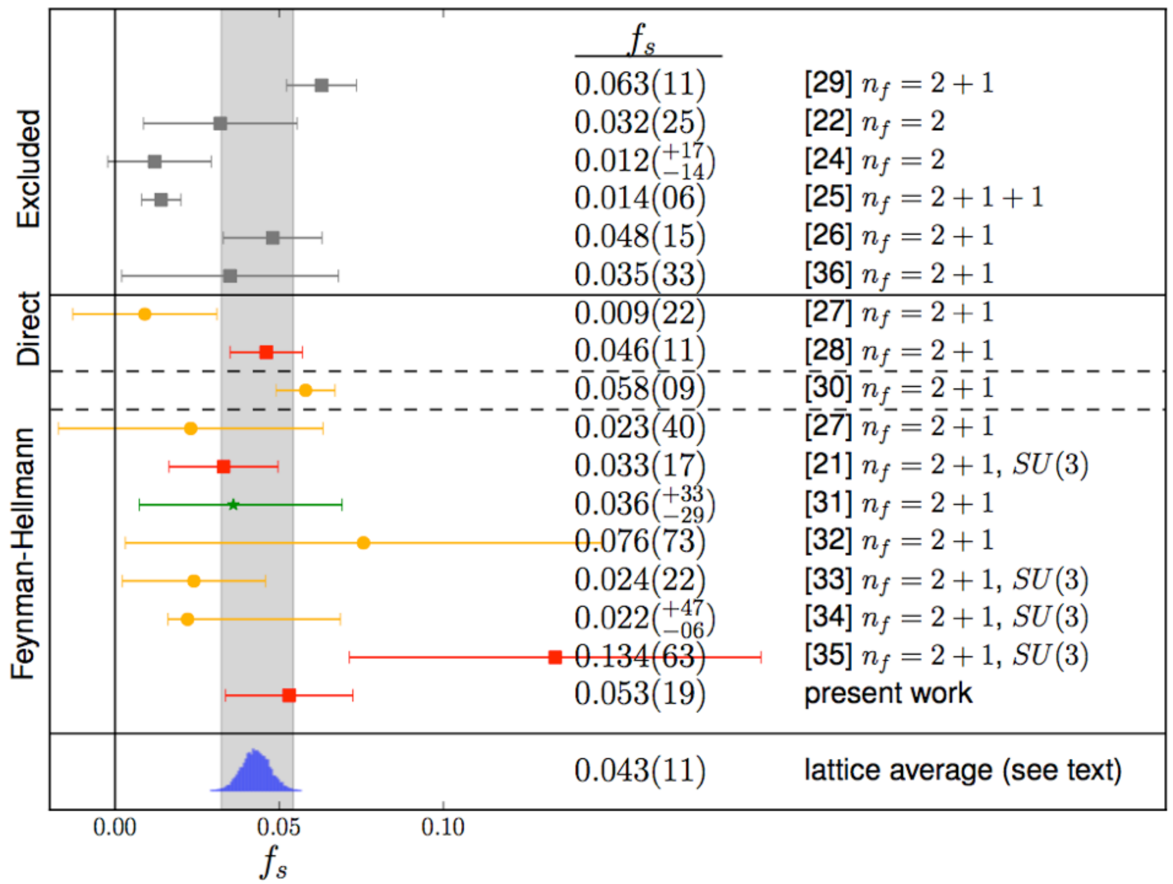


- Recent analysis : Shanahan *et al*, **arXiv:1403.6537**

Lattice QCD:
Results - Nucleon Strangeness

Pari Junnarkar's PhD thesis @ UNH (Beane)

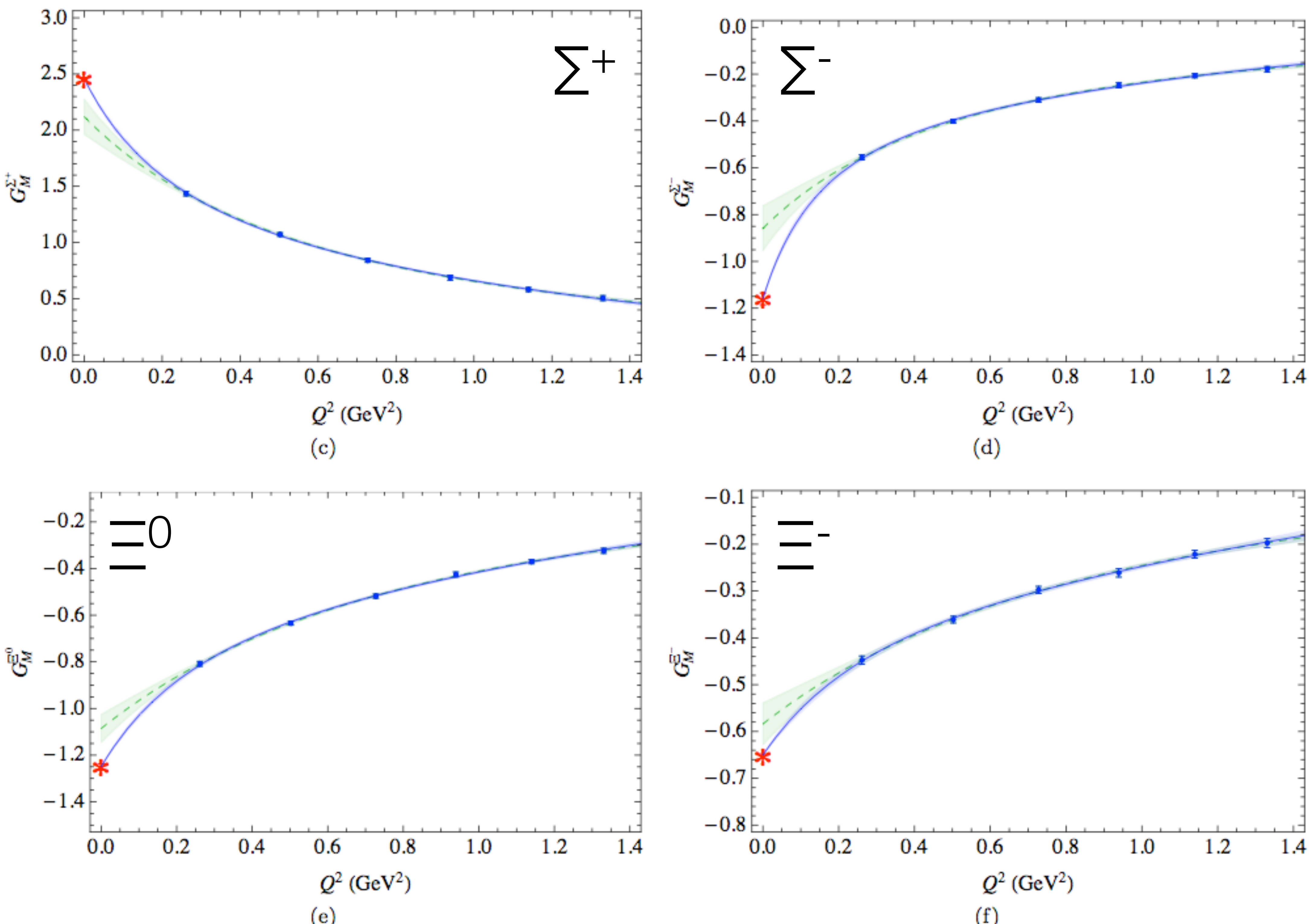
Junnarkar and Walker-Loud, Phys.Rev. D87 (2013) 11, 114510



$$m_s\langle N|\bar{s}s|N\rangle = 48 \pm 10 \pm 15 \text{ MeV},$$
$$f_s = 0.051 \pm 0.011 \pm 0.016$$

- Feynman-Hellmann - 2pt function
  - M_N as a function of m_s
  - multiple ensembles of lattices
- Operator Insertion
  - multiple propagator calculations

Lattice QCD:
Results - Hyperon Magnetic Form Factors



Shanahan *et al*
QCDSF/UKQCD

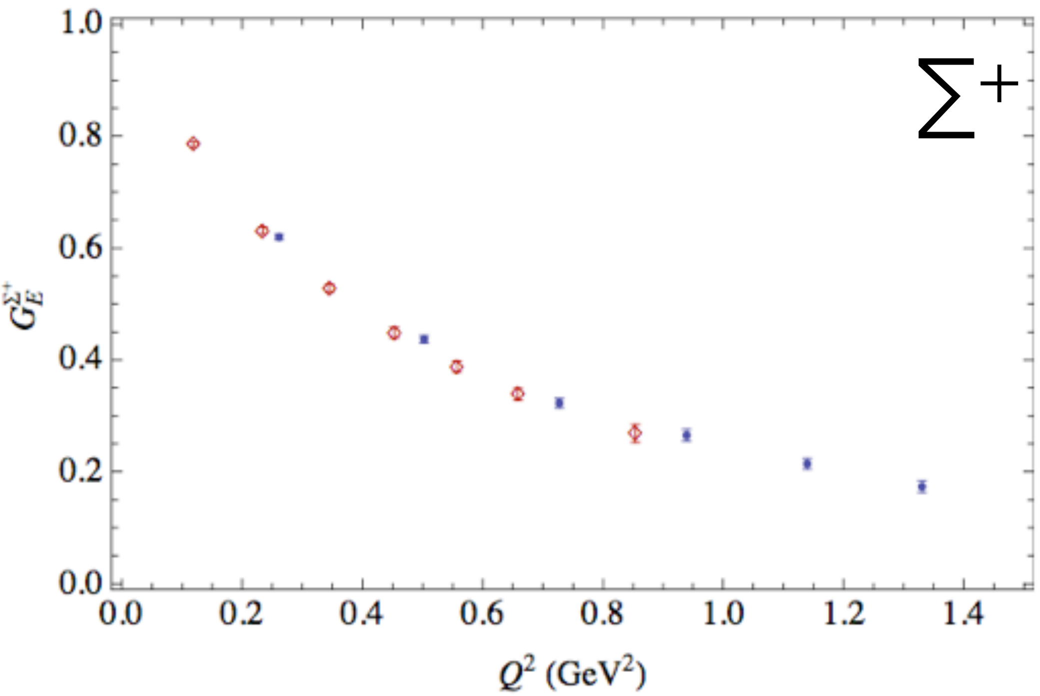
Chirally extrapolated

connected parts only

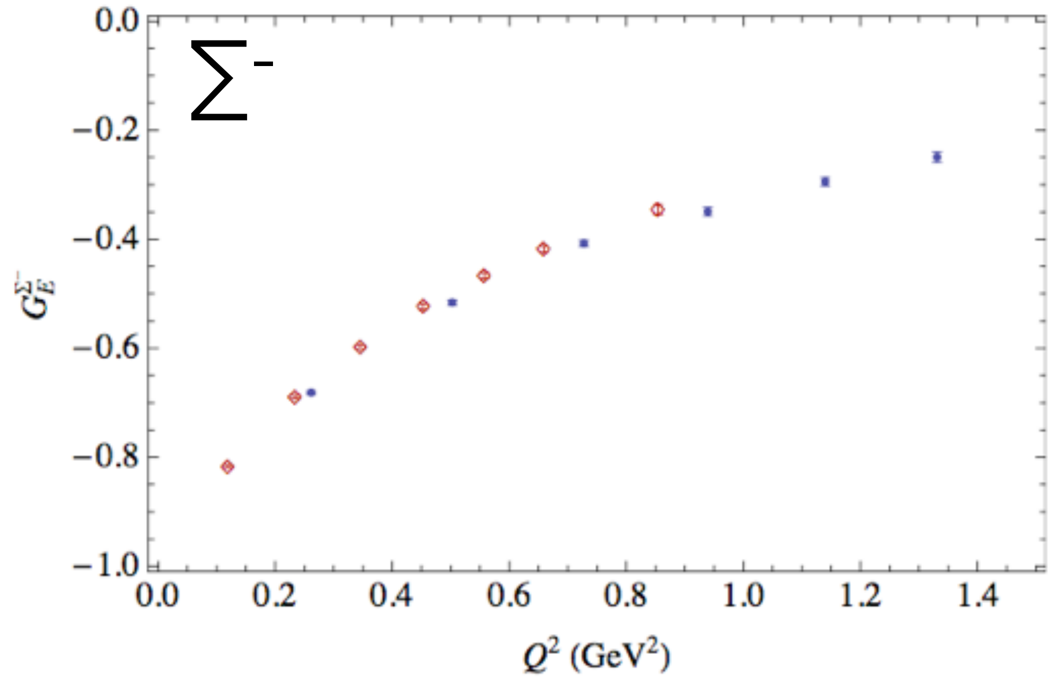
Lattice QCD:

Results - Hyperon Electric Form Factors

Shanahan *et al*
QCDSF/UKQCD

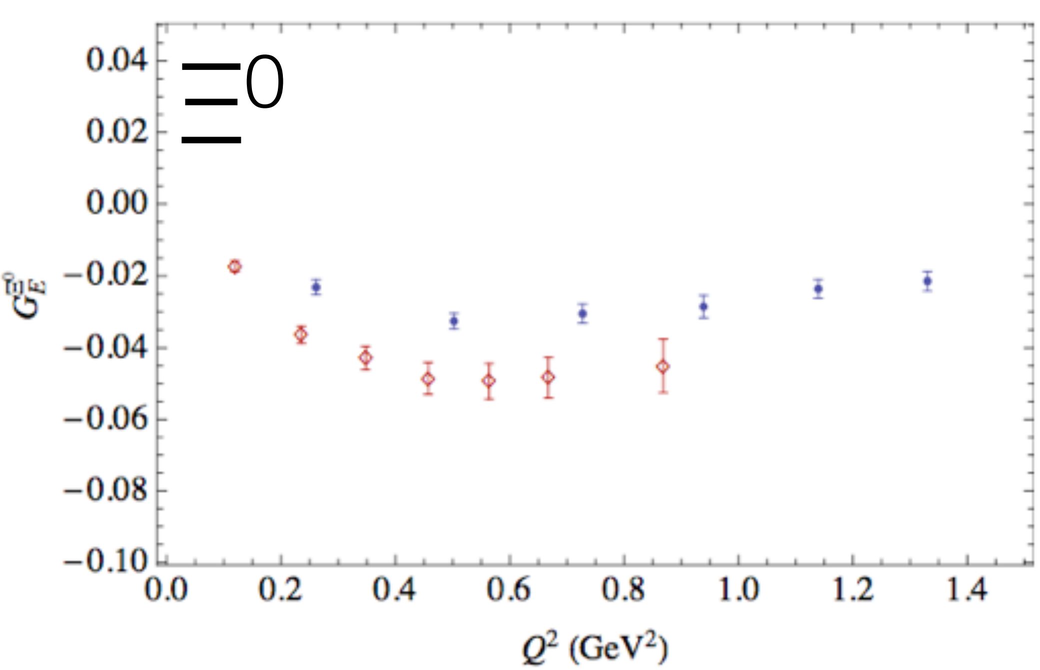


(c)

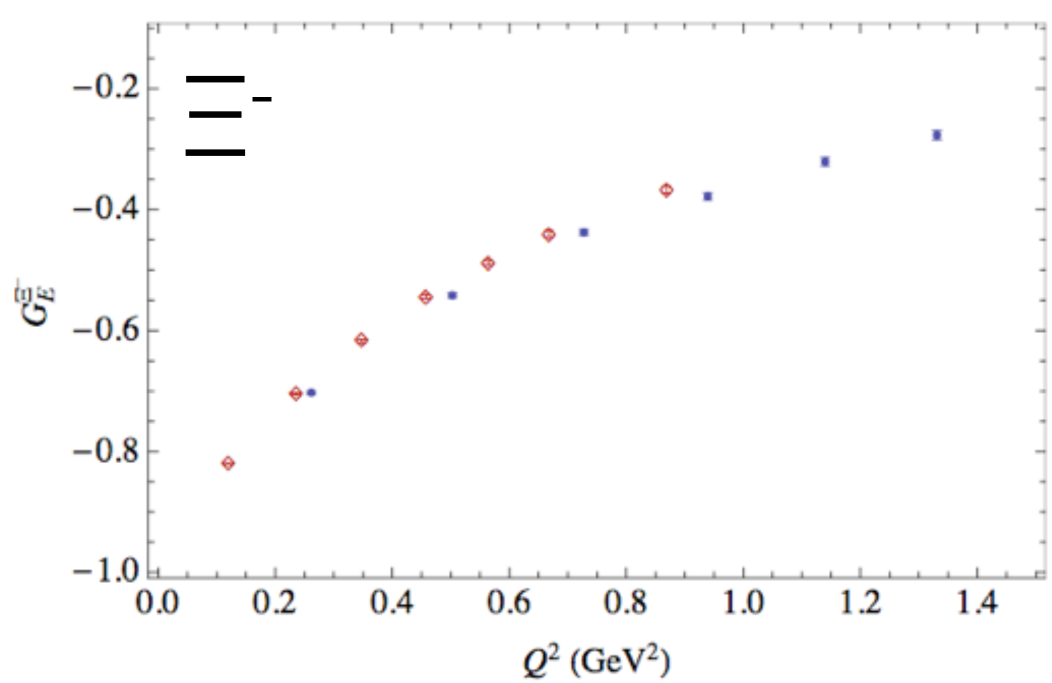


(d)

m_π ~ 220 MeV



(e)

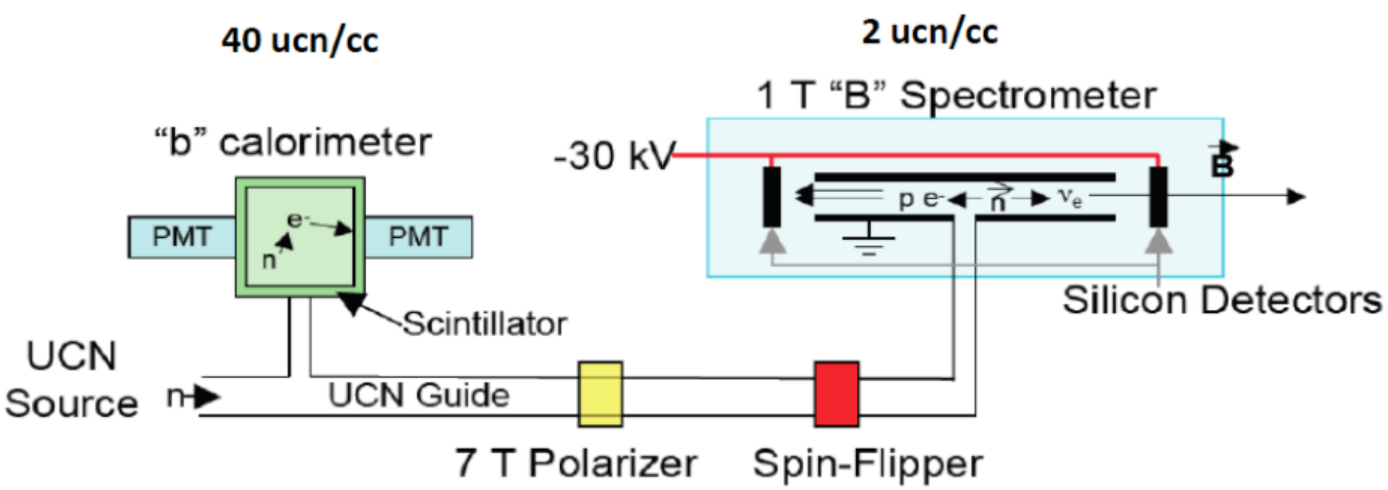


(f)

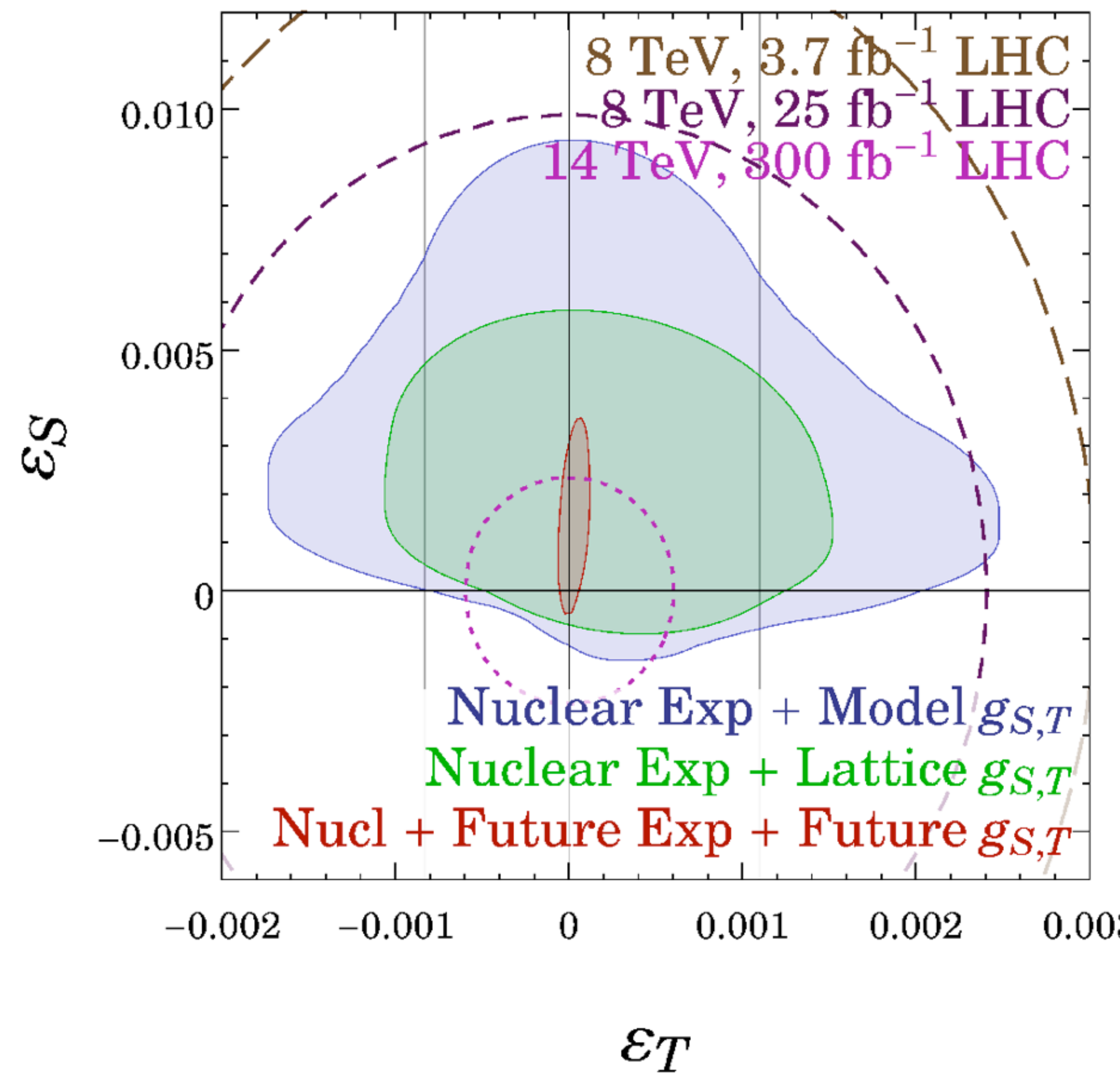
connected parts only

Lattice QCD:

Results - Neutron Beta-Decay - Constraining New Physics



LANL experiment

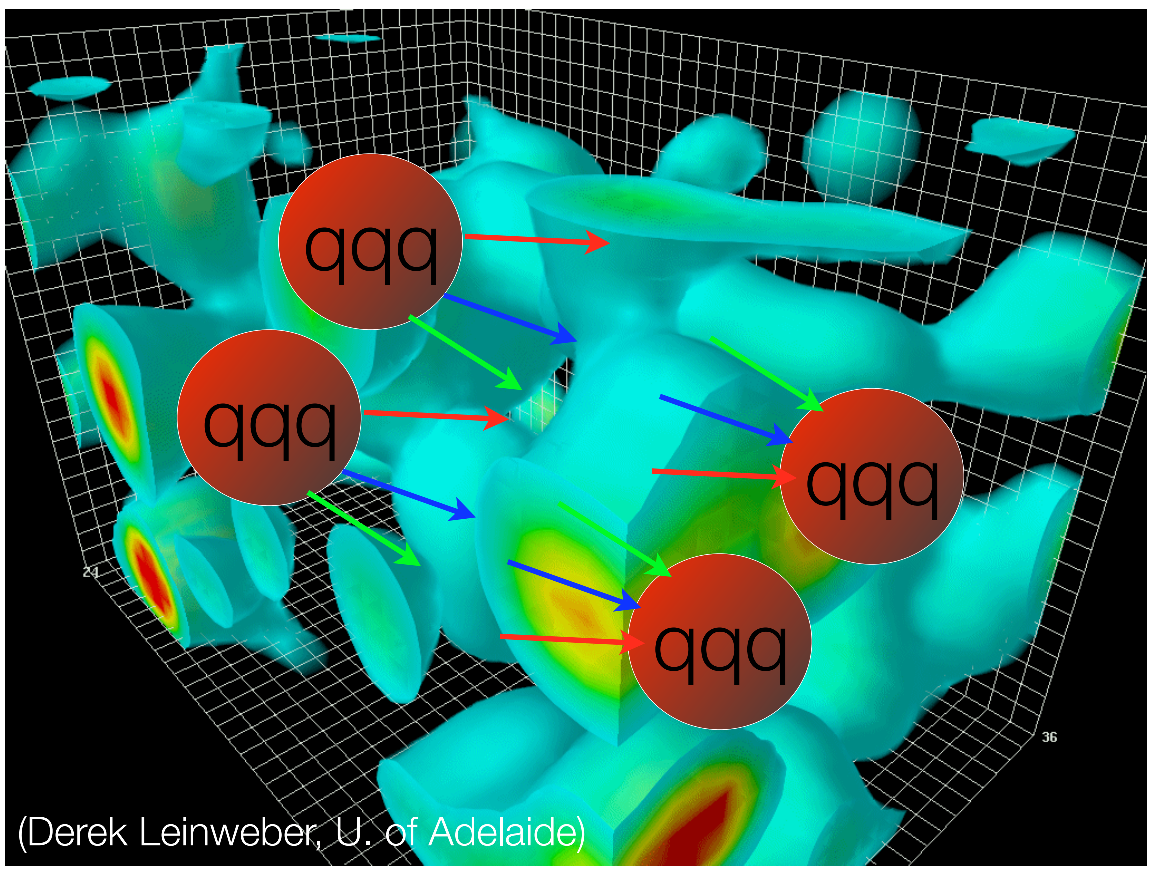


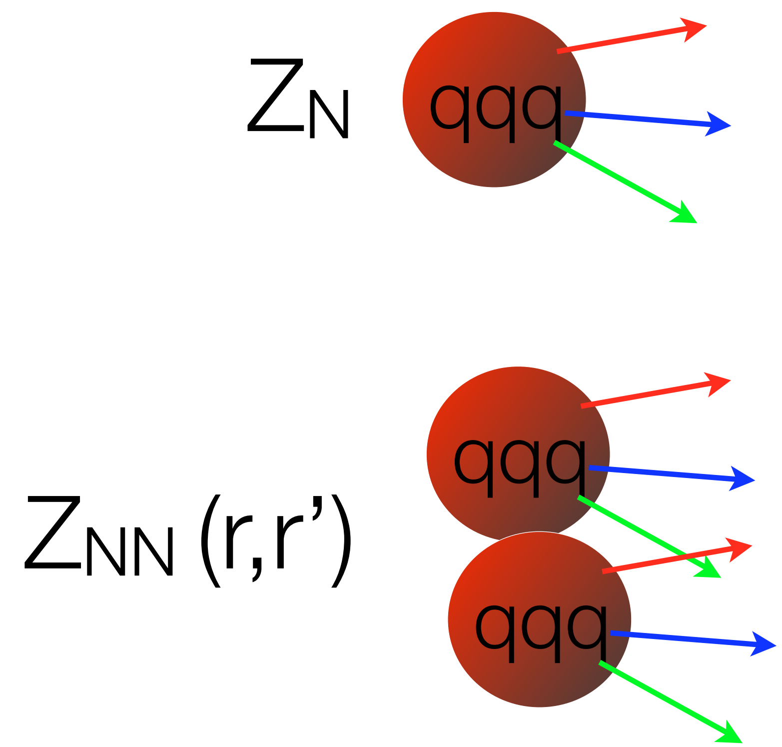
PNDME collab

- LQCD calcs at pion mass of 220 MeV
- Looking toward 140 MeV

Bhattacharya et al, Phys.Rev. D89 (2014) 9, Phys.Rev. D85 (2012) 054512

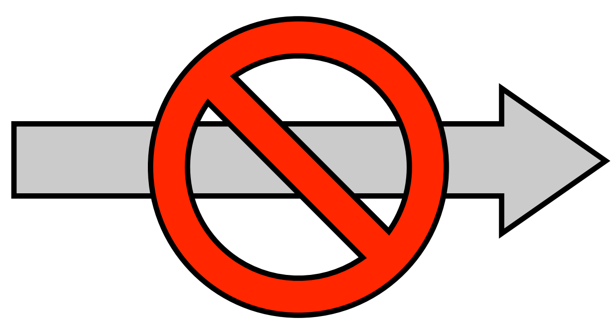
Lattice QCD:
Results - n-Body Physics





- Self-consistent extraction of S-matrix elements, with uncertainty quantification
- V(r) not possible without Modeling

Lattice QCD:
Results - Maiani-Testa Theorem

$G_{NN}(s)^{Euclidean}$  $G_{NN}(s)^{Minkowski}$

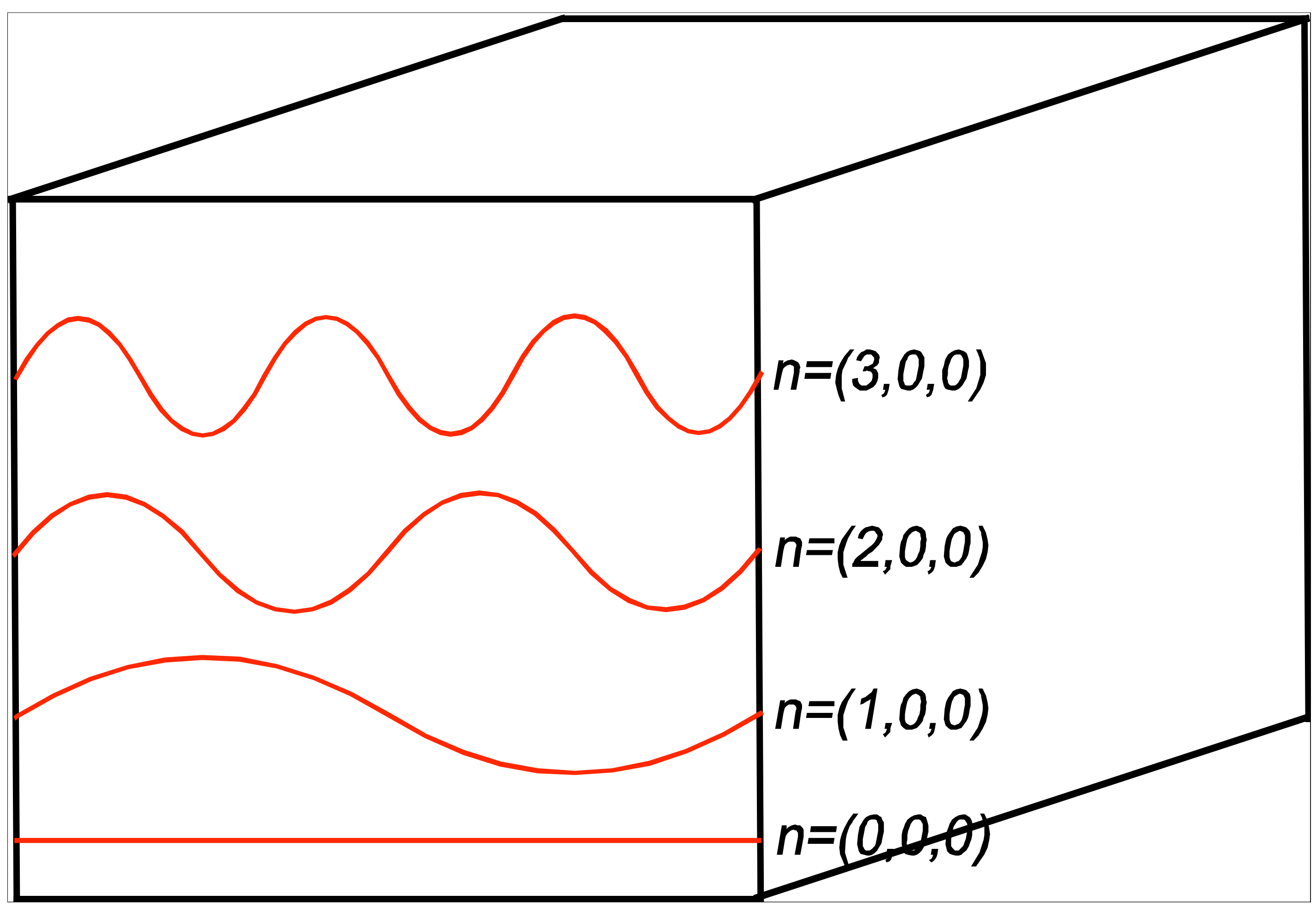
$\delta(s)$?

Lattice QCD:

Results - Luscher’s Quantization Conditions

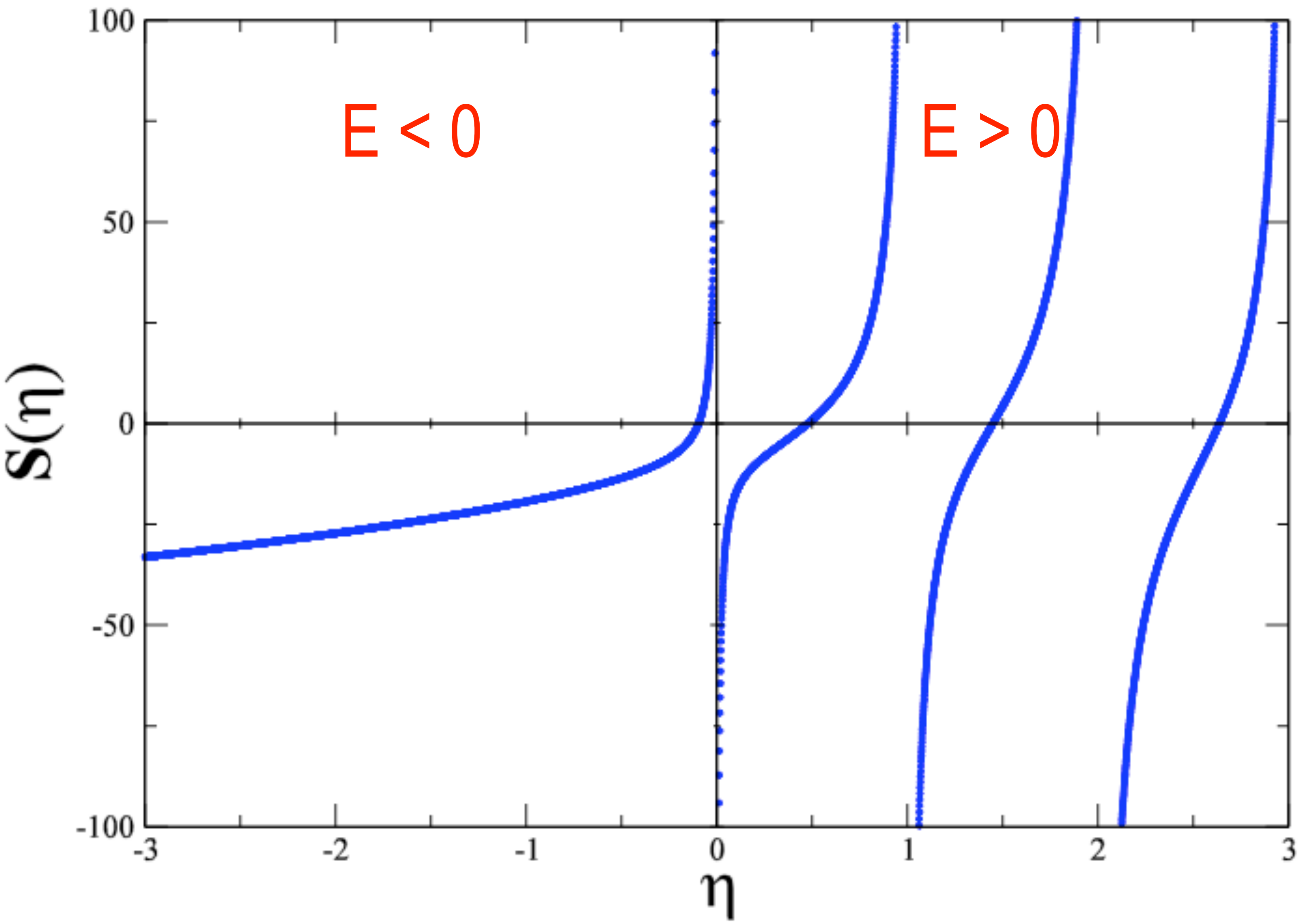
Below Inelastic Thresholds :

Measure on lattice ➡ $$\delta E = 2\sqrt{p^2 + m^2} - 2m$$



Lattice QCD:

Results - Luscher's Quantization Conditions



A_1^+

Bound-state or Scattering state ?

$$p \cot \delta(p) = \frac{1}{\pi L} \mathbf{S}\left(\left(\frac{Lp}{2\pi} \right)^2 \right)$$

$$k = \frac{2\pi}{L} n$$

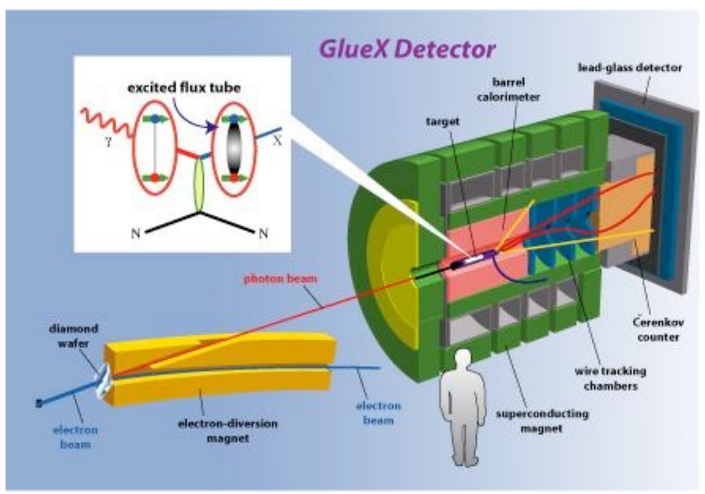
$$n = (nx, ny, nz)$$

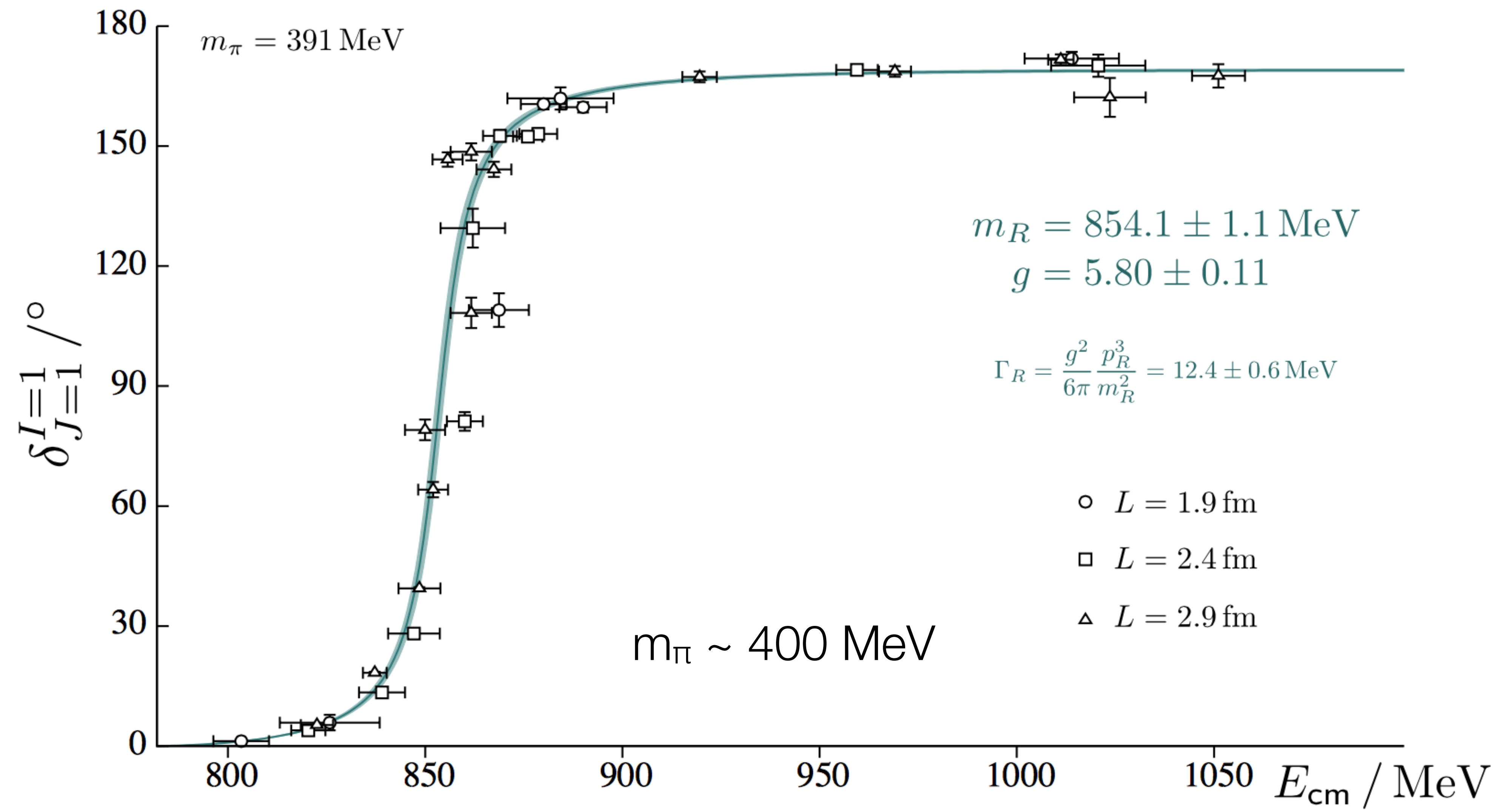
Non-interacting particles

$$V = 0 \quad \rightarrow \quad a = r = 0$$
$$S = \infty$$

Lattice QCD:
Results - Resonances

Dudek *et al*, Phys.Rev. D87 (2013) 3, 034505

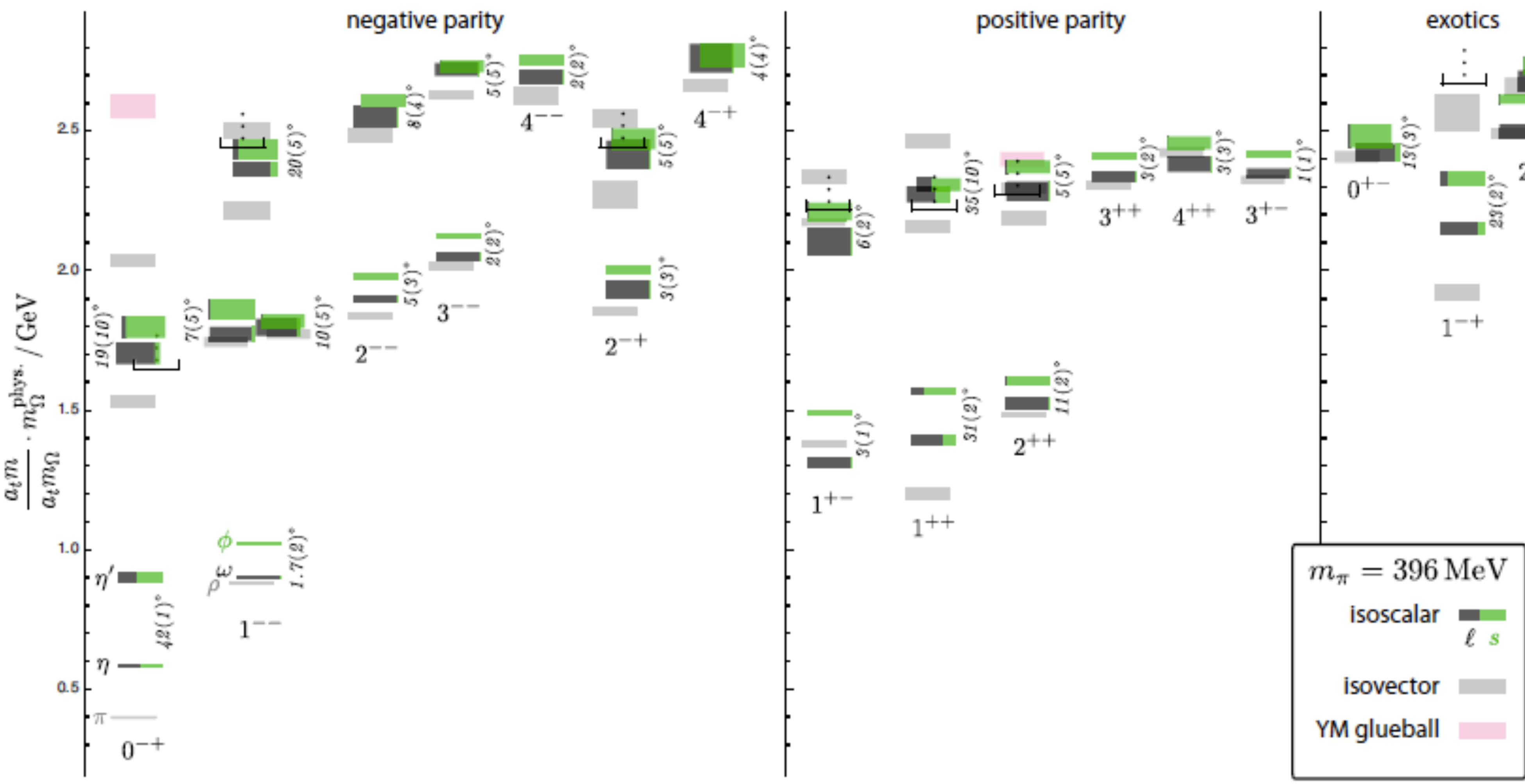


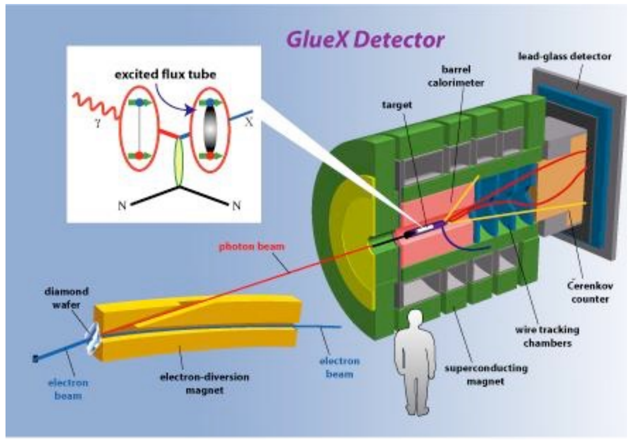


ρ- resonance successfully determined

Lattice QCD:

Results - Excited Meson Spectrum





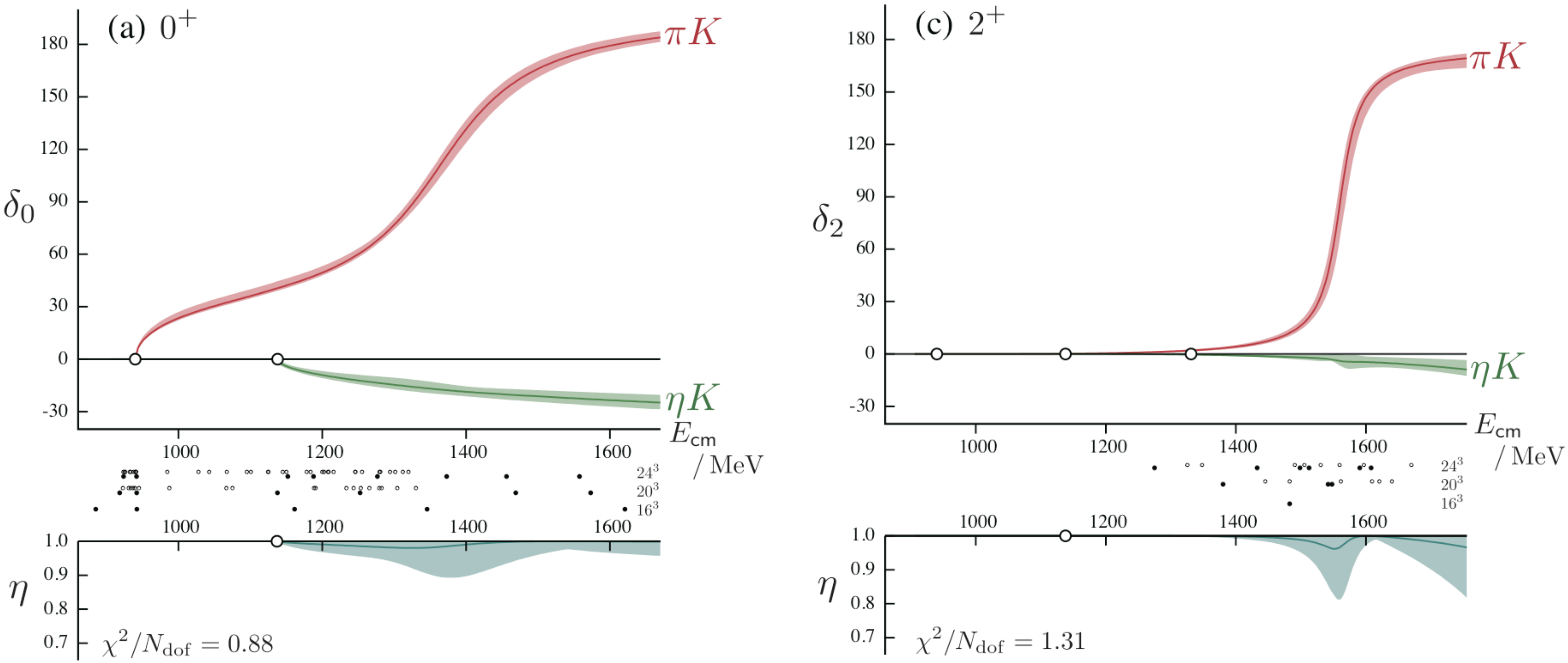
Dudek *et al* , arXiv: 1102.4299

Lattice QCD will predict the exotic spectrum before or during the GlueX experiment

Lattice QCD:
Results - Coupled Channels

m_π ~ 390 MeV

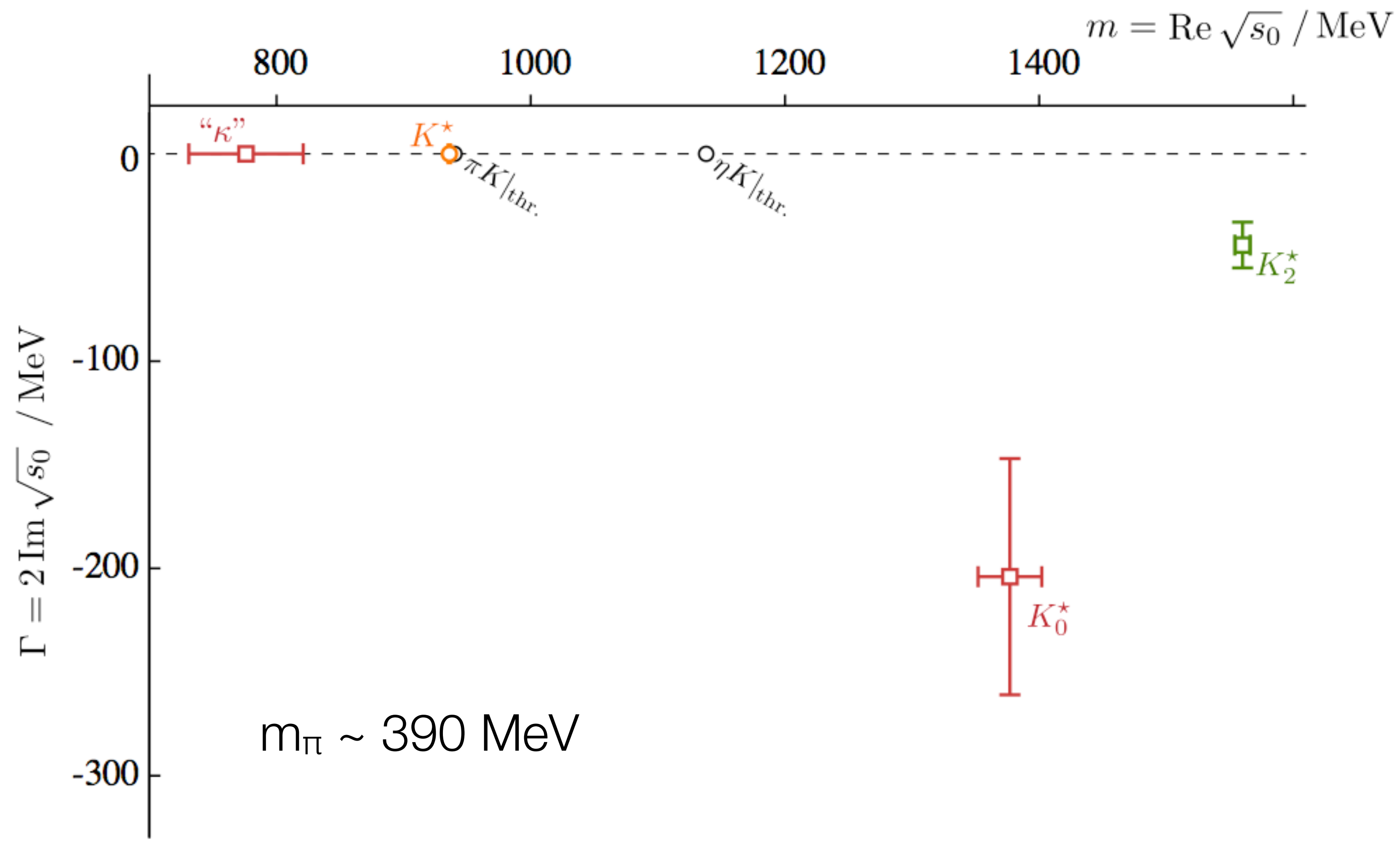
Dudek *et al*



- Parameterization of the T-matrix required
- Regions include systematics from many different params.

Lattice QCD:
Results - Coupled Channels

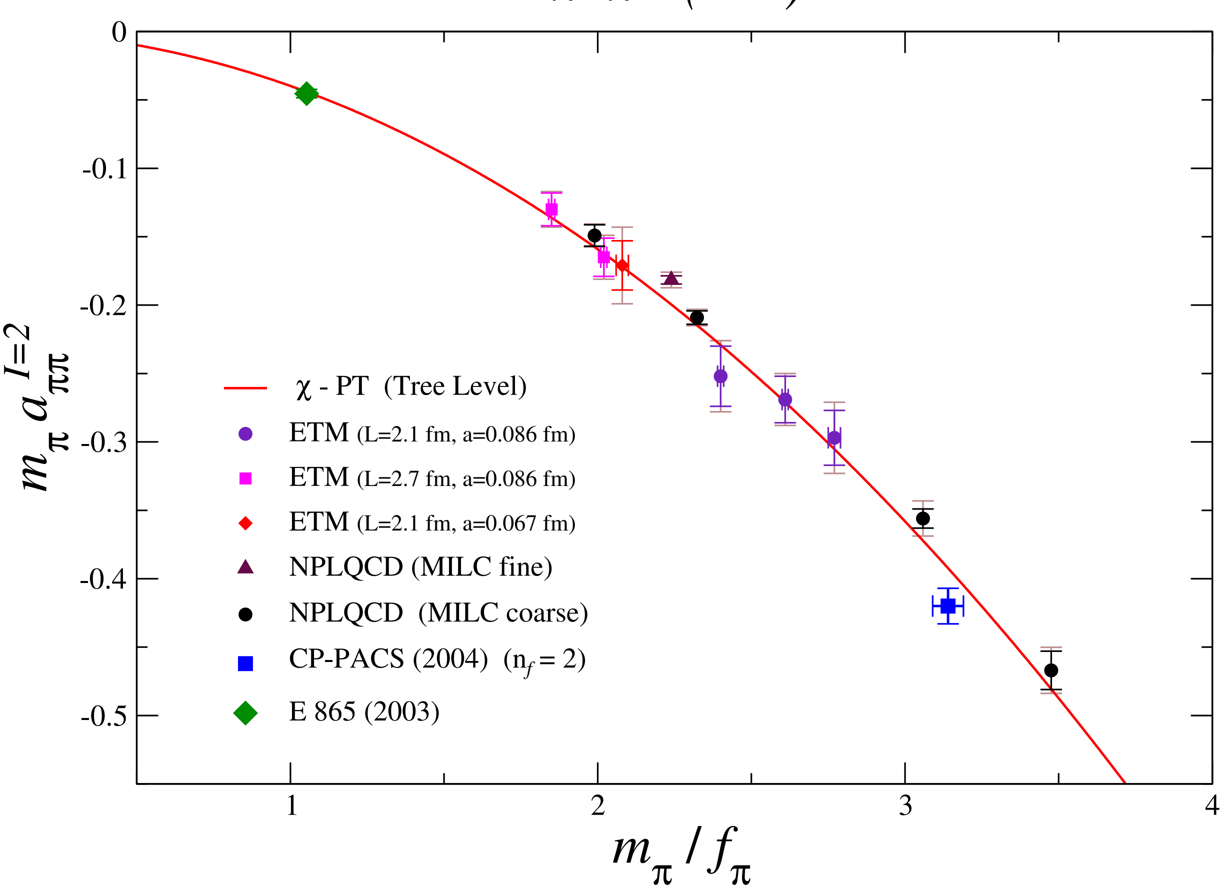
Dudek *et al.*



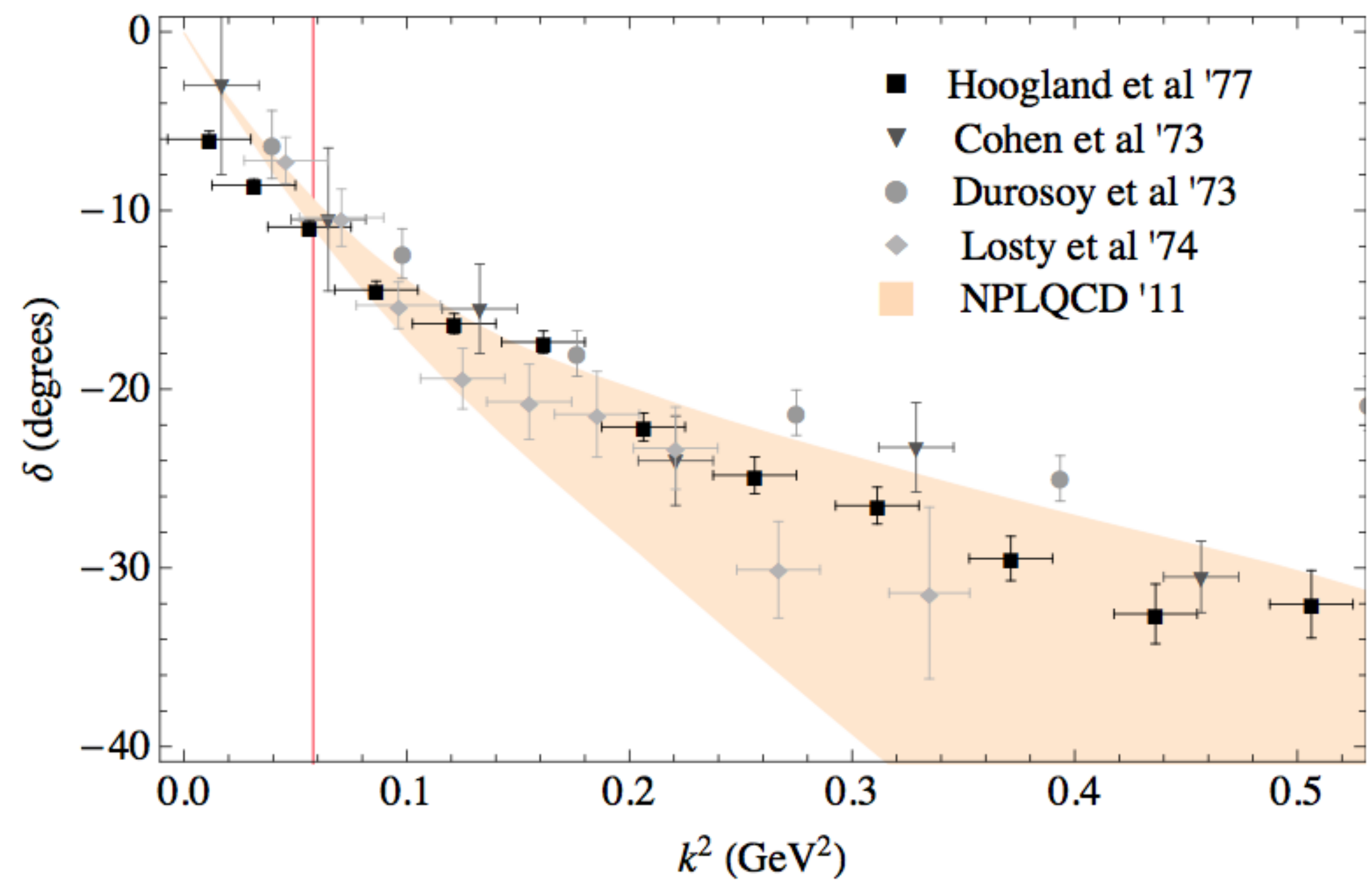
- Bound states and Resonances from T-matrix
- QCD predictions at these quark masses
- Efforts to extend to multi-hadron coupled channels
- Extended to KK systems, but less developed

Lattice QCD:
Results - I=2 pion-pion Scattering

$\pi^+\pi^+$ $(I=2)$

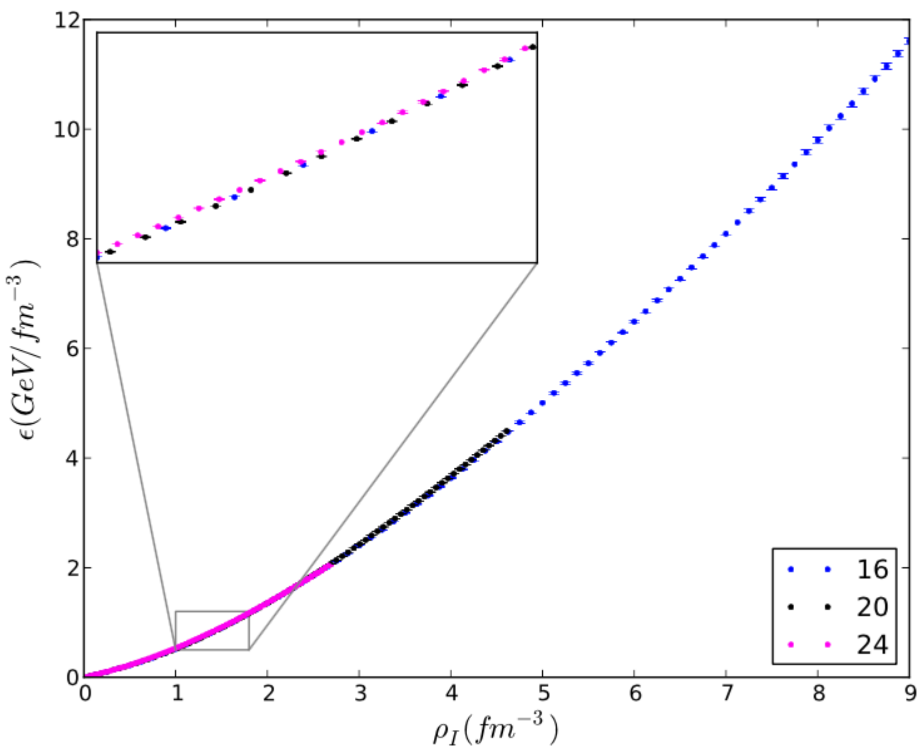


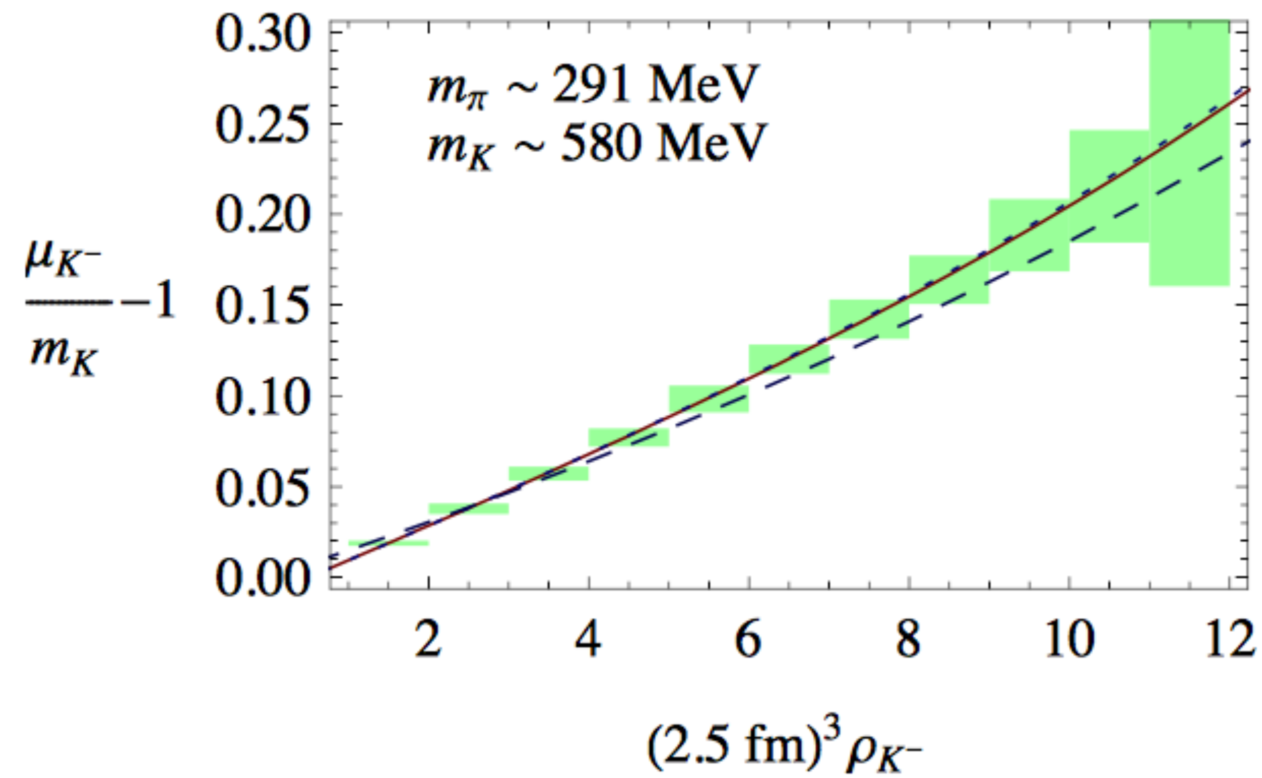
χPT extrapolation to nature



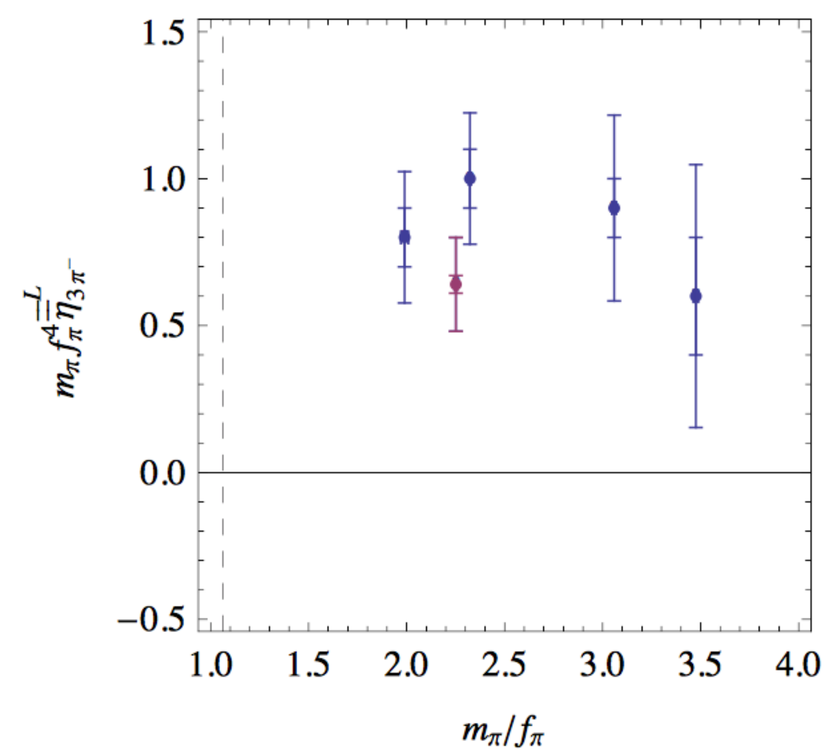
Lattice QCD:

Results - Multi-Meson Systems



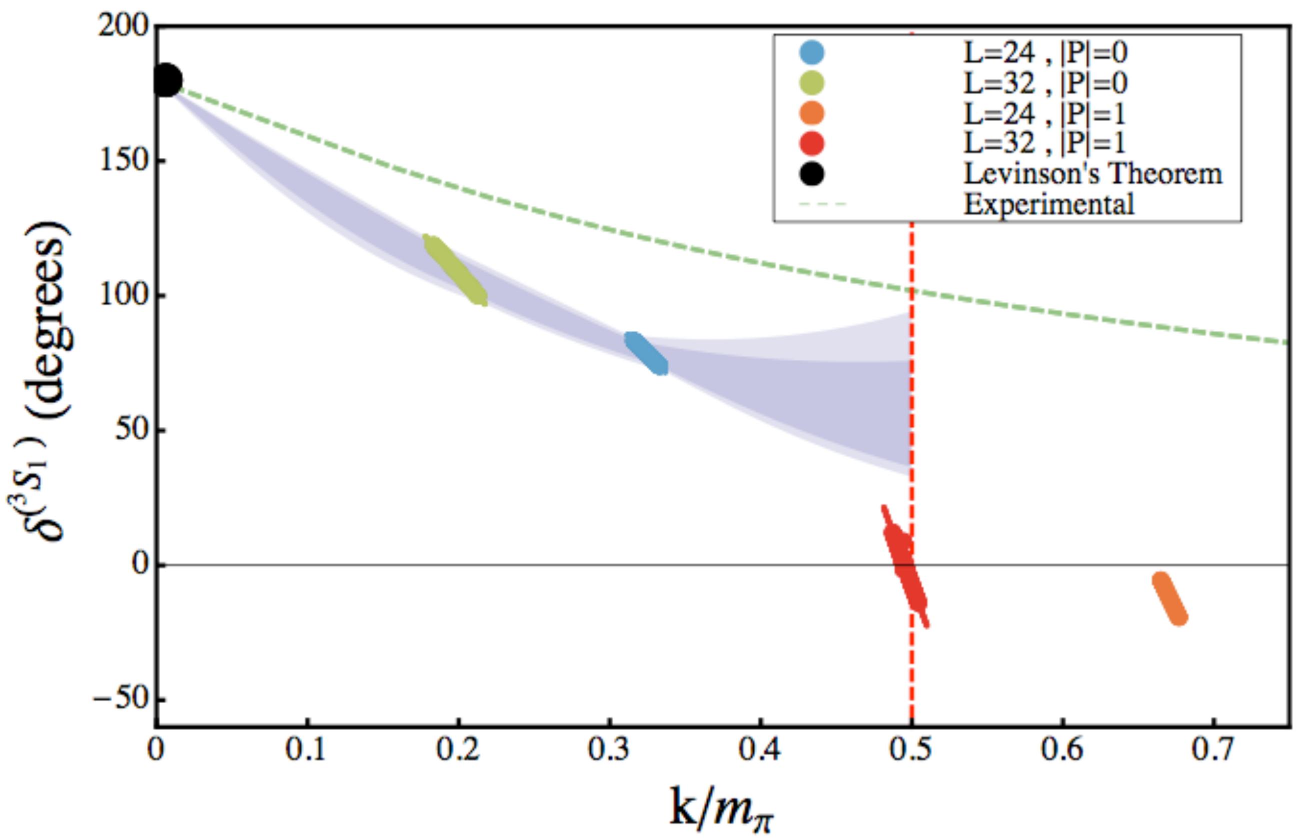


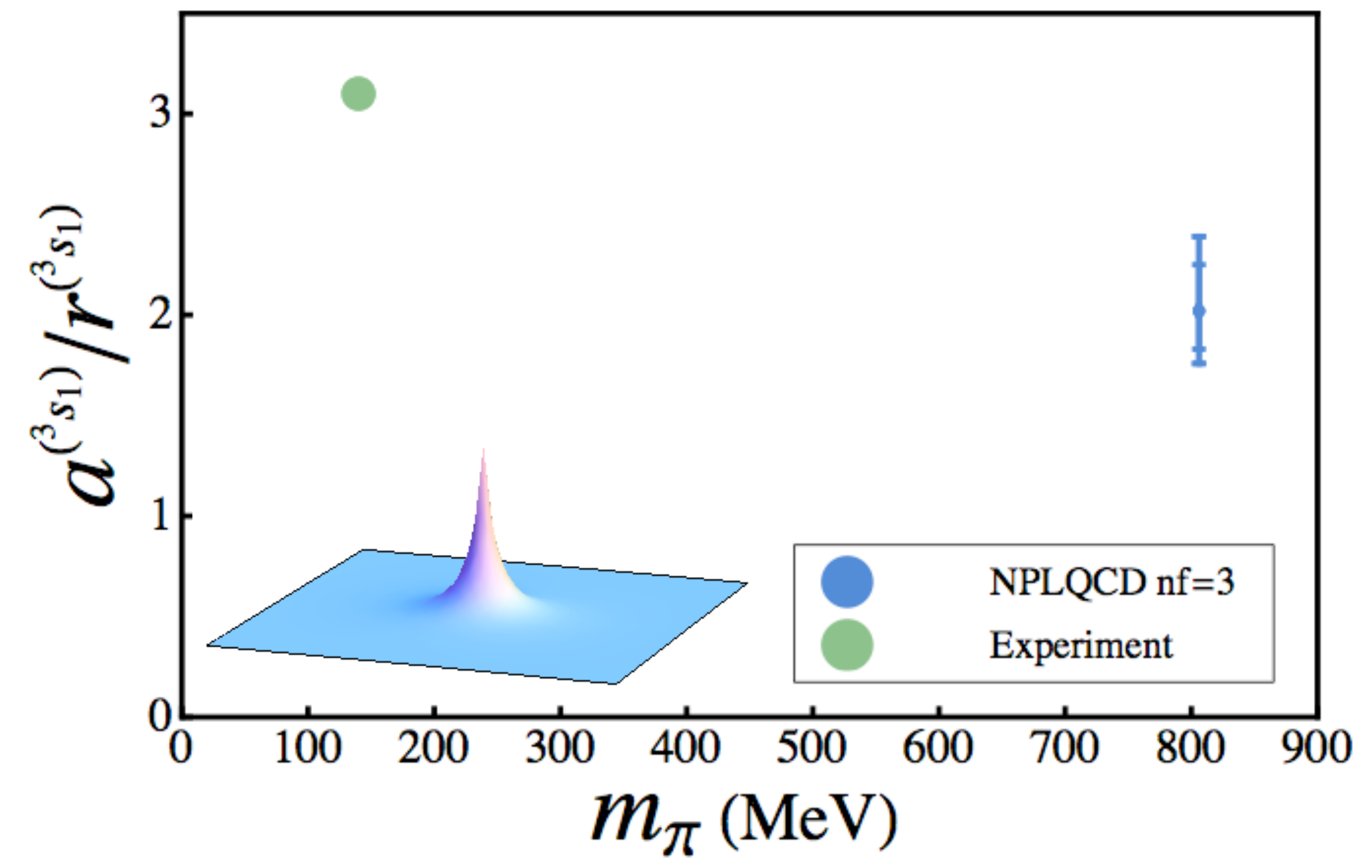
$$\Delta E_n = \frac{4\pi\,\bar{a}}{M\,L^3}\,{}^nC_2\left\{1 - \left(\frac{\bar{a}}{\pi\,L}\right)\mathcal{I} + \left(\frac{\bar{a}}{\pi\,L}\right)^2\left[\mathcal{I}^2 + (2n-5)\mathcal{J}\right]\right.$$
$$- \left(\frac{\bar{a}}{\pi\,L}\right)^3\left[\mathcal{I}^3 + (2n-7)\mathcal{I}\mathcal{J} + \left(5n^2 - 41n + 63\right)\mathcal{K}\right]$$
$$+ \left(\frac{\bar{a}}{\pi\,L}\right)^4\left[\mathcal{I}^4 - 6\mathcal{I}^2\mathcal{J} + (4+n-n^2)\mathcal{J}^2 + 4(27-15n+n^2)\mathcal{I}\,\mathcal{K}\right.$$
$$\left.\left. + (14n^3 - 227n^2 + 919n - 1043)\mathcal{L}\,\right]\right\}$$
$$+\ {}^nC_3\left[\frac{192\,\bar{a}^5}{M\pi^3L^7}\left(\mathcal{T}_0 + \mathcal{T}_1\,n\right) + \frac{6\pi\bar{a}^3}{M^3L^7}\,(n+3)\,\mathcal{I}\right]$$
$$+\ {}^nC_3\,\frac{1}{L^6}\,\bar{\bar{\eta}}_3^{L} + \mathcal{O}\left(L^{-8}\right) \quad ,$$



Lattice QCD:

Results - Nucleon-Nucleon Scattering



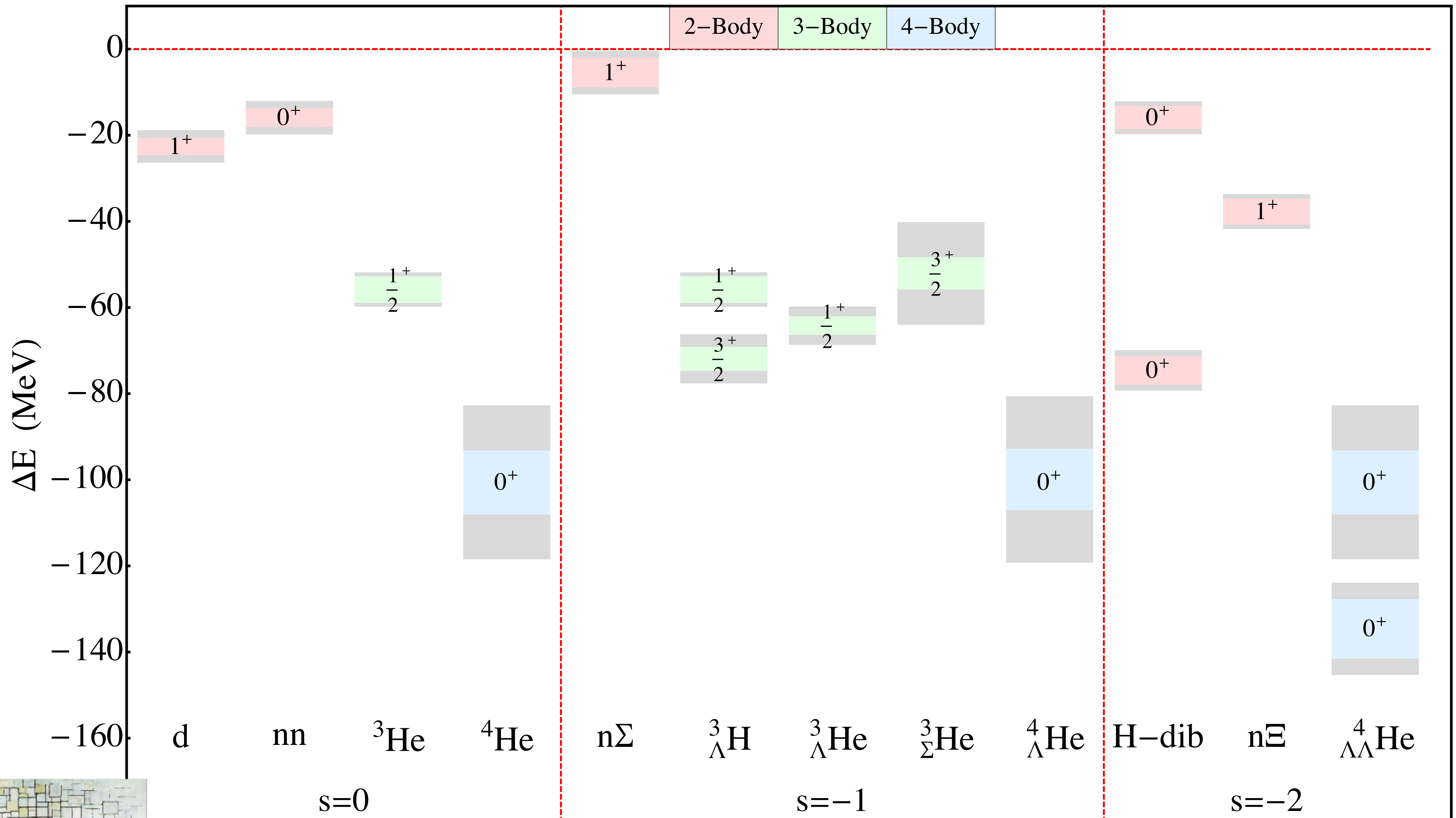


m_π ~ 800 MeV

Deuteron appears to be unnatural but not finely-tuned ??

Generic feature of YM with n_f=3

Lattice QCD:
Results - Nuclei



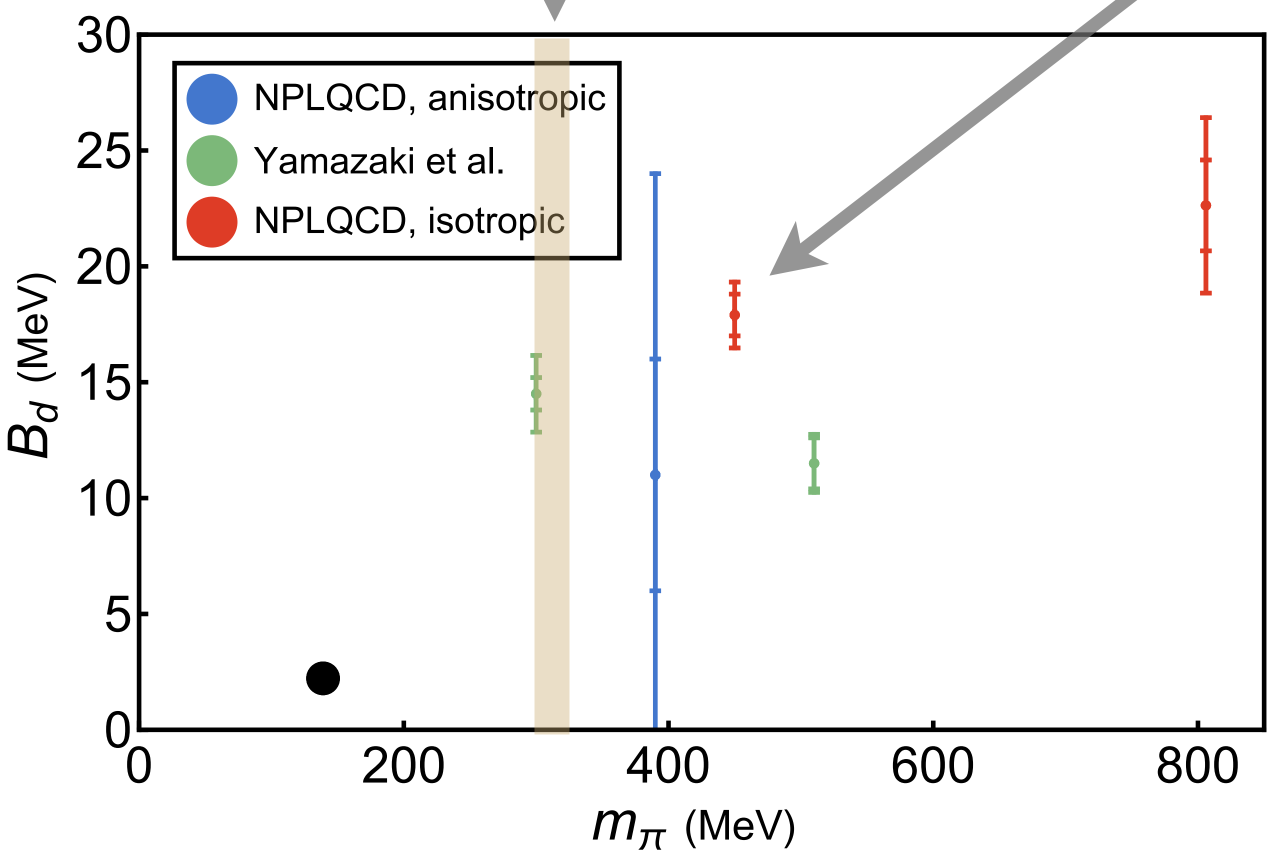
m_π ~ 800 MeV

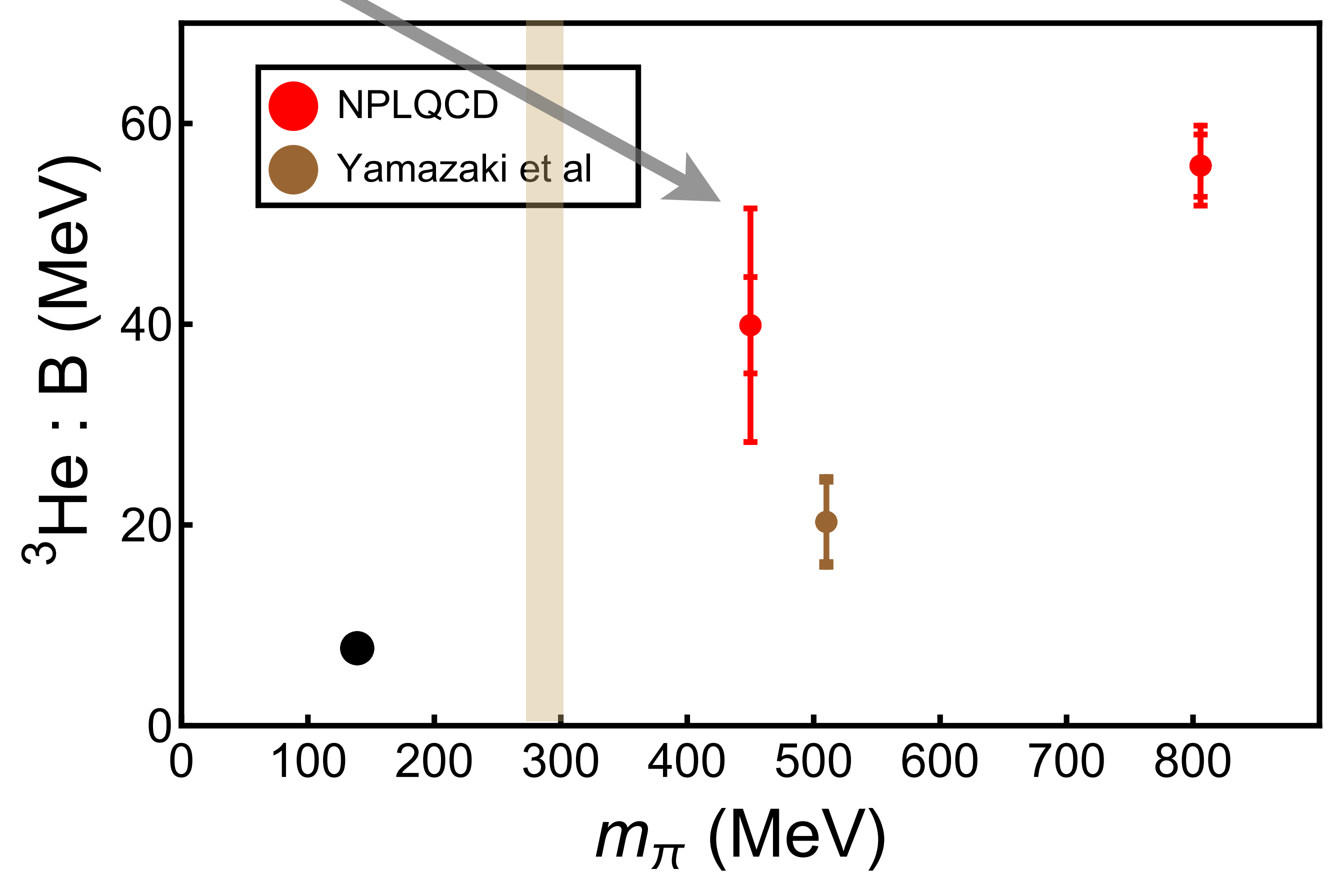
Lattice QCD:

Results - Nuclei - Quark-Mass Dependence

current production

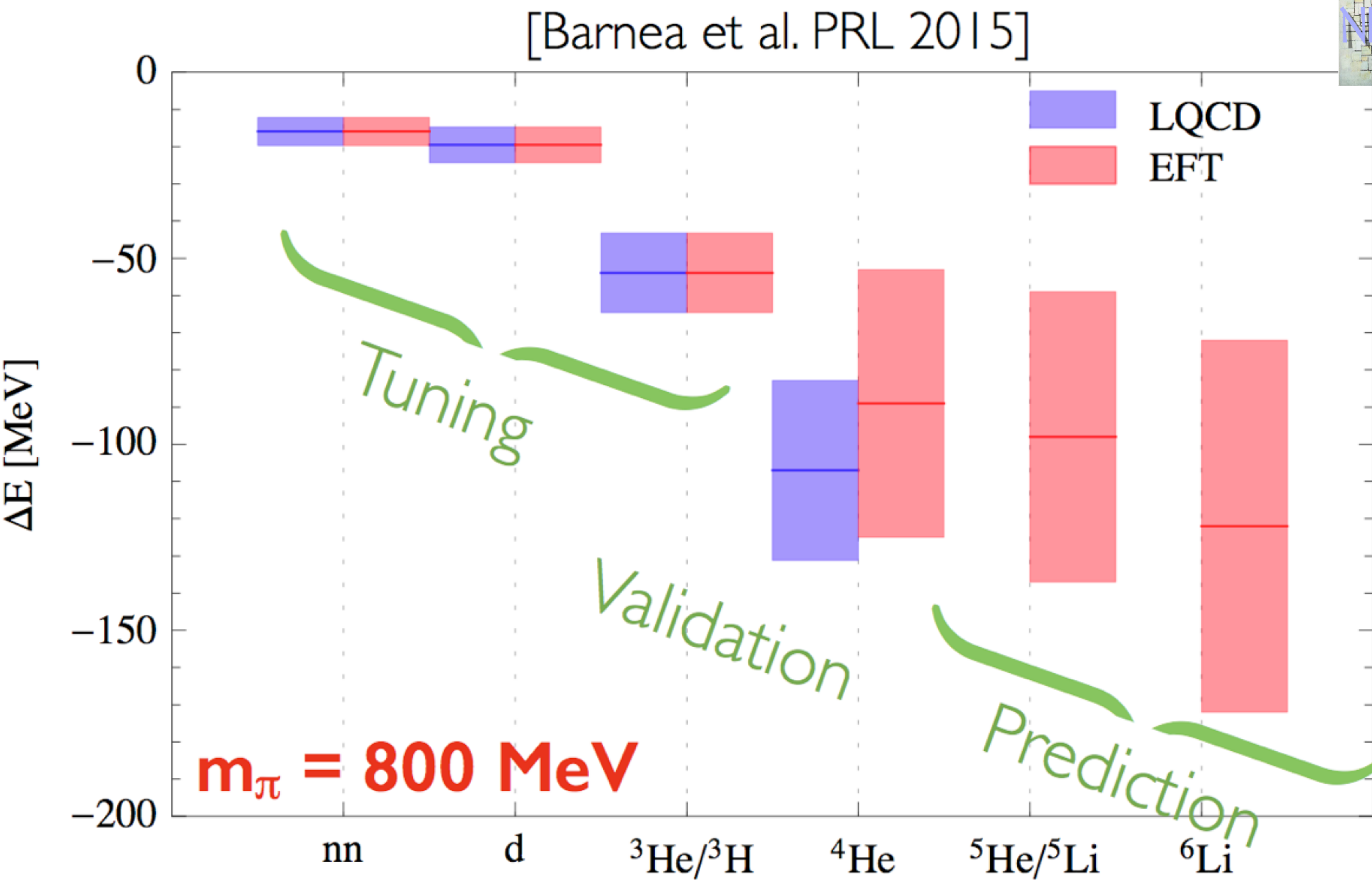
preliminary





Lattice QCD:

Results - Nuclei - Toward the Periodic Table



Lattice QCD:

Results - Nuclei - Dark Matter Interactions(?)

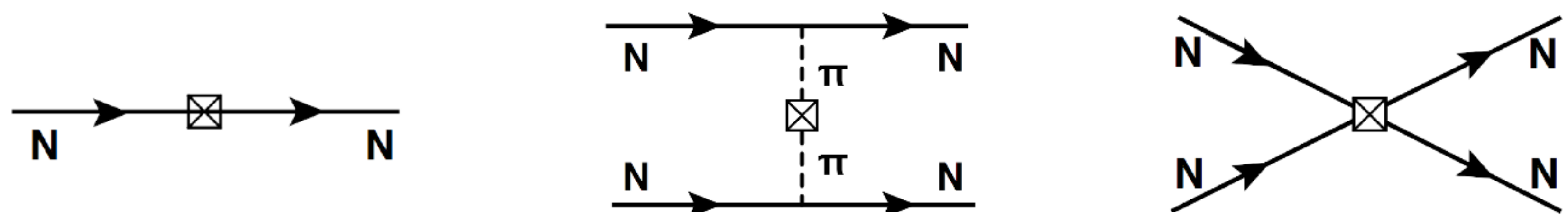
Nuclear σ-terms

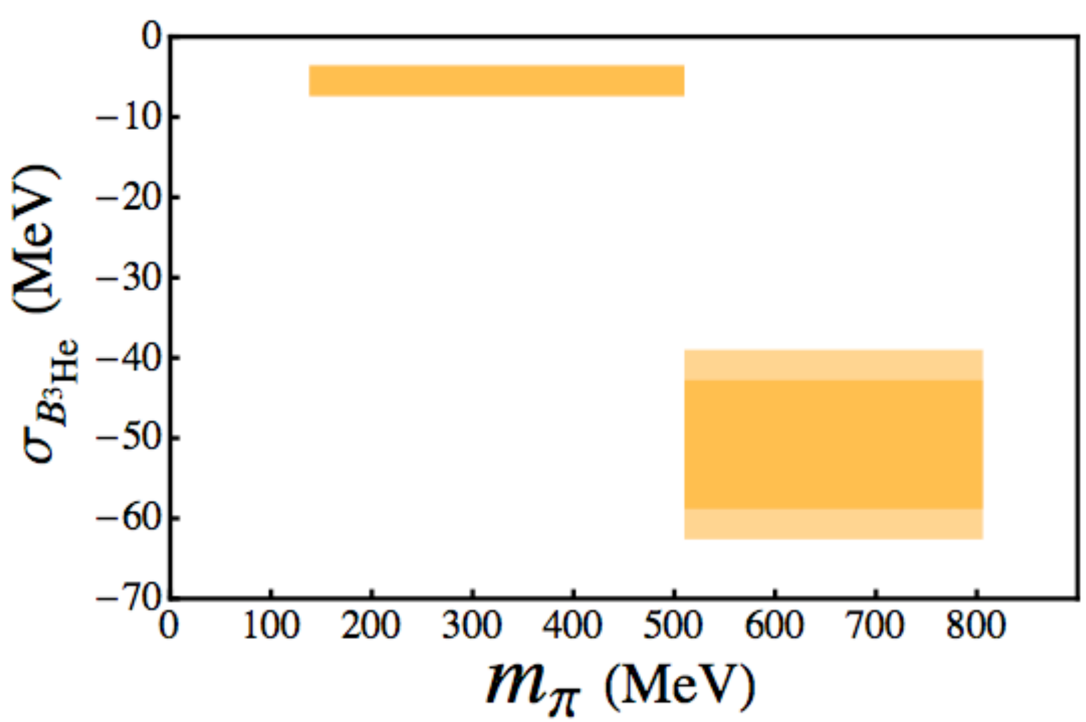
(Beane *et al*, Phys.Rev. D89 (2014) 074505)

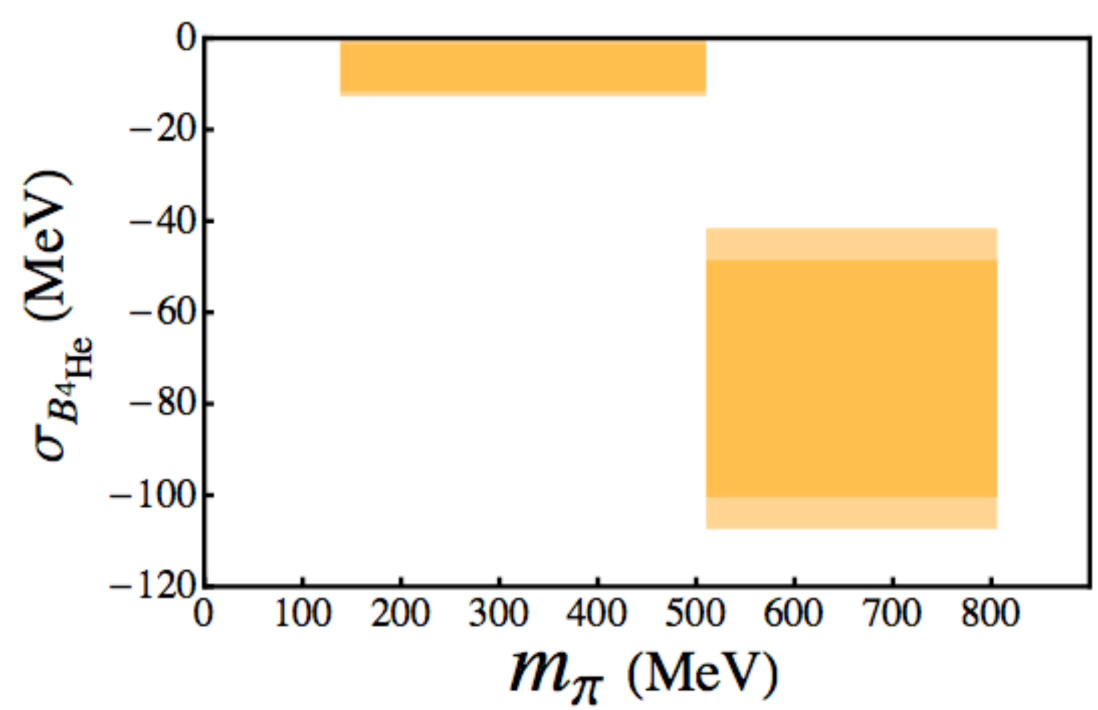
$$\sigma_{Z,N} = \overline{m}\langle Z,N(\mathrm{gs})|\ \overline{u}u + \overline{d}d\ |Z,N(\mathrm{gs})\rangle = \overline{m}\frac{d}{d\overline{m}}E^{(\mathrm{gs})}_{Z,N}$$

$$= \left[\ 1\ +\ \mathcal{O}\left(m_\pi^2\right)\ \right]\frac{m_\pi}{2}\frac{d}{dm_\pi}E^{(\mathrm{gs})}_{Z,N}$$

σ-term from binding only



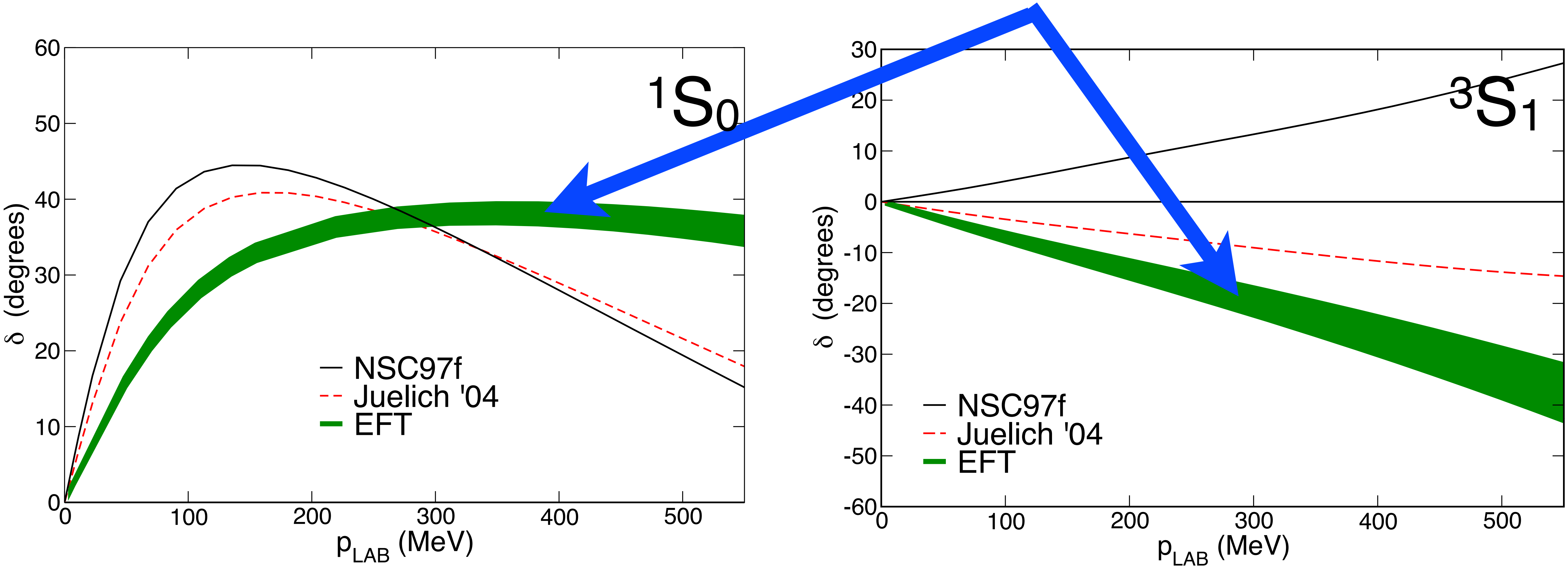




Lattice QCD:

Results - Hyperon-Nucleon Interactions

Meissner+Haidenbauer - Experiment + YN-EFT (LO)

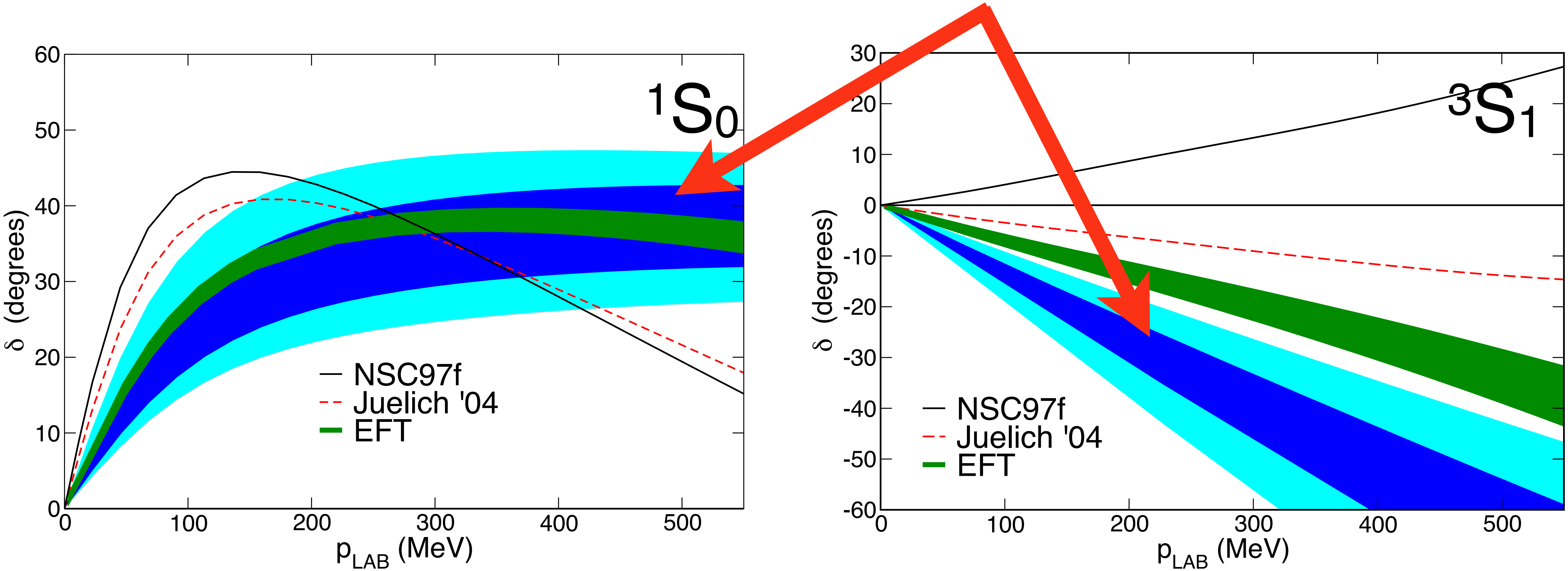


Cancellation between channels in dense matter energy-shift of hyperon

Lattice QCD:

Results - Hyperon-Nucleon Interactions

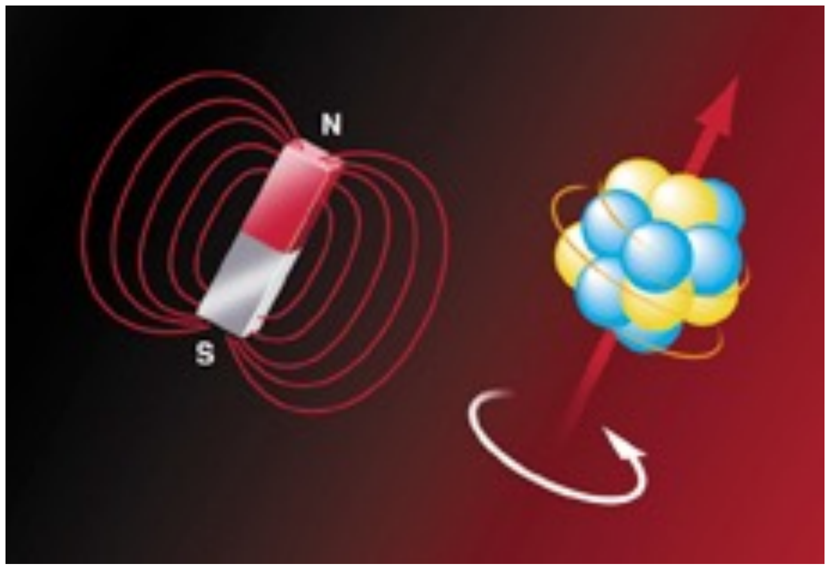
NPLQCD - Lattice QCD + YN-EFT (LO)



Cancellation between channels in dense matter energy-shift of hyperon

Lattice QCD:

Results - Nuclear Magnetic Moments

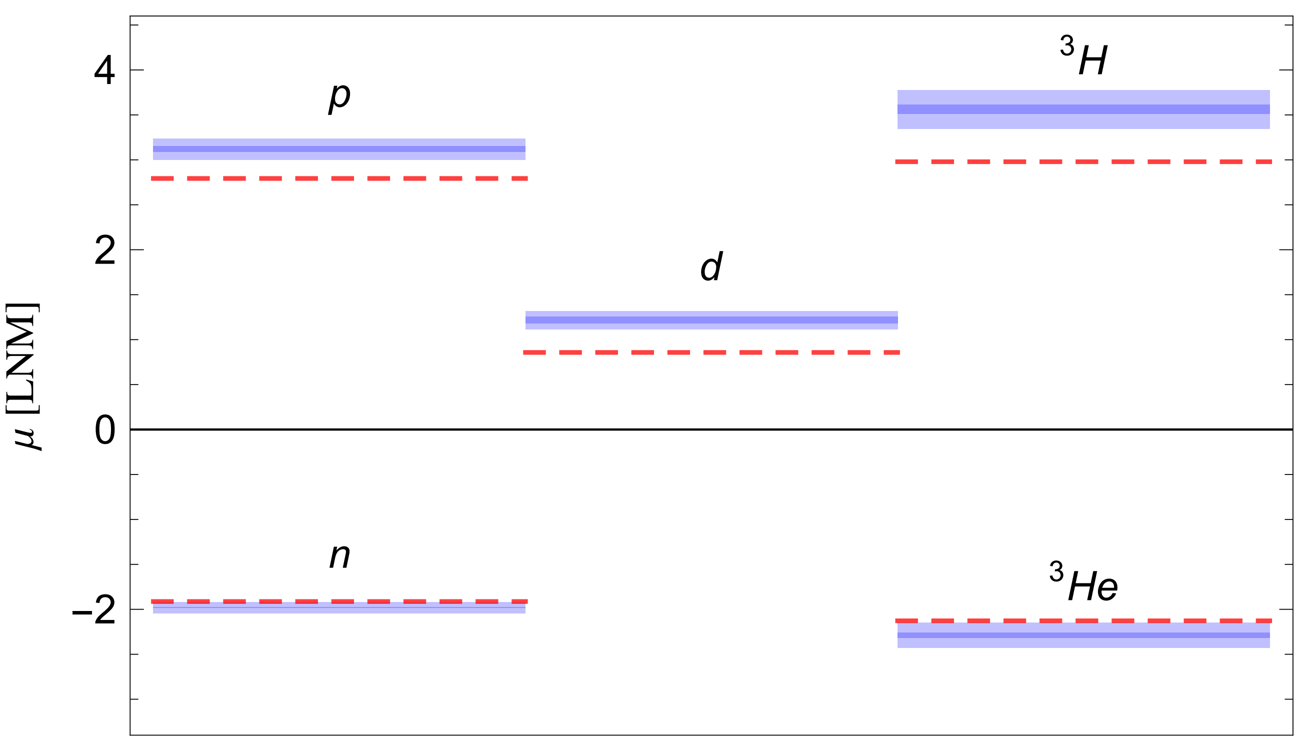


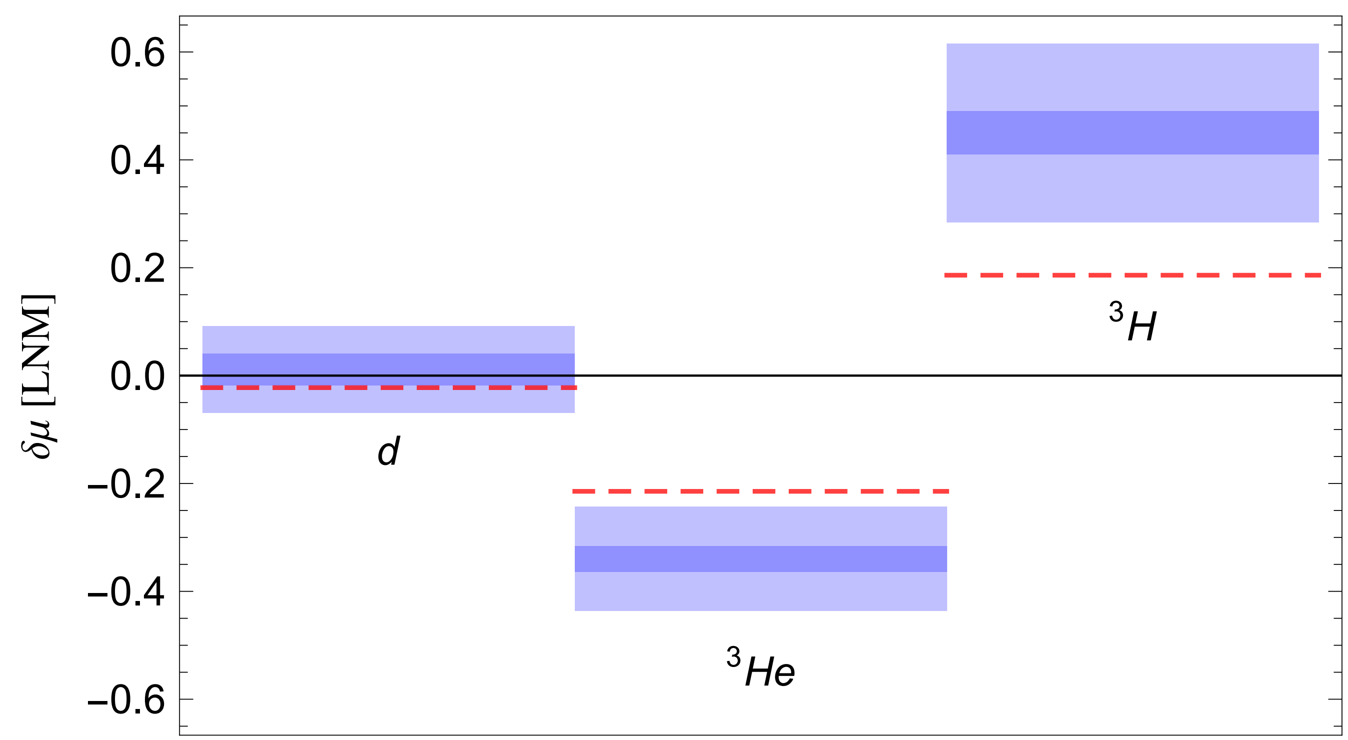
Magnetic moments of light nuclei from lattice quantum chromodynamics

S.R. Beane, E. Chang, S. Cohen, W. Detmold, H.W. Lin, K. Orginos, A. Parreno, M.J. Savage, B.C. Tiburzi

Published in **Phys.Rev.Lett. 113 (2014) 25, 252001**
e-Print: **arXiv:1409.3556 [hep-lat]**

$m_\pi \sim 800$ MeV Vs Nature

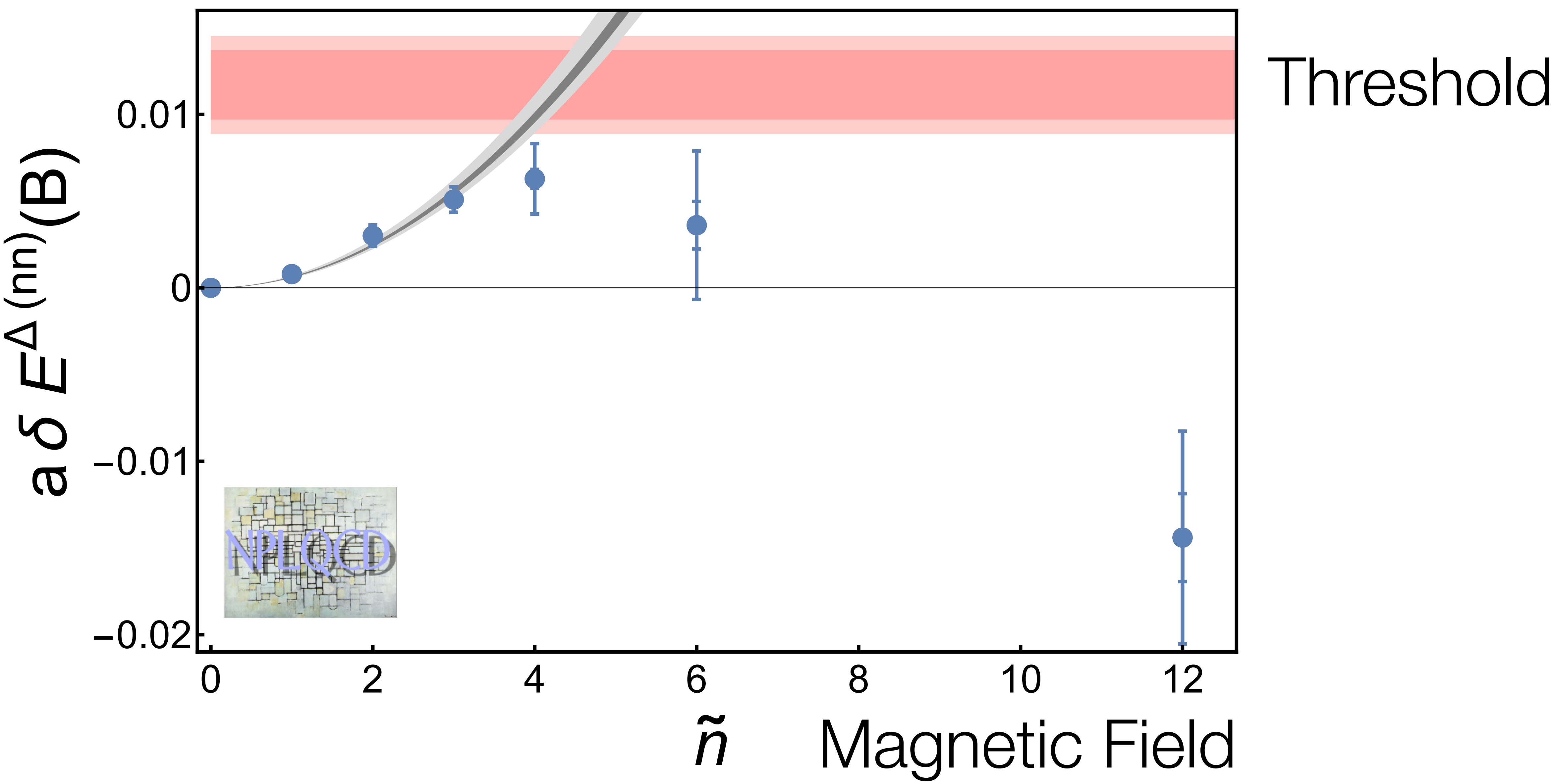




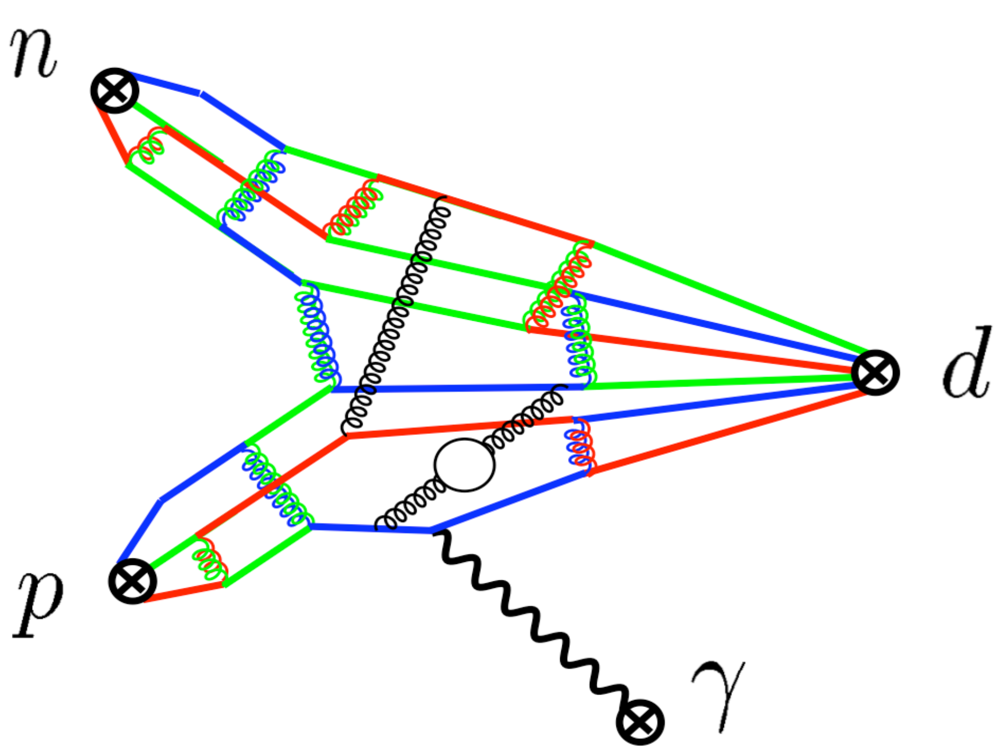
Nuclei are collections of nucleons
- shell model phenomenology!

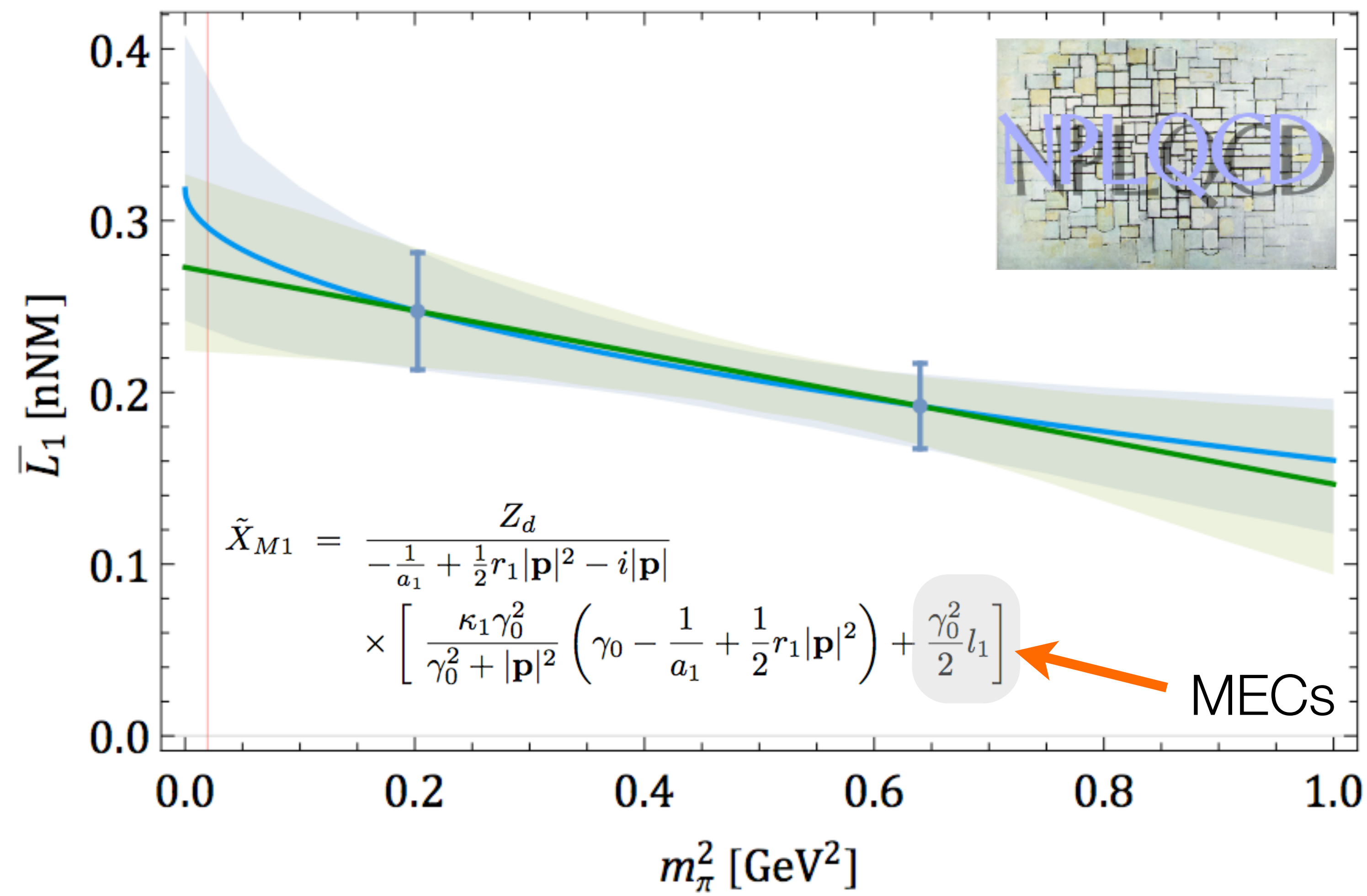
Lattice QCD:

Results - A Feshbach Resonance!



Lattice QCD:
Results - $np \to d\gamma$



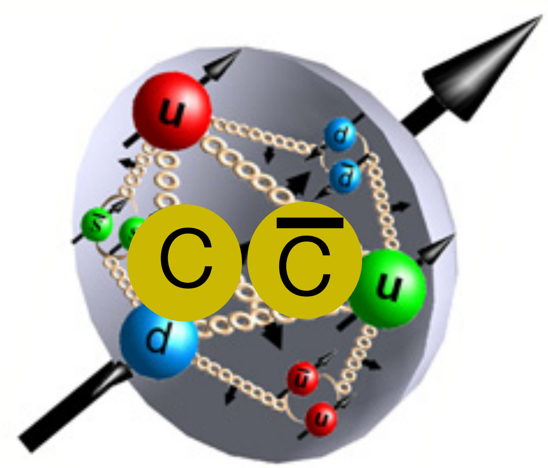


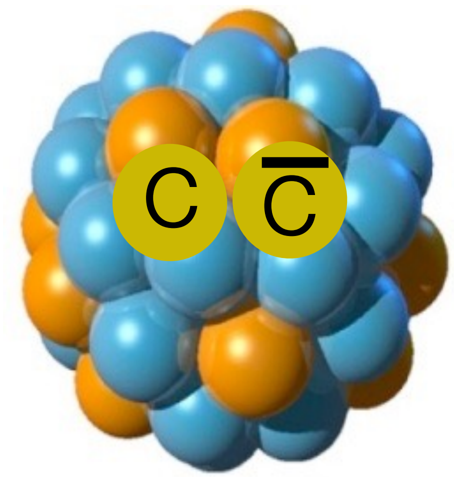
postdiction at the physical point (verification) :

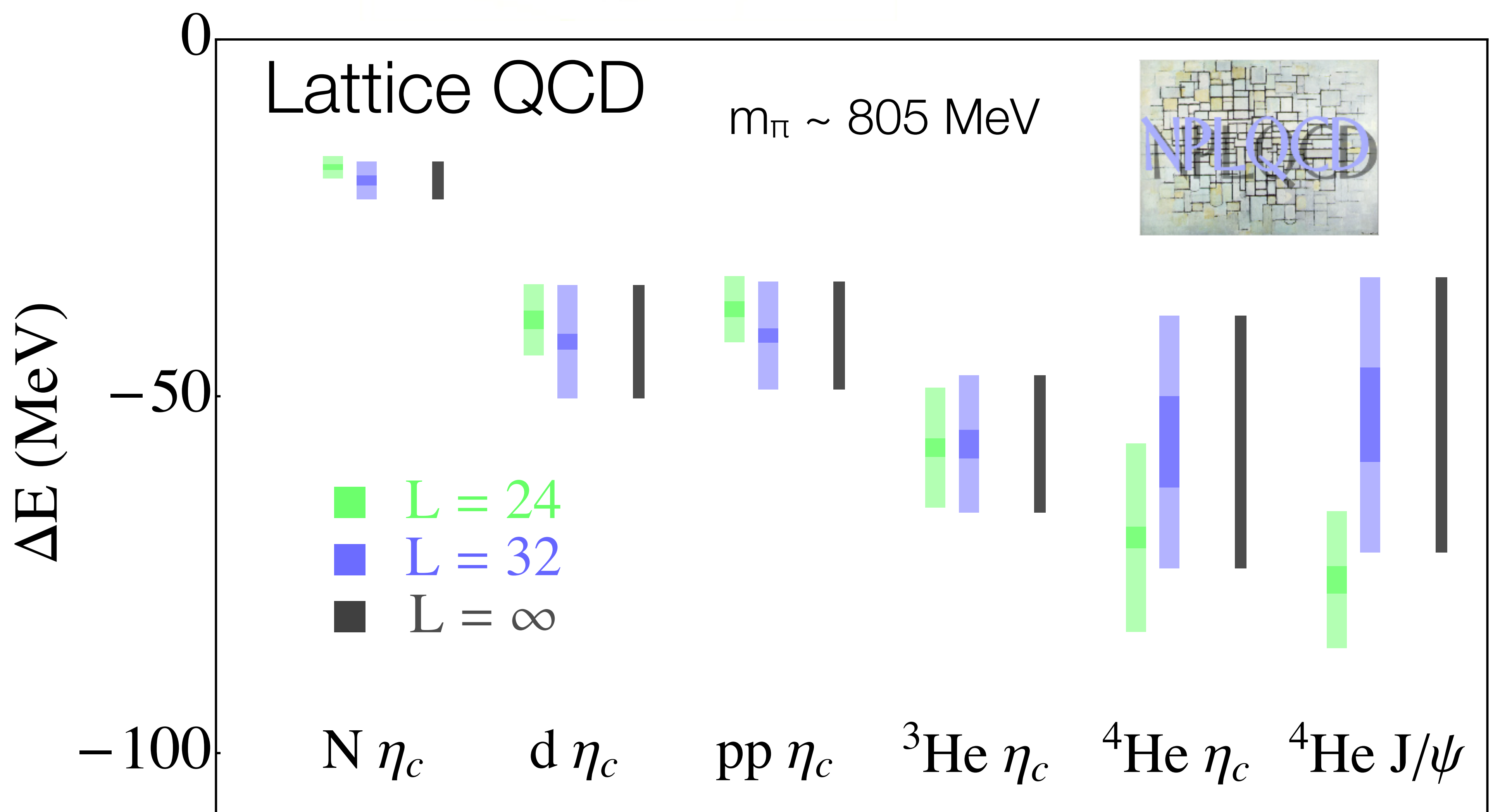
$$\sigma^{\rm lqcd} = 332.4\left({}^{+5.4}_{-4.7} \right)\ {\rm mb} \qquad v = 2,200\ {\rm m/s}$$

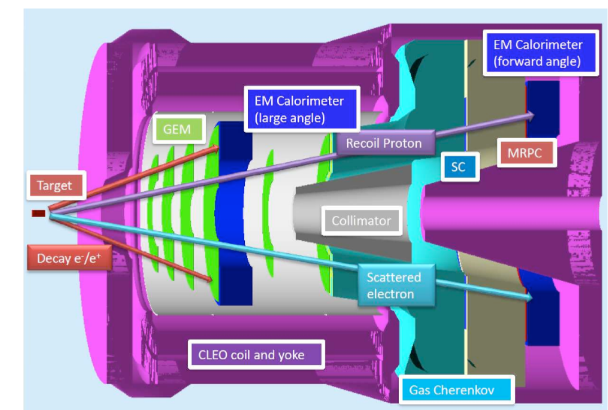
$$\sigma^{\rm expt}(np \to d\gamma) = 334.2(0.5)\ {\rm mb}$$

Lattice QCD:
Results - Exotic Nuclei









Athenna

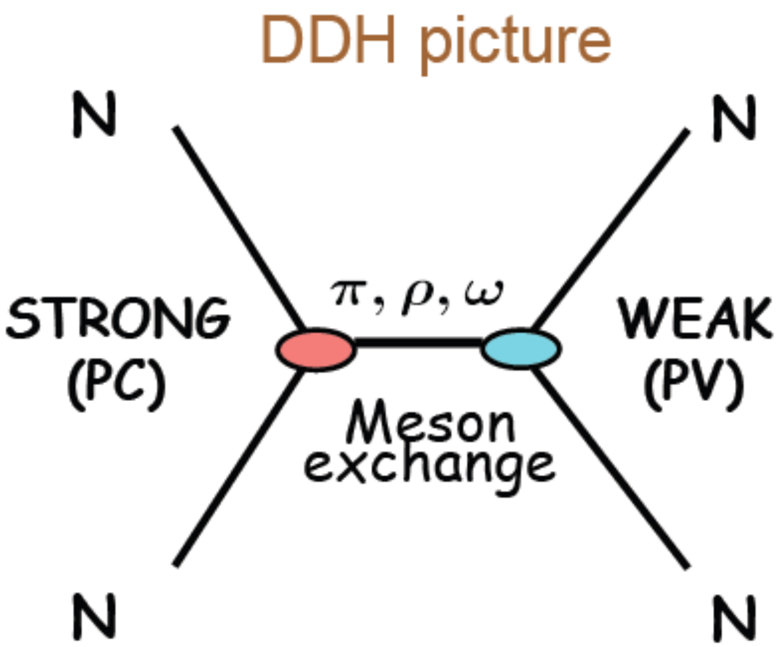
Jefferson Lab
EXPLORING THE NATURE OF MATTER

experimental effort led by
Zein-Eddine Meziani
Temple

(Beane, Chang, Cohen, Detmold, Lin, Orginos, Parreno, MJS , arXiv:1410.7069)

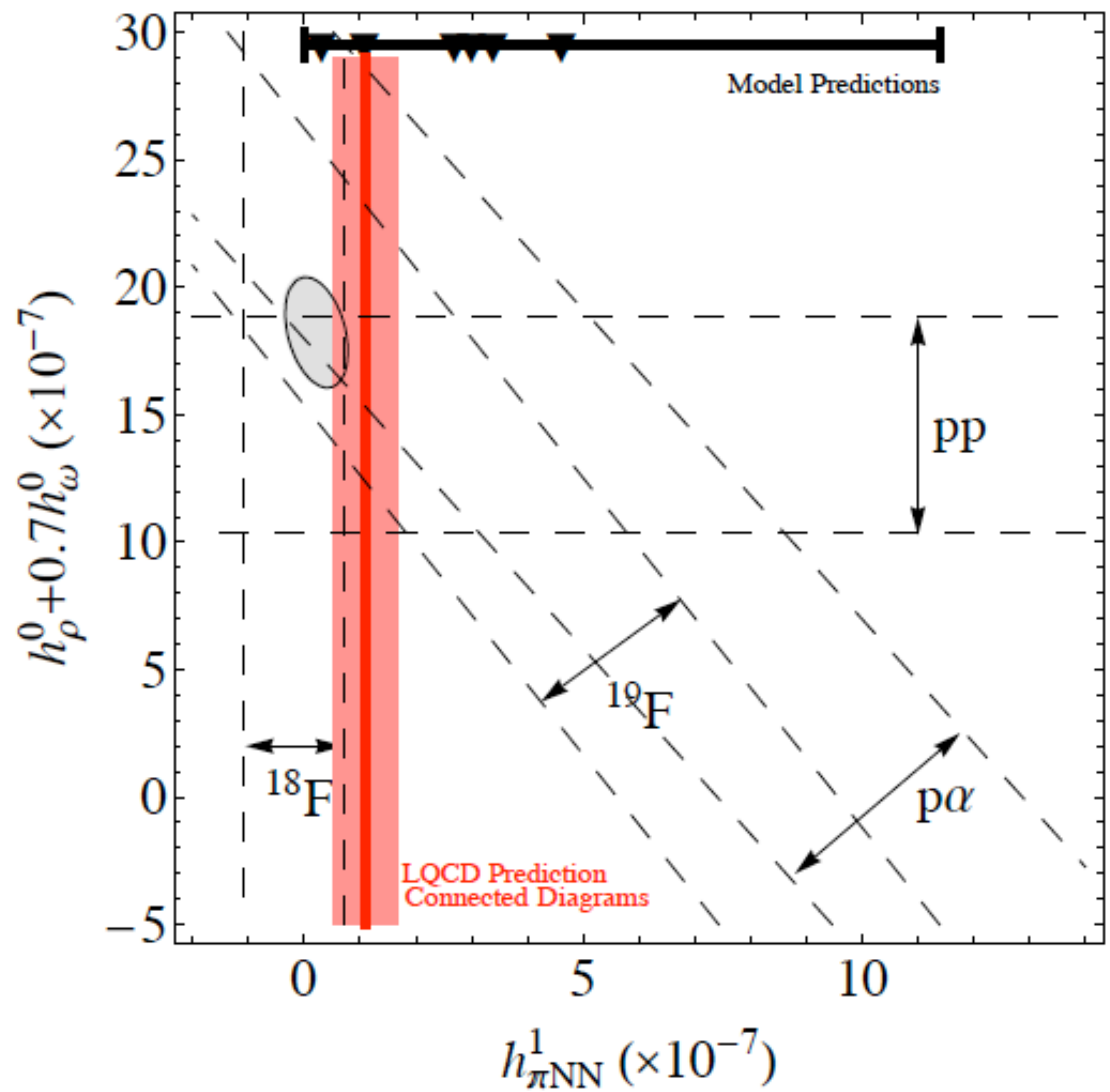
Lattice QCD:

Results - Nuclear Parity Violation



$$\frac{e^2}{M_W^2} / \frac{g^2}{m_\pi^2} \approx 10^{-7}$$

(Wasem (UW/LLNL) 2011)



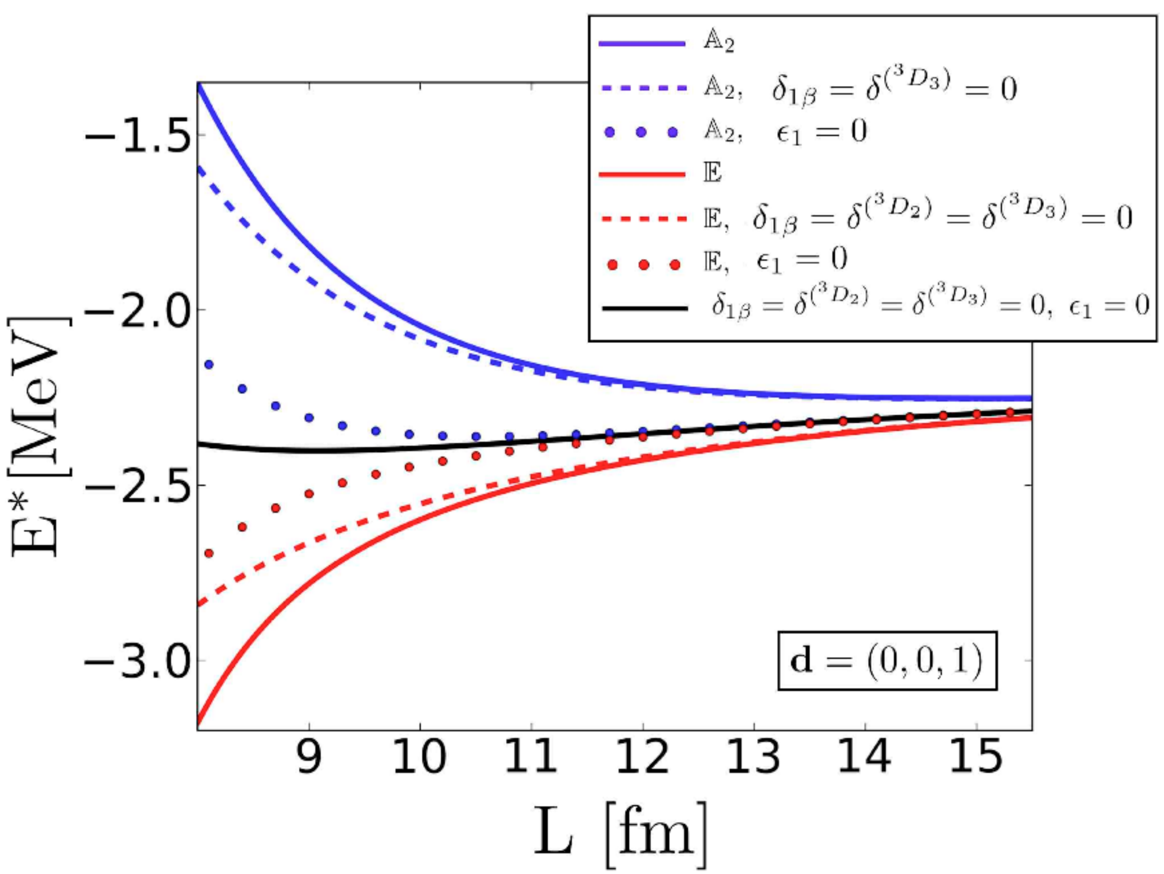
Presently incomplete

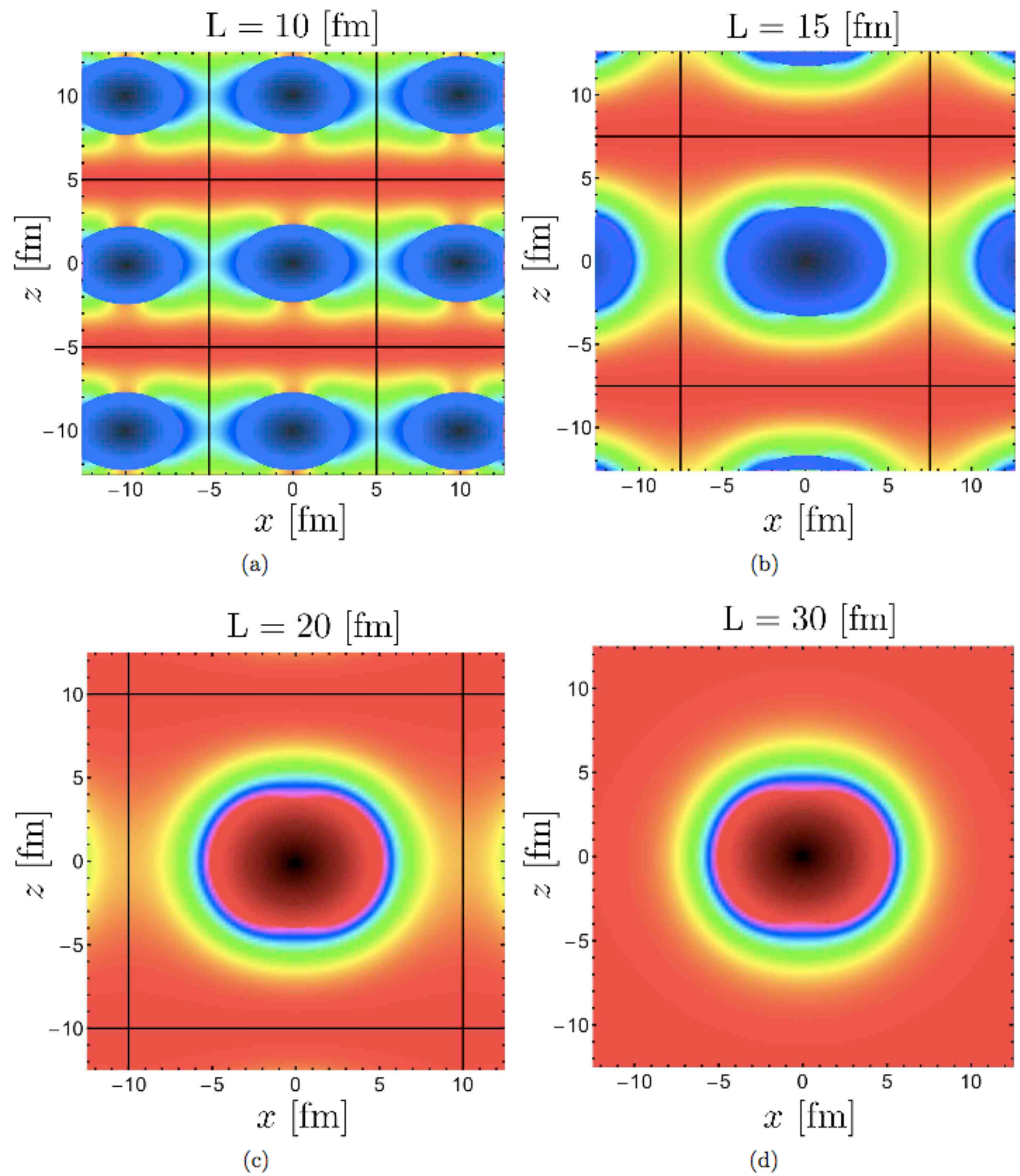
- unphysical quark masses
- operator matching
- LQCD interpolators

Lattice QCD:
Recent Formal Developments

Two-Nucleon Systems in a Finite Volume:
(II) 3S1-3D1 Coupled Channels and the Deuteron
Raul A. Briceno, Zohreh Davoudi, Thomas Luu, MJS

Mass density of boosted deuteron d=(0,0,1)



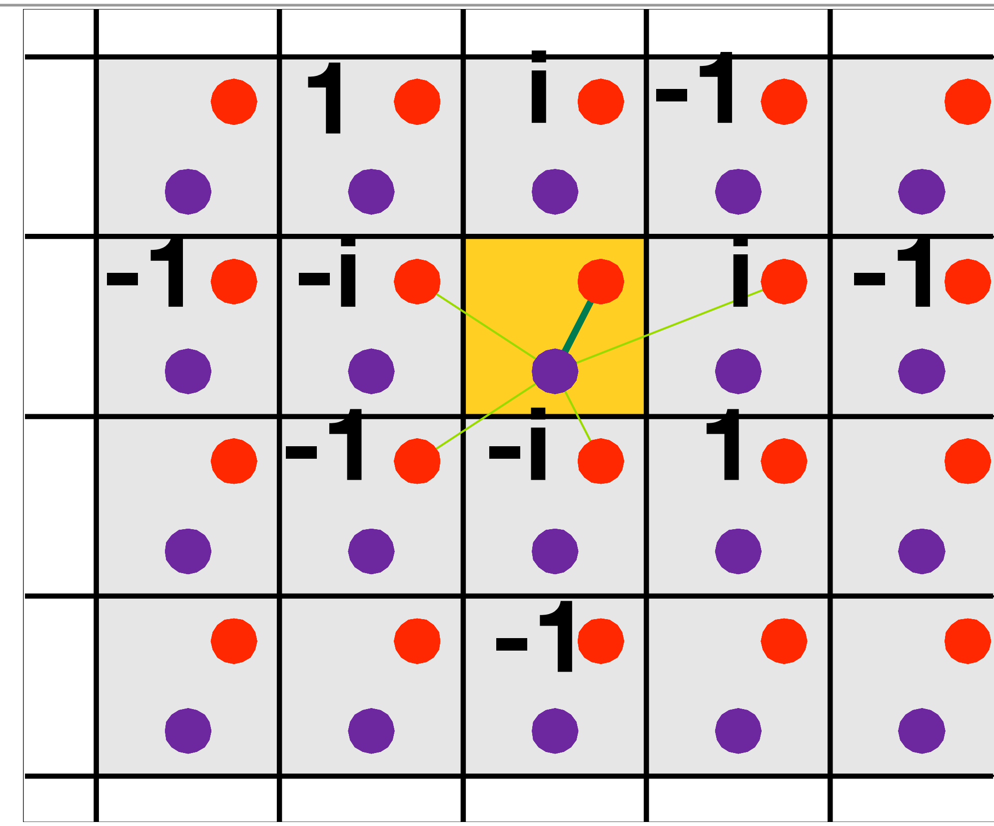


Lattice QCD:

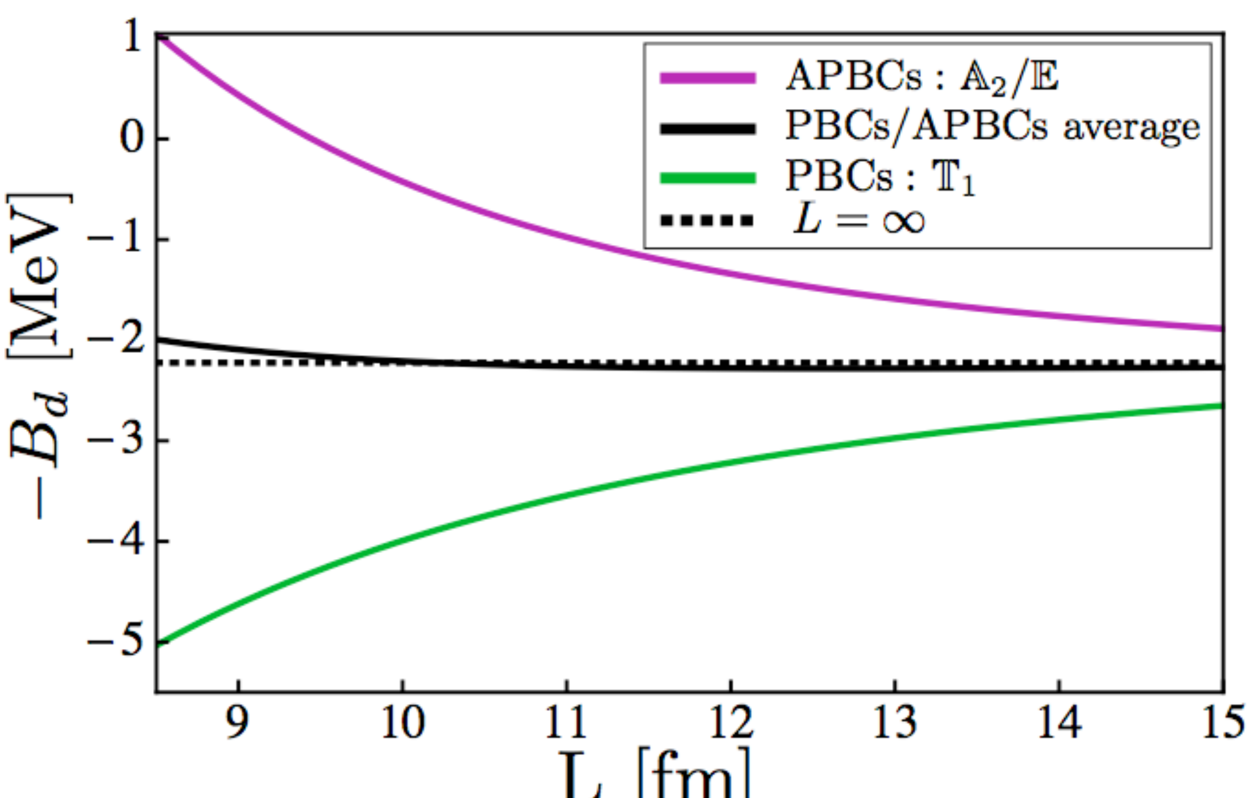
Recent Formal Developments - i-Periodic Boundary Conditions

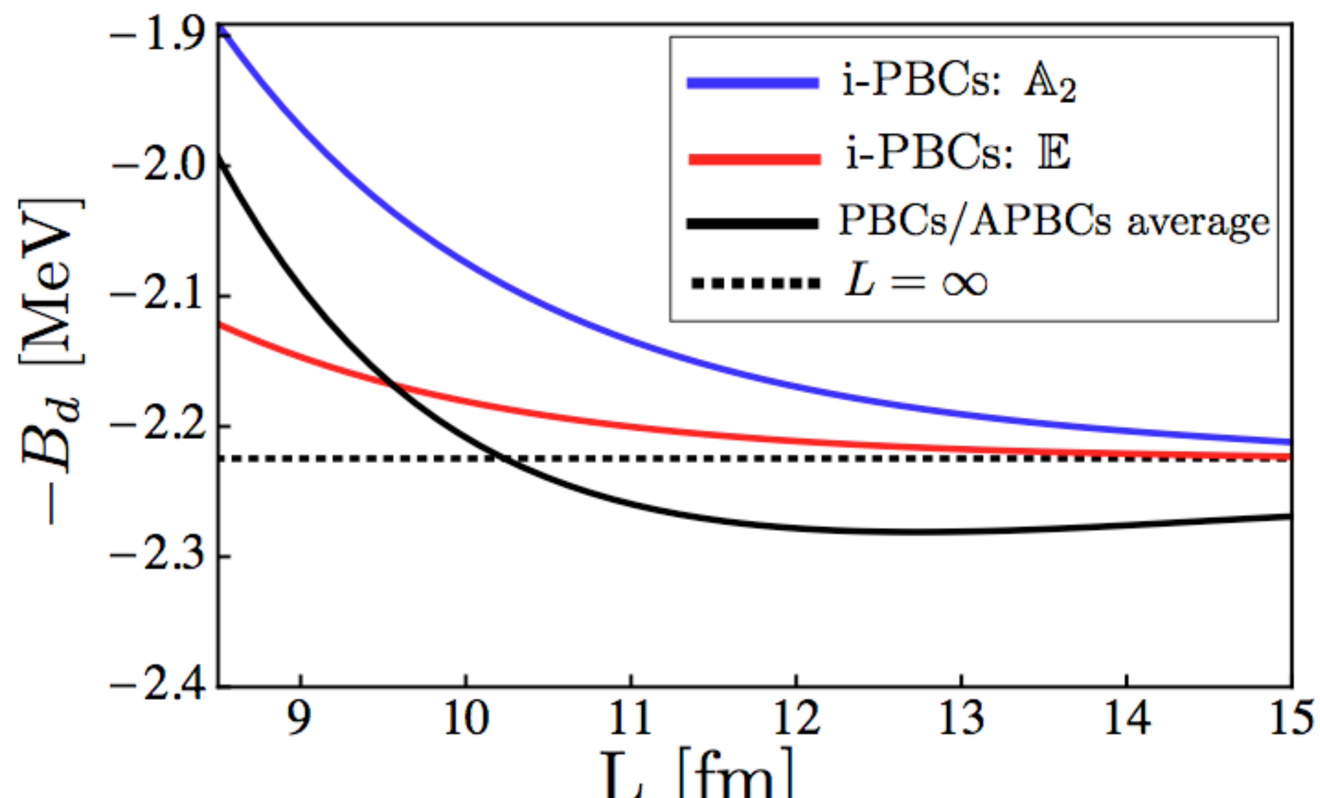
Raul A. Briceno, Zohreh Davoudi, Thomas Luu, MJS
Phys.Rev. D89 (2014) 7, 074509

INT Program : Quantitative Large Amplitude Shape Dynamics:
fission and heavy ion fusion



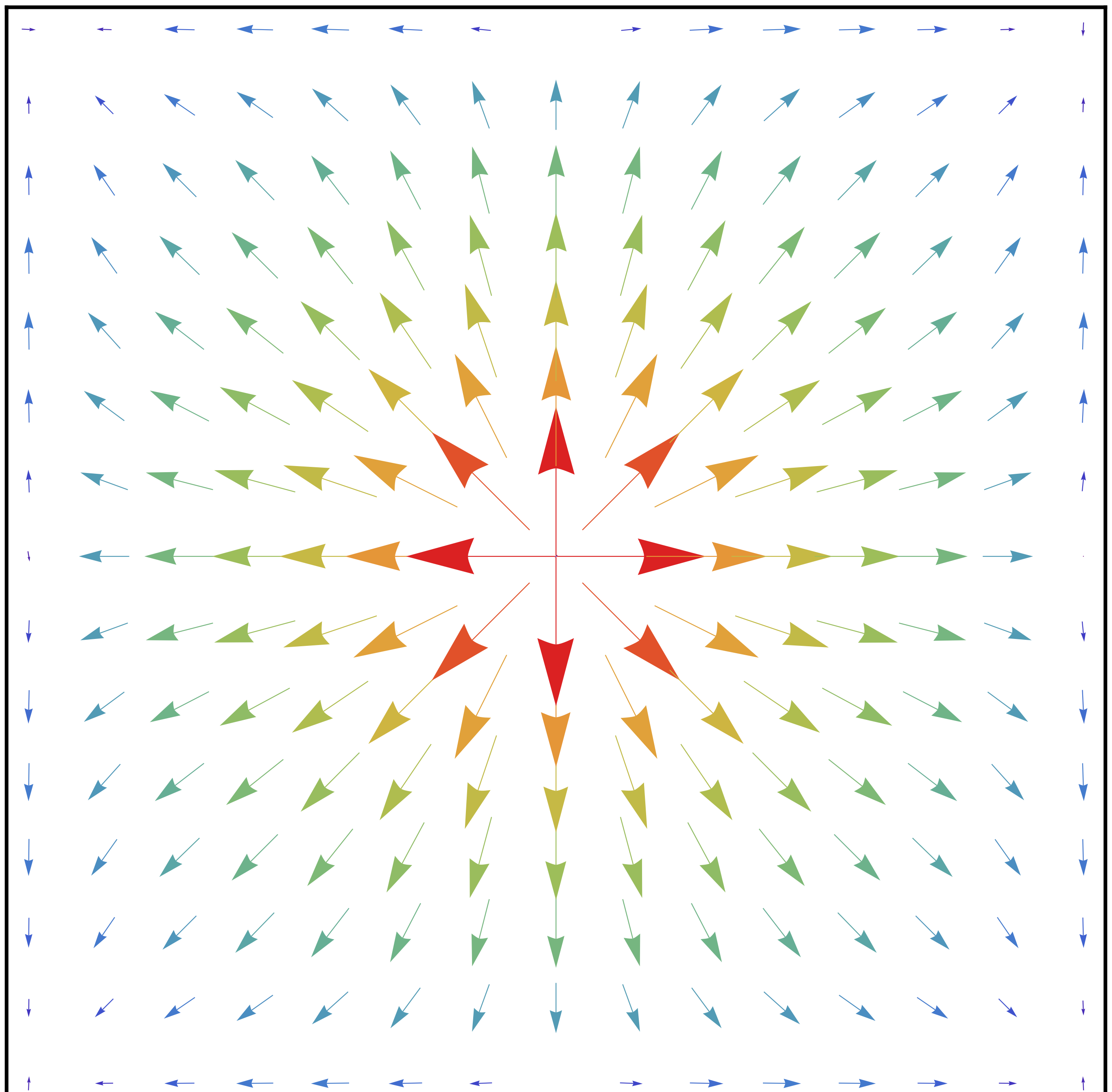
i-PBCs

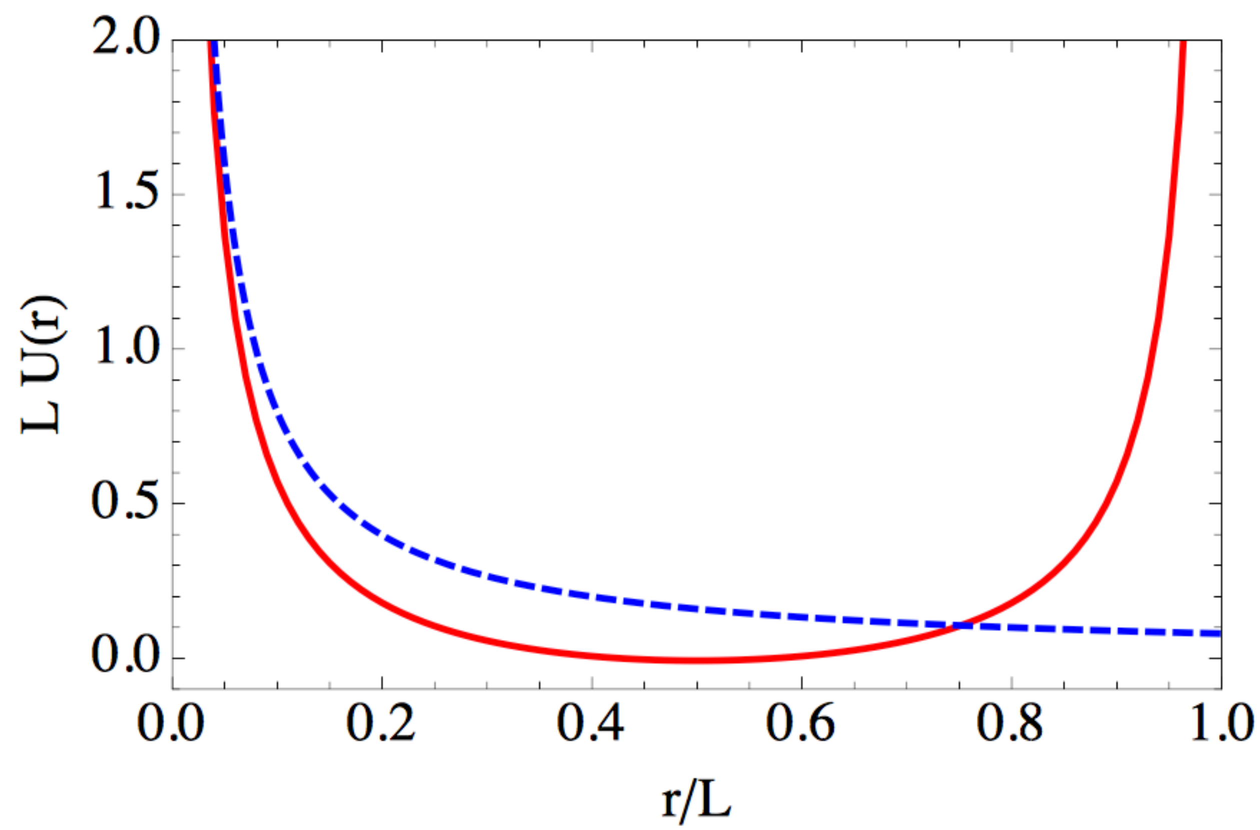




Lattice QCD:
Recent Formal Developments - QED

The potential with periodic BCs

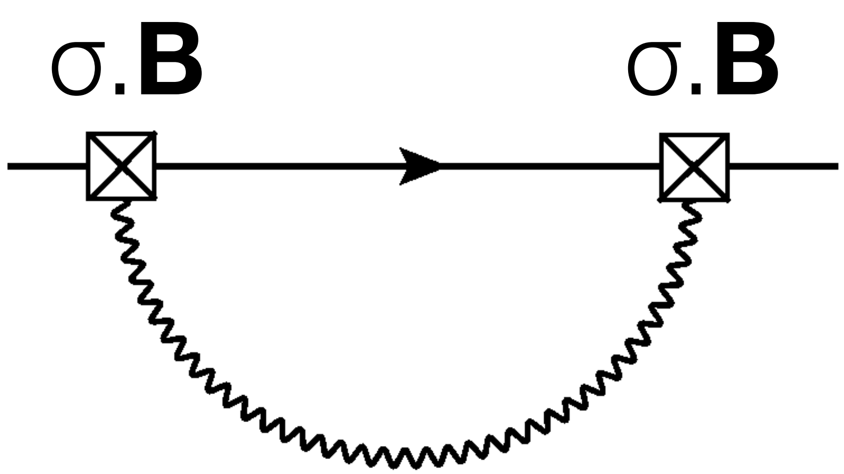


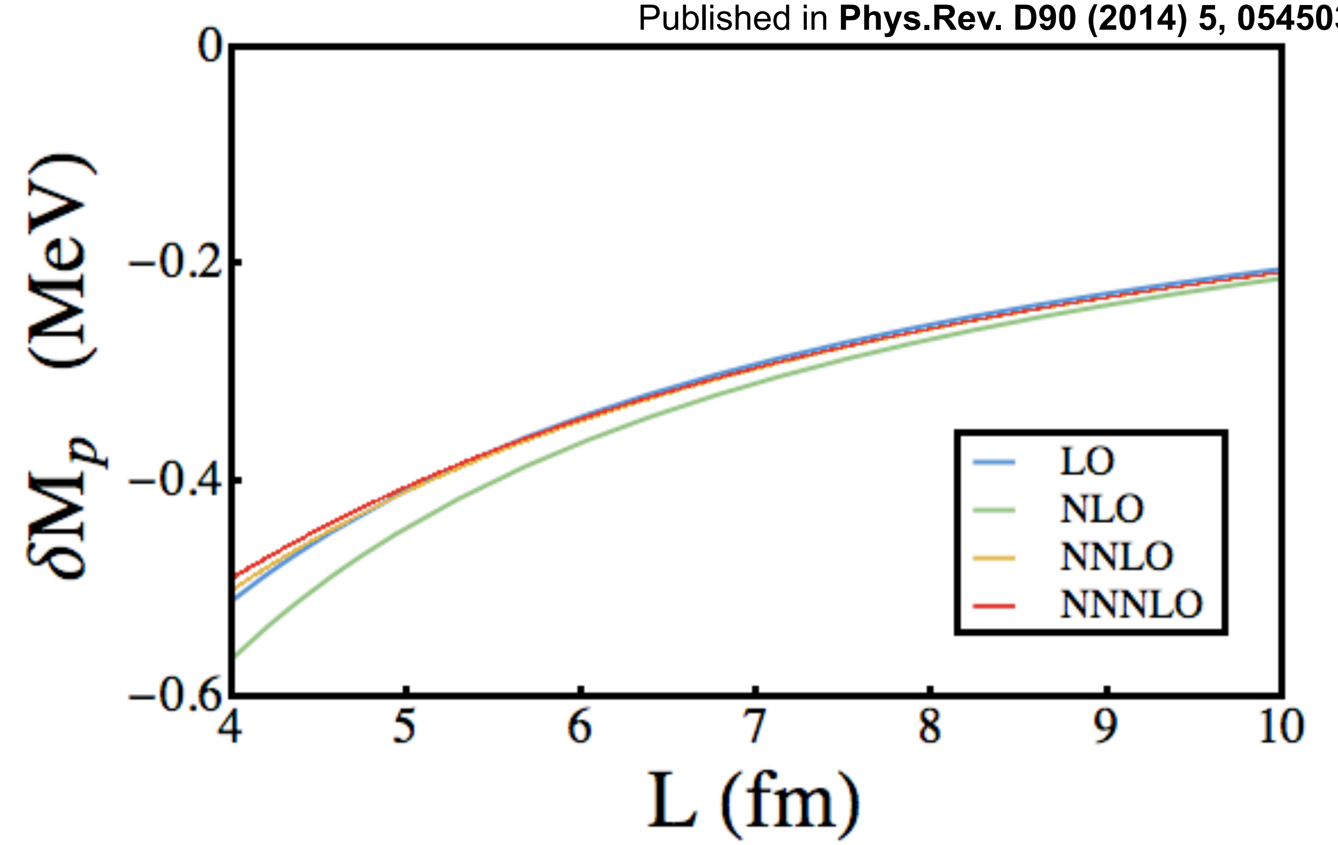


Lattice QCD:
Recent Formal Developments - QED

Zohreh Davoudi and MJS
Published in **Phys.Rev. D90 (2014) 5, 054503**

FV NRQED, e.g.,



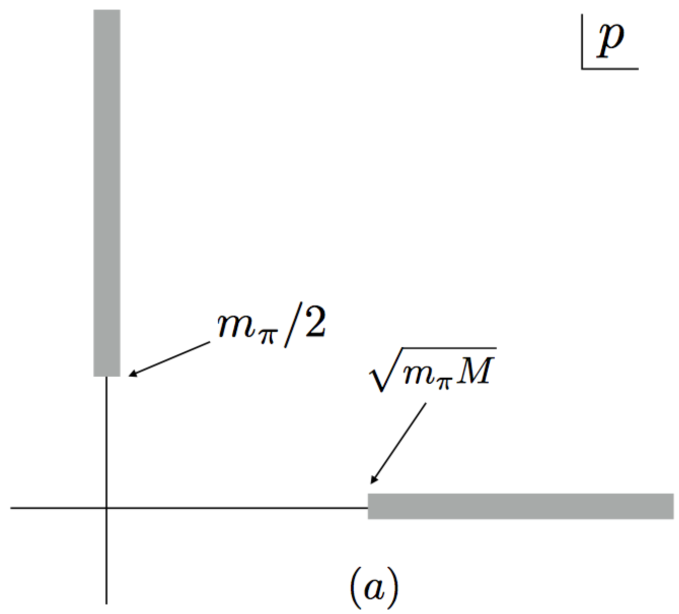


$$\delta M_p = \frac{\alpha_e}{2L} c_1 \left(1 + \frac{2}{M_p L}\right) + \frac{2\pi\alpha_e}{3L^3}\left(1 + \frac{4\pi}{M_p L} c_{-1}\right)\langle r^2\rangle_p + \frac{\pi\alpha_e}{M_p^2 L^3}\left(\frac{1}{2} + (1+\kappa_p)^2\right)$$
$$- \frac{4\pi^2}{L^4}\left(\alpha_E^{(p)} + \beta_M^{(p)}\right) c_{-1} - \frac{2\pi^2 \alpha_e \kappa_p}{M_p^3 L^4} c_{-1},$$

$$\delta M_n = \kappa_n^2 \frac{\pi\alpha_e}{M_n^2 L^3} - \frac{4\pi^2}{L^4}\left(\alpha_E^{(n)} + \beta_M^{(n)}\right) c_{-1},$$

Lattice QCD:

Recent Formal Developments - QED - Scattering



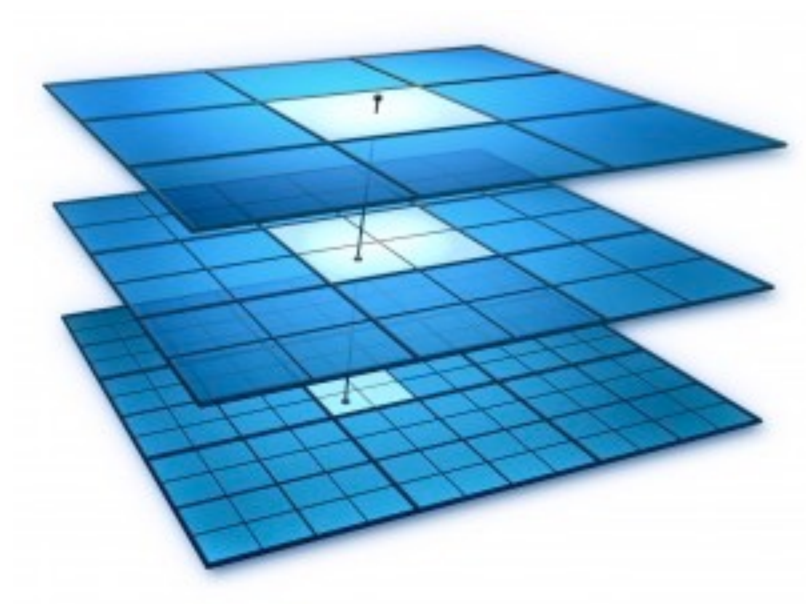
$$-\frac{1}{a'_C} + \frac{1}{2} r'_0 p^2 + \ldots = \frac{1}{\pi L} \mathcal{S}^C(\tilde{p}) + \alpha M \left[\ln\left(\frac{4\pi}{\alpha M \mathrm{L}} \right) - \gamma_E \right] + \ldots$$

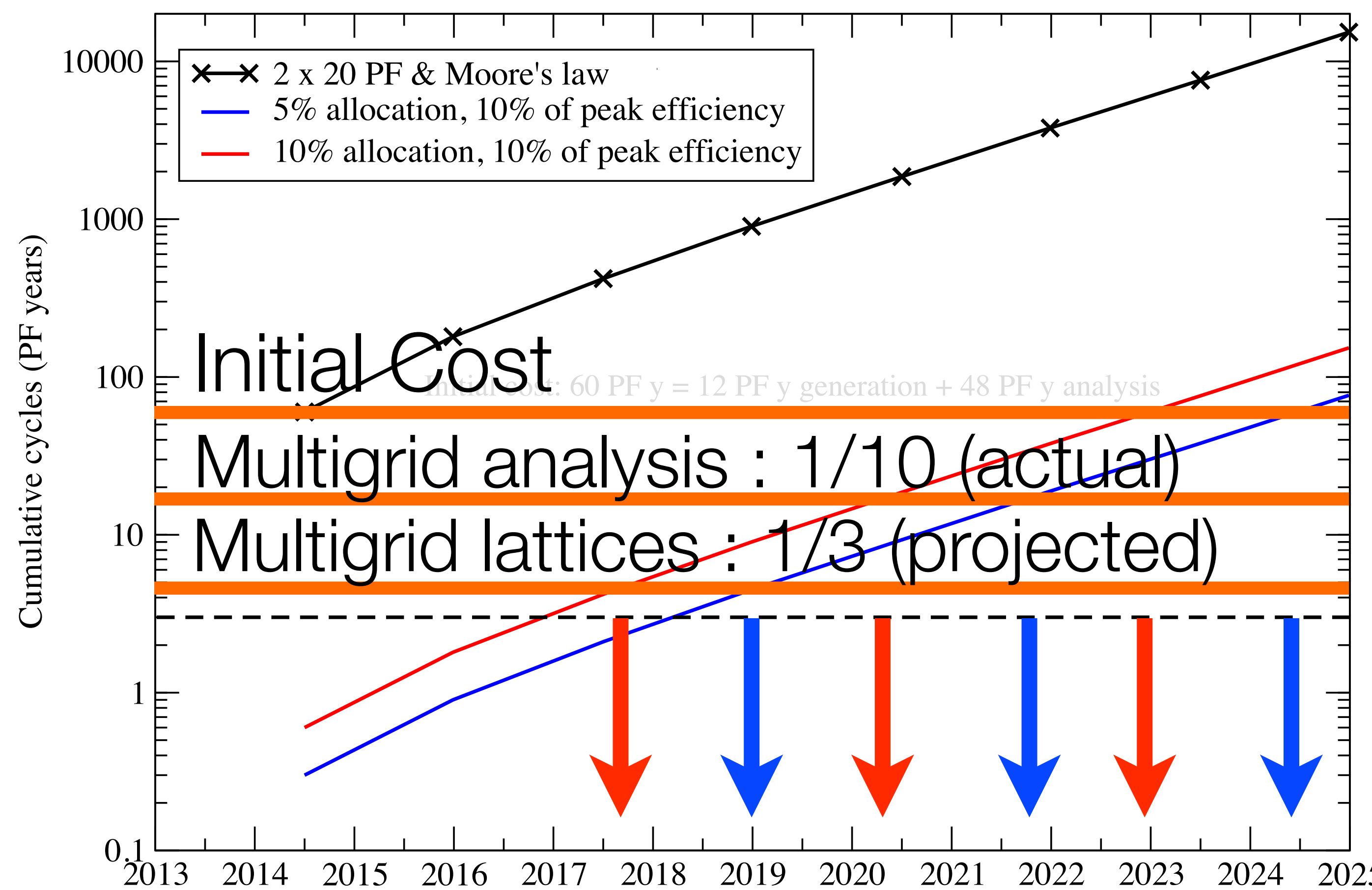
$$\begin{aligned}
\Delta E_0^C = \; & \Delta E_0 + \Delta E_0^{(\alpha)} \\
= & \frac{4\pi\, a'}{M\, L^3} \left\{ 1 - \left(\frac{a'}{\pi\, L} \right) \mathcal{I} + \left(\frac{a'}{\pi\, L} \right)^2 \left[\mathcal{I}^2 - \mathcal{J} \right] + \ldots \right\} \\
& - \frac{2\alpha\, a'}{L^2 \pi^2} \left\{ \mathcal{J} + \left(\frac{a'}{\pi\, L} \right) \left[\mathcal{K} - \mathcal{I}\mathcal{J} - \mathcal{R}/2 \right] \right. \\
& \quad + \left(\frac{a'}{\pi\, L} \right)^2 \left[\mathcal{R}\mathcal{I} + \mathcal{I}^2 \mathcal{J} - 2\mathcal{J}^2 - 2\mathcal{I}\mathcal{K} + \mathcal{L} - \mathcal{R}_{24} \right] \\
& \quad \left. + \frac{2 a' r'_0 \pi^2}{L^2} \mathcal{I} + \ldots \right\} ,
\end{aligned}$$

Lattice QCD:
Quantified Impact of Algorithms

How to solve **optimally** ?

A.x=b

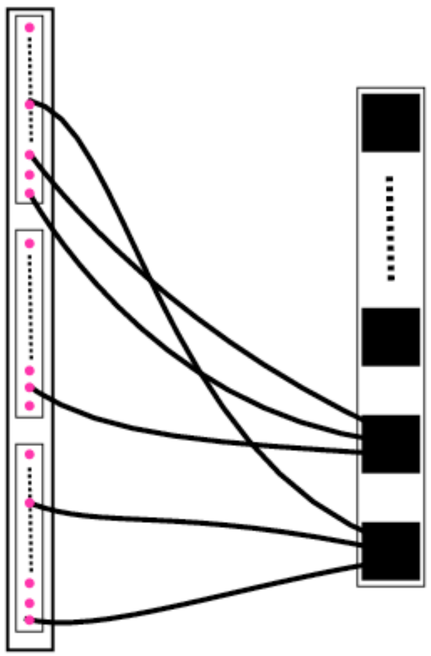




- Multigrid is current (new) technology...
- What is next ?
- Requires talking/collaboration with CS and AM researchers

Lattice QCD:

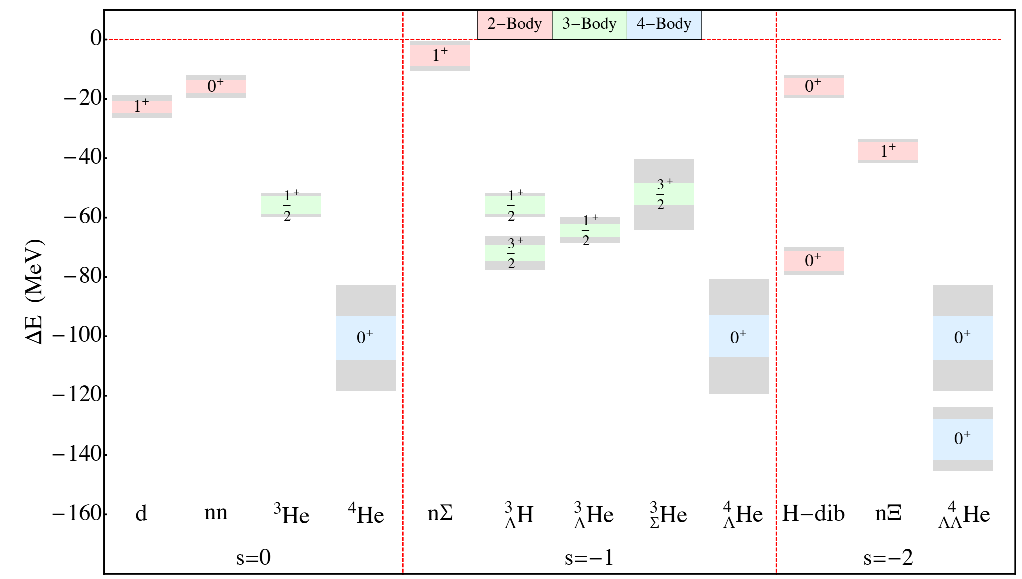
Roadblocks of the Past



Contractions - 2012

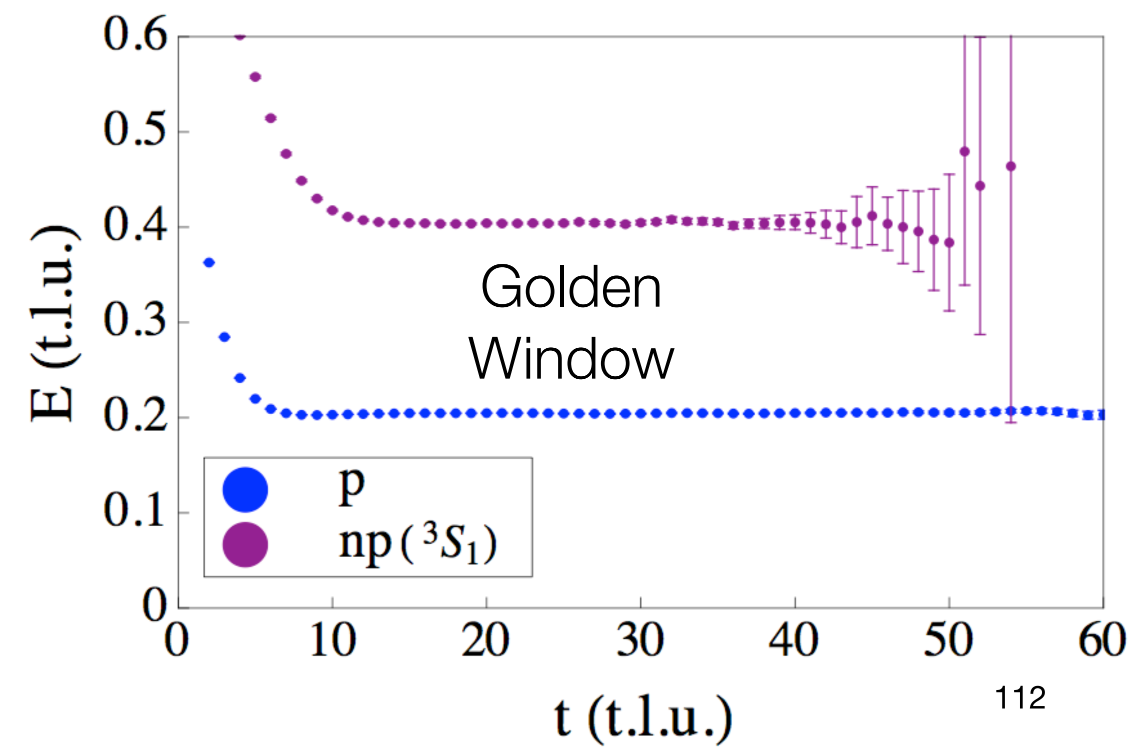
no longer an issue for light nuclei

e.g. ^{4}He : 0.8 core-seconds per time-slice
Orginos+Detmold algorithm
Phys.Rev. D87 (2013) 11, 114512
see also, **Doi and Endres,**
Comput.Phys.Commun. 184 (2013) 117

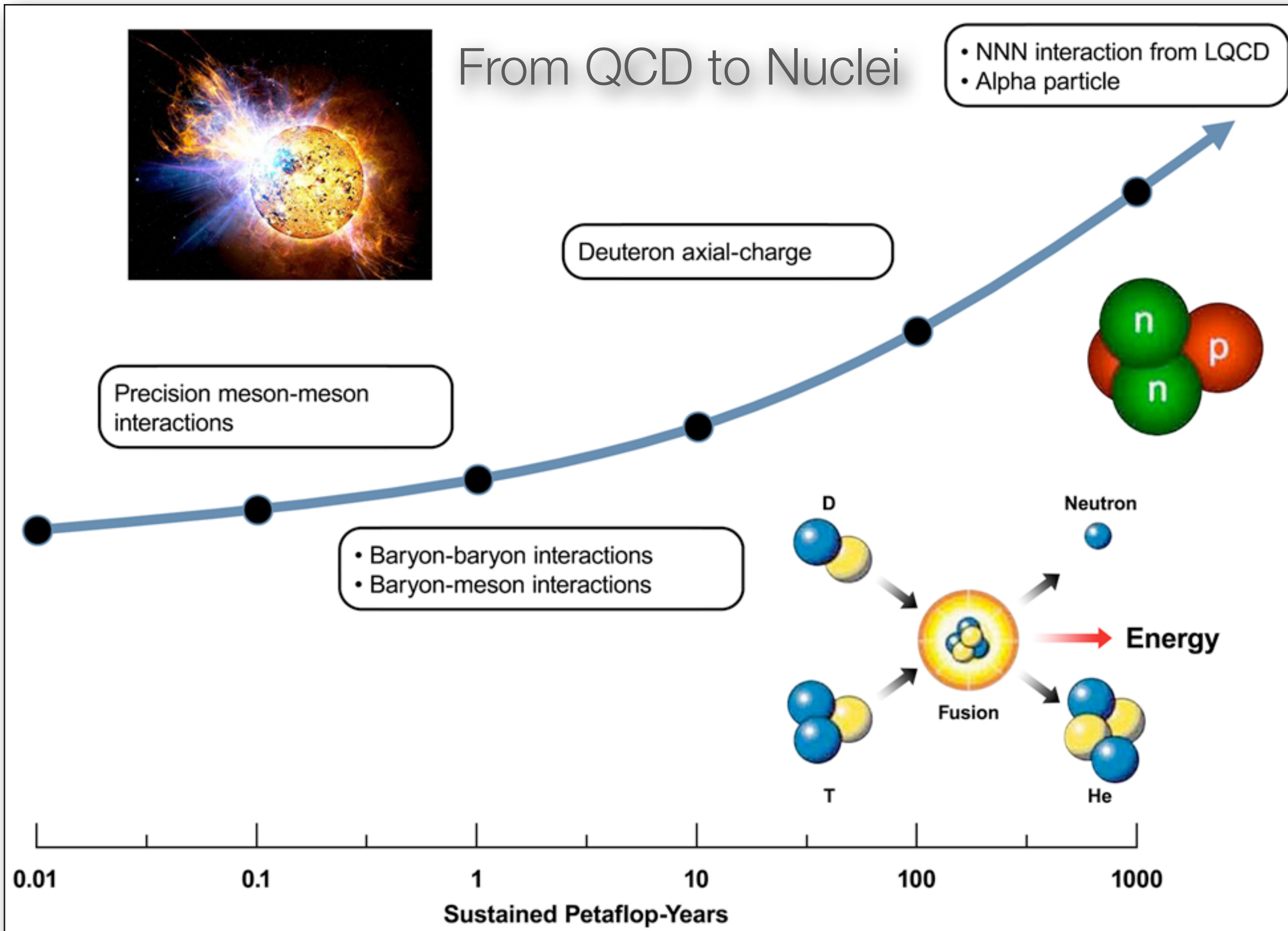


Signal to noise

Large numbers of measurements



Lattice QCD:
Resource Estimates



Electromagnetism
Isospin Breaking
The Real Deal !

Lattice QCD:

How much is that ?

~ 1 Gigaflop

~ 9 thousand core-hours/year

1 Exaflop = 10^3 Petaflops = 10^6 Teraflops = 10^9 Gigaflops

Tianhe-2 [china]

~33.9 Petaflops, 17.6 MWatts

~3 million compute cores

(32K Ivy Bridges, 48K Xeon Phi)

US will deploy ~100 Pflop machines ~ 2017-18

expect ~ 1 Eflop machines ~ 2022

Lattice QCD:
Status as of 2014

2007-2014 ...

Structure of the Baryons

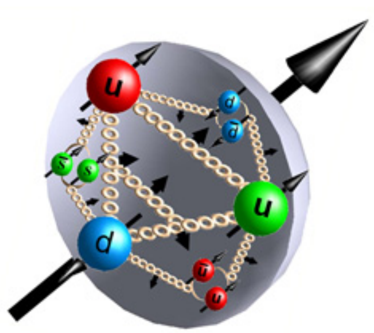
multiple L,T, lattice spacings
multiple discretizations
N predictions for mq(phys)

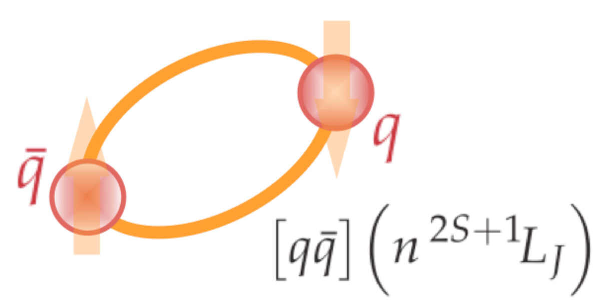
Meson and Baryon Spectroscopy

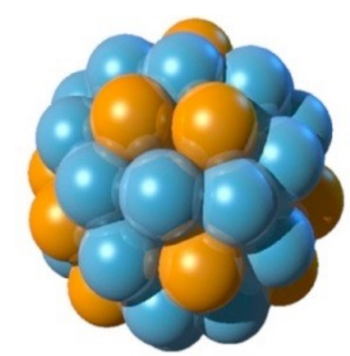
multiple L,T
one lattice spacing
resolved spectrum
mapped out resonances

Nuclei and Nuclear Forces

multiple L,T
one lattice spacing
light (hyper-)nuclei, scattering
simple properties of nuclei





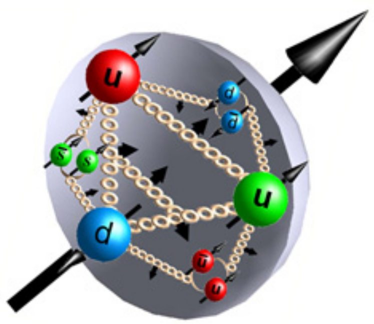
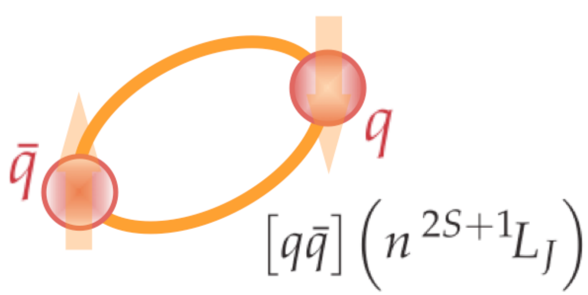


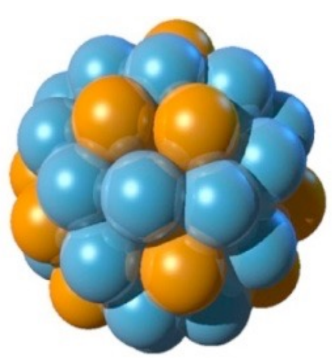
140 MeV | 300 MeV | 800 MeV

Pion Mass

Lattice QCD:
Next Few years

Before 2022 ...

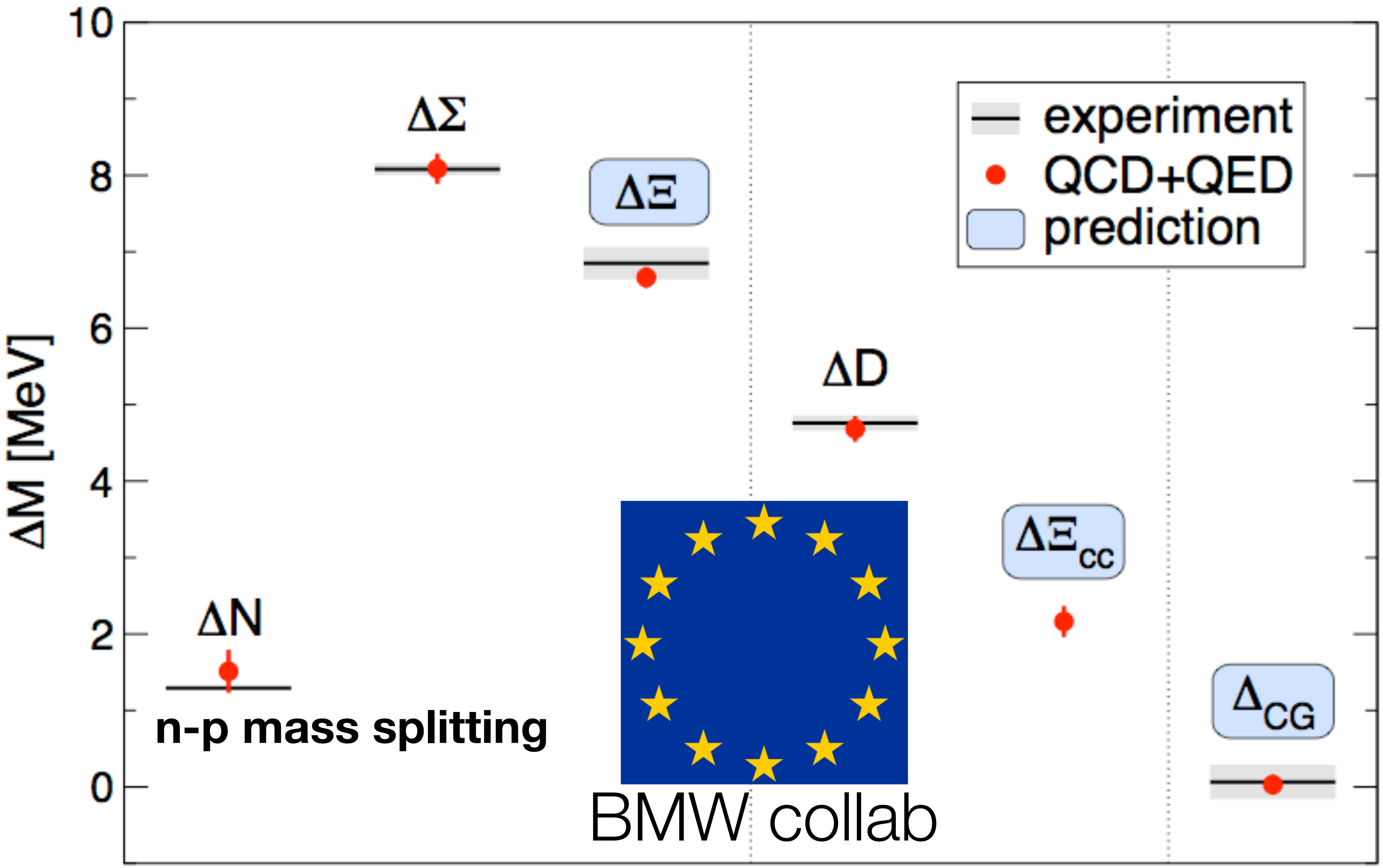


- physical pion mass with $n_f = 1+1+1+1$
- electromagnetism
- precision calculations
- multiple lattices volumes with large T
- multiple lattice spacings
- multiple discretizations
- fully quantified uncertainties
- complement experimental program
- guide future experimental program
- provide critical inputs for theory

140 MeV — 300 MeV — 800 MeV

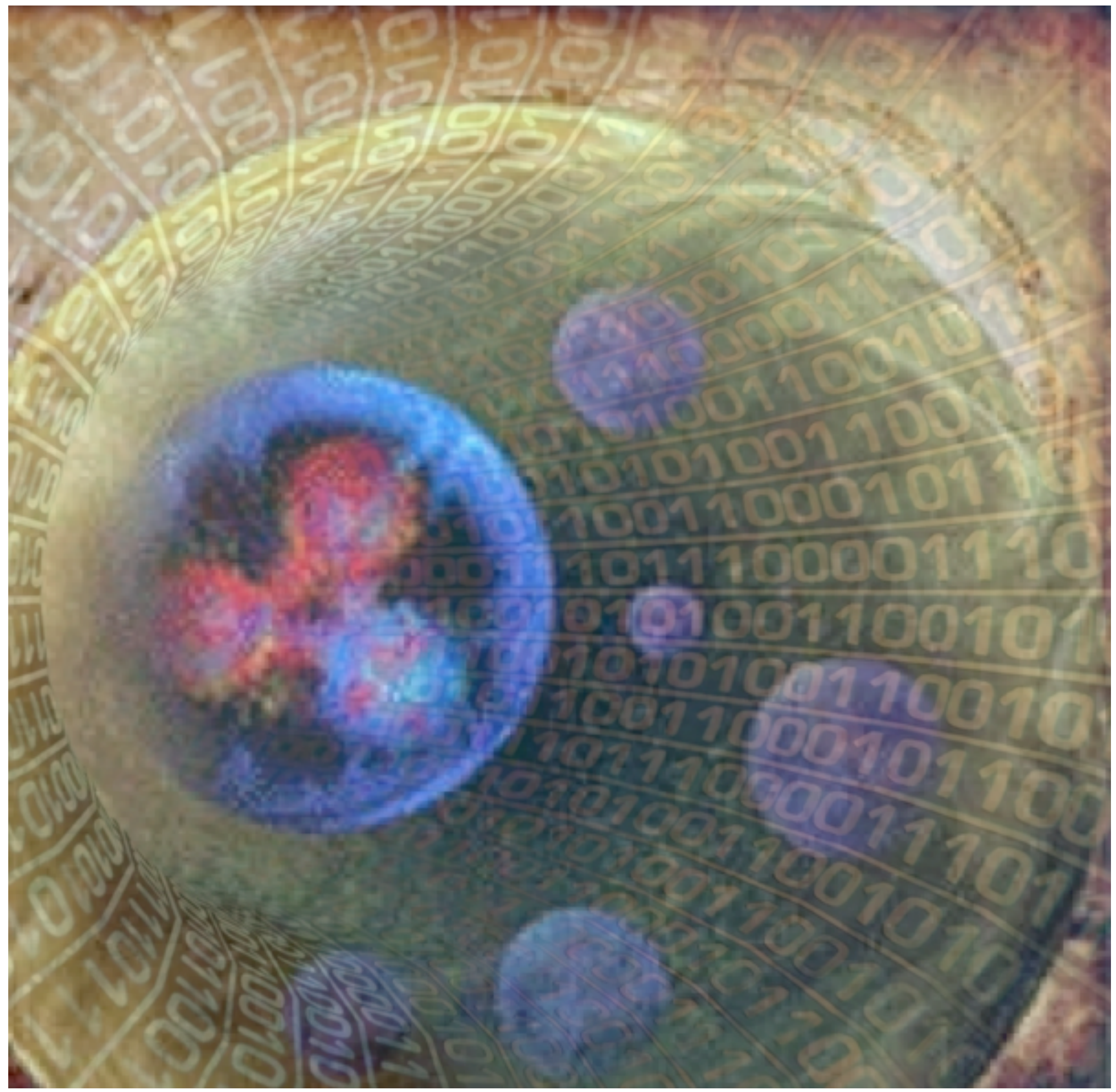
Pion Mass

Lattice QCD:
The Bleeding Edge



- Physical up, down, strange and charm quark masses
- Fully dynamical QCD+QED

Lattice QCD:
Closing Remarks



Lattice QCD is beginning to provide first principles predictive capabilities for nuclear physics

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