Lattice QCD, the Isotensor Amplitude and Beyond

Hadronic Parity Nonconservation
15-16 March 2018
KITP

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LBNL

Lattice QCD for Hadronic Parity Nonconservation

- Introduction to Lattice QCD (LQCD)
- Lattice QCD Challenges for Nuclear Physics
- Lattice QCD Challenges for Parity Nonconservation (PNC)
- g_A - a success story
  - convergence of SU(2) baryon chiral perturbation theory
- Inspiration for Lattice QCD Calculations of I=2 PNC
  - New method for 4-quark operators
  - New method for two-nucleon calculations

Introduction to LQCD

$$C(t) = \left\langle \mathcal{O}(t)\mathcal{O}^\dagger(0) \right\rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\psi \, \mathcal{D}\bar{\psi} \, \mathcal{D}U \; \mathcal{O}(t)\mathcal{O}^\dagger(0) e^{-S[\bar{\psi},\psi,U]}$$

$$= \frac{1}{\mathcal{Z}} \int \mathcal{D}U \det\left(\not{D} + M\right) e^{-S[U]} \; \mathcal{O}(t)\mathcal{O}^\dagger(0)$$

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lattice
finite volume

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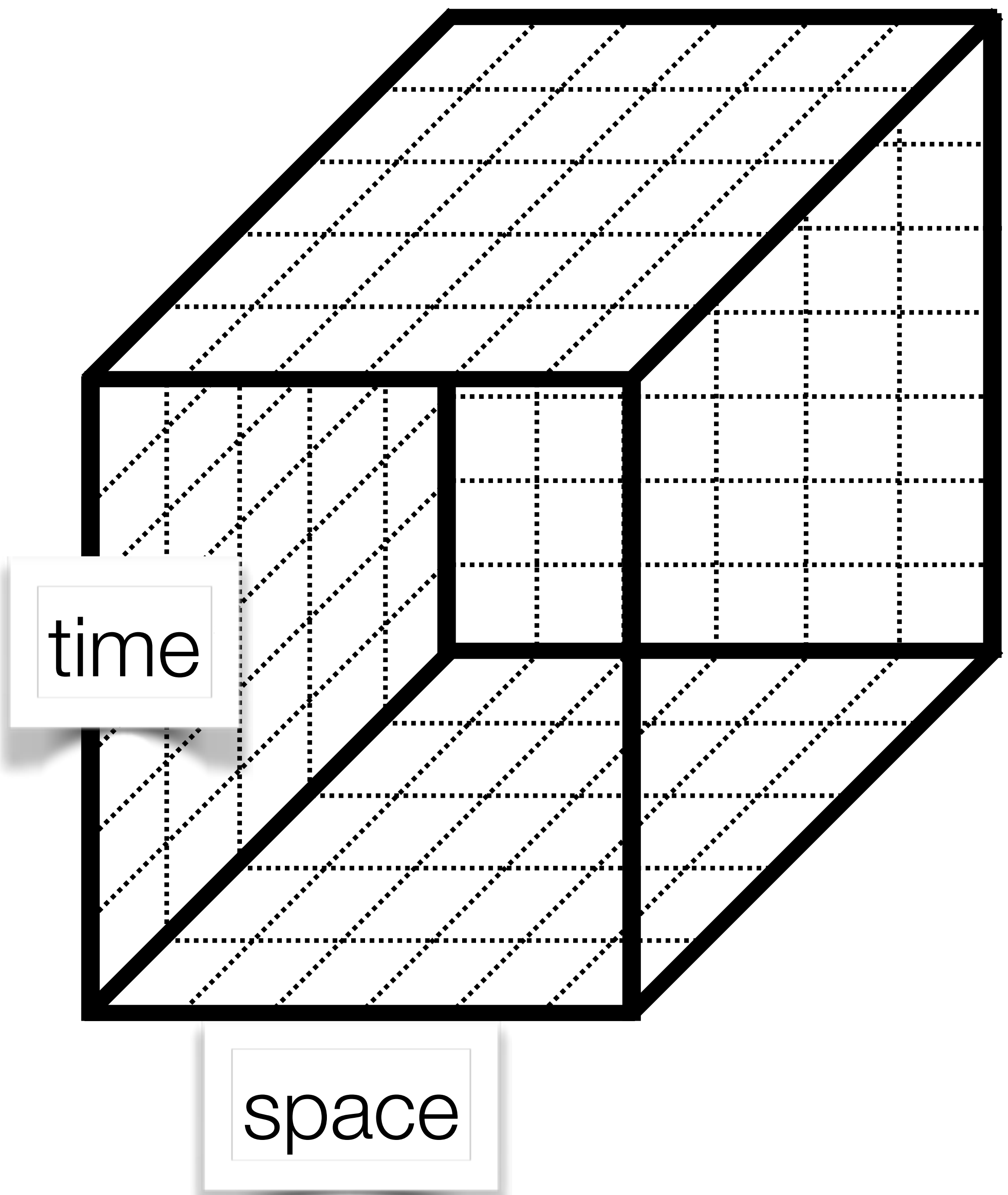

lattice
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Introduction to LQCD

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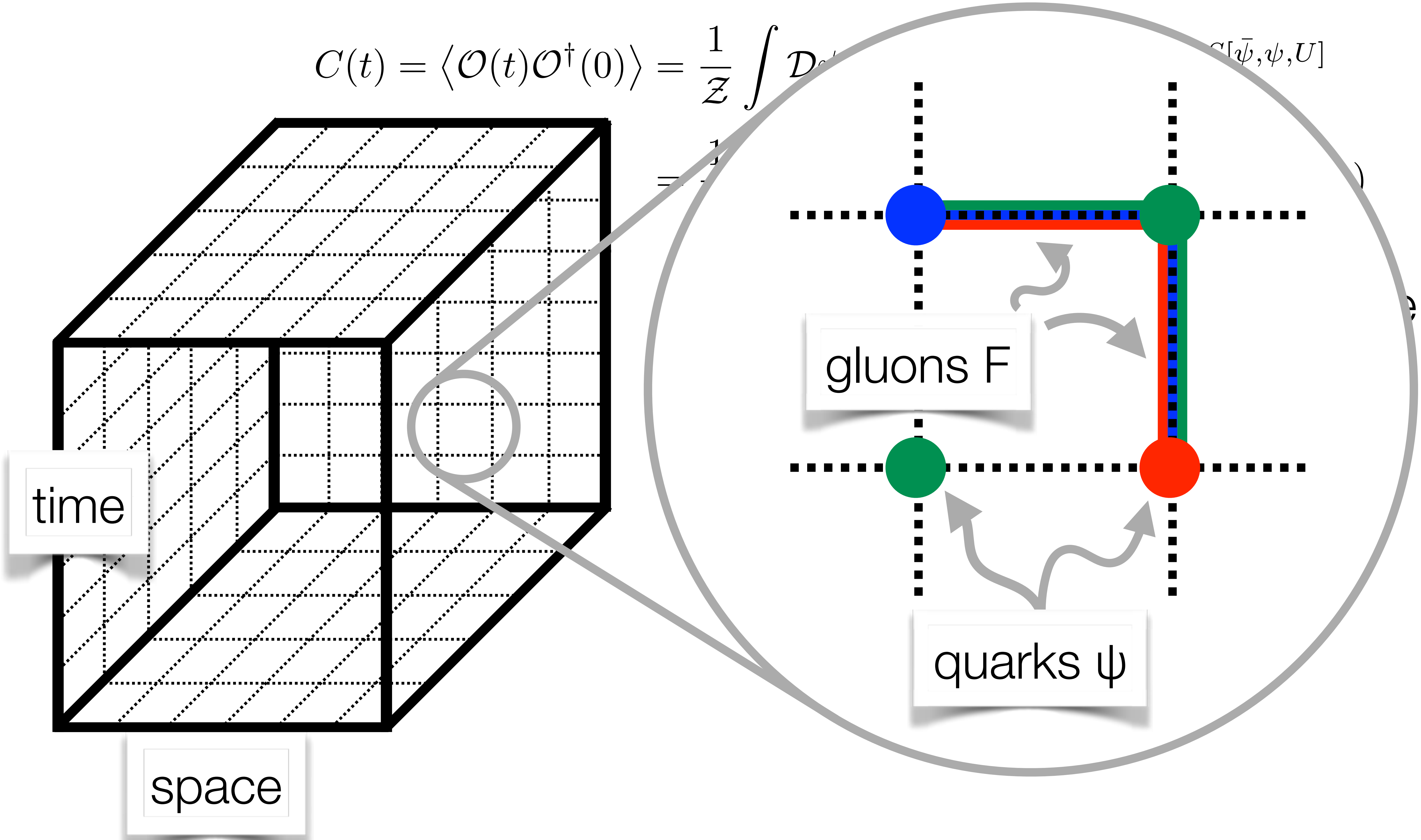

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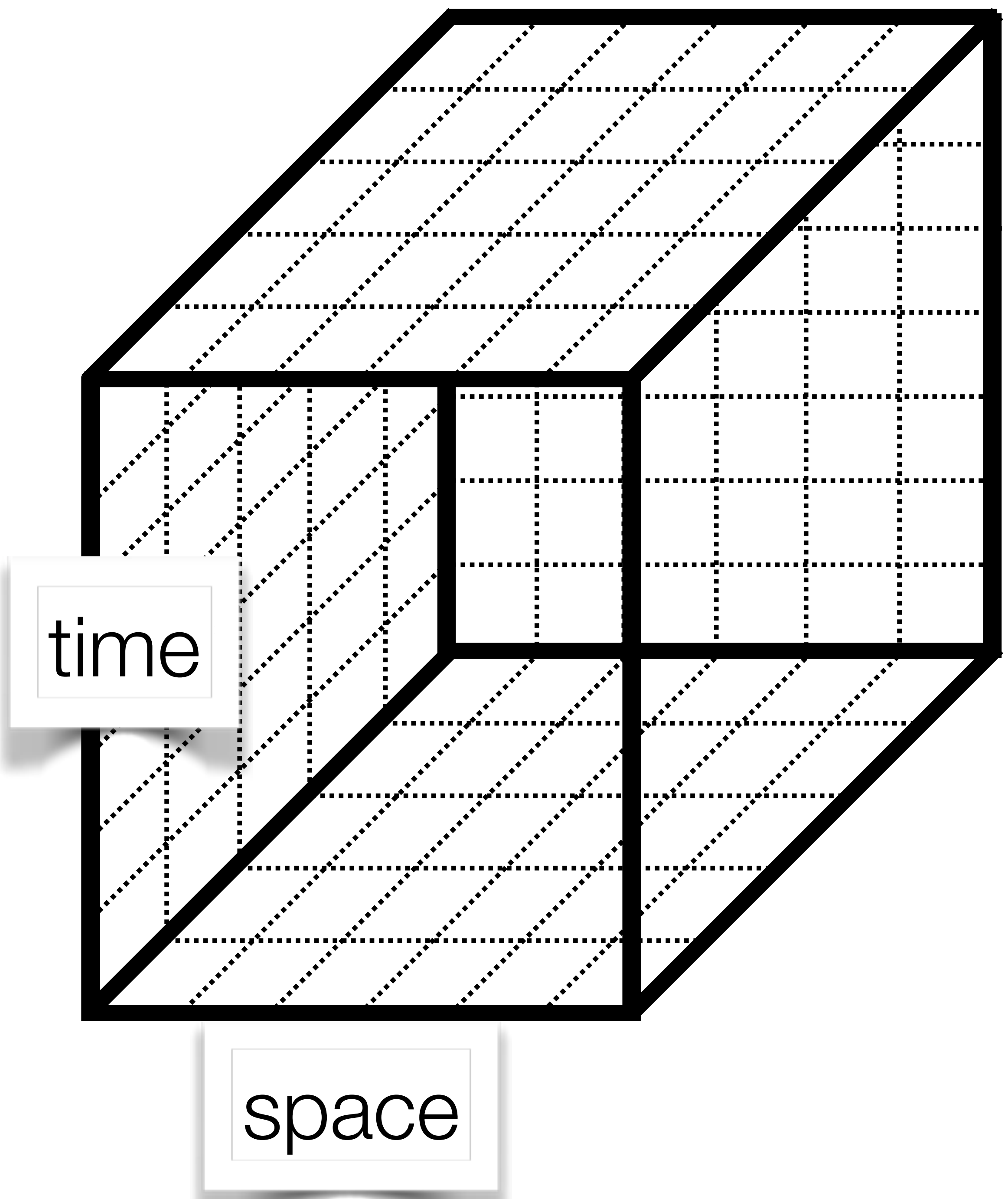

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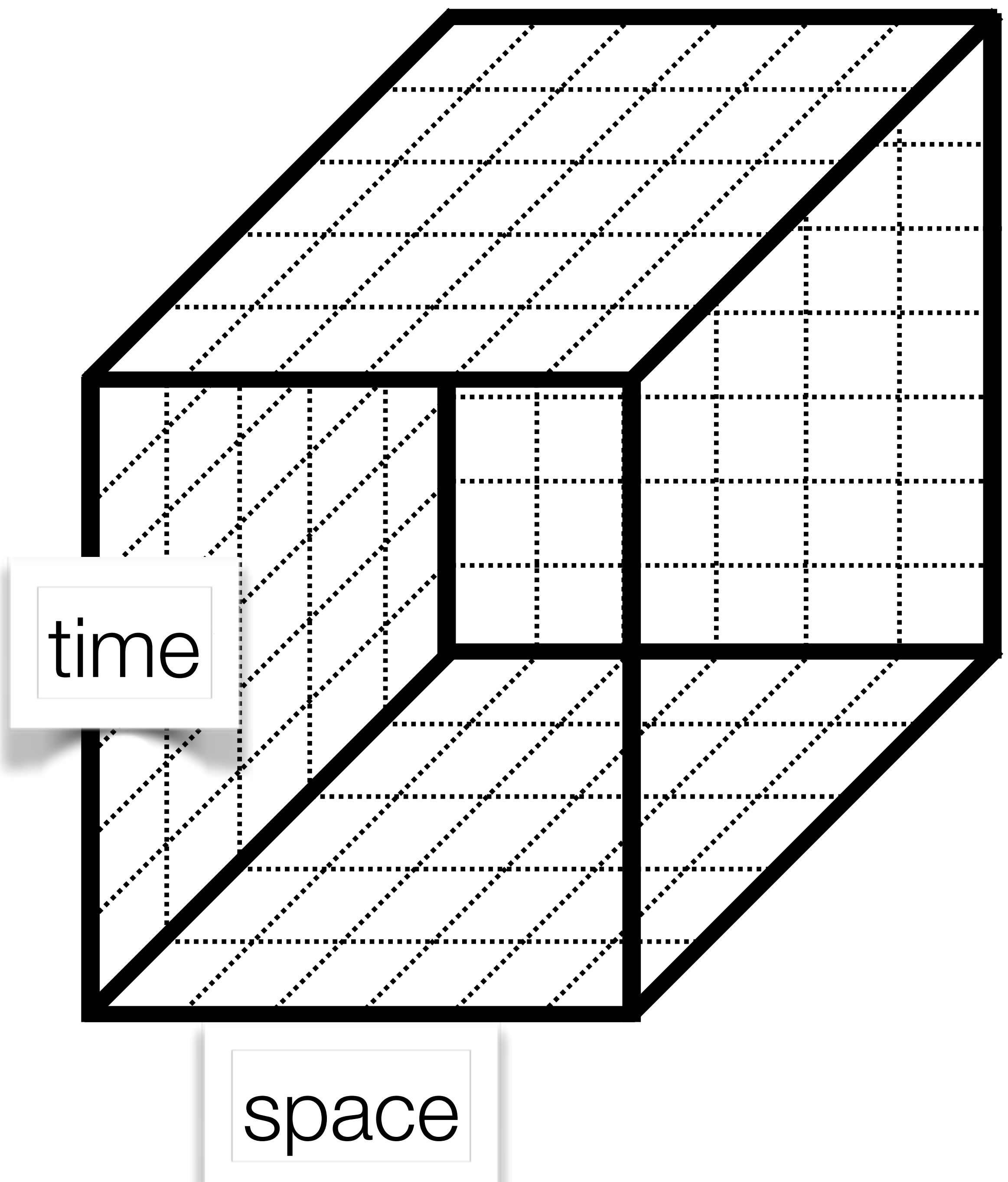

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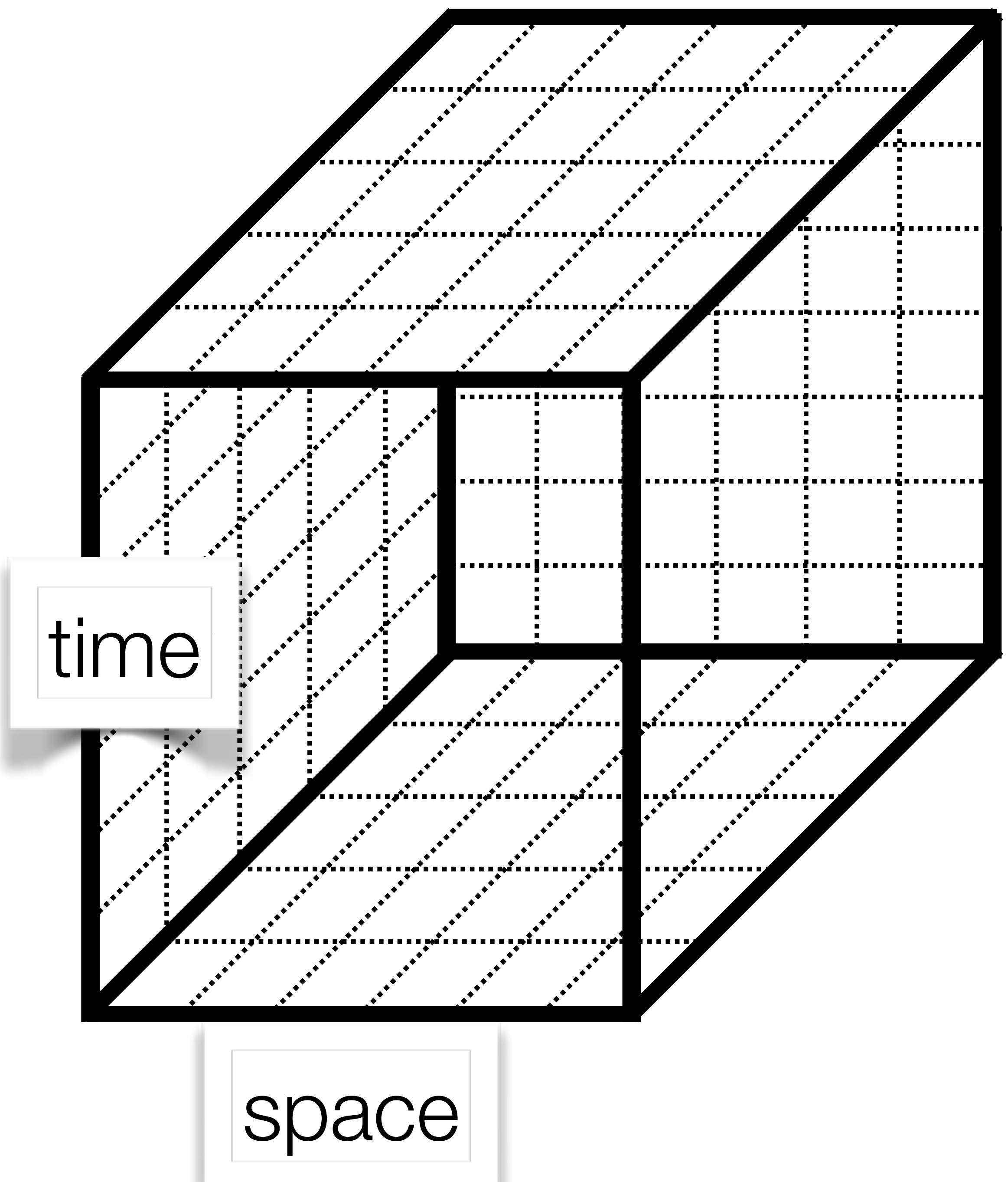

$$\{U_1, U_2, U_3, \ldots, U_N\}$$

Markov Chain Monte Carlo

Introduction to LQCD

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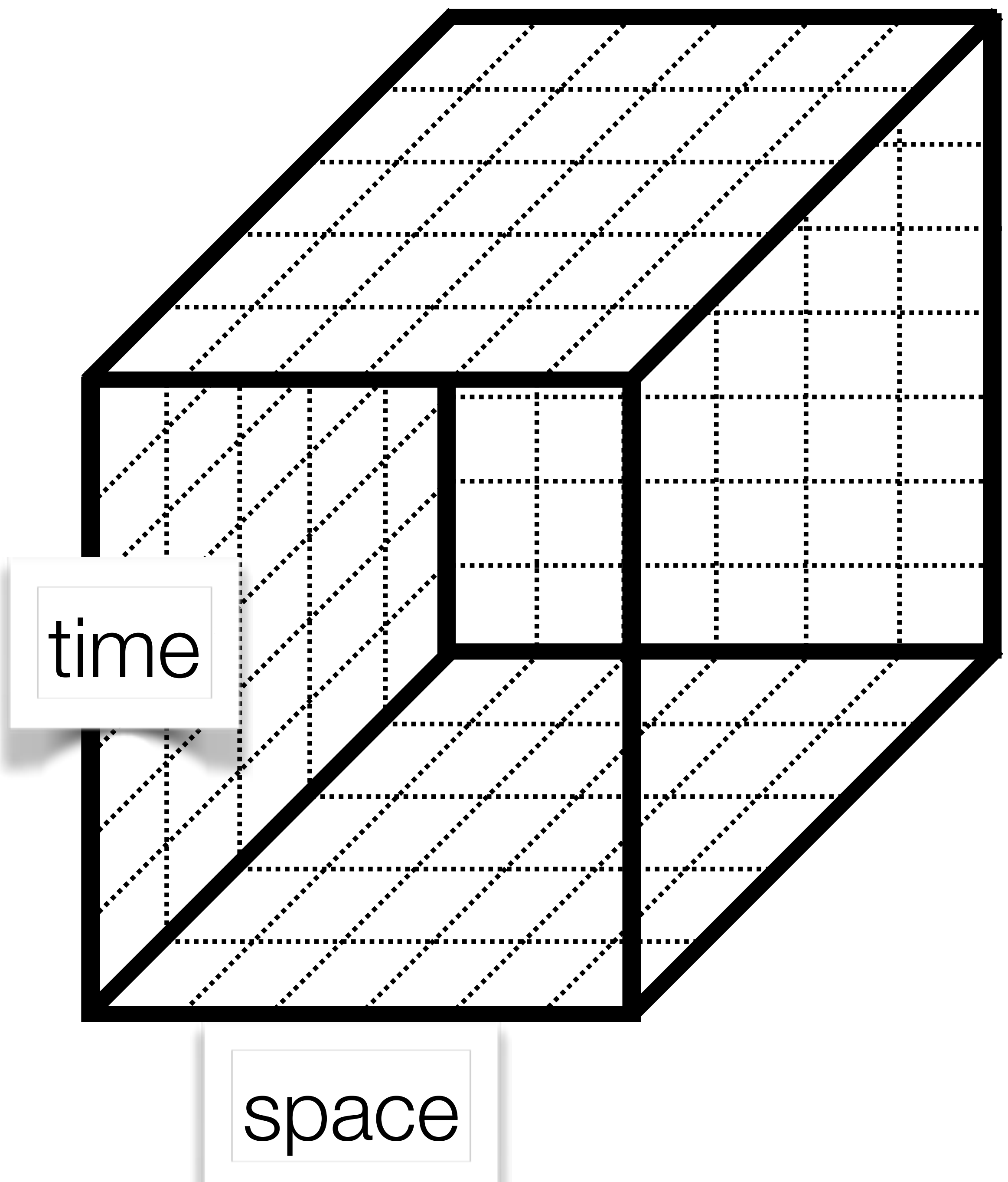


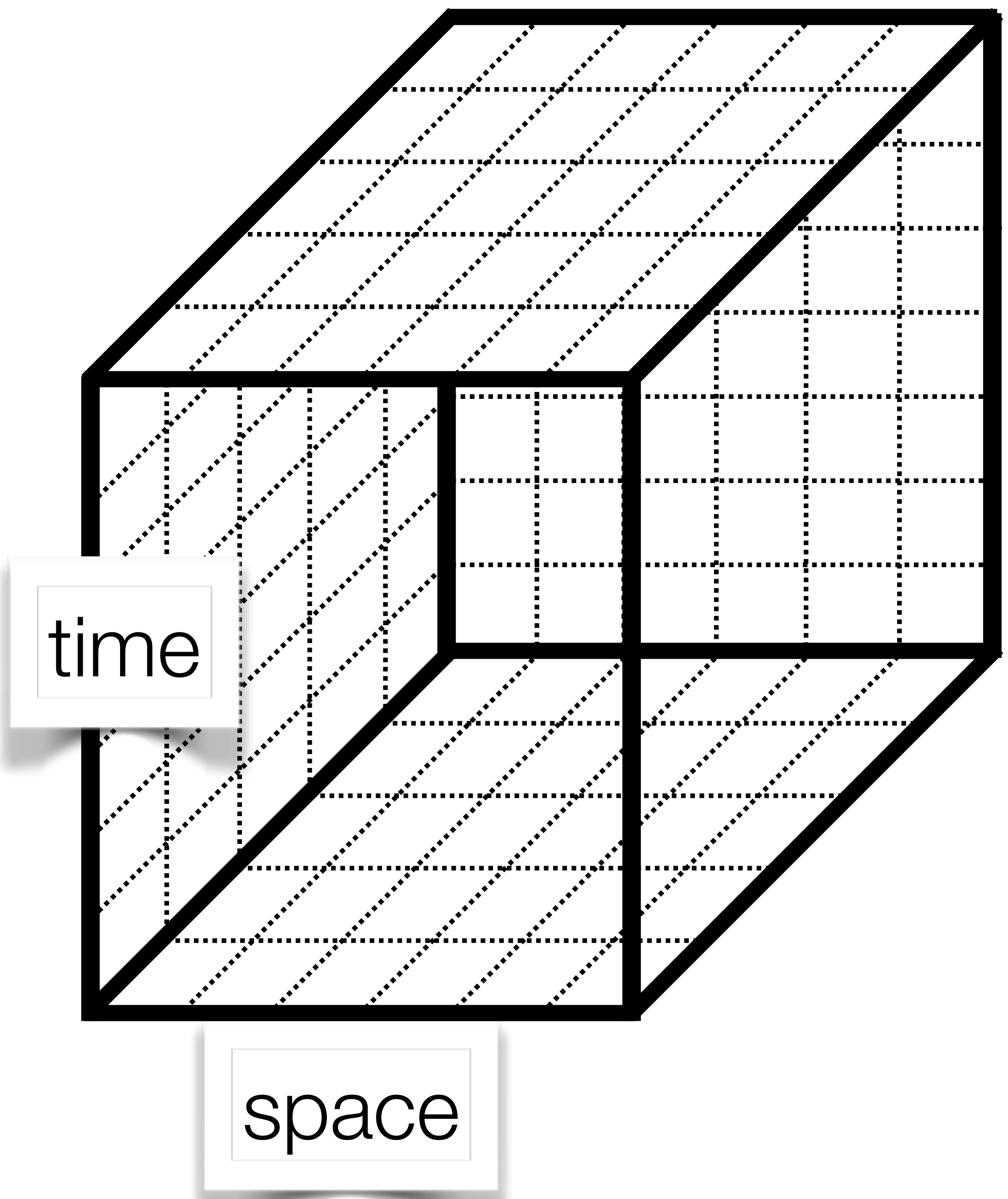
Probability

$$\{U_1, U_2, U_3, \ldots, U_N\}$$

Markov Chain Monte Carlo

$$\approx \frac{1}{N}\sum_{i=1}^{N} \mathcal{O}(t)\mathcal{O}^\dagger(0)[U_i]$$

Introduction to LQCD



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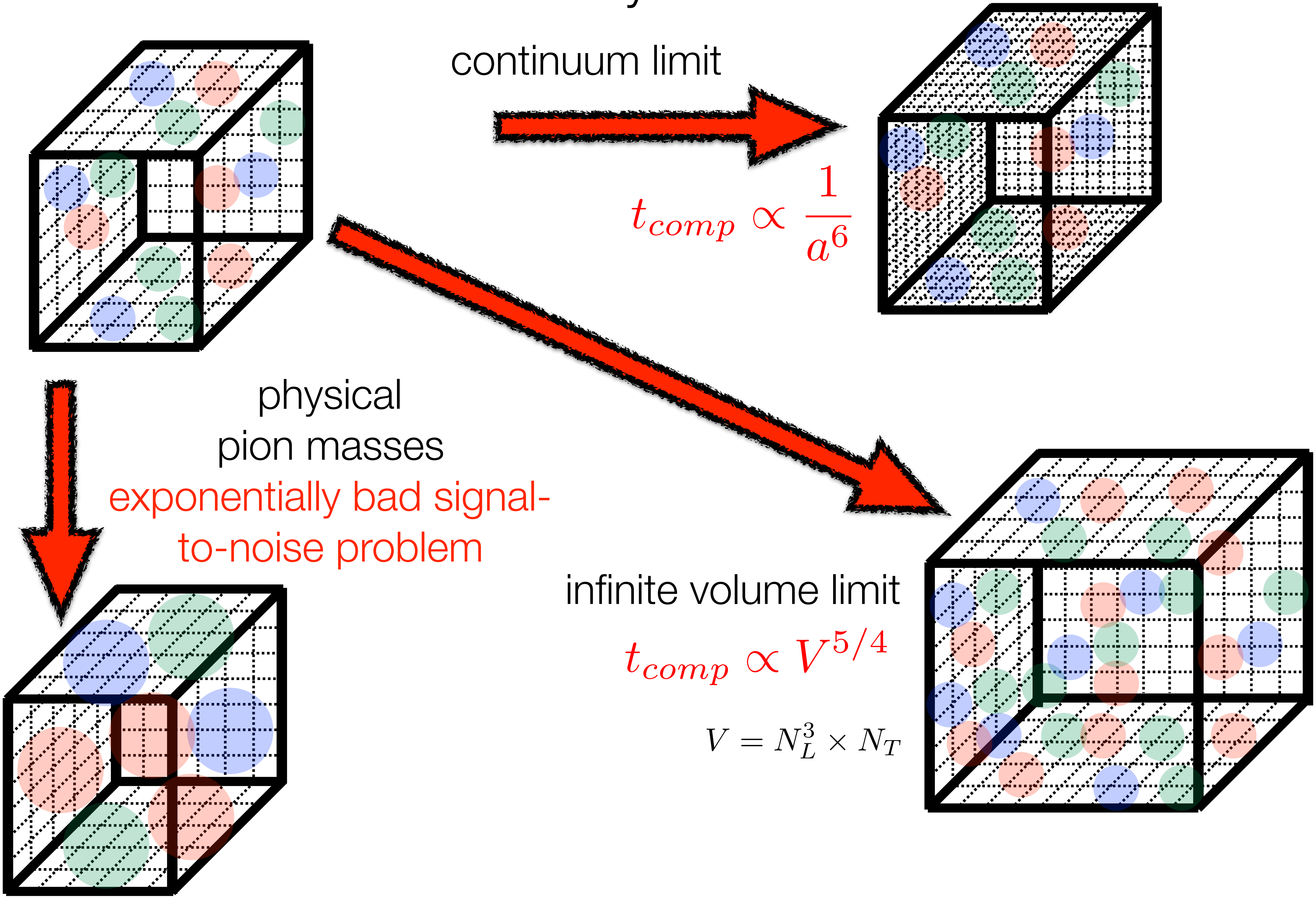
Probability

$$\{U_1, U_2, U_3, \ldots, U_N\}$$

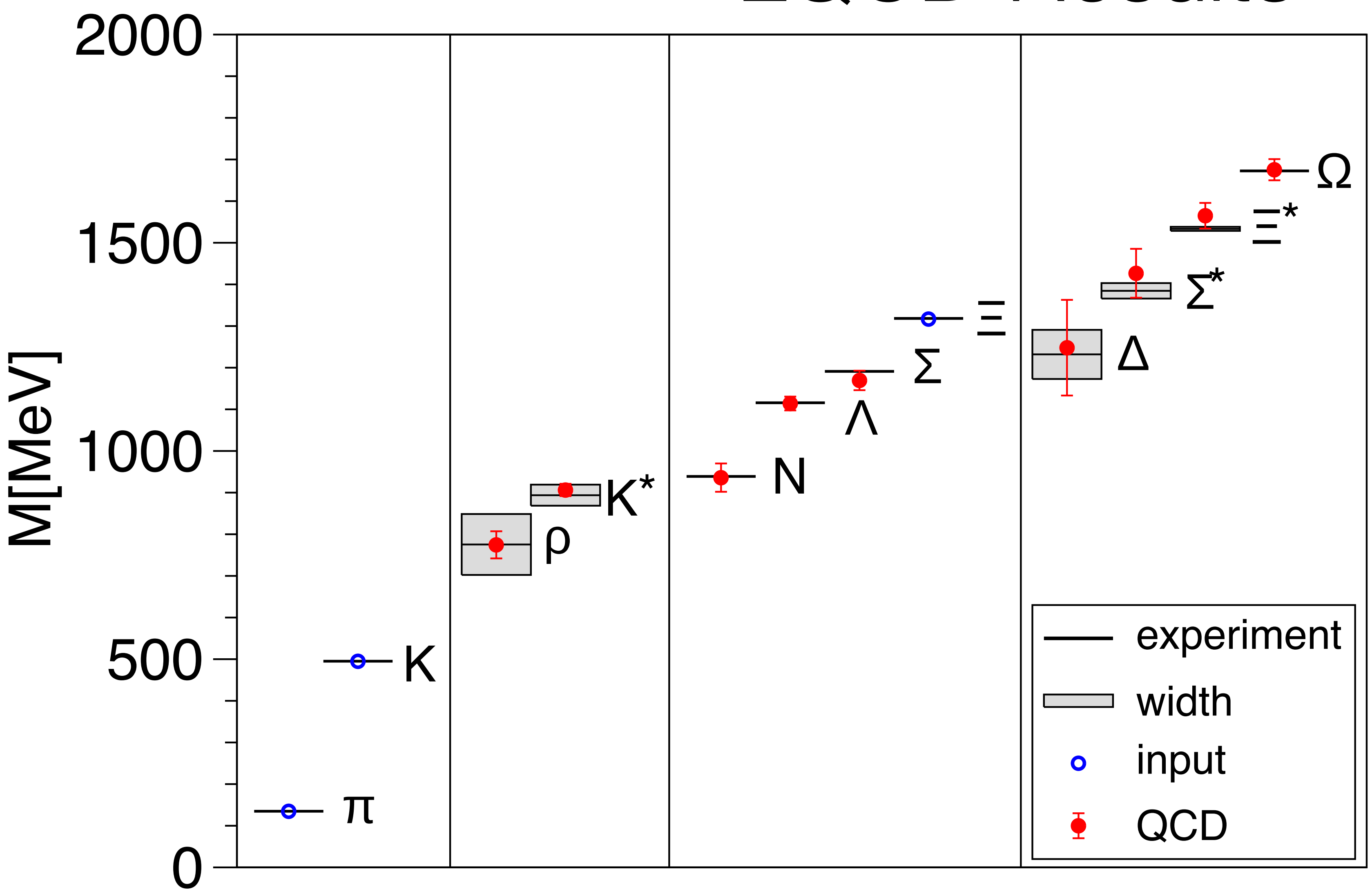
Markov Chain Monte Carlo

$$\approx \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}(t)\mathcal{O}^\dagger(0)[U_i] + O\left(\frac{1}{\sqrt{N}}\right)$$

LQCD Systematics



LQCD Results



Durr et al., Science 322 (2008) [arXiv:0906.3599]

Pion mass is used to fix the physical light quark mass $M_\pi^2 = 2B_0\hat{m}_l + \cdots$

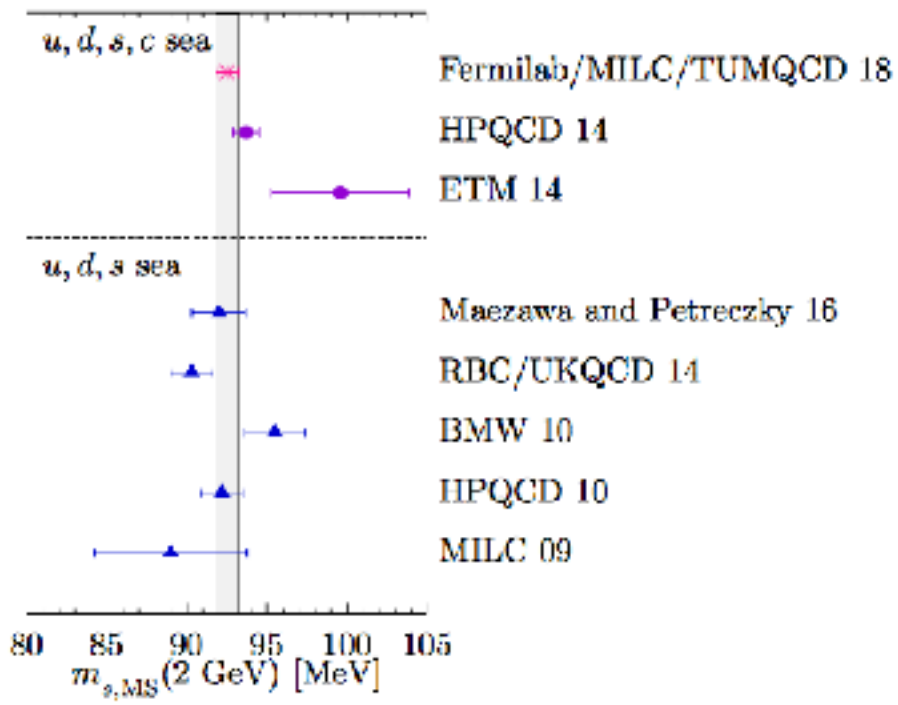
Kaon mass is used to fix the physical strange quark mass $M_K^2 = B_0(m_s + \hat{m}_l) + \cdots$

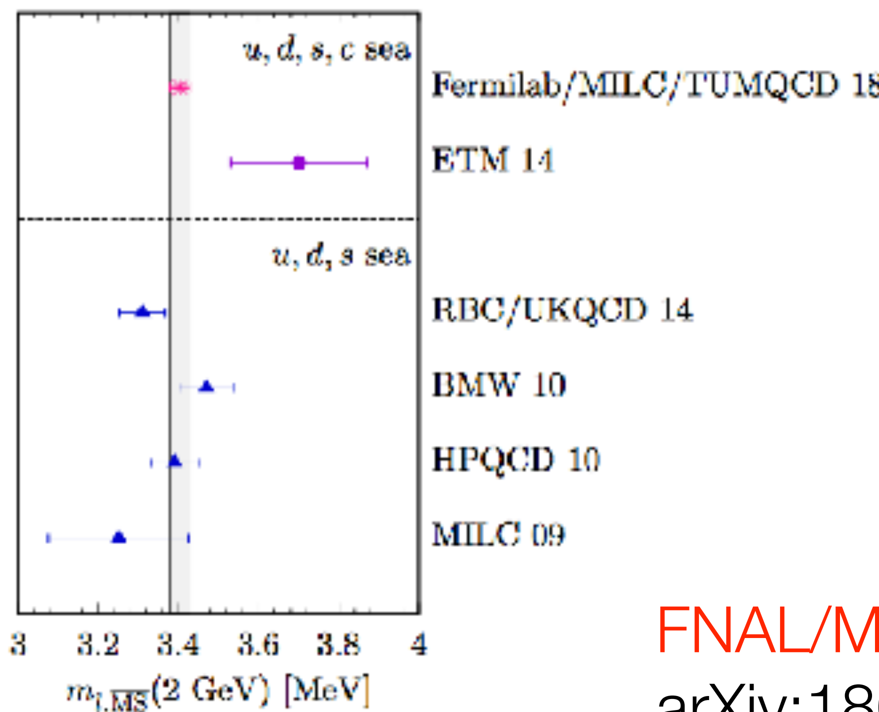
Hadronic quantity is used to set the scale in MeV $M_\Sigma[\mathrm{MeV}] \leftrightarrow a[\mathrm{fm}]$

Everything else is a prediction!

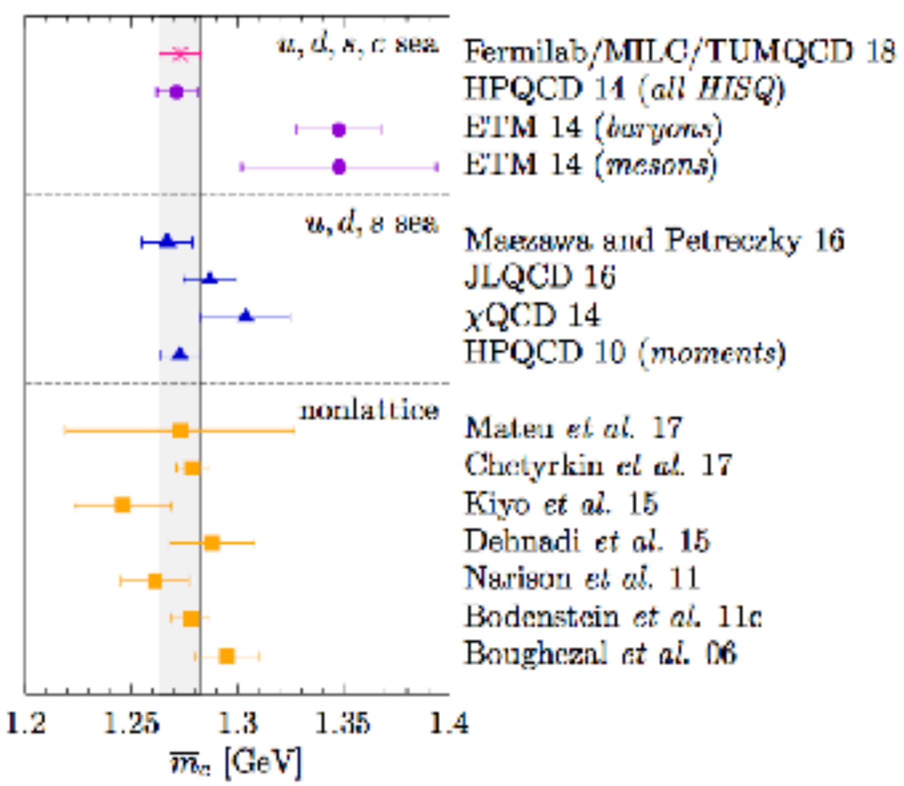
(need 1 new quantity for each new input)

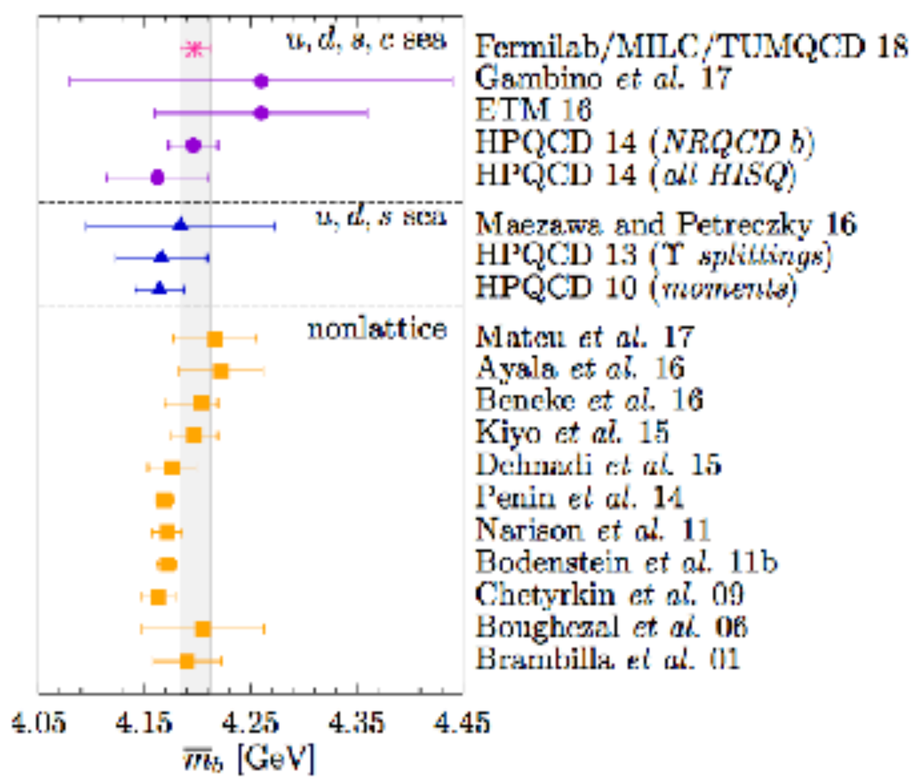
LQCD Results





FNAL/MILC/TUMQCD Collaborations
arXiv:1802.04248

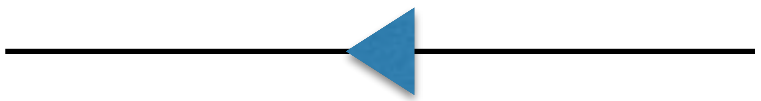




Most precise determination of quark masses now comes from LQCD

LQCD Challenges for NP

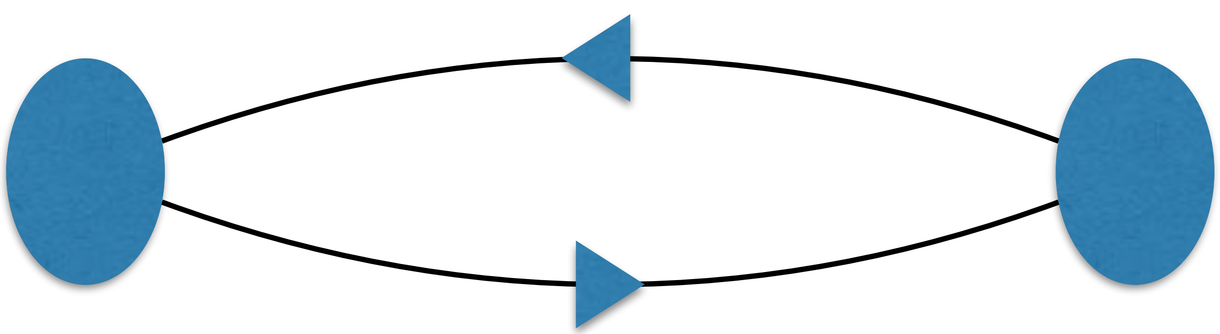
- The most difficult challenge in applying LQCD to NP is an exponentially bad signal-to-noise problem for nucleons



$$\sim e^{-\frac{1}{2}m_\pi t} + e^{-\frac{1}{3}m_N t} + \cdots$$

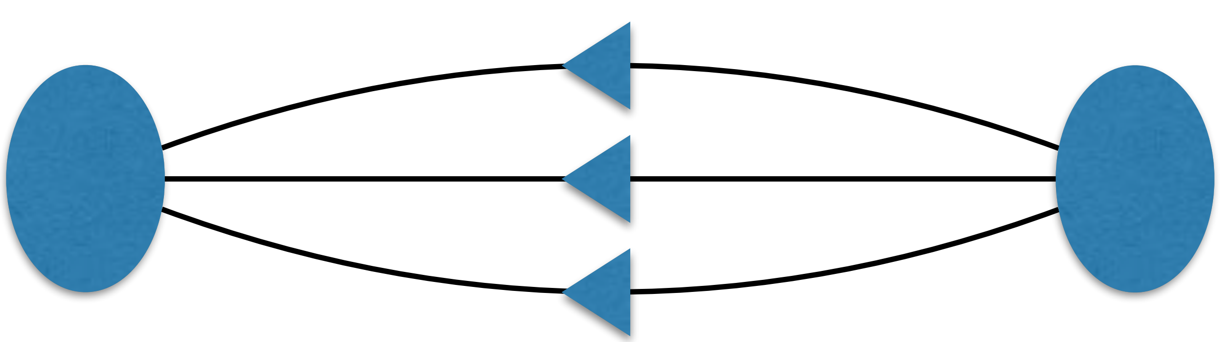
each quark carries information about pions and nucleons

$$\lambda_\pi(t) \gg \lambda_N(t)$$



$$\bar{d}\gamma_5 u : C(t) = A_\pi e^{-m_\pi t} + \cdots$$

For the nucleon - the large pion eigenvalues must cancel to expose the small nucleon eigenvalues



$$(u^T C\gamma_5 d)u : C(t) = A_N e^{-m_N t} + \cdots$$

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Lepage Argument

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Lepage Argument

- signal-to-noise ratio of correlation functions

$$\mathrm{SNR} \sim \frac{\langle N\bar{N}\rangle}{\sqrt{\langle (N\bar{N})(N\bar{N})^\dagger\rangle - \langle N\bar{N}\rangle^2}}$$

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Lepage Argument

- signal-to-noise ratio of correlation functions
- numerator $\sim \exp(-m_N t)$

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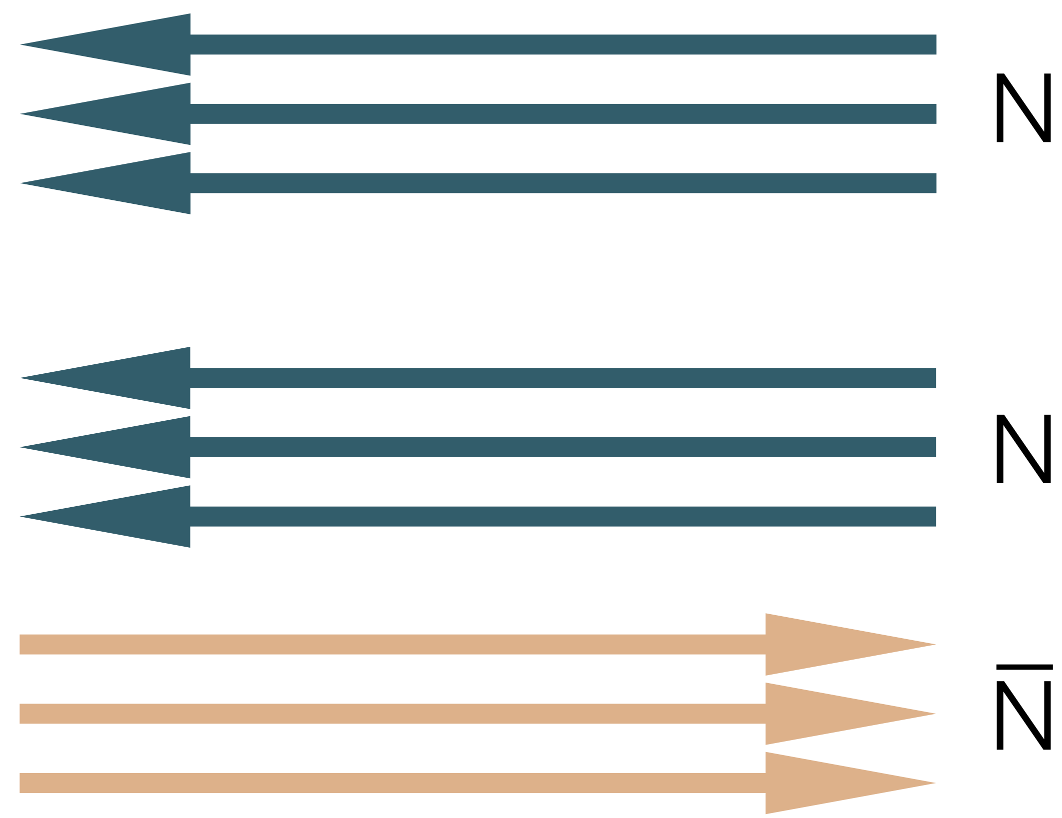
- numerator
  $\sim \exp(-m_N t)$

- denominator



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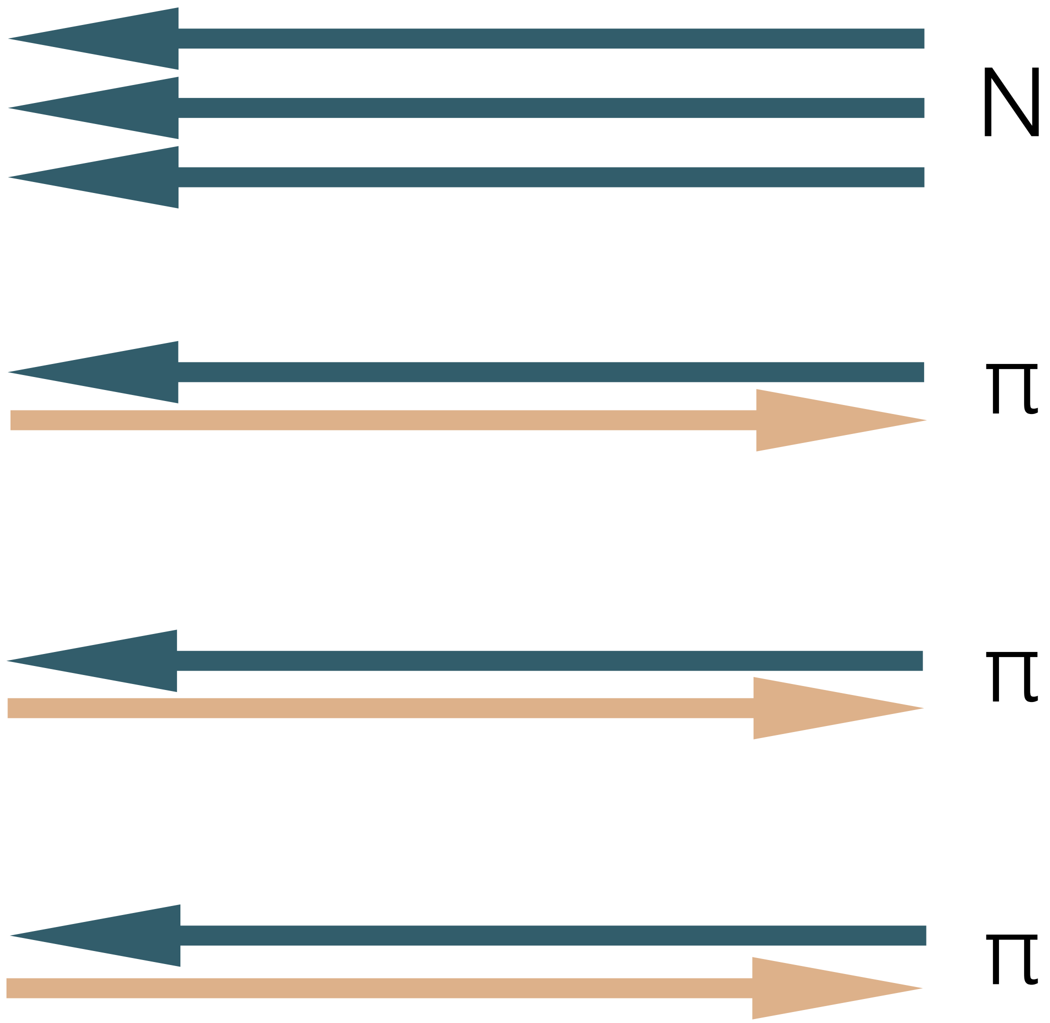
- denominator $\sim \exp\left(-\frac{3}{2}m_\pi t\right)$



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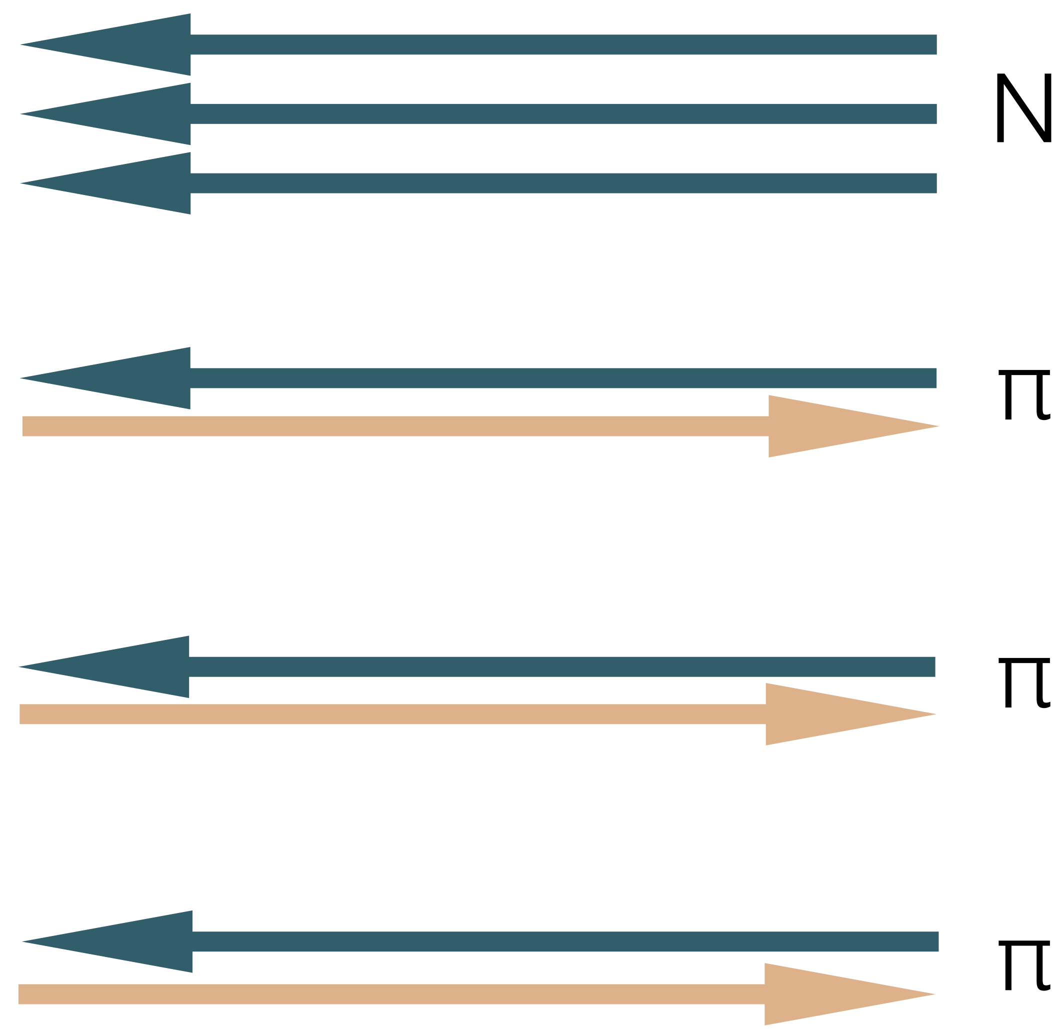
- signal-to-noise ratio of correlation functions
- numerator $\sim \exp(-m_N t)$
- denominator $\sim \exp\left(-\frac{3}{2}m_\pi t\right)$
- time-dependence of SNR

$$\sim \sqrt{N}\exp\left[-A\left(m_N - \frac{3}{2}m_\pi\right)t\right]$$



exponential noise
power-law statistics

LQCD Challenges for NP

- Consider a 2-point correlation function

$$C(t) = \sum_{\mathbf{x}} \langle \Omega | \mathcal{O}(t, \mathbf{x}) \mathcal{O}^\dagger(0, \mathbf{0}) | \Omega \rangle$$

all we do with LQCD is compute 2, 3, 4 point functions

$$1 = \sum_n |n\rangle\langle n|$$

multiply by 1

$$C(t) = \sum_n z_n z_n^\dagger e^{-E_n t}$$

$$z_n = \langle \Omega | \mathcal{O} | n \rangle$$

overlap factor

$$C(t) = z_0 z_0^\dagger e^{-E_0 t} \left[1 + \delta_{10}^z e^{-\Delta_{10} t} + \cdots \right]$$

$$\Delta_{10} = E_1 - E_0$$

$$\delta_{10}^z = \frac{z_1 z_1^\dagger}{z_0 z_0^\dagger}$$

$$\lim_{t \to \infty} C(t) = z_0 z_0^\dagger e^{-E_0 t}$$

The ground state spectrum is what we can compute with better control than any other quantity

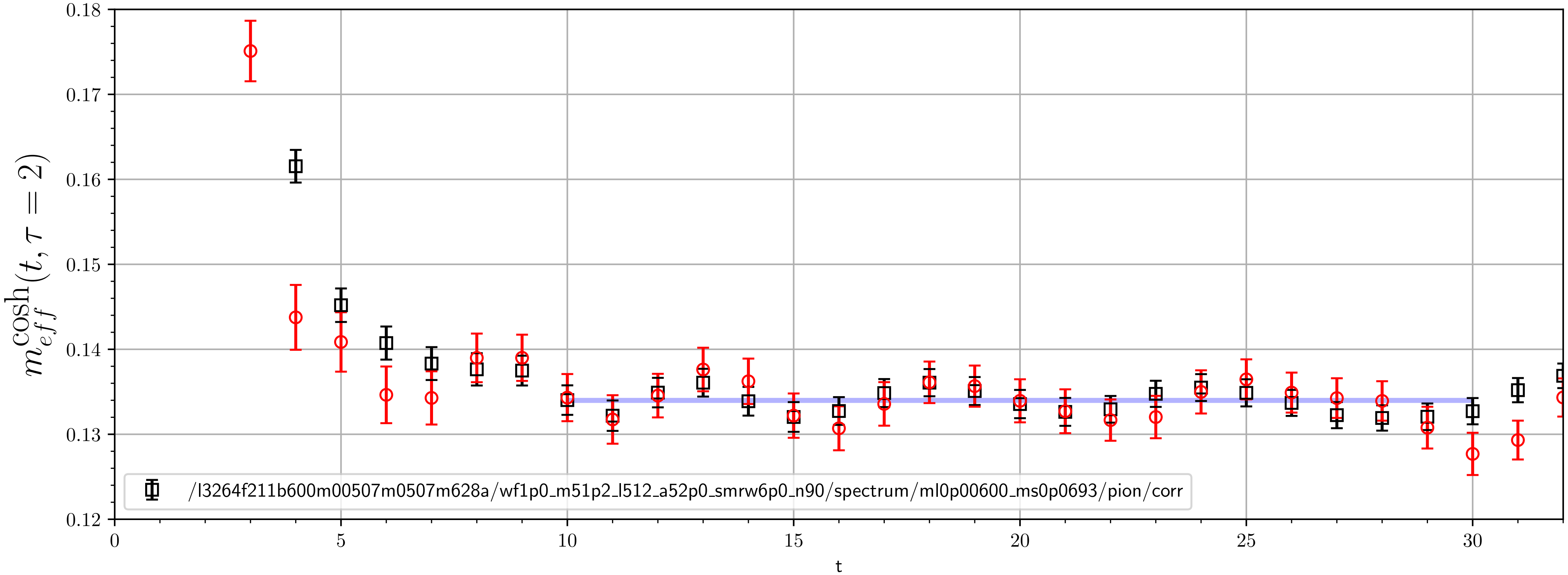
$$m_{eff}(t) = \frac{1}{\tau} \ln \left(\frac{C(t)}{C(t+\tau)} \right)$$

$$\lim_{t \to \infty} m_{eff}(t) = E_0$$

A useful quantity is the effective mass

LQCD Challenges for NP

- Consider a 2-point correlation function

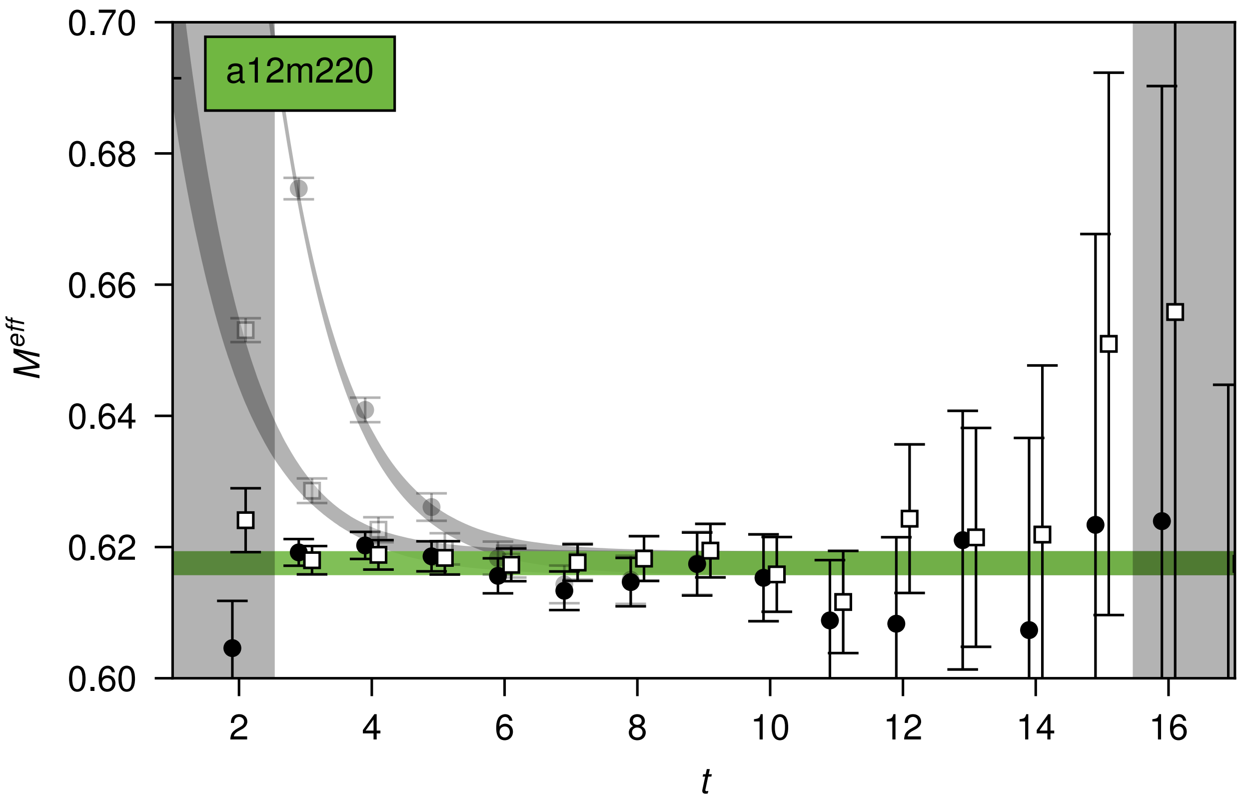


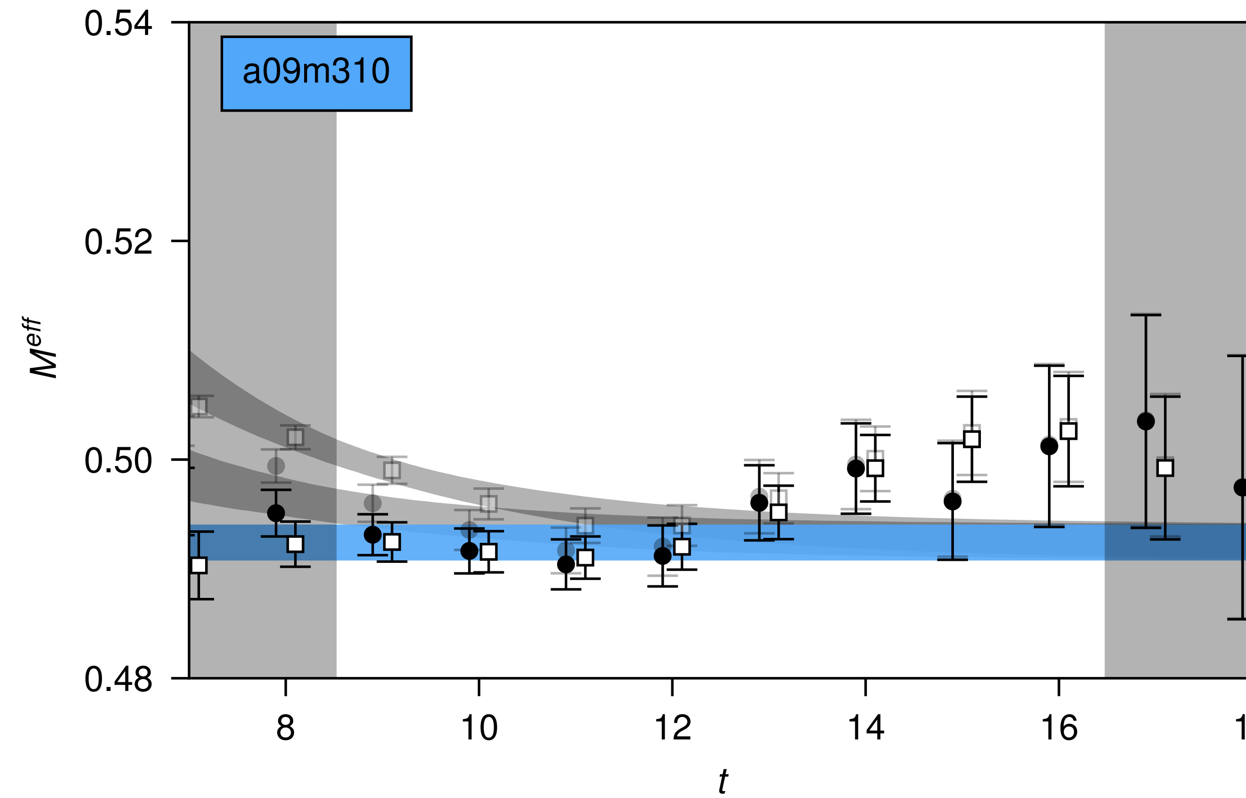
Effective mass of Pion 2-point correlation function
red and black "data" are from different choices of overlap operators

Noise is constant in time - can determine very clean ground state (blue band)

LQCD Challenges for NP

- Consider a 2-point correlation function





Two examples of nucleon effective mass

Noise is growing in time - can not simply go to the long-time limit without exponentially increasing the amount of statistics needed

$$\frac{Signal}{Noise} \to \sqrt{N_{state}} e^{-(m_N - \frac{3}{2} m_\pi)t}$$

Correlated late-time fluctuations… what is the ground state?

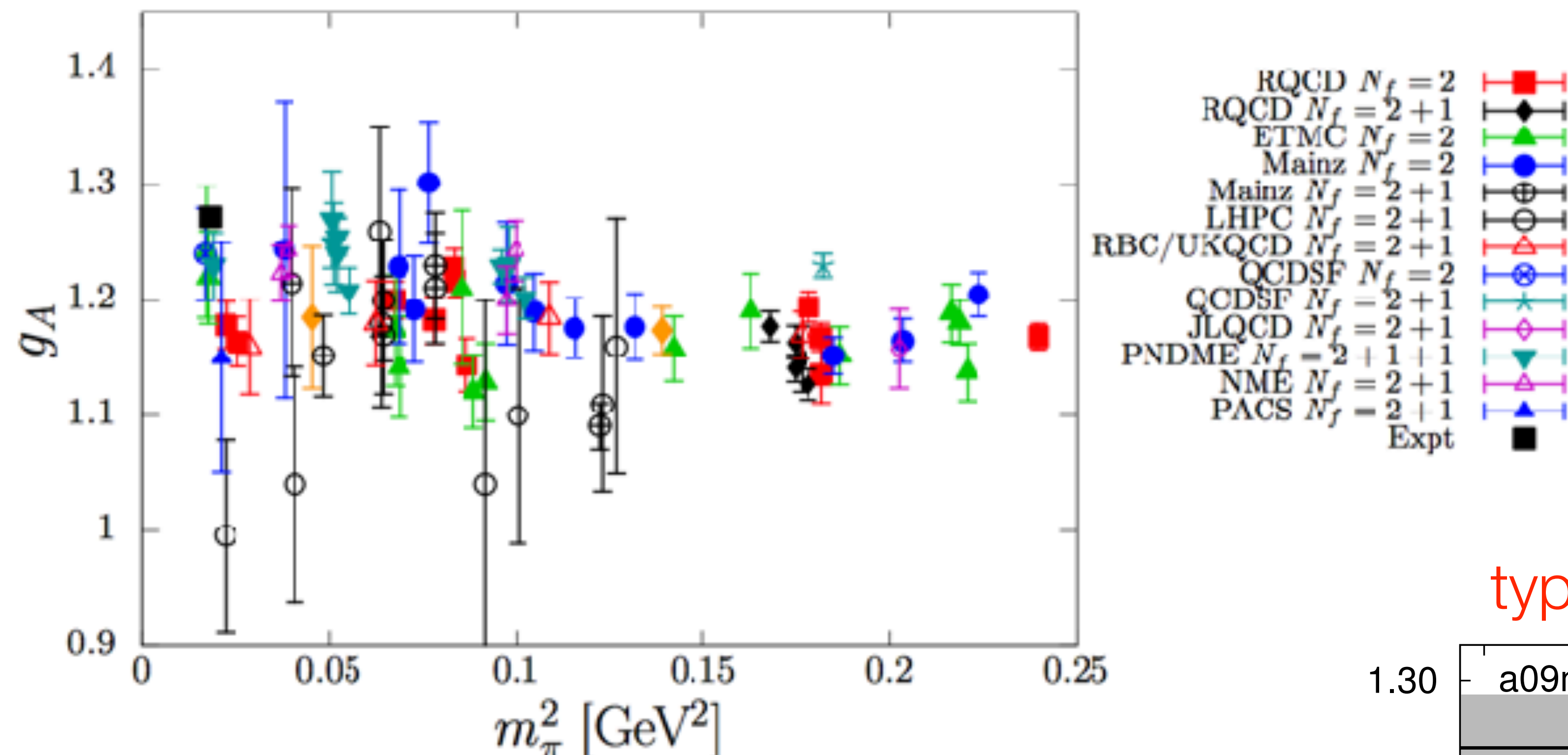
Need sophisticated analysis to ensure you are not susceptible to correlated fluctuations

This problem is exacerbated with 2+ nucleons and form-factor calculations (g_A)

LQCD Challenges for NP

Nucleon axial charge - S. Collins - Lattice 2016 Plenary

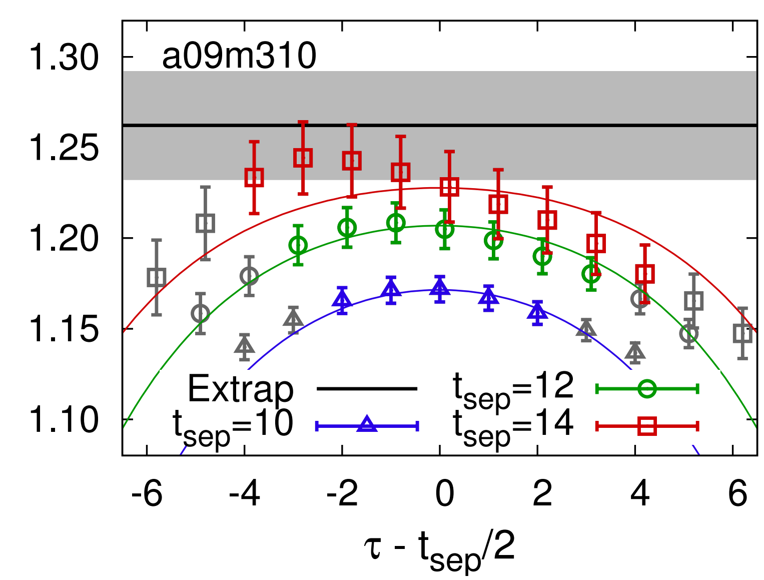
Benchmark quantity sensitive to systematics.



g_A is an important benchmark quantity - very challenging for LQCD to get under control

Presented 2016:
PNDME, NME, Mainz, RQCD, ETMC, PACS, χQCD, QCDSF, …

typical calculation



in long-time limit - should be flat

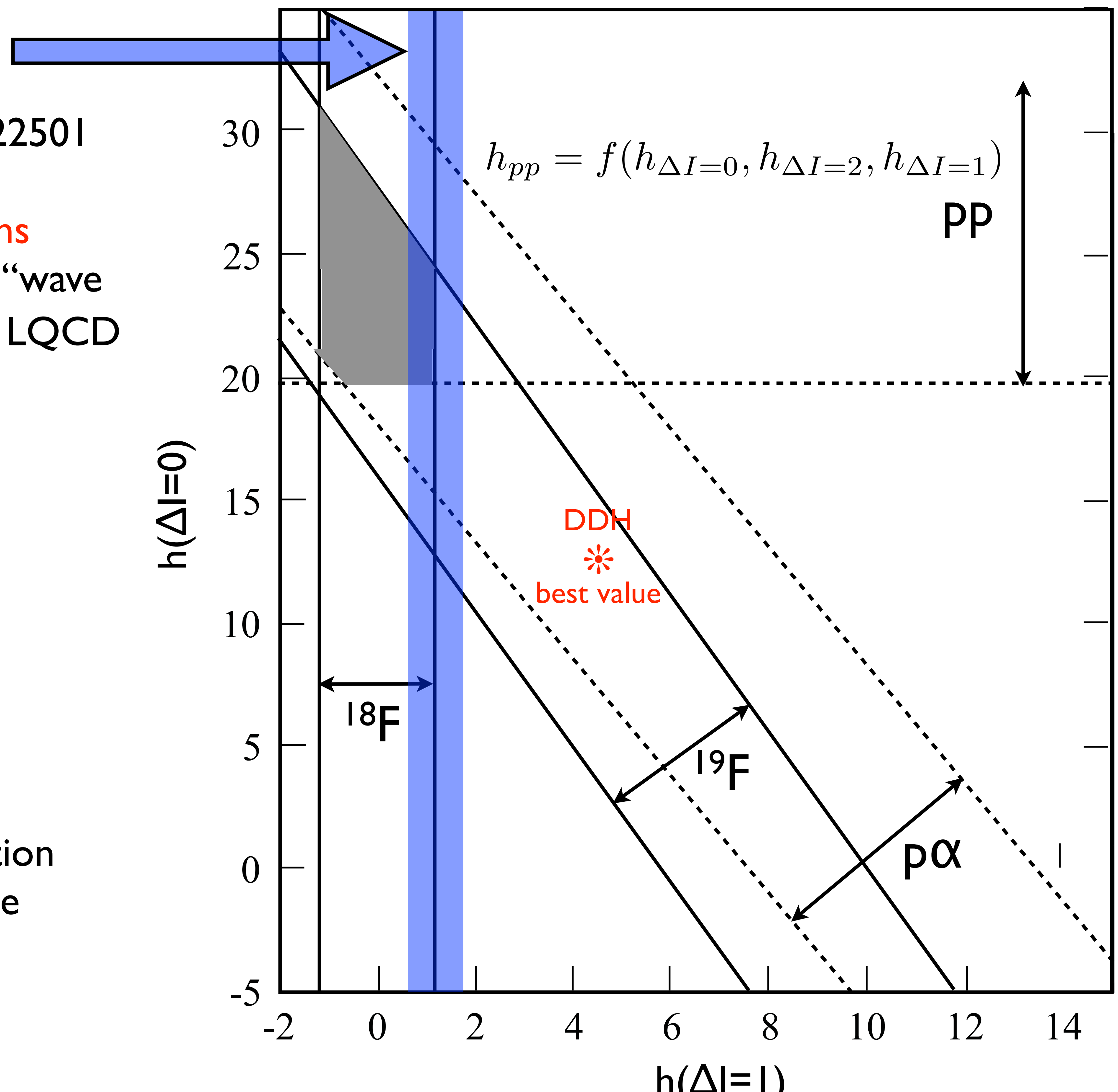
LQCD Challenges for Parity Nonconservation

first LQCD calculation of h_π^1 for
L=2.5 f a=0.123f m_π= 389 MeV
J. Wasem Phys. Rev. C85 (2012) 022501

Several unquantified approximations

- assumption about coupling of "wave function" used to Nπ state in LQCD calculations
- "disconnected" quark loops neglected
- single lattice spacing
- single pion mass
- single volume
- no renormalization

- This was a tour-de-force calculation carried out single handedly by Joe Wasem



LQCD Challenges for Parity Nonconservation

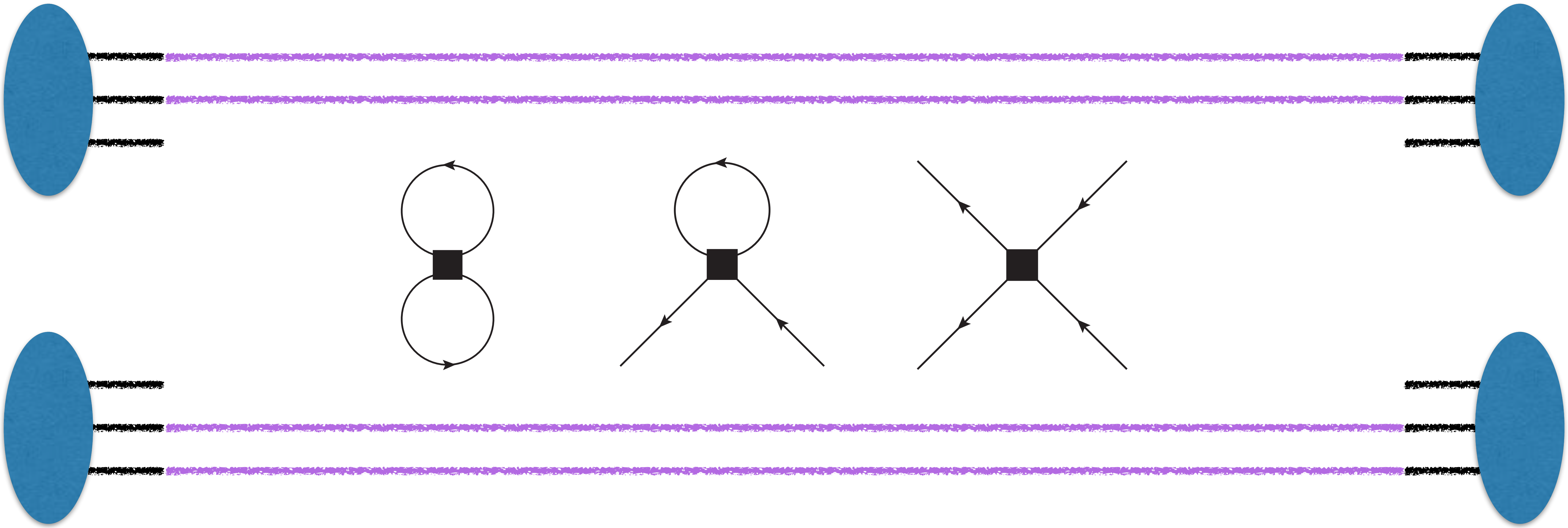
- Signal-to-noise is exponentially worse than single nucleon

$$\frac{S_{NN}}{\sigma_{NN}} \sim \left(\frac{S_N}{\sigma_N}\right)^2 = \left(\sqrt{N_{samples}}\; e^{(m_N - \frac{3}{2}m_\pi)t}\right)^2$$

- Either need all-to-all quark propagators (1 or more orders of magnitude more expensive) or
  - can not do I=0 and I=1 PNC amplitudes
  - lose a Volume factor in statistics in I=2

- Wick contraction cost of connecting all quark lines is ~100 times more than for two-nucleons

LQCD Challenges for Parity Nonconservation



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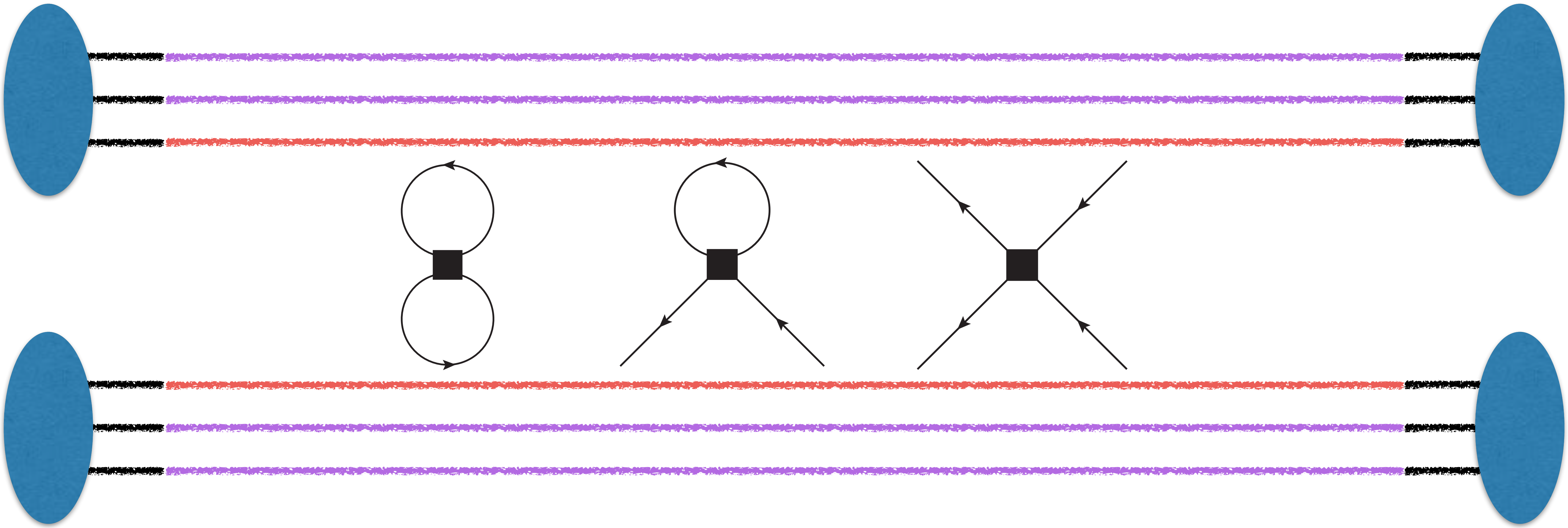
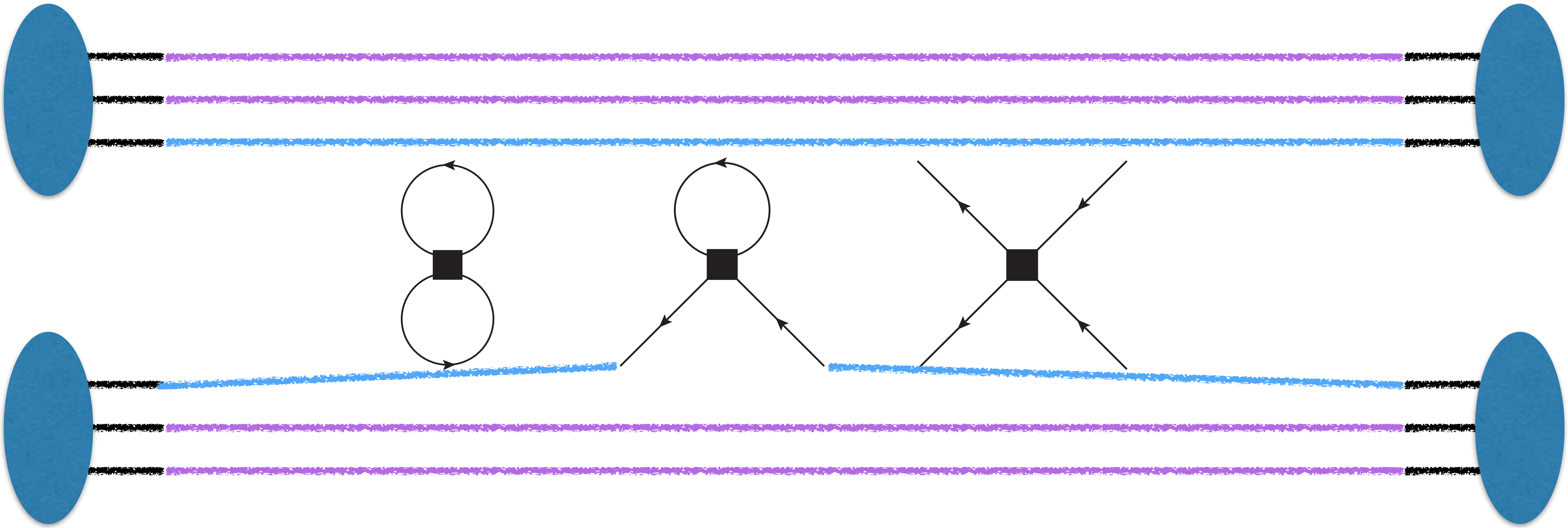


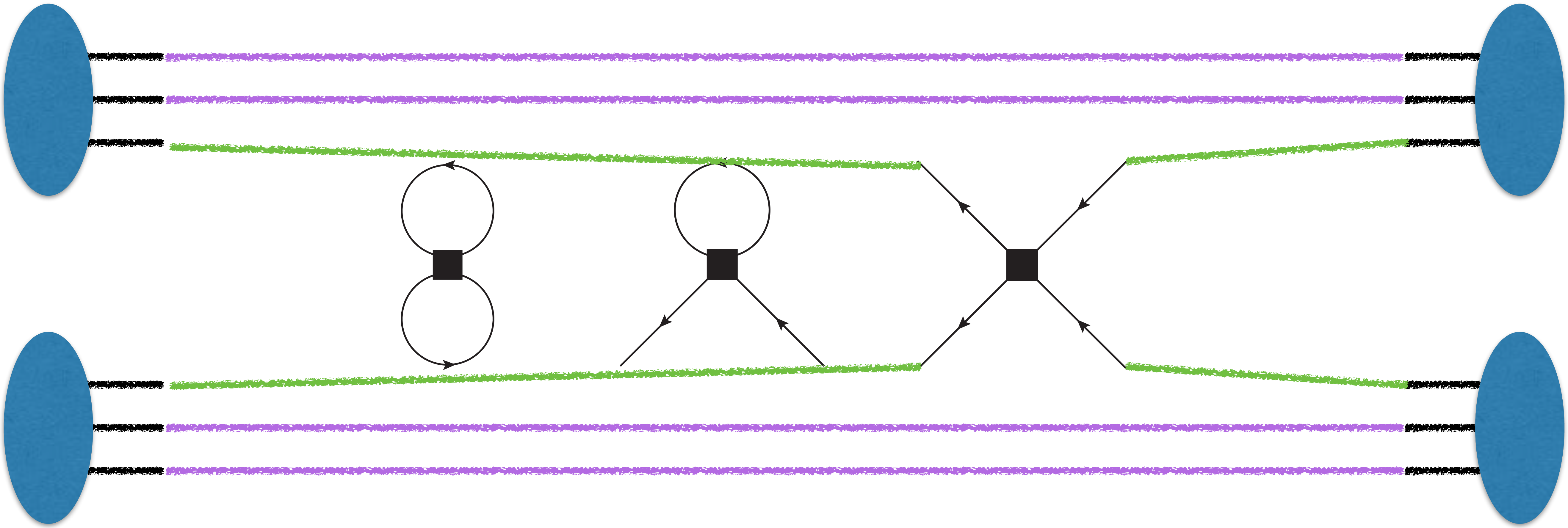
ΔI=0

LQCD Challenges for Parity Nonconservation



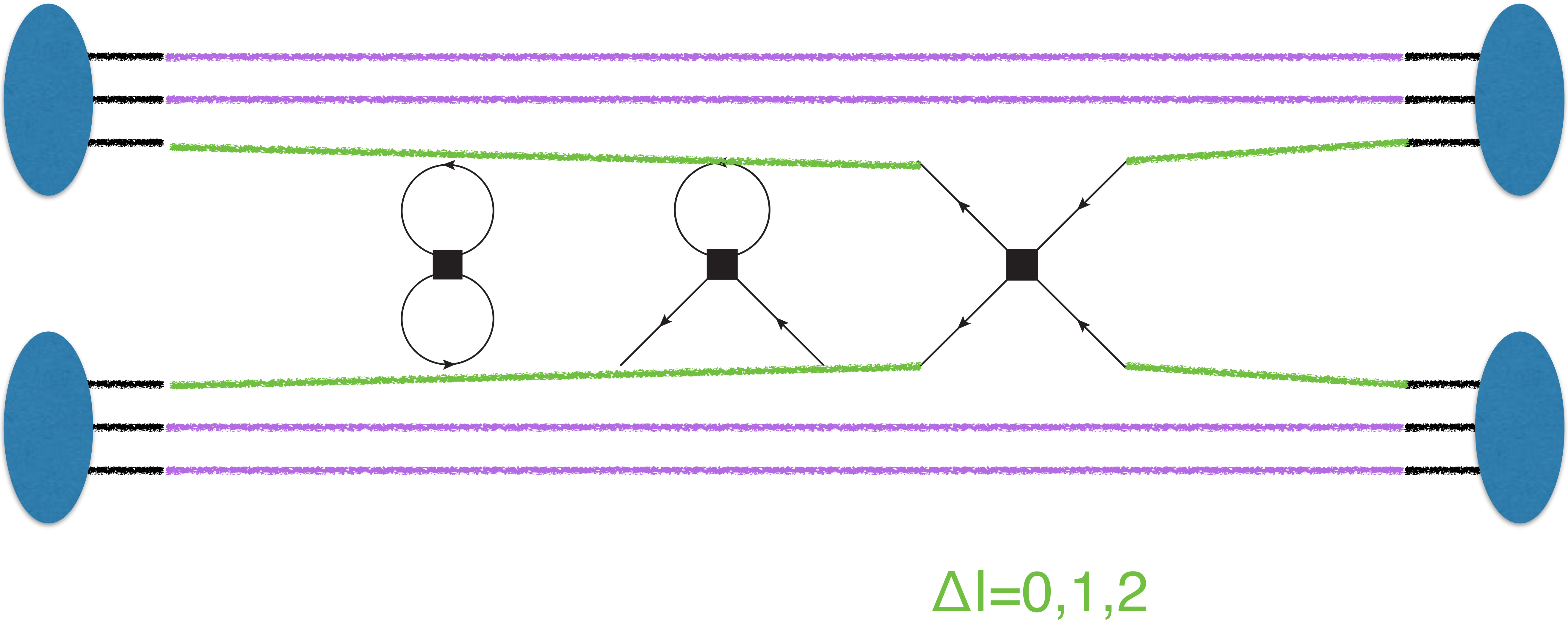
ΔI=0,1

LQCD Challenges for Parity Nonconservation



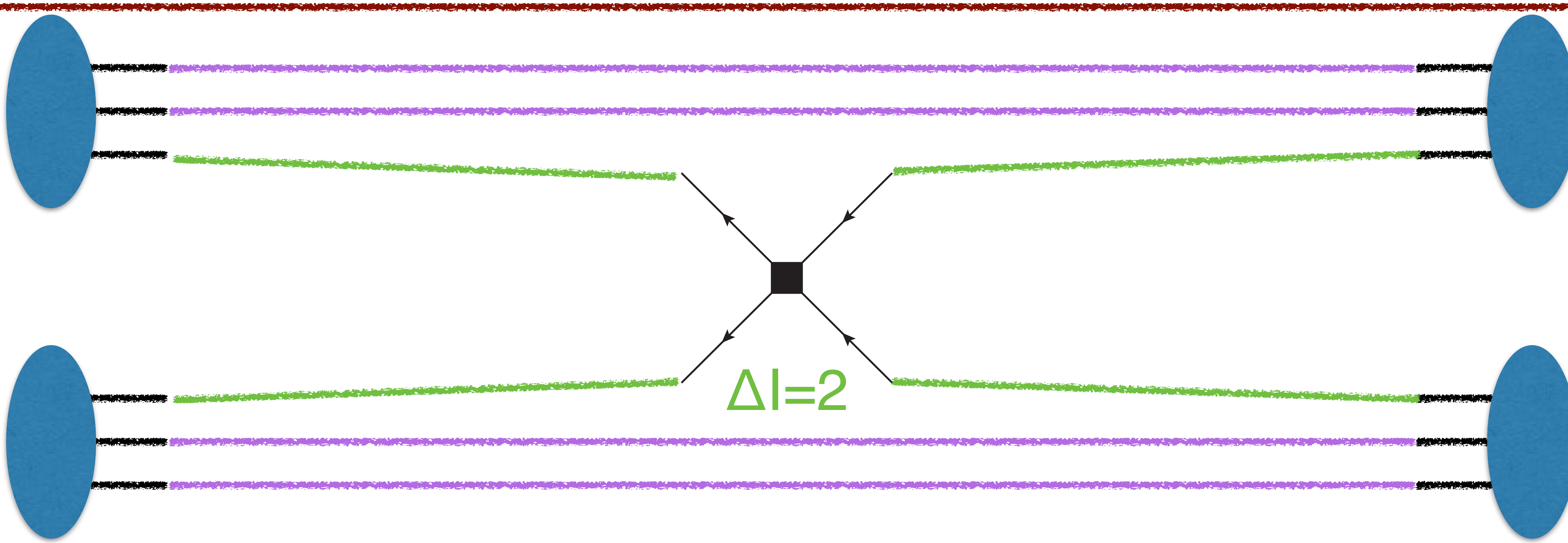
ΔI=0,1,2

LQCD Challenges for Parity Nonconservation



- The "disconnected" quark loops are numerically more expensive, and stochastically noisier
- LQCD calculations can project onto definite ΔI

LQCD Challenges for Parity Nonconservation



$NN(t, \mathbf{x})$ $\qquad$ $\mathcal{O}(t_{\mathcal{O}}, \mathbf{z})$ $\qquad$ $N^\dagger N^\dagger(0, \mathbf{0})$

- To project the operator, *O*, onto definite momentum, and to project the final NN state onto definite momentum, we need all-to-all propagators (expensive): $\sum_{\mathbf{x}}, \sum_{\mathbf{z}}$
- For now - fix source-sink separation (t) and do NOT sum over **x**, loss of spatial volume in statistics

Hadronic Parity Violation

- 2 Baryon „s-wave“ source

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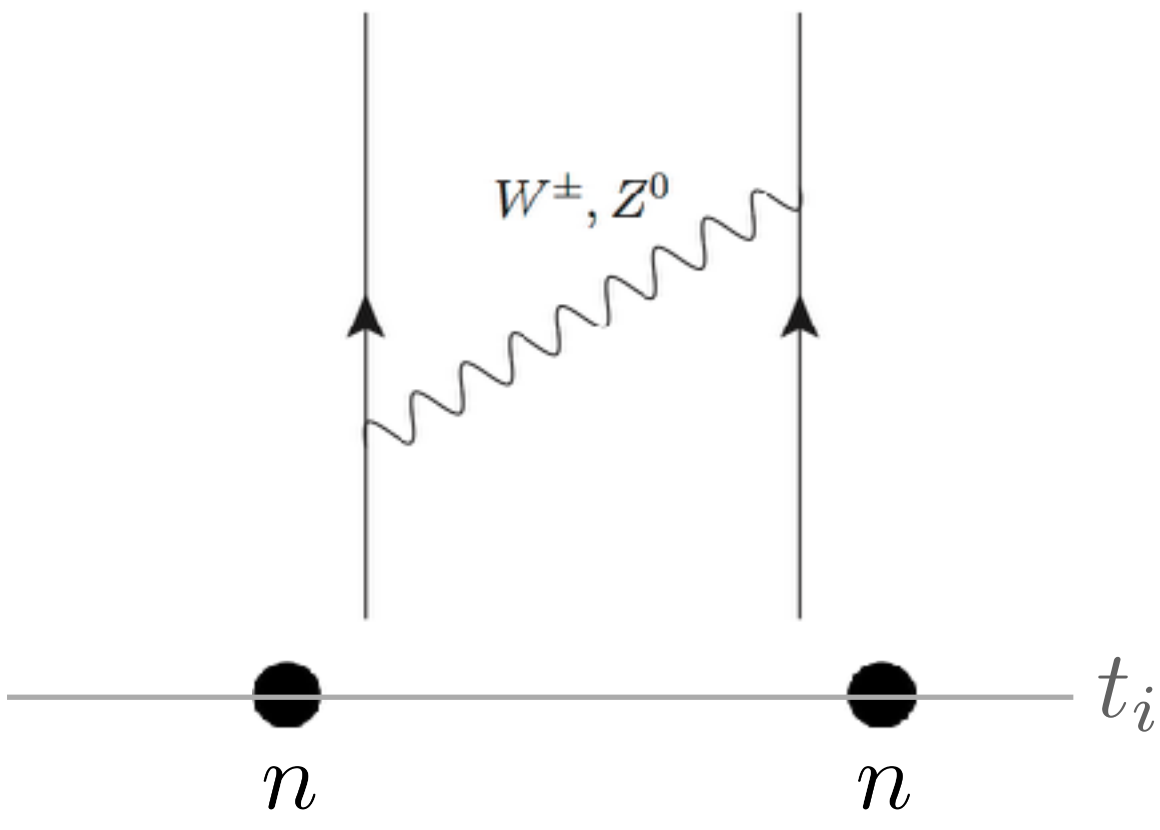
- 2 Baryon „s-wave“ source

- EW vertices ⇒ 4-quark operator insertion



Hadronic Parity Violation

- 2 Baryon „s-wave“ source

$$\mathcal{O}^{\Delta I=2} \equiv \sum_{\mathbf{x}} \left[(\bar{q}\tau^3 q)_A (\bar{q}\tau^3 q)_V - \frac{1}{3} (\bar{q}\vec{\tau} q)_A (\bar{q}\vec{\tau} q)_V \right] (\mathbf{x})$$

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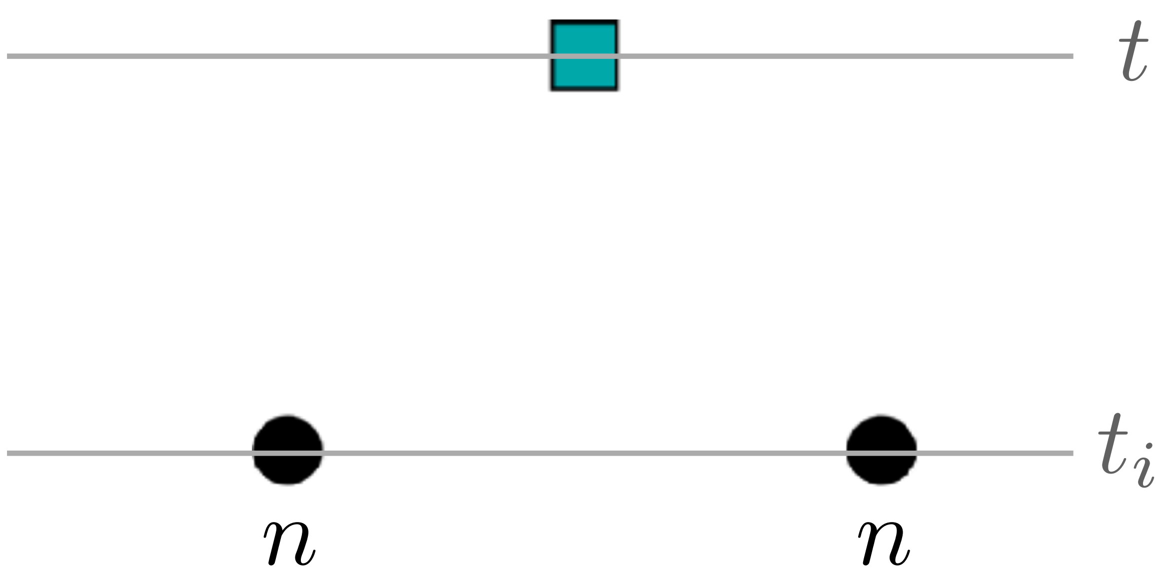

Hadronic Parity Violation

- 2 Baryon „s-wave“ source
- EW vertices ⇒ 4-quark operator insertion
- 2 Baryon „p-wave“ sink
- In total there are 4896 contractions
- isospin limit reduces this number to 2208

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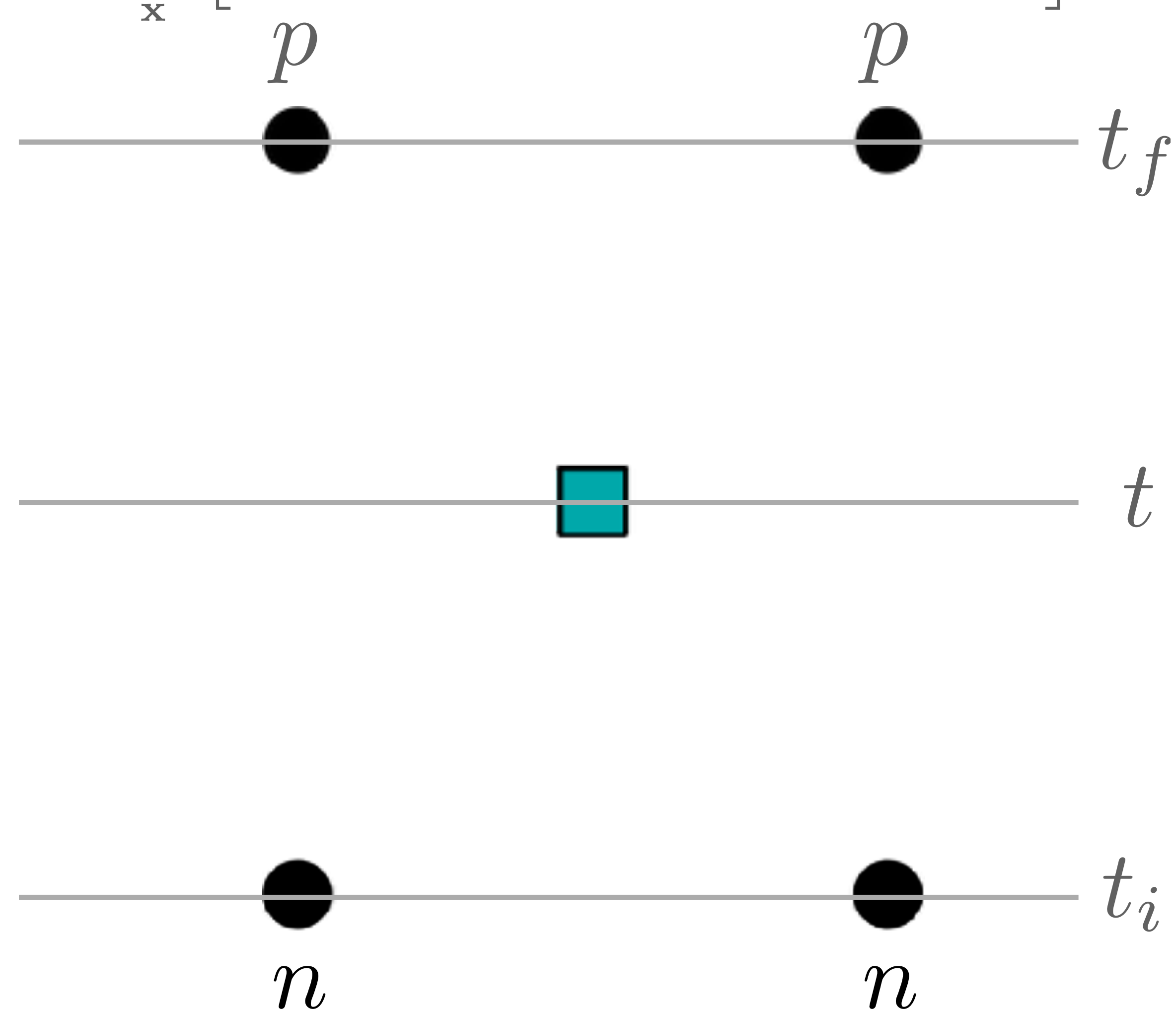

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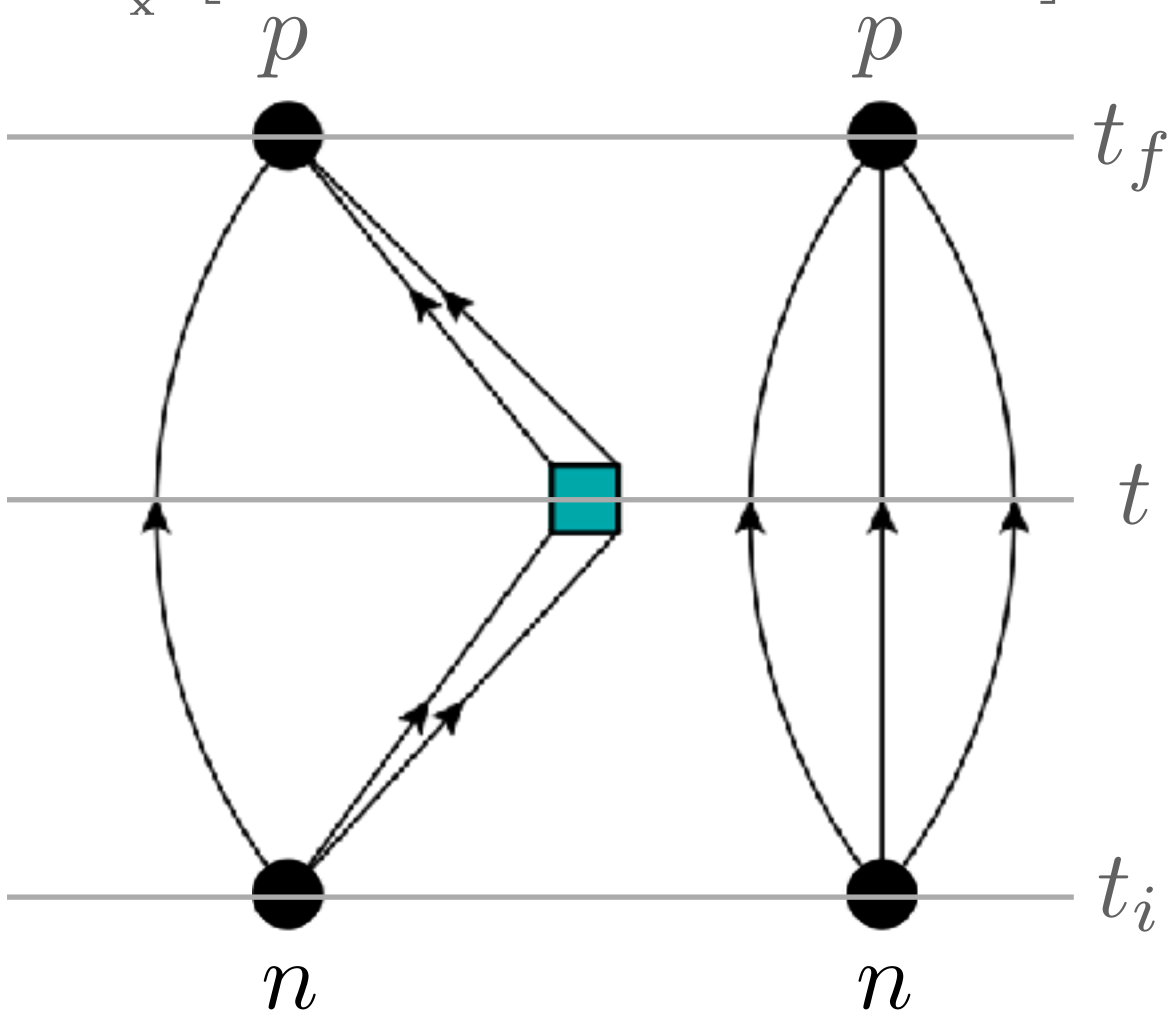
$$\mathcal{O}^{\Delta I=2} \equiv \sum_{\mathbf{x}} \left[(\bar{q}\tau^3 q)_A (\bar{q}\tau^3 q)_V - \frac{1}{3}(\bar{q}\vec{\tau} q)_A (\bar{q}\vec{\tau} q)_V \right](\mathbf{x})$$



Hadronic Parity Violation

- 2 Baryon „s-wave“ source
- EW vertices ⇒ 4-quark operator insertion
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- In total there are 4896 contractions
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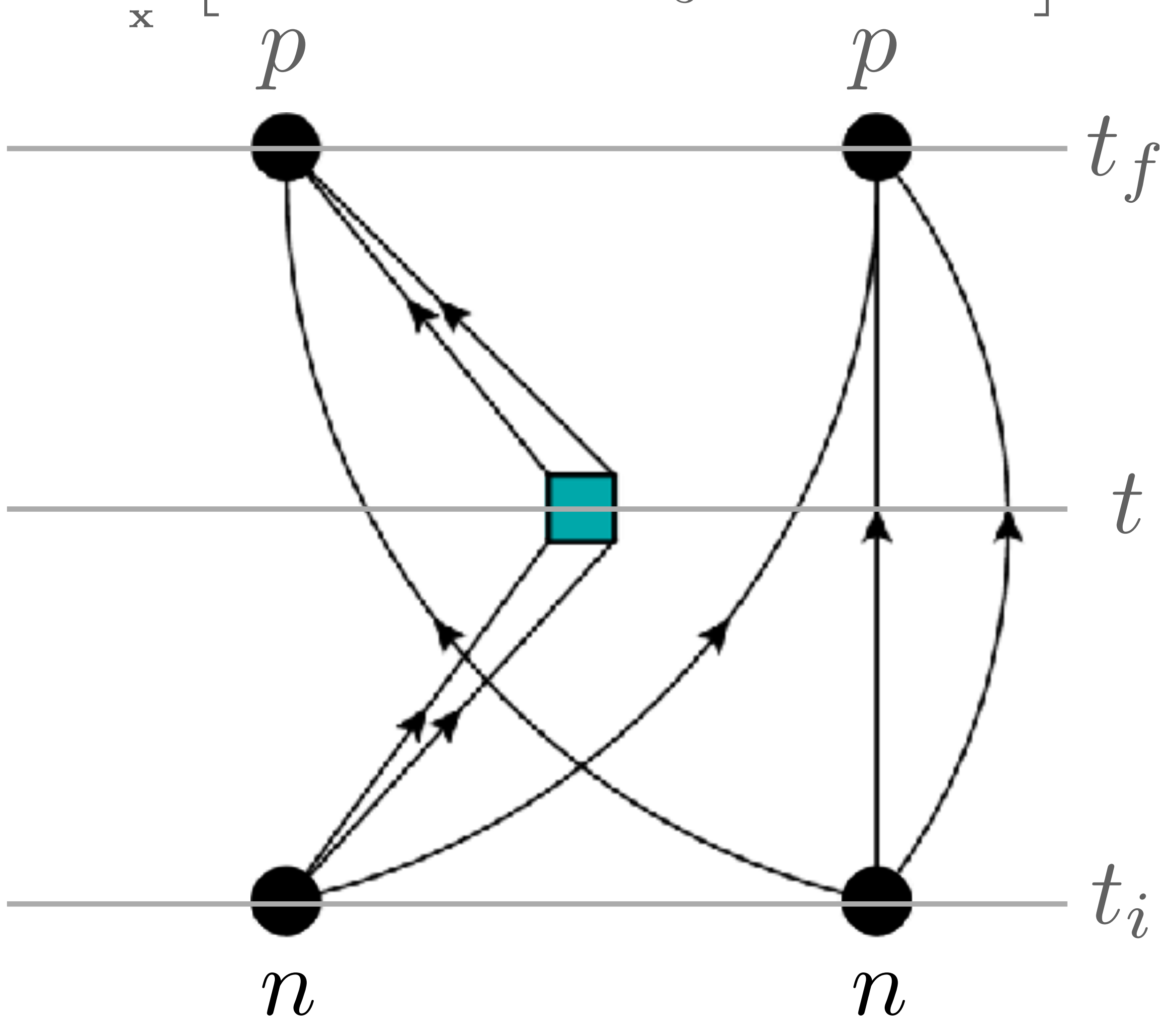

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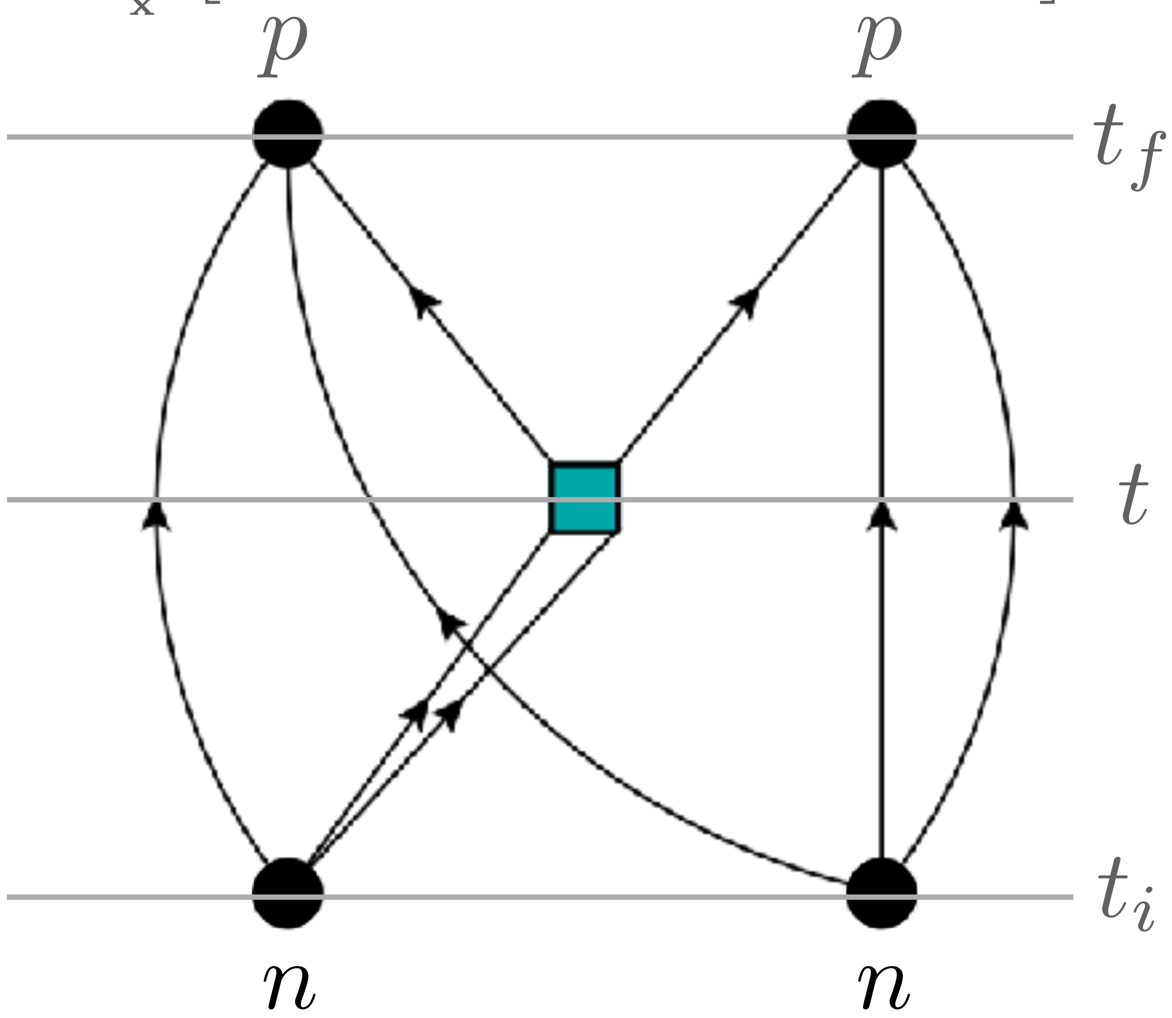

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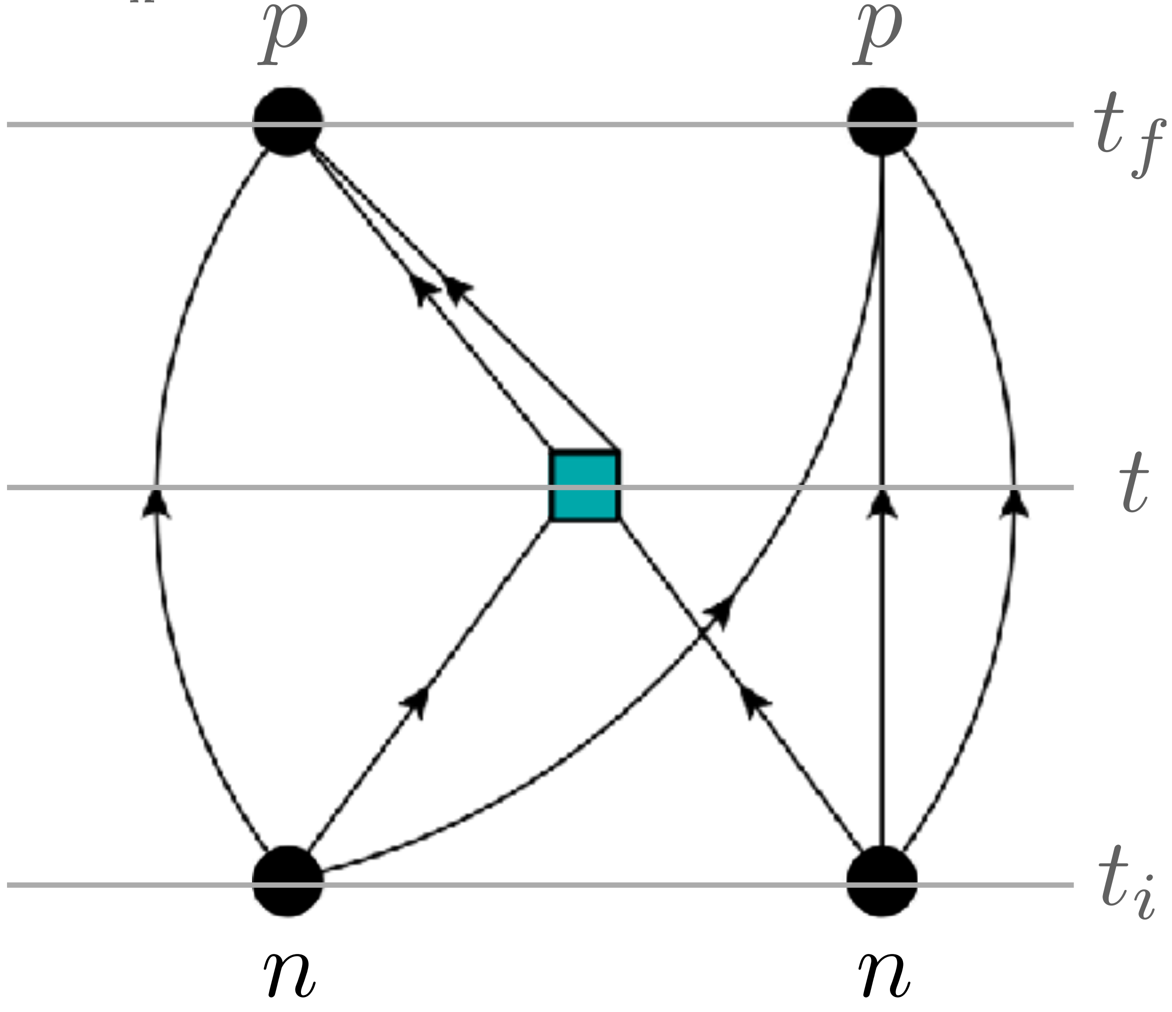

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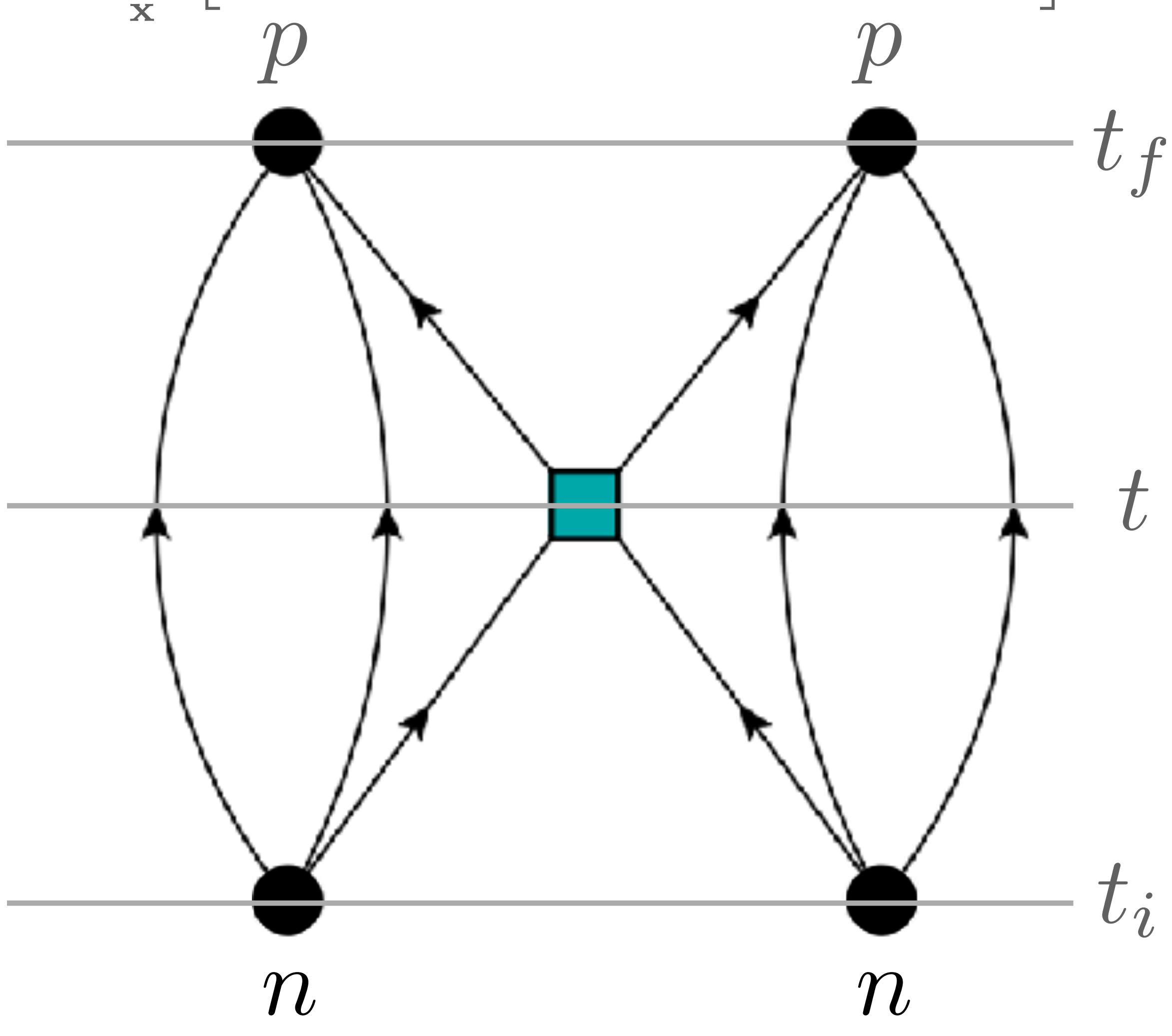

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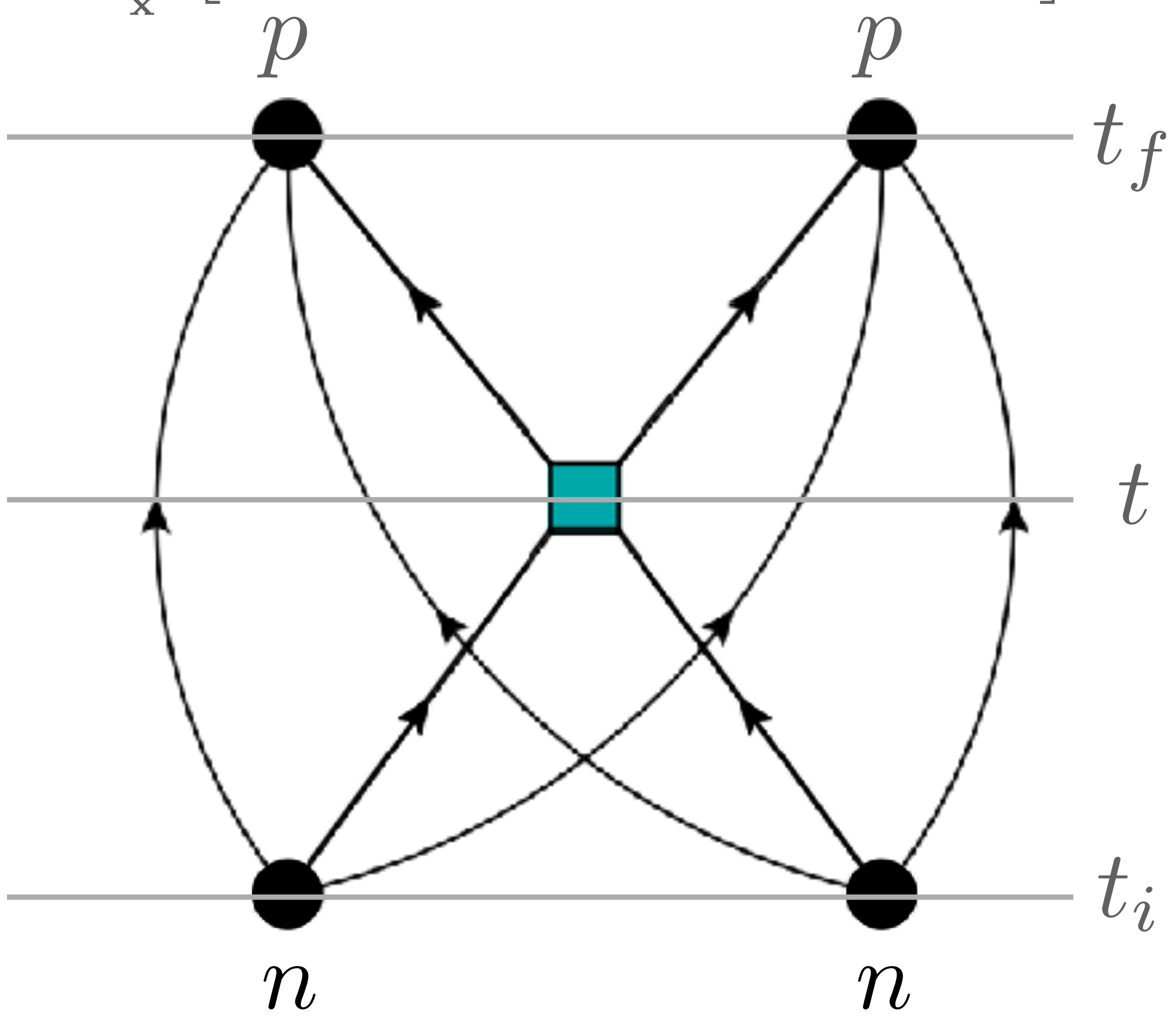

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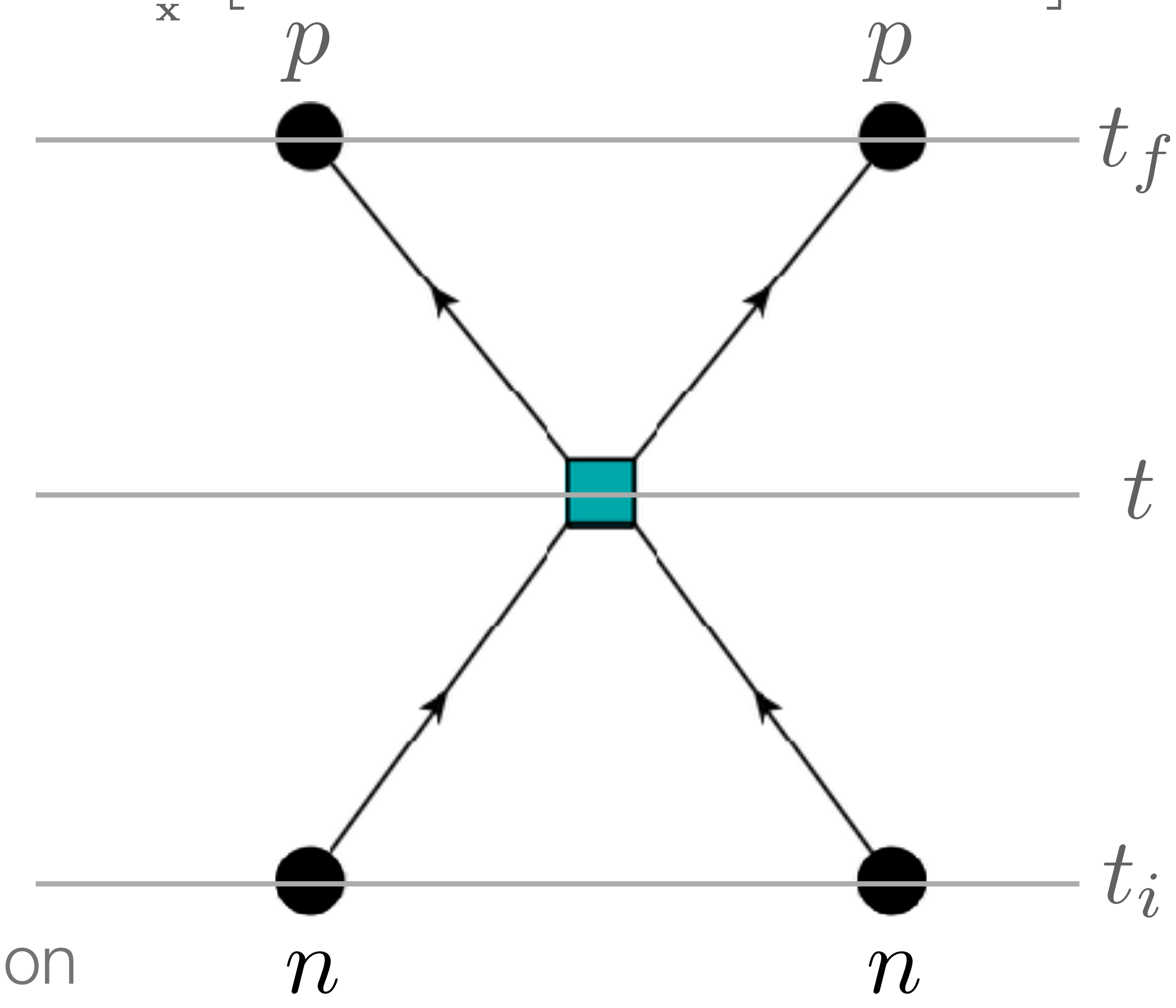

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- Partial wave scattering needed as well

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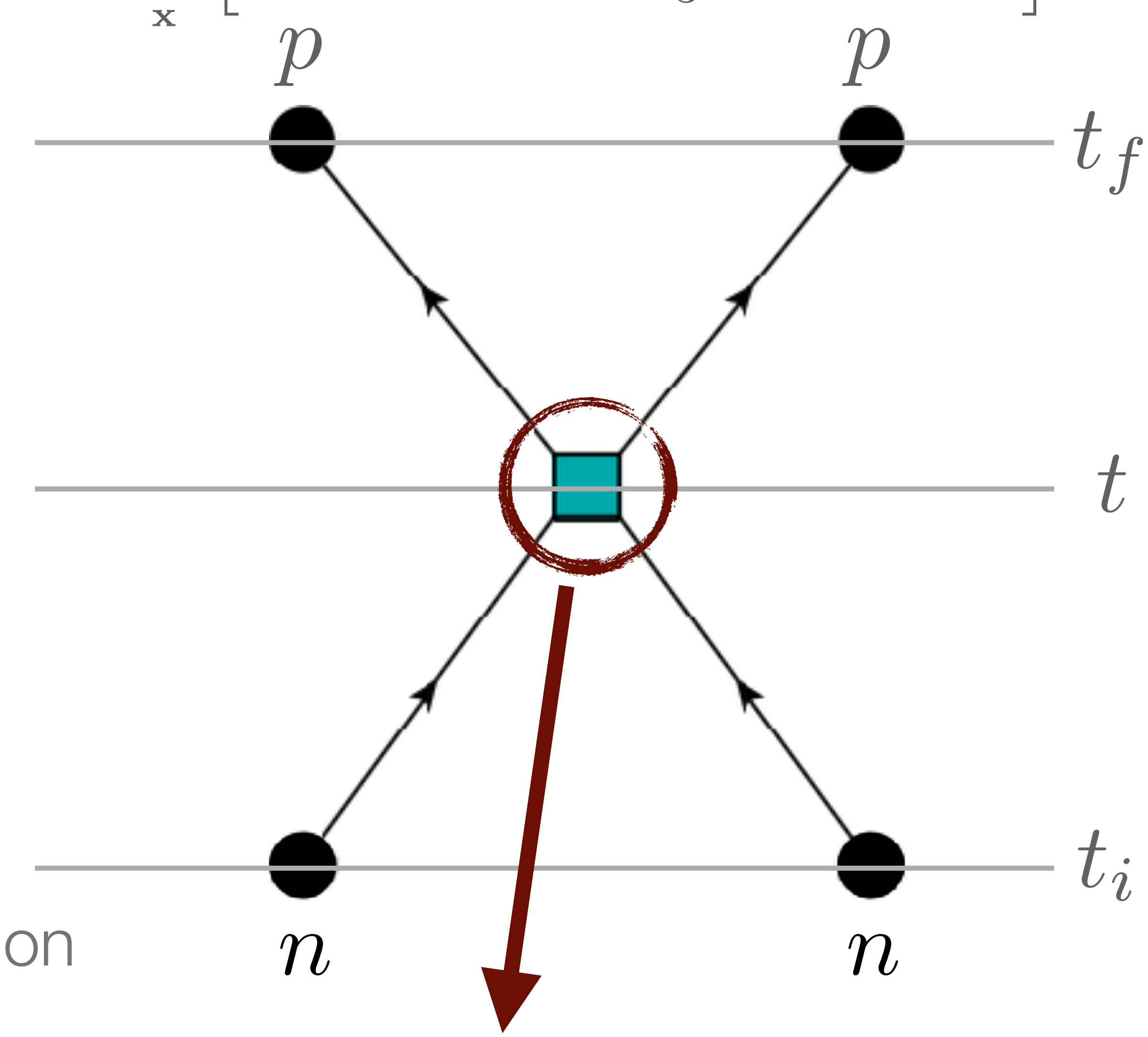
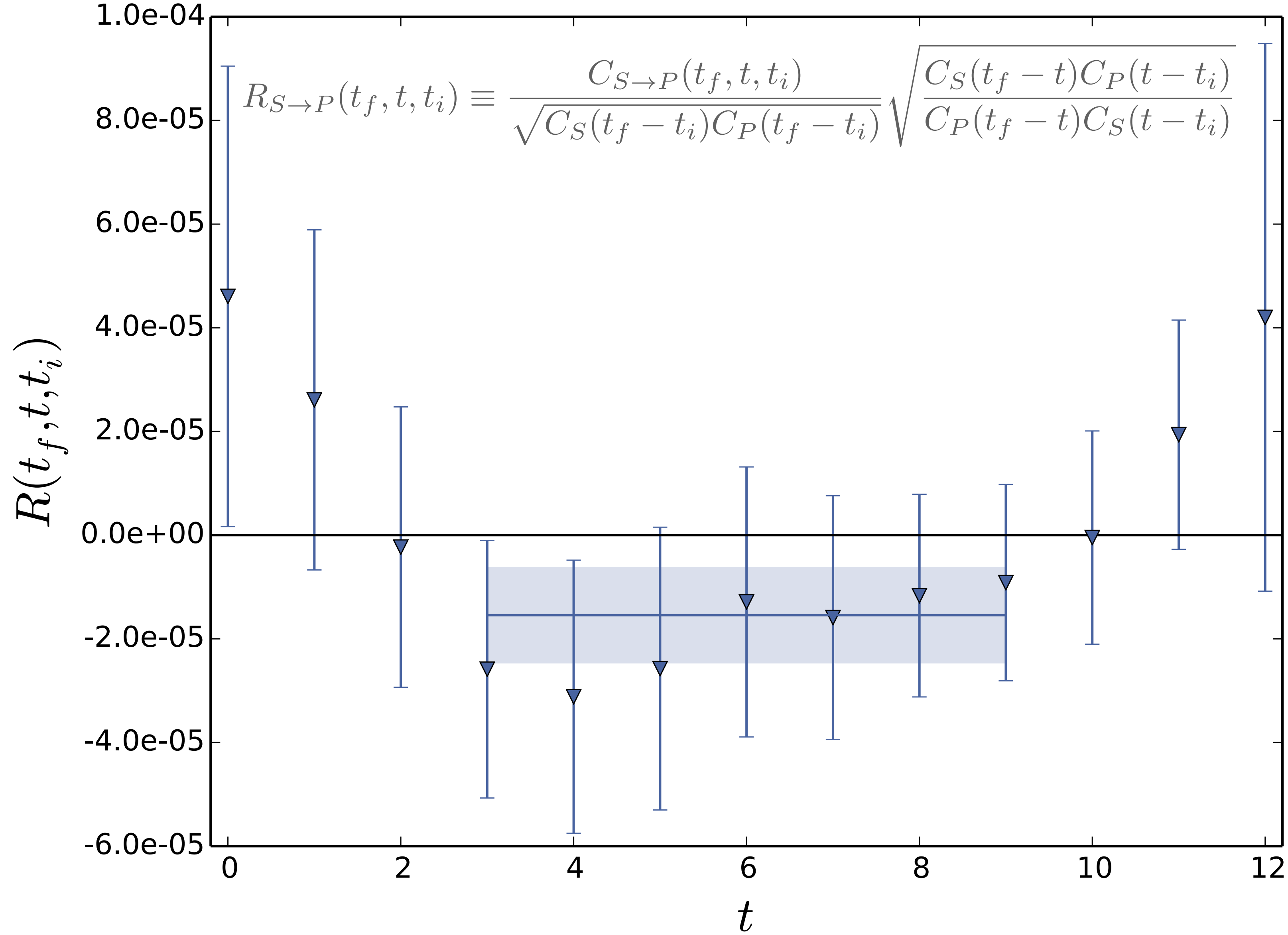


$$\langle {}^3P_0 | H_{\mathrm{EW}} | {}^1S_0 \rangle_\infty = f\left(\delta^{(S)}, \partial_E \delta^{(S)}, \delta^{(P)}, \partial_E \delta^{(P)}\right) \times \langle {}^3P_0 | H_{\mathrm{EW}} | {}^1S_0 \rangle_{\mathrm{FV}}$$

Hadronic Parity Violation

Normalized Ratio



Preliminary!

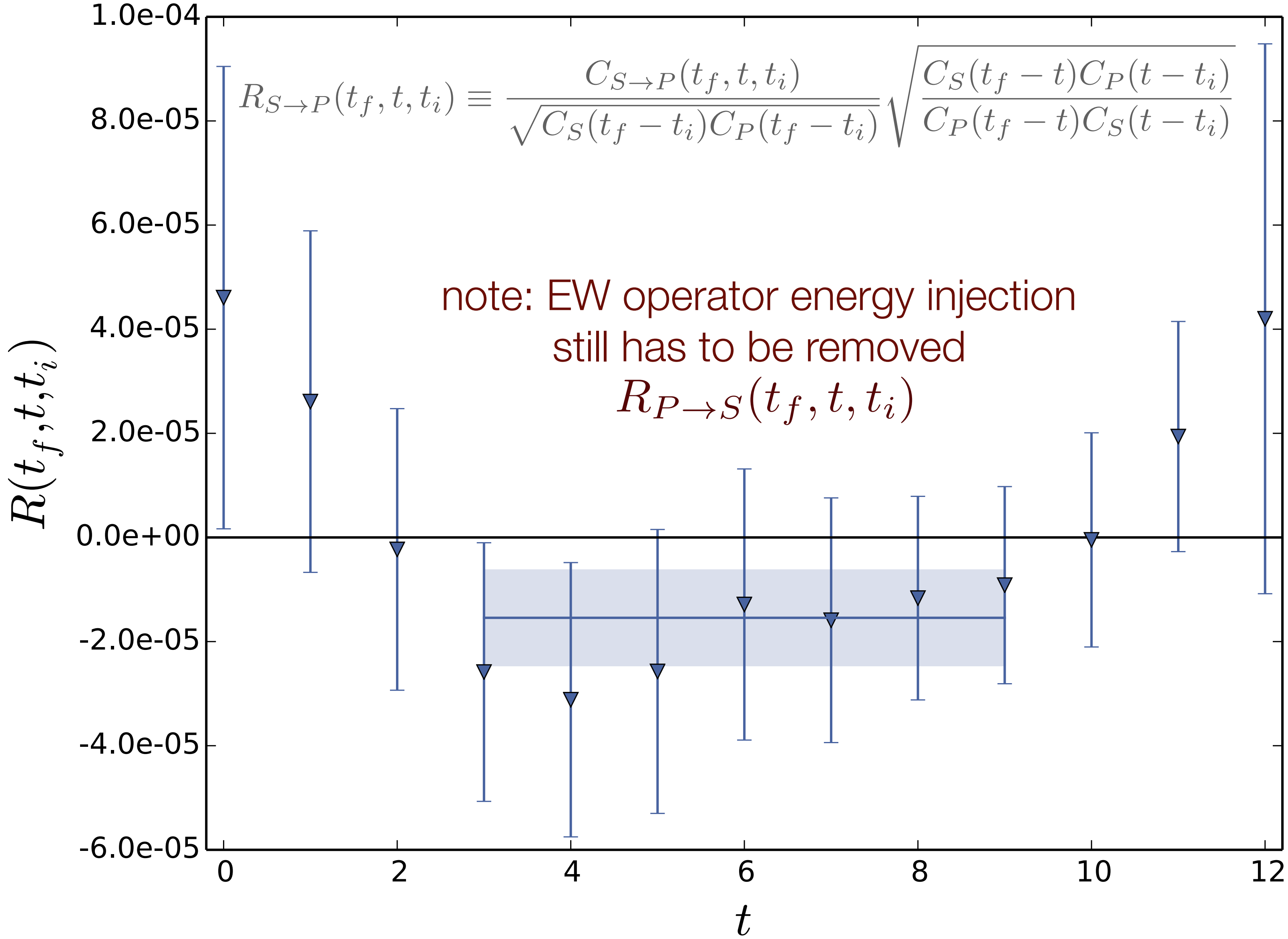
m_π=800 MeV

only 200 samples

The most challenging aspect of this calculation is the NN interaction

Hadronic Parity Violation

Normalized Ratio



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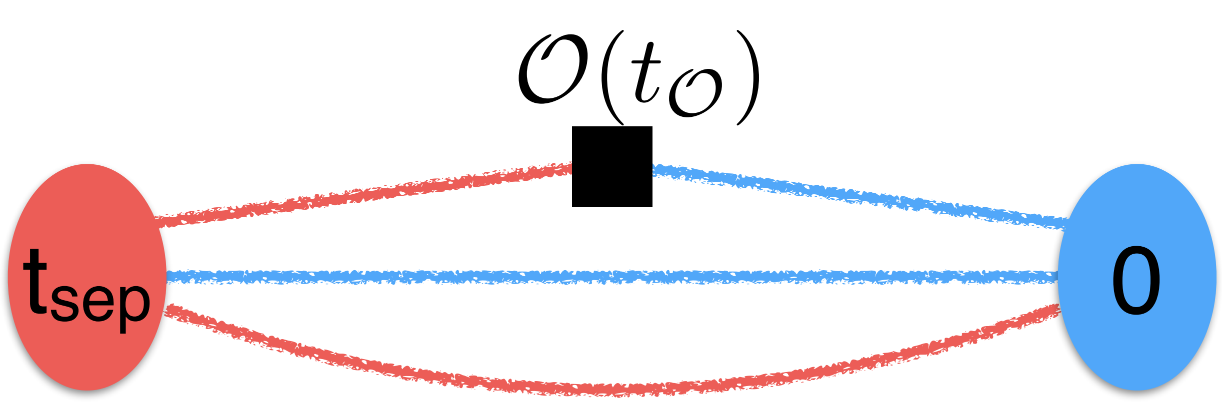
g_A - a success story

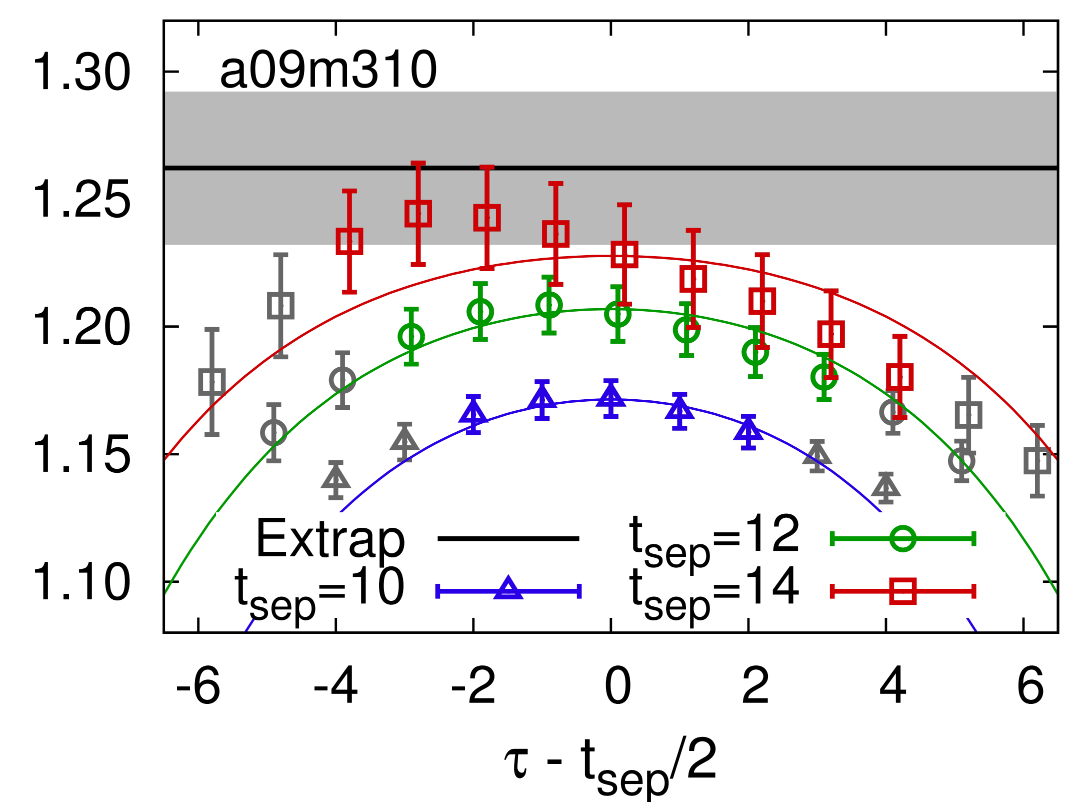
- Our success required a few key components:
  - Access to **publicly available** lattice QCD gauge configurations (MILC Collaboration) with multiple lattice spacings, multiple volumes, near physical pion masses
  - ***ludicrously fast*** GPU code (Quda library)
  - access to leadership class computing (Titan via INCITE)
  - a new strategy motivated by the Feynman-Hellmann Theorem

standard method



fixed source-sink separation time

PNDME arXiv:1606.07049



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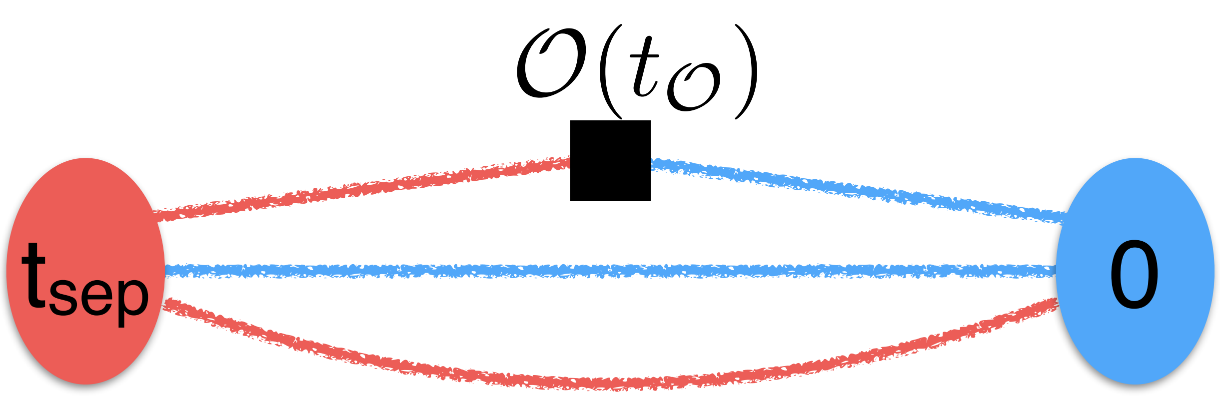

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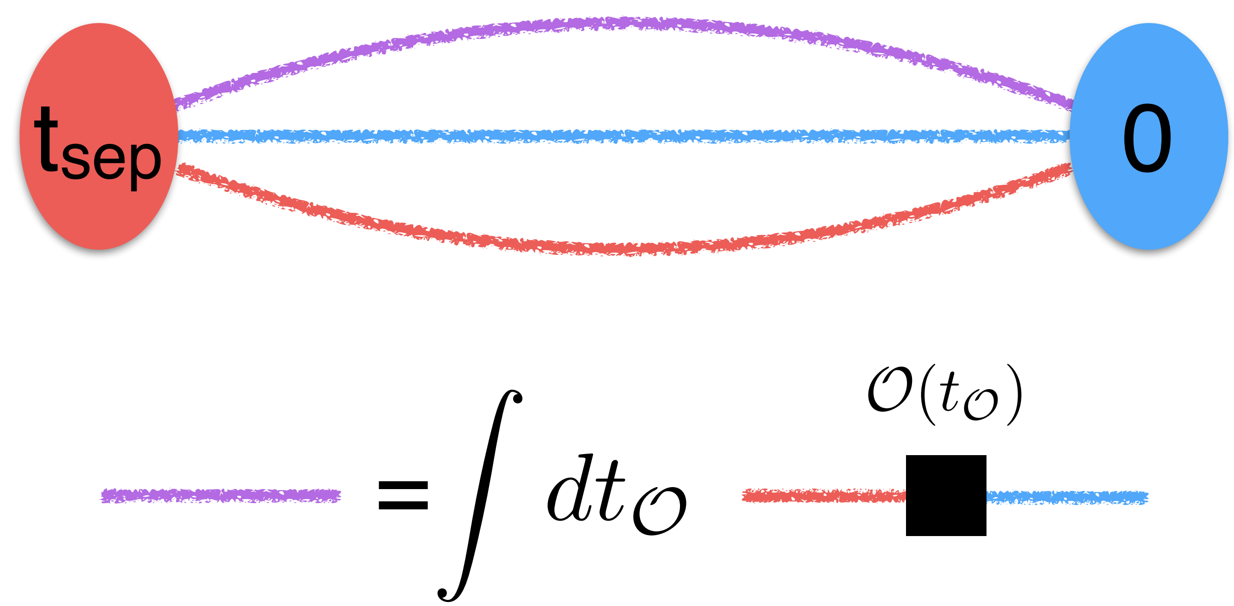
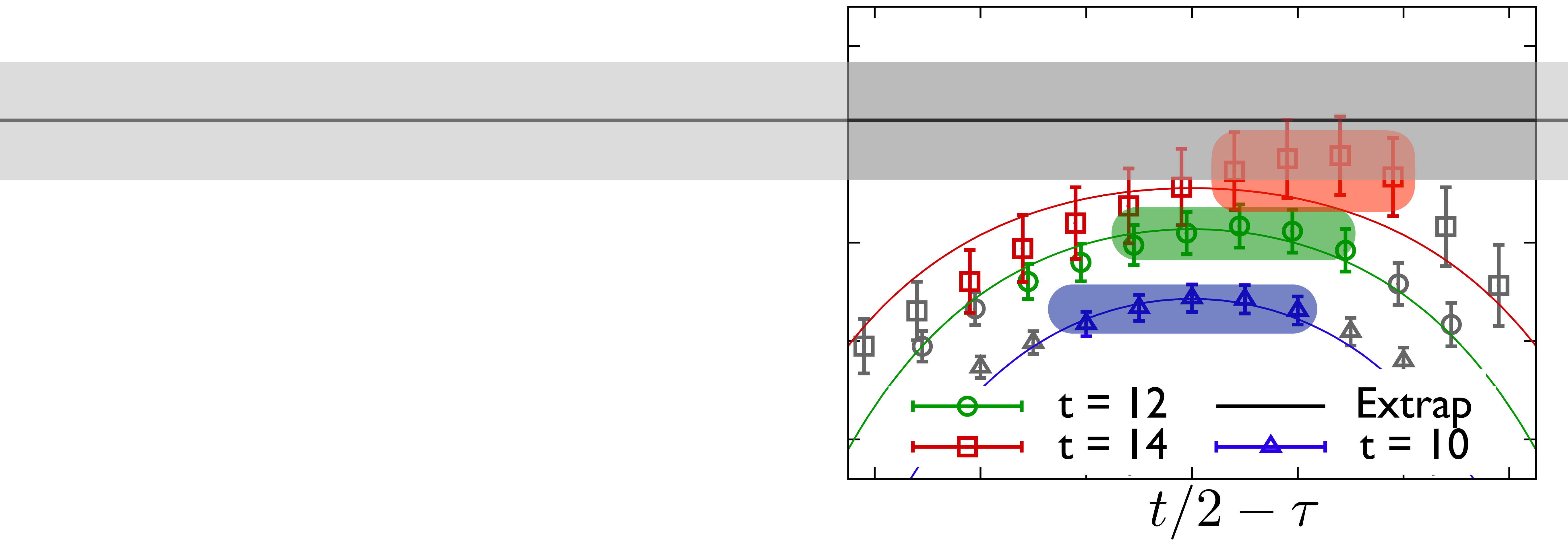


Comparison with a Standard Method

PNDME Phys. Rev. D94 (2016) arXiv:1606.07049



Slides adapted from A. Nicholson adapted from E. Berkowitz

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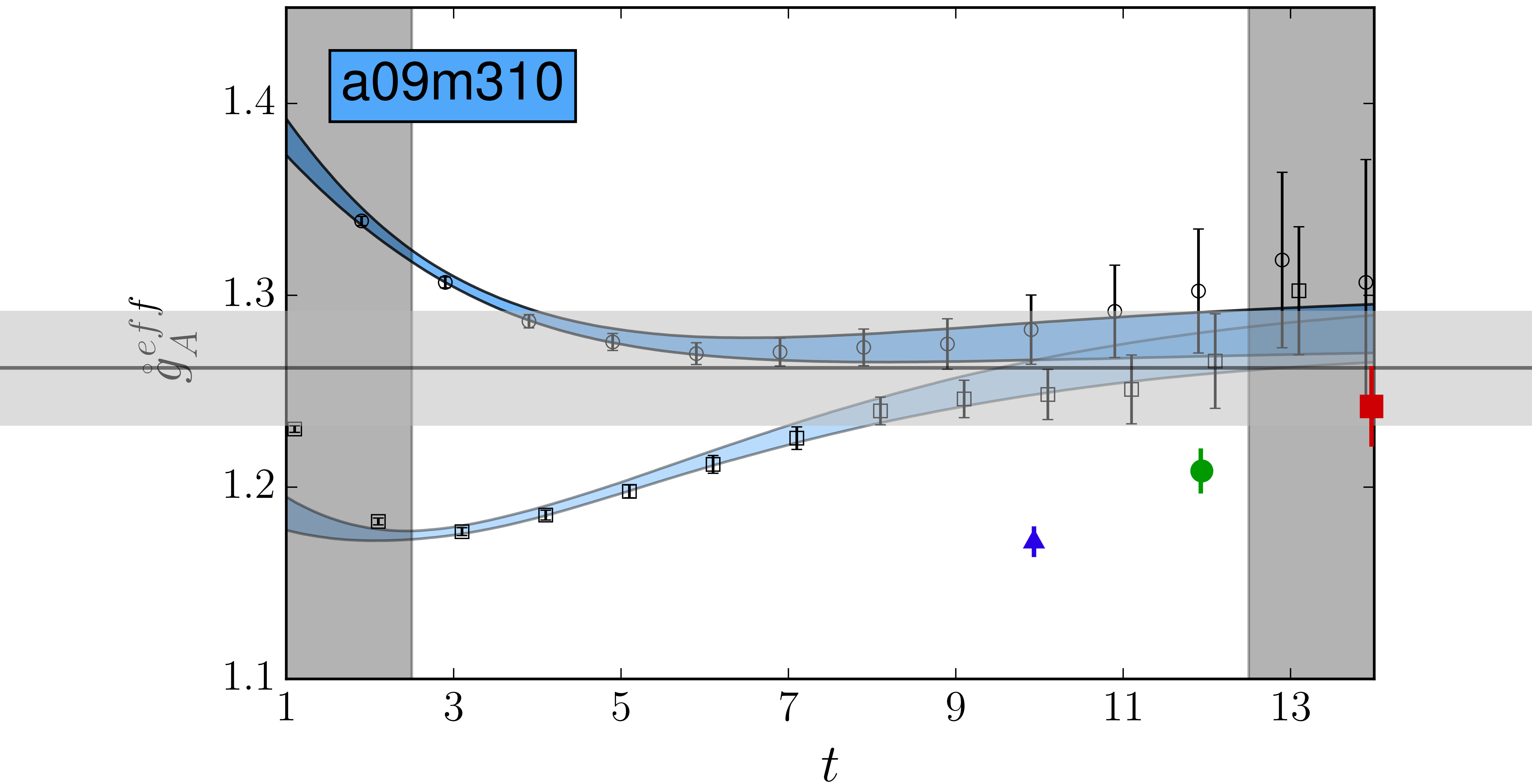

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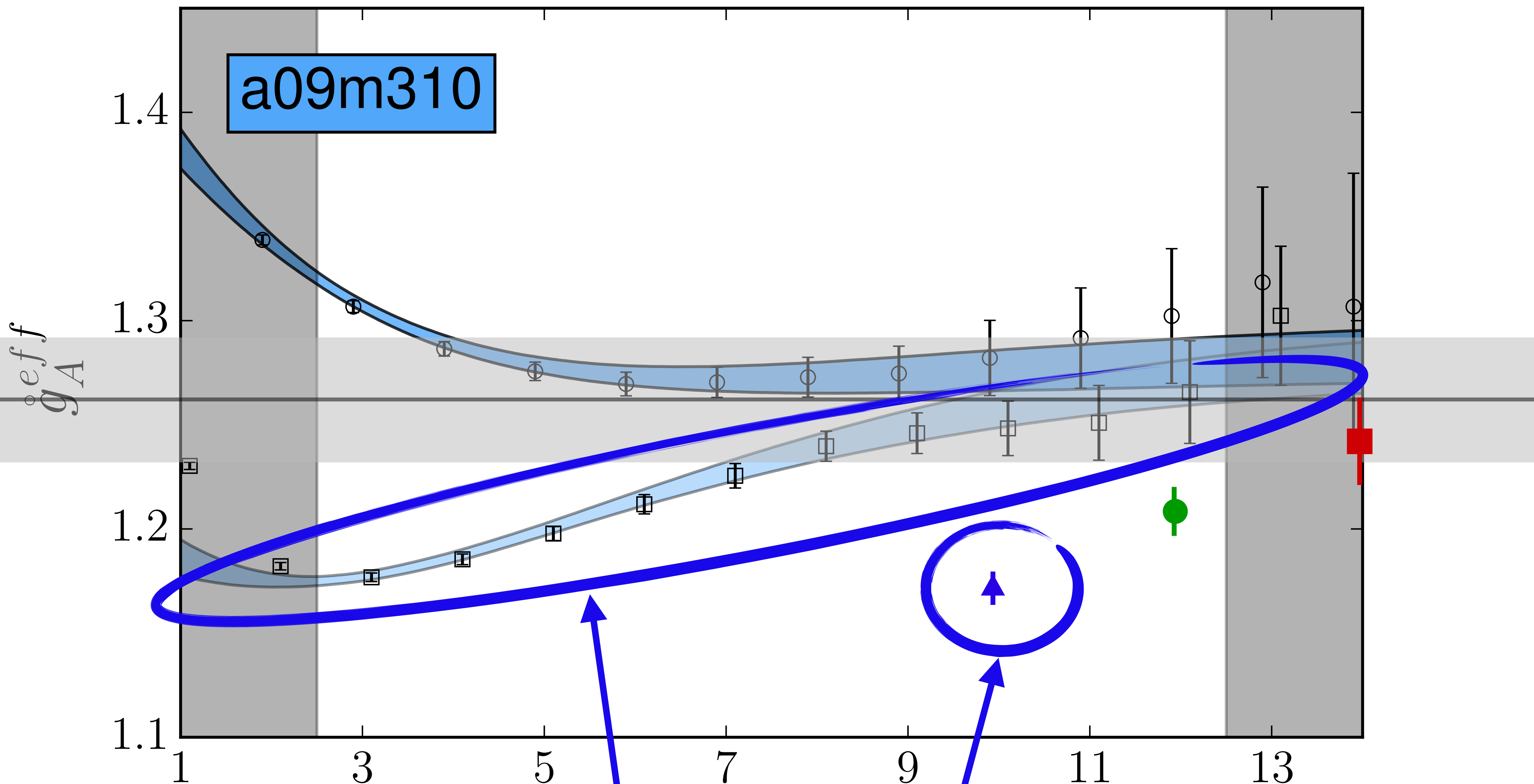
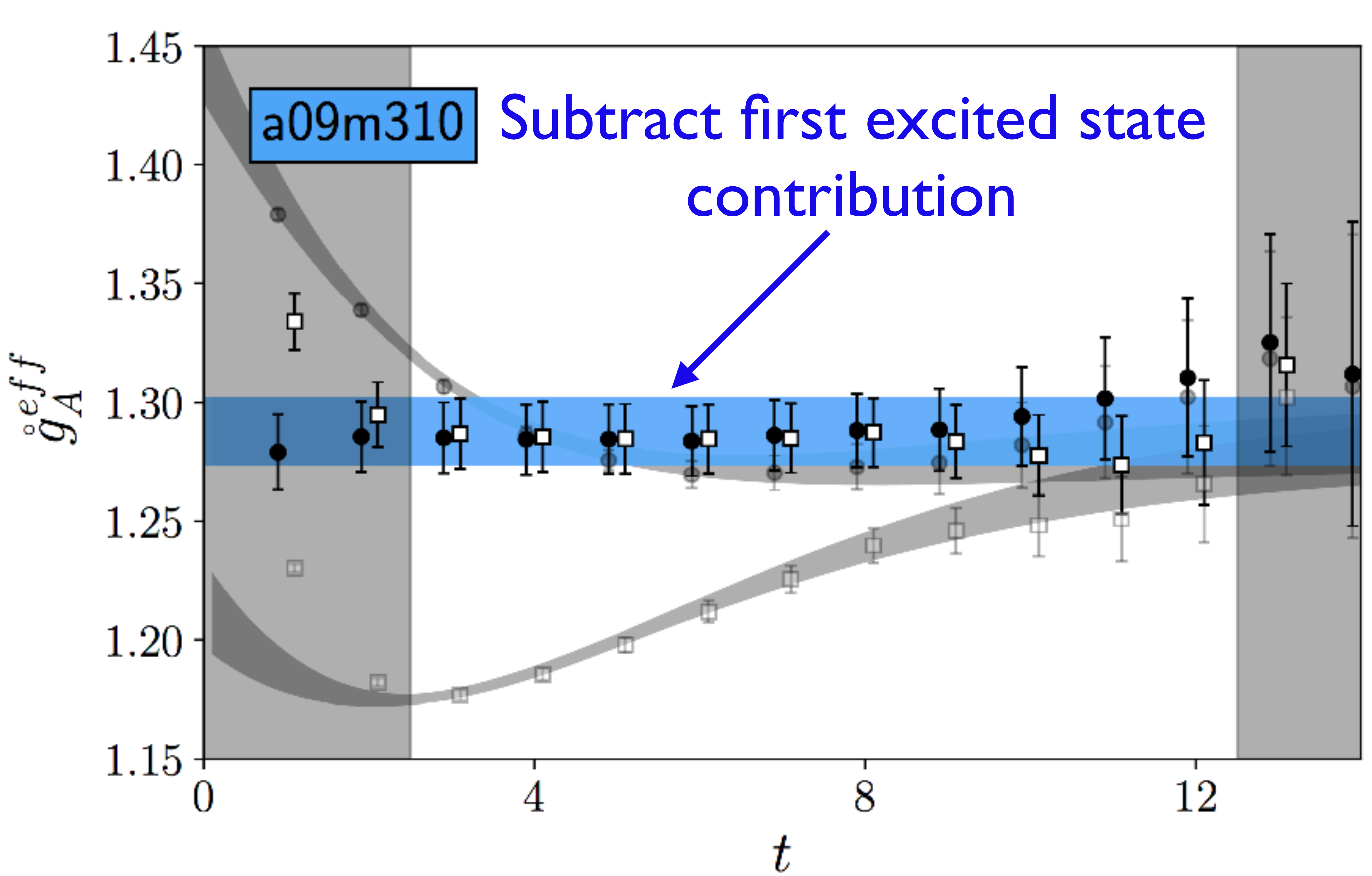


Each one of these points costs the same as all times for one source in our calc

Slides adapted from A. Nicholson adapted from E. Berkowitz

Comparison with a Standard Method



Slides adapted from A. Nicholson

A percent-level determination of the nucleon axial coupling from QCD

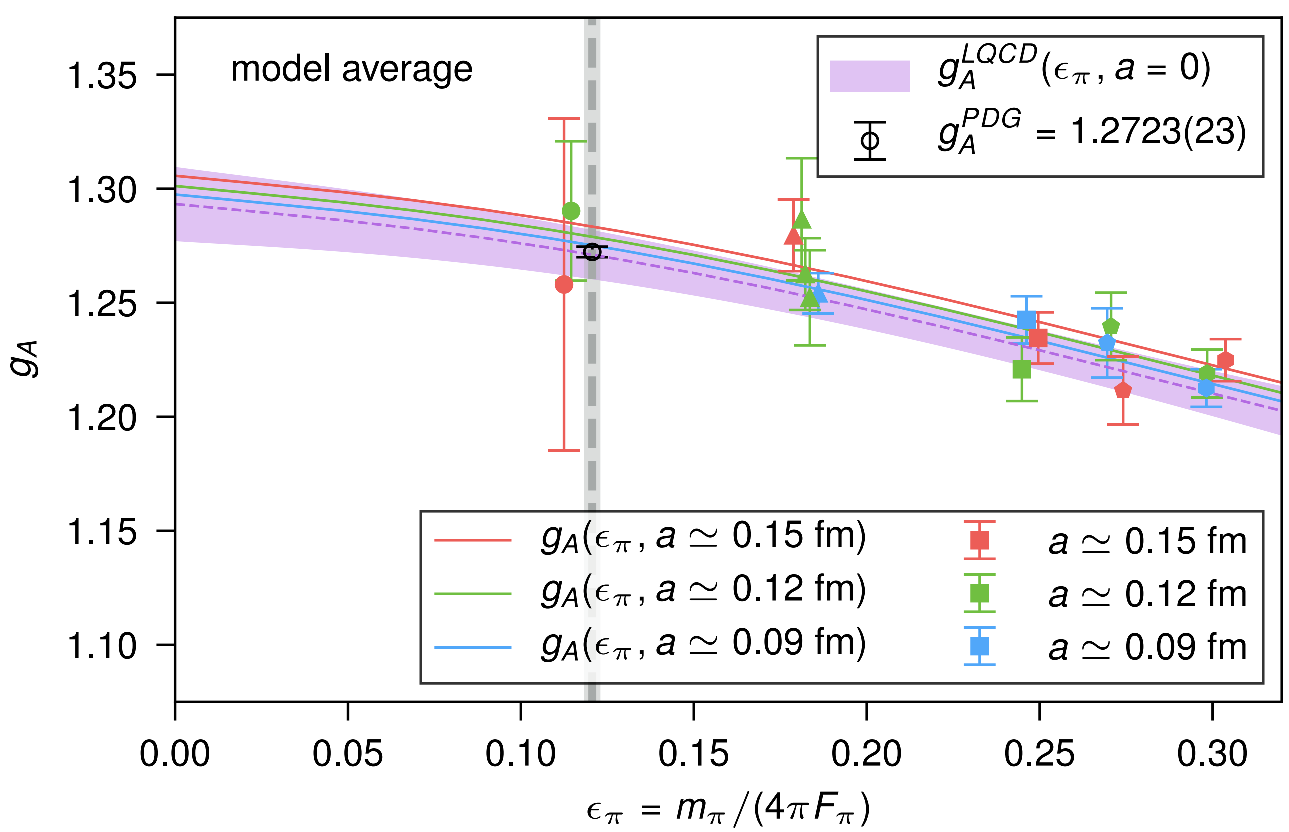
Lattice QCD Team

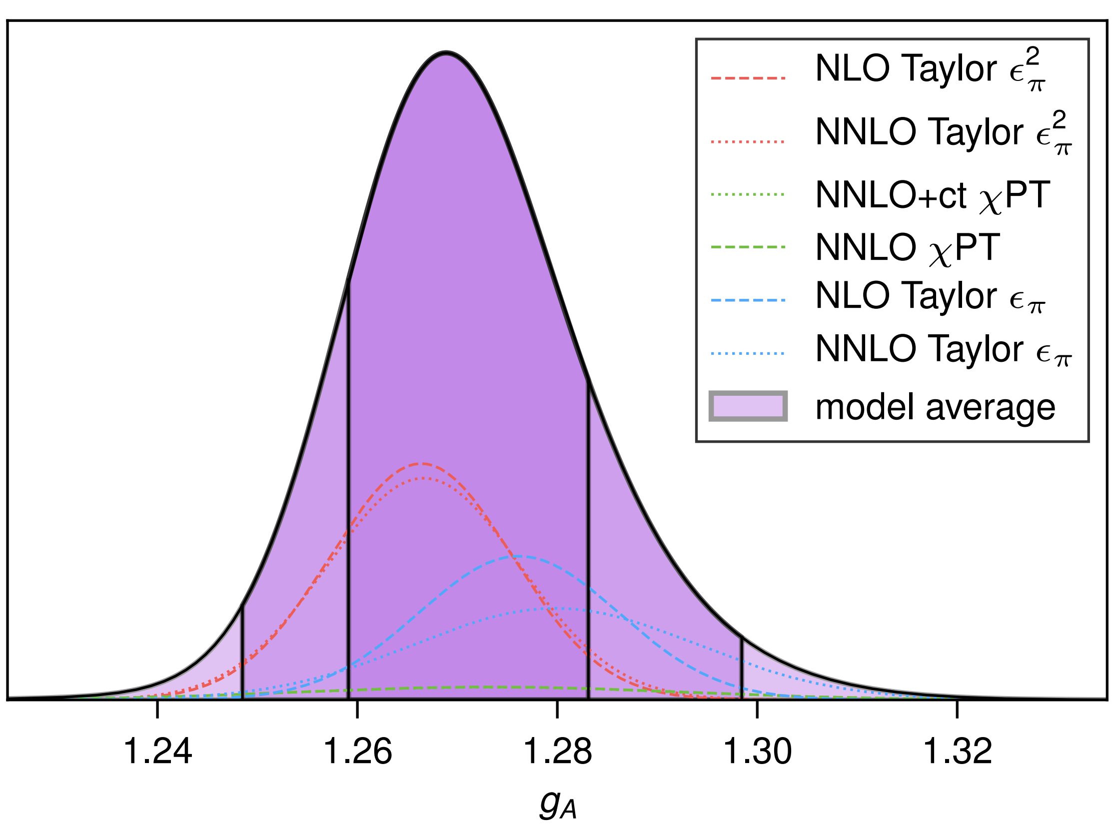
Glasgow:	Chris Bouchard
INT:	Chris Monahan
JLab:	Balint Jóo
Jülich:	Evan Berkowitz
LBL/UCB:	David Brantley, Chia Cheng (Jason) Chang, T. Kurth (NERSC), Henry Monge-Camacho, AWL
LLNL:	Pavlos Vranas
Liverpool:	Nicolas Garron
NVIDIA:	Kate Clark
RIKEN/BNL:	Enrico Rinaldi
UNC:	Amy Nicholson
William and Mary:	Kostas Orginos

plus a few others

$$g_A^{\mathrm{QCD}} = 1.2711(103)^s(39)^\chi(15)^a(19)^V(04)^I(55)^M$$
$$= 1.2711(126)$$
$$g_A^{\mathrm{UCNA}} = 1.2772(020)$$

experiment factor of 6 more precise





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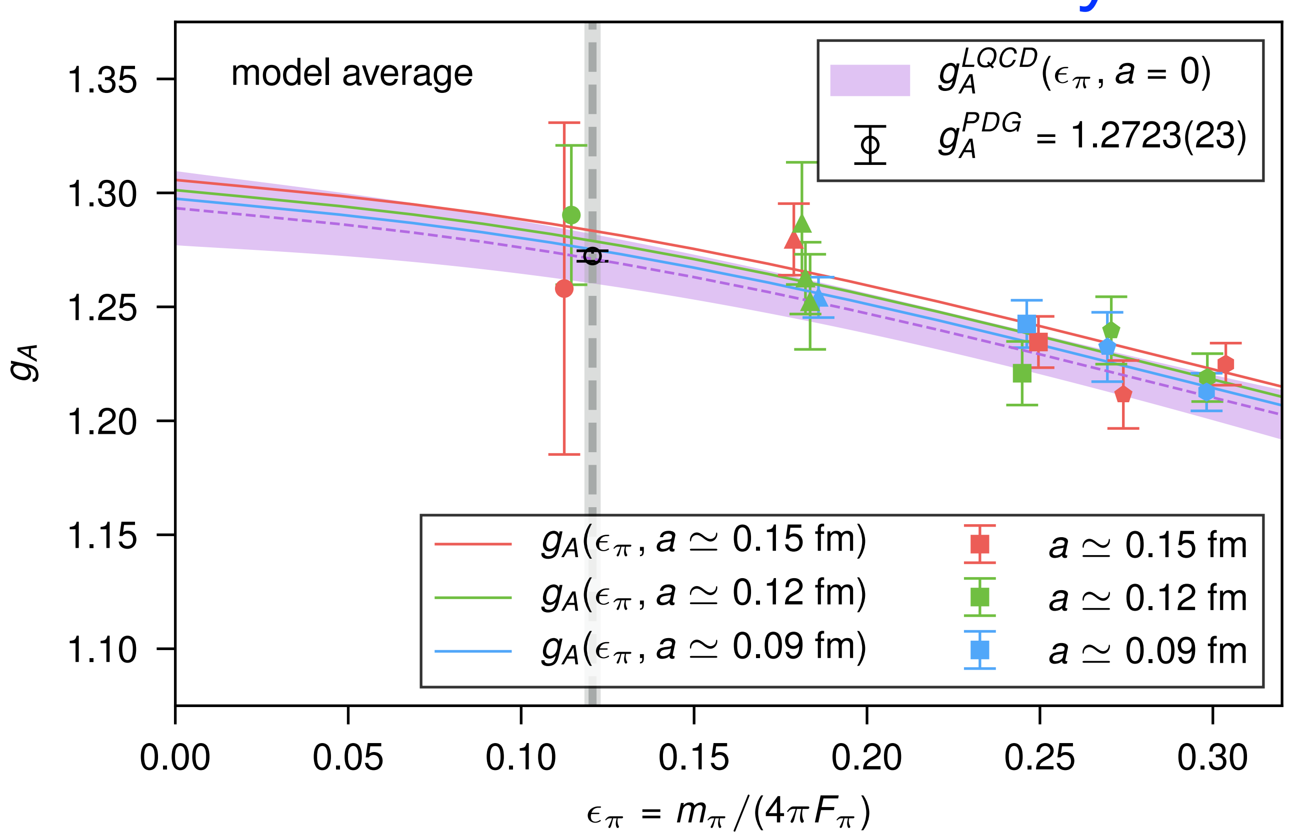
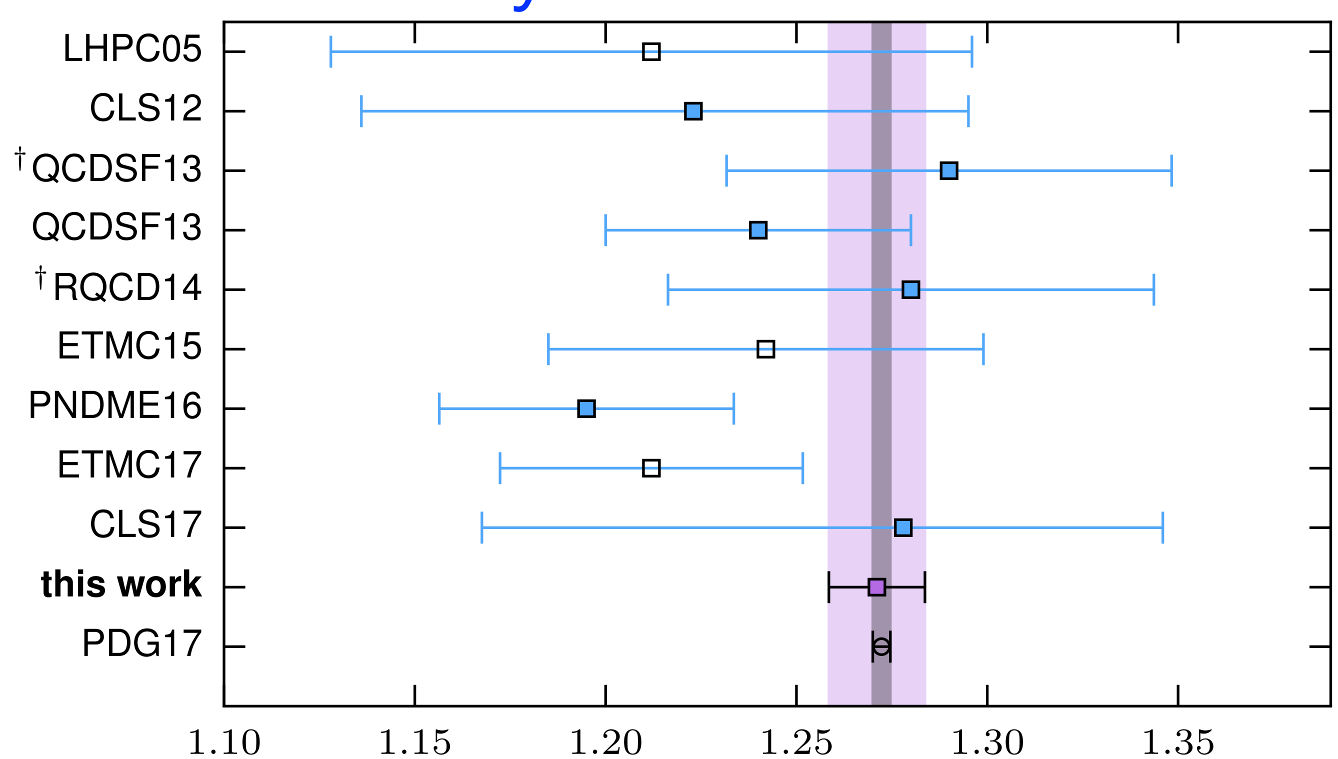
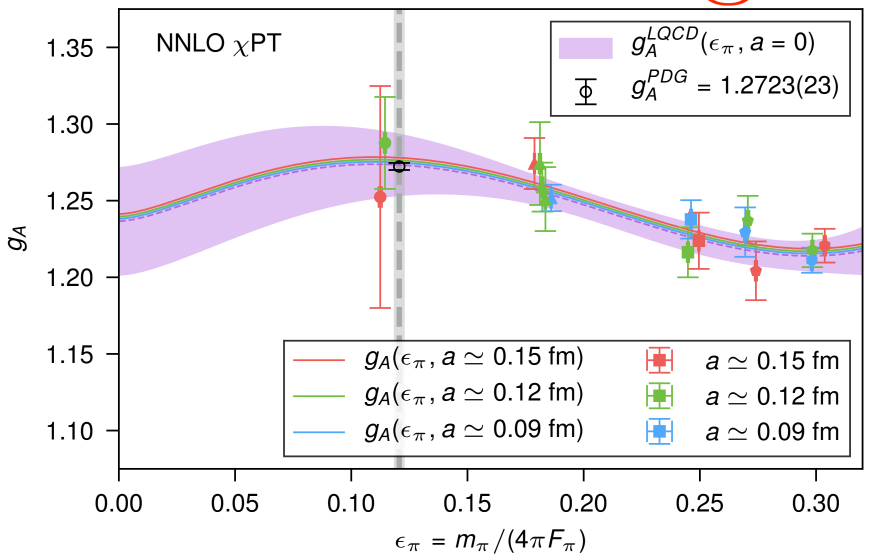
Lattice community estimated 2% by 2020

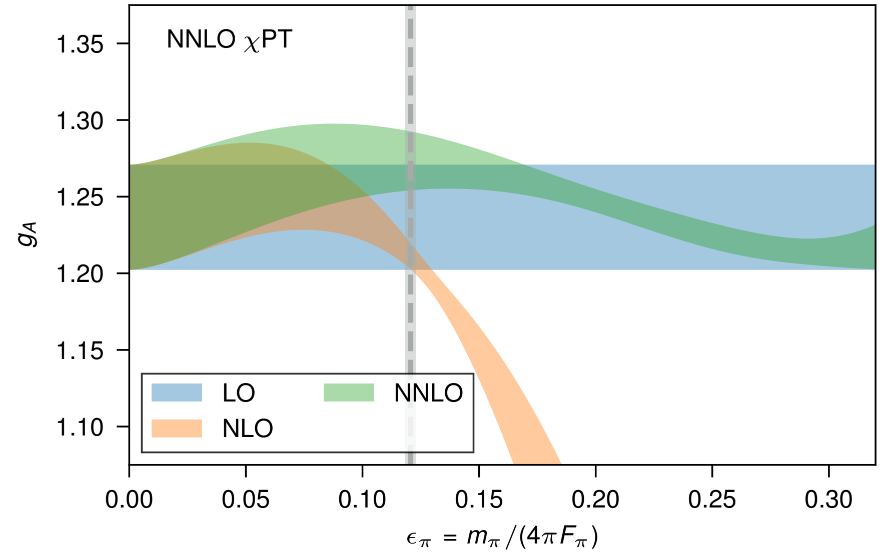


LQCD results



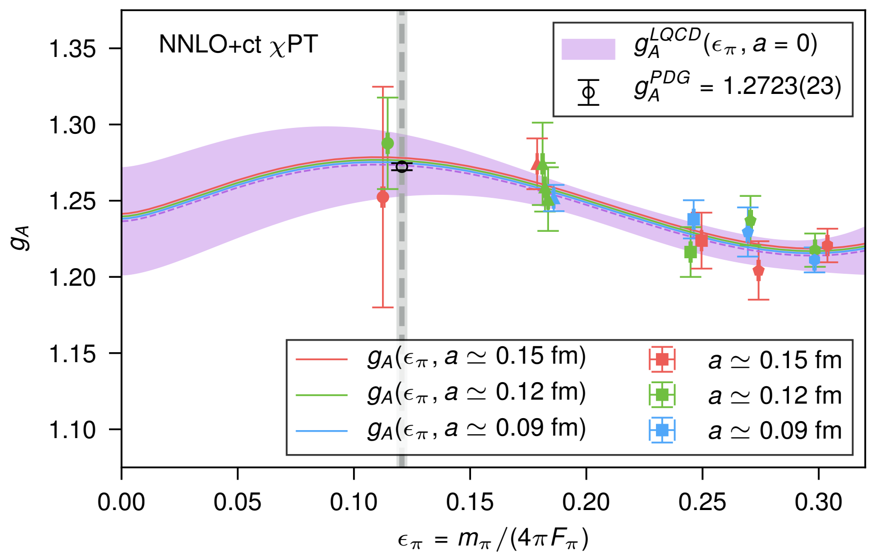
convergence of the chiral expansion…

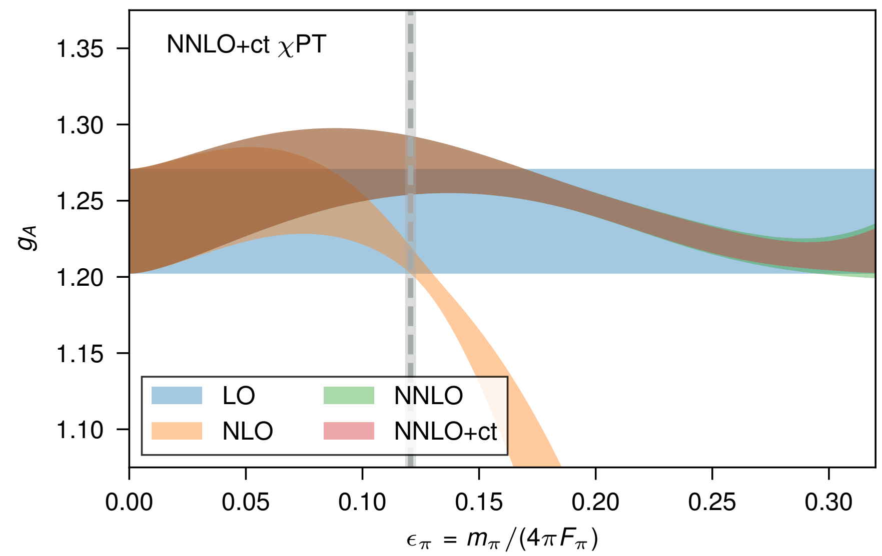




$$g_A = g_0 - \epsilon_\pi^2(g_0 + 2g_0^3)\ln(\epsilon_\pi^2) + c_2\epsilon_\pi^2 + g_0 c_3 \epsilon_\pi^3$$

$$\epsilon_\pi = \frac{m_\pi}{4\pi F_\pi}$$





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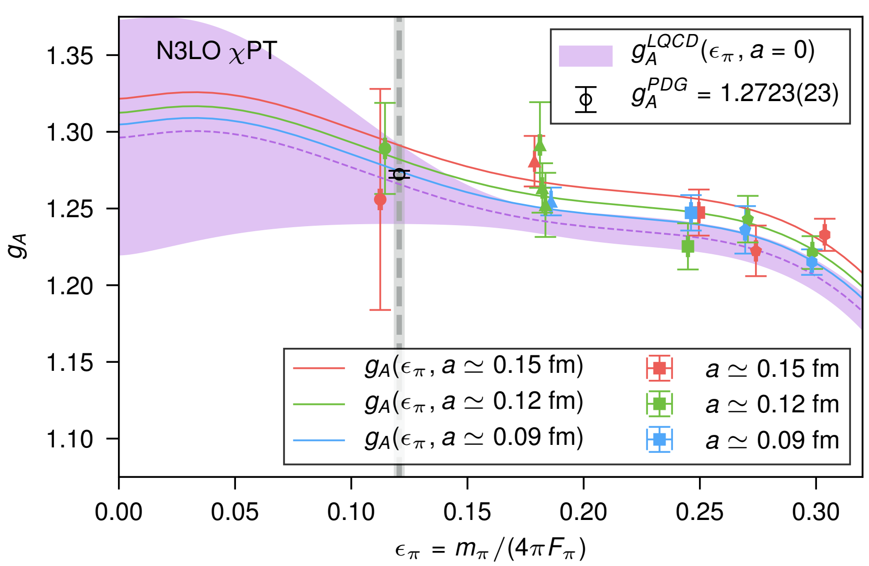

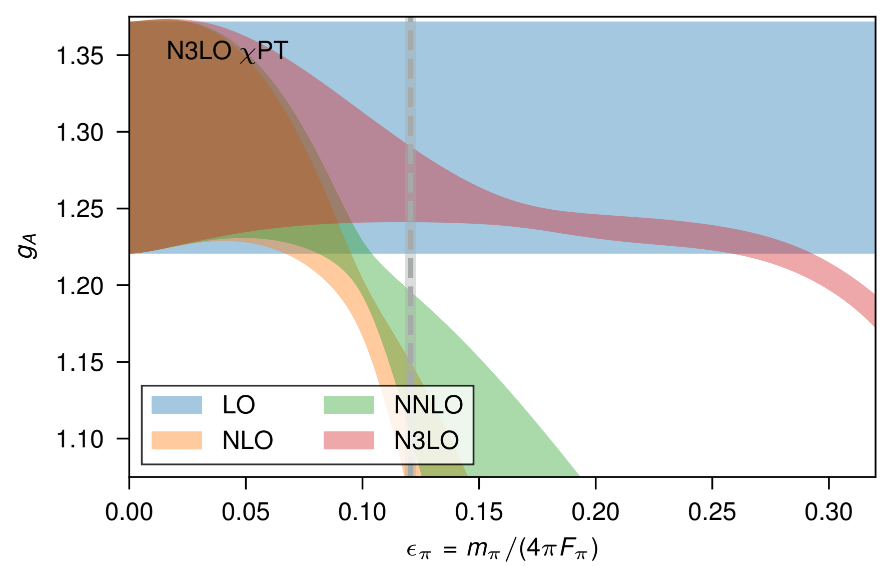

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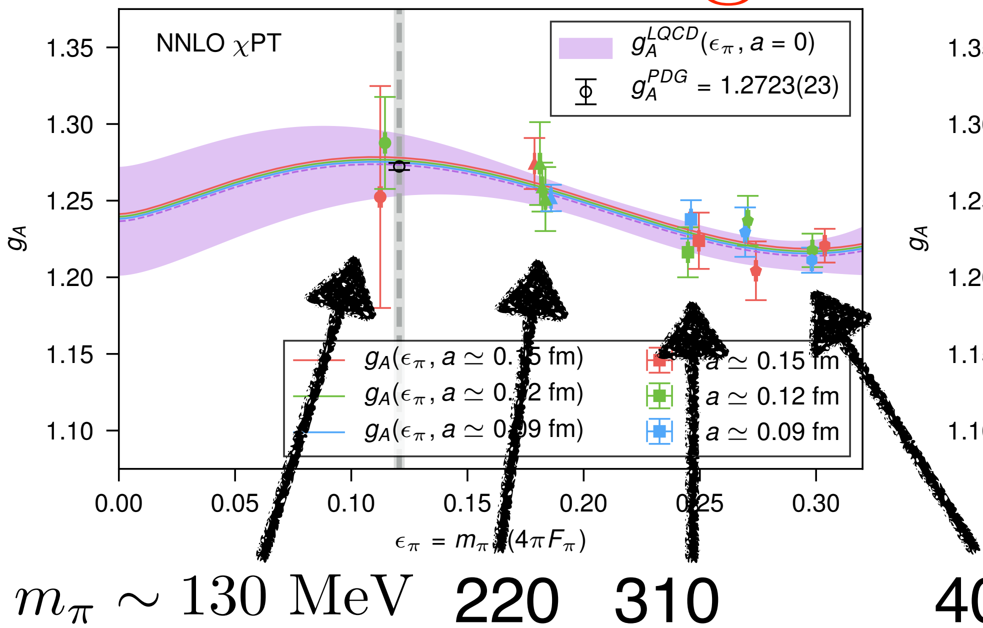

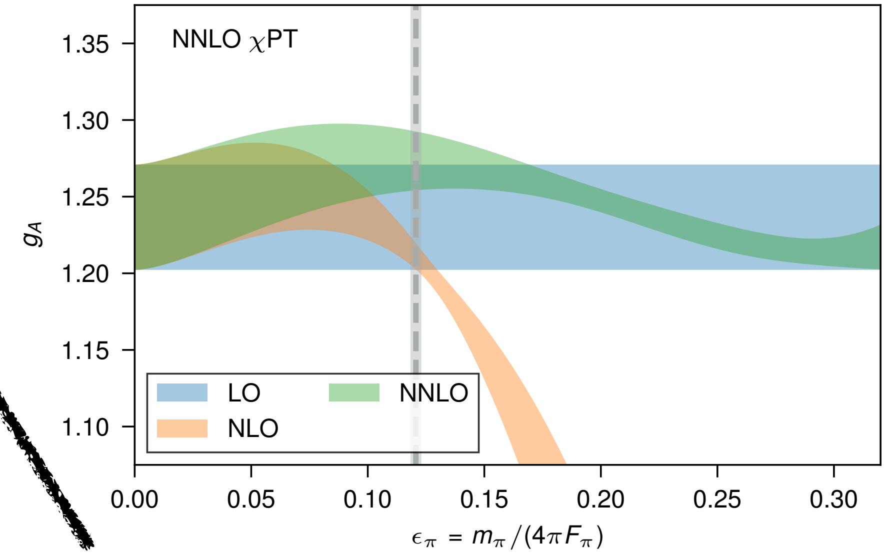

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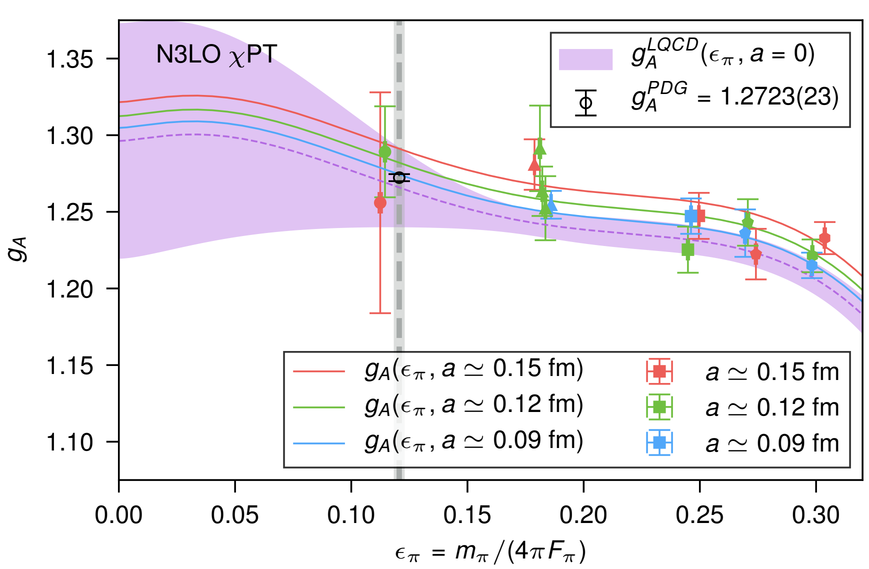
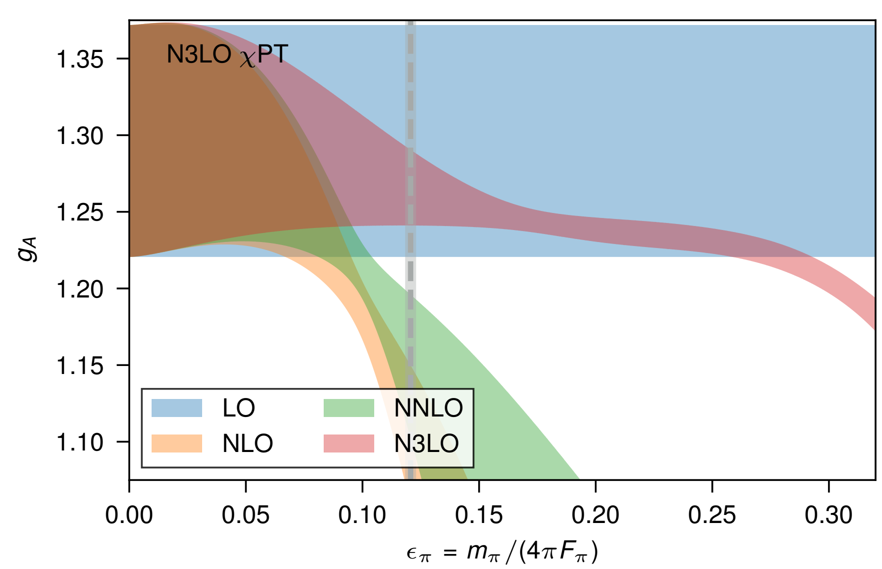
if the single nucleon is not converging, would you trust chiral extrapolations of two or more nucleons?





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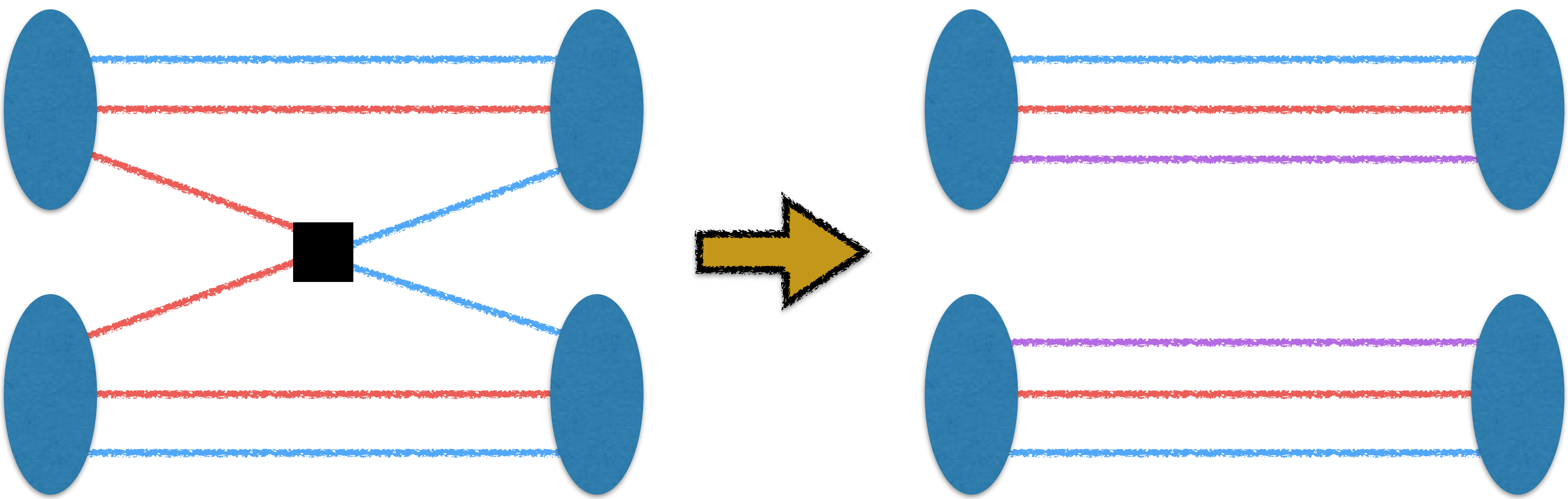
Inspiration for LQCD calculations of ΔI=2 PNC

- The method we developed to compute gA is only applicable to quark bi-linear currents $\bar{q}\,\Gamma\,q$
- This has inspired us - we believe we know how to generalize this method to 4-quark operators - if successful, it will substantially simplify the calculations



- We will hopefully know soon if this new idea works

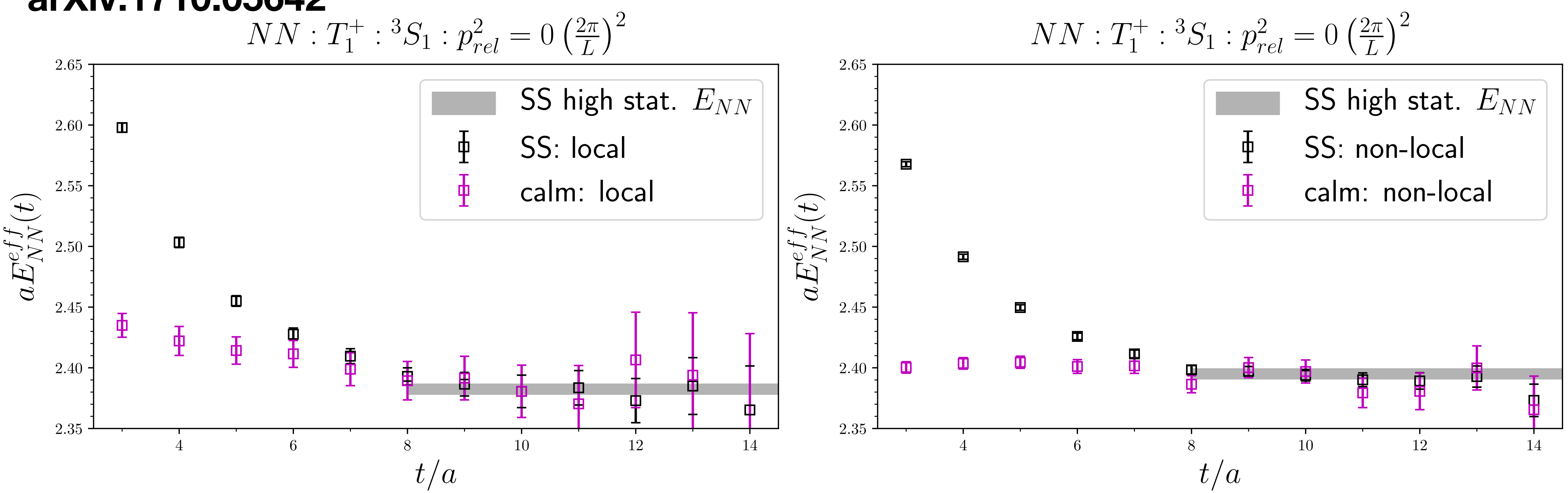
Inspiration for LQCD calculations of ΔI=2 PNC

- Two-nucleon LQCD calculations are the most substantial challenge to making progress in two-nucleon matrix element calculations
- We have cooked up a simple idea that offers the promise of exponentially improving the calculations

Calm Multi-Baryon Operators

E.Berkowitz, A. Nicholson, C.C. Chang, E. Rinaldi, M.A. Clark, B. Joo, T. Kurth, P. Vranas, AWL

arXiv:1710.05642



Matrix Prony

arXiv.org > hep-lat > arXiv:0903.2990

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High Energy Physics – Lattice

High Statistics Analysis using Anisotropic Clover Lattices: (I) Single Hadron Correlation Functions

Silas R. Beane, William Detmold, Thomas C. Luu, Kostas Orginos, Assumpta Parreno, Martin J. Savage, Aaron Torok, Andre Walker-Loud

- In this work, we applied for the first time, the Matrix Prony method for analyzing two-point correlation functions.
- Idea: construct linear combination of correlation functions to remove excited state contamination

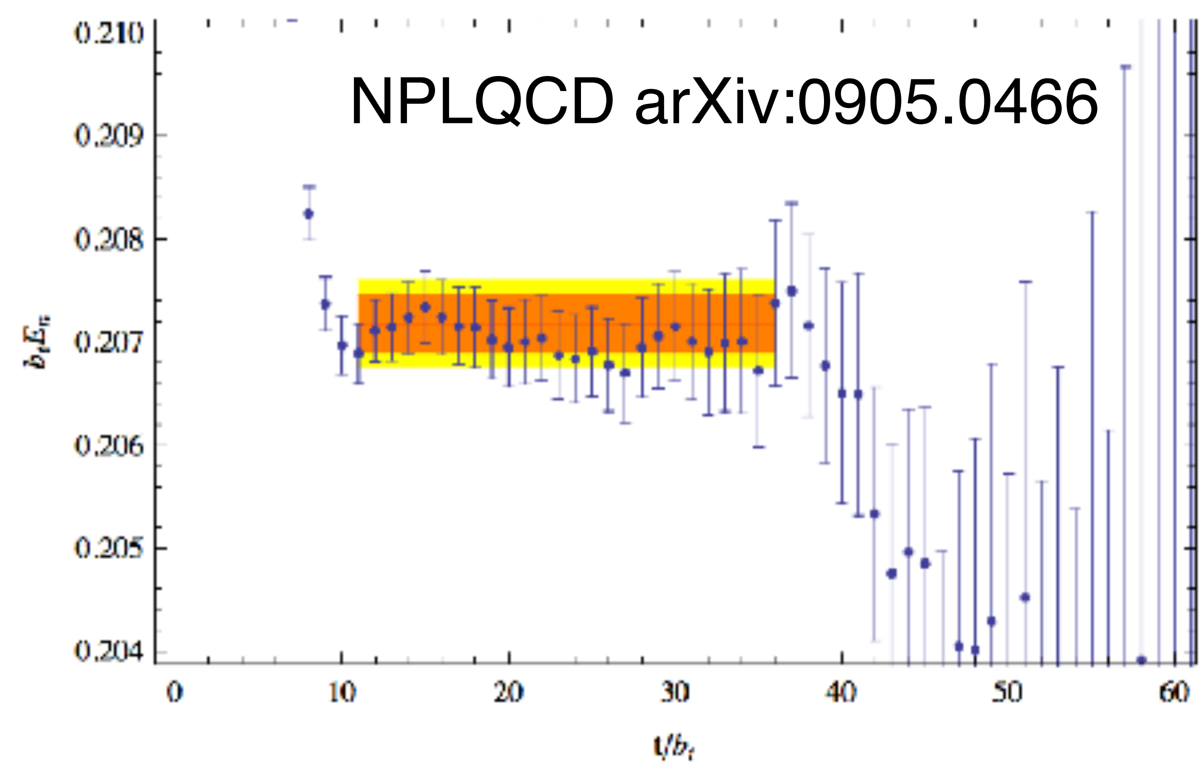
$$C_A(t) = A_0 e^{-E_0 t} + A_1 e^{-E_1 t} + \cdots$$

$$C_B(t) = B_0 e^{-E_0 t} + B_1 e^{-E_1 t} + \cdots$$

$$C_0 = \alpha_0 C_A + \beta_0 C_B$$

$$\alpha_0 A_1 + \beta_0 B_1 = 0$$

Find α_0 and β_0 with black-box method (Matrix Prony)



Matrix Prony: Improved NN

What is the new idea?

- Previously, Matrix Prony has been used to analyze linear combinations of correlation functions in B, BB, BBB, BBBB systems after they were generated
- We realized we could instead use Matrix Prony to form an optimal linear combination of single-nucleon correlation sinks, that could then be inserted into the two(multi)-nucleon contraction code

$$B^{\mu} = \alpha_0 B^{\mu}_{SS} + \beta_0 B^{\mu}_{PS}$$

- This is a "poor man's" version of the more sophisticated variational methods used by Hadspec, Bulava et. al., etc.
- The numerical cost is less than the standard method in which both SS and PS two-nucleon correlation functions are generated
  - only single set of contractions/FFT required

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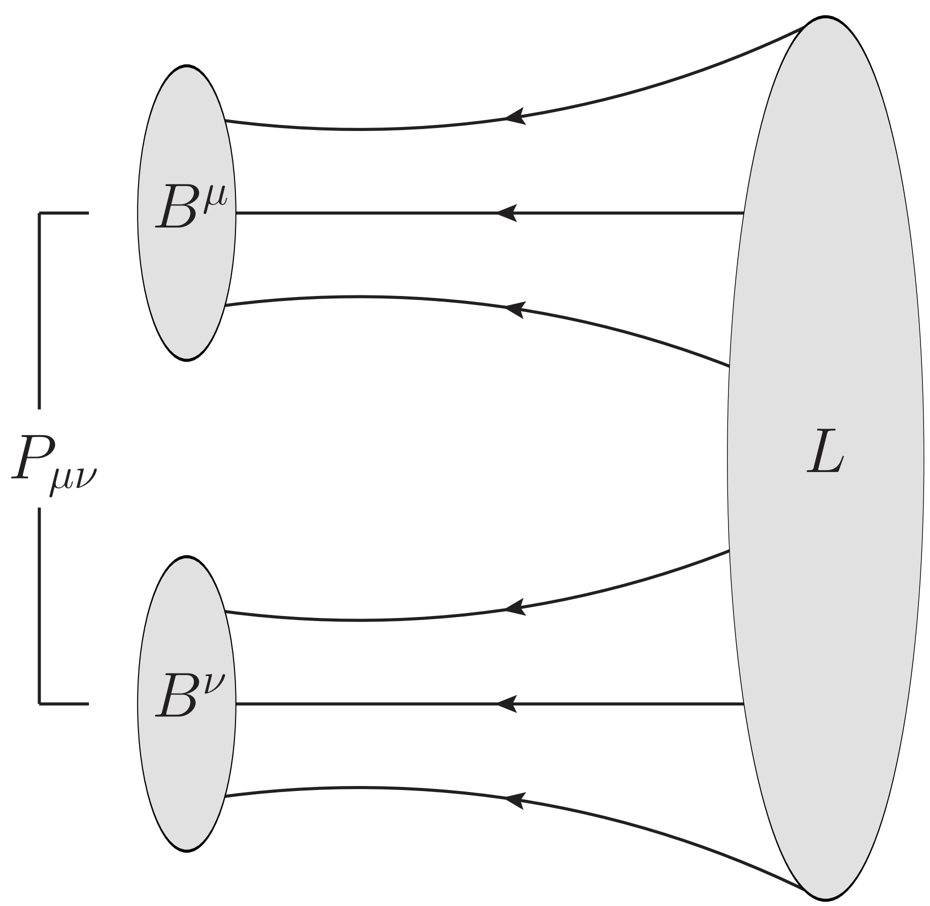

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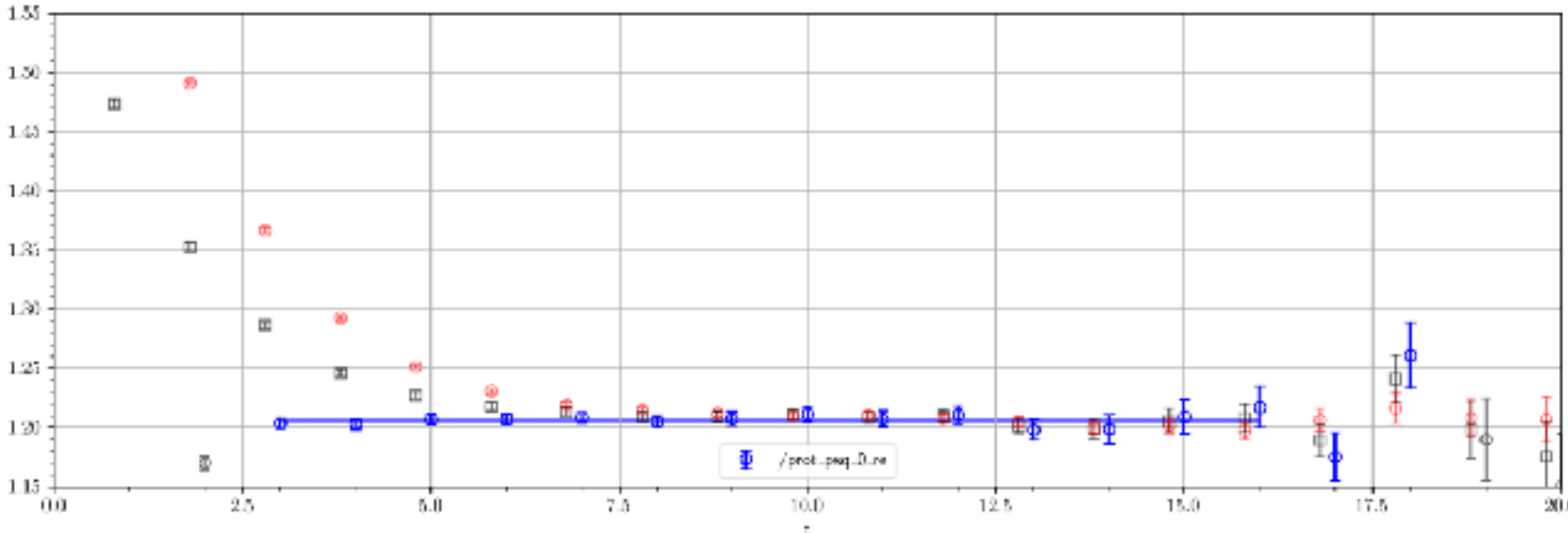
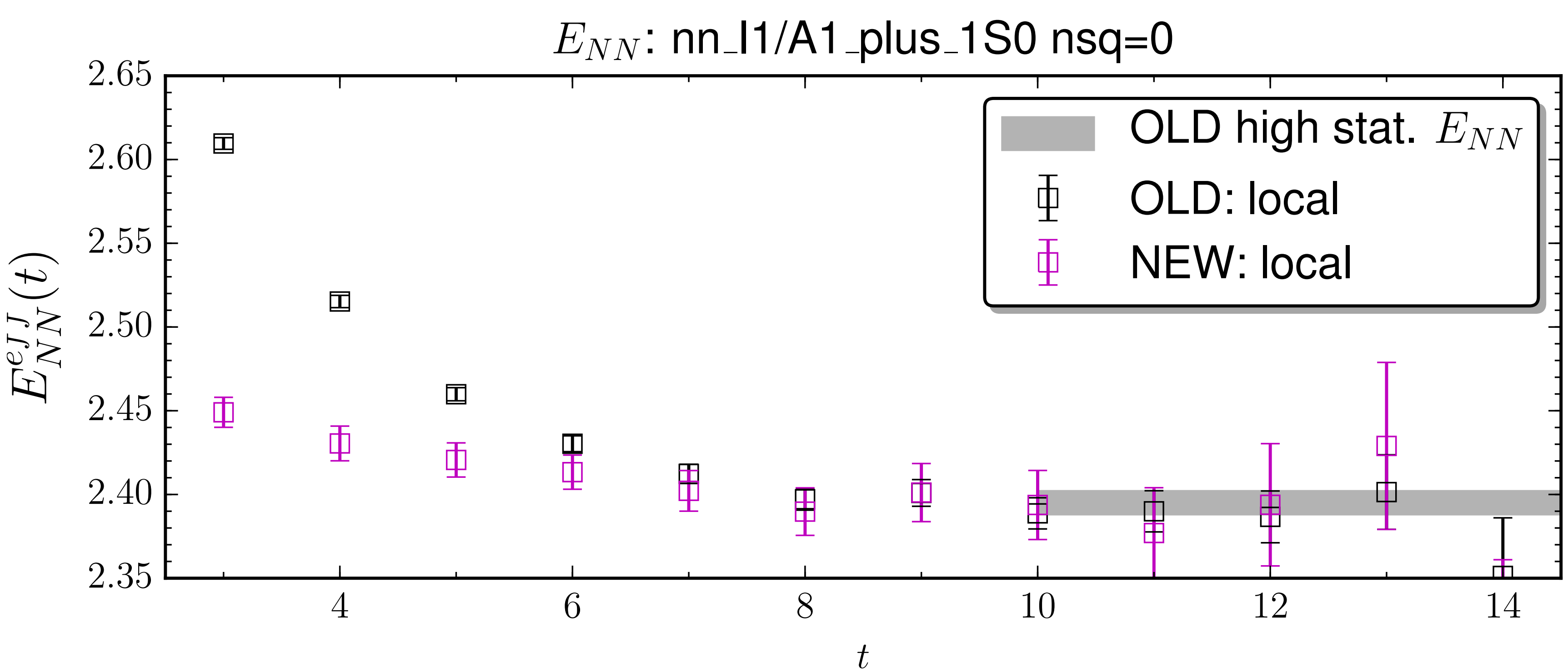
Matrix Prony: Improved NN

- How well does it work?
  - Test the idea out on mπ~800 MeV data - iso-clover WM/JLab cfgs



single nucleon pulled in 6 time slices



used with local NN interpolating fields

$$N^{\dagger}(0,x_i)N^{\dagger}(0,x_i)$$

we observe a reduction in the excited state contamination

Matrix Prony: Improved NN

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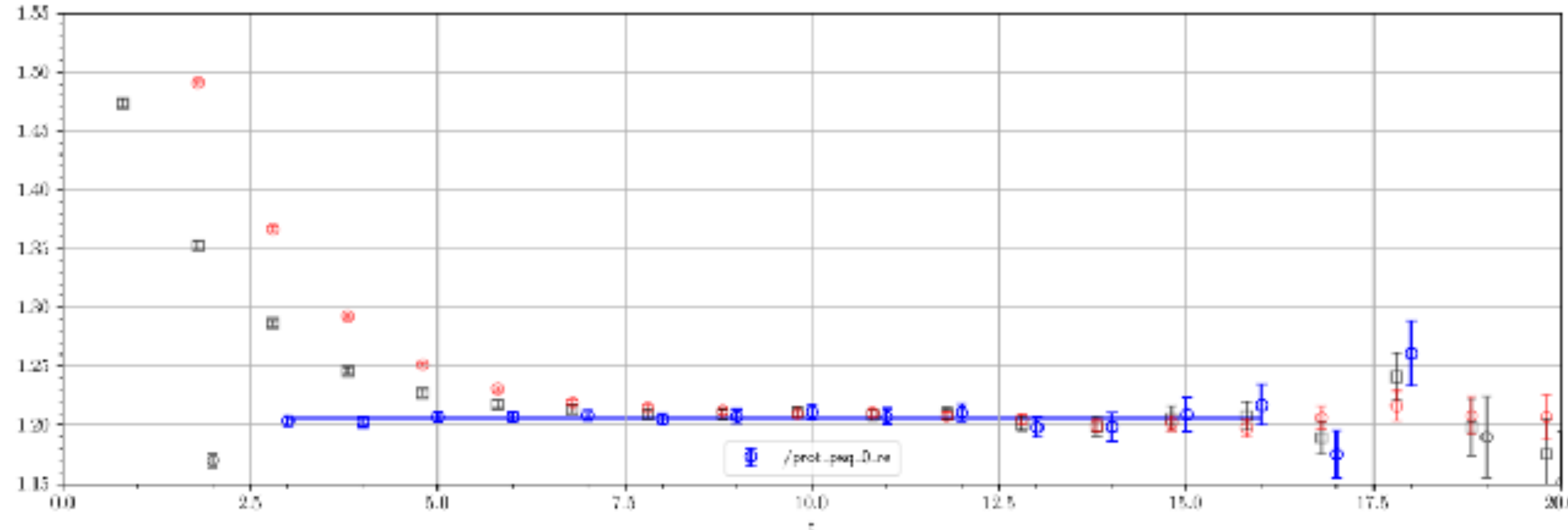

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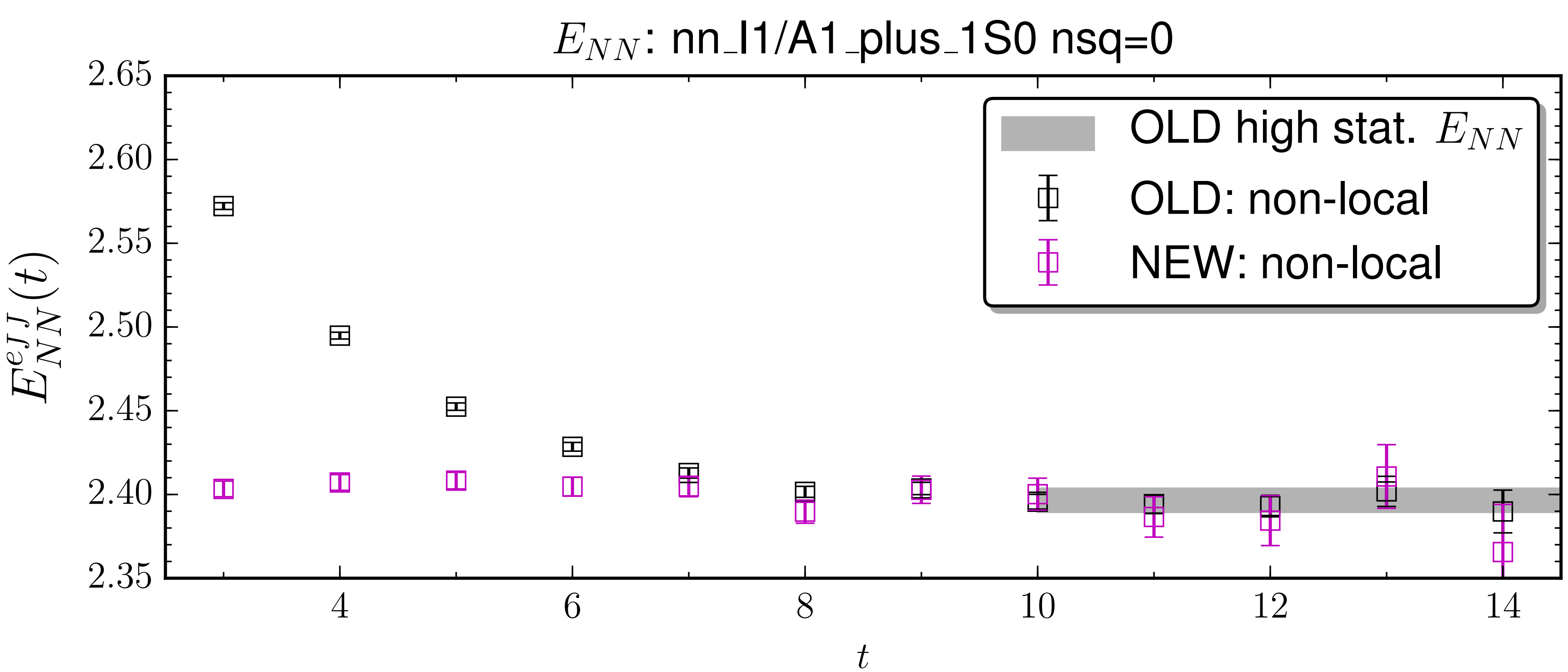


used with non-local NN interpolating fields

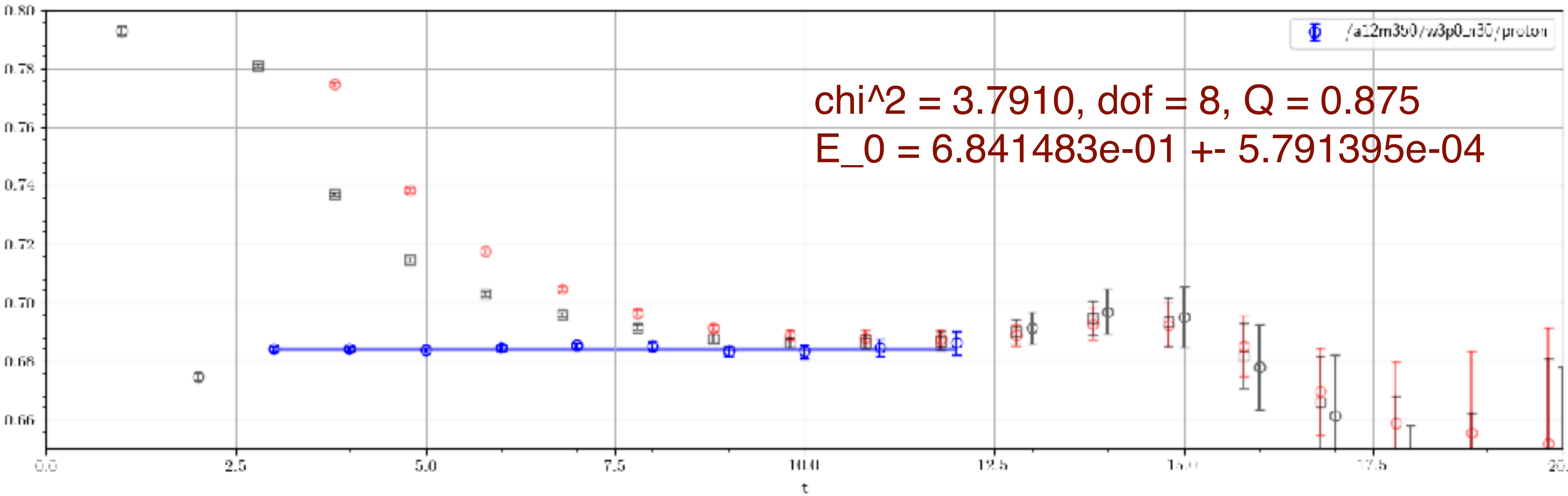
$$N^\dagger(0, x_i) N^\dagger(0, x_i + \Delta)$$

we observe a more significant reduction in the excited state contamination

Matrix Prony: Improved NN

- How well does it work with an interesting pion mass?
  - Application with MDWF on gradient-flowed HISQ

    $m\pi$~350 MeV, Nsrc = 20,000 (2 srcs/cfg, 10K cfgs)



$$am_N = 0.68417(58)$$ ~ 0.085%, g.s. pulled in 8 time slices ~ 0.96 fm

NOTE: this is one of the ensembles used for our gA calculation - this demonstrates from the numerical data (no fits) that there are only 2 states meaningfully contributing to the correlation function all the way down to t = 3 (0.36 fm)

Matrix Prony: Improved NN

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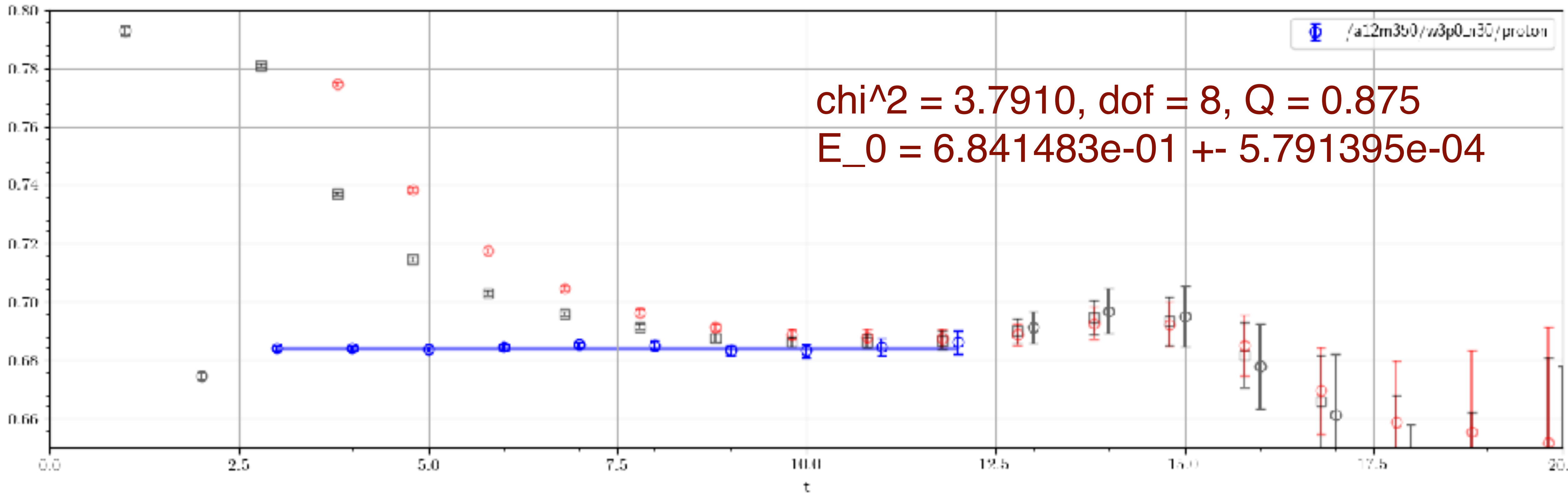
    $m\pi \sim 350$ MeV, Nsrc = 20,000 (2 srcs/cfg, 10K cfgs)



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NPLQCD [arXiv:0903.2990] $m\pi \sim 400$ MeV

$$a_t m_N = 0.20693(33)$$

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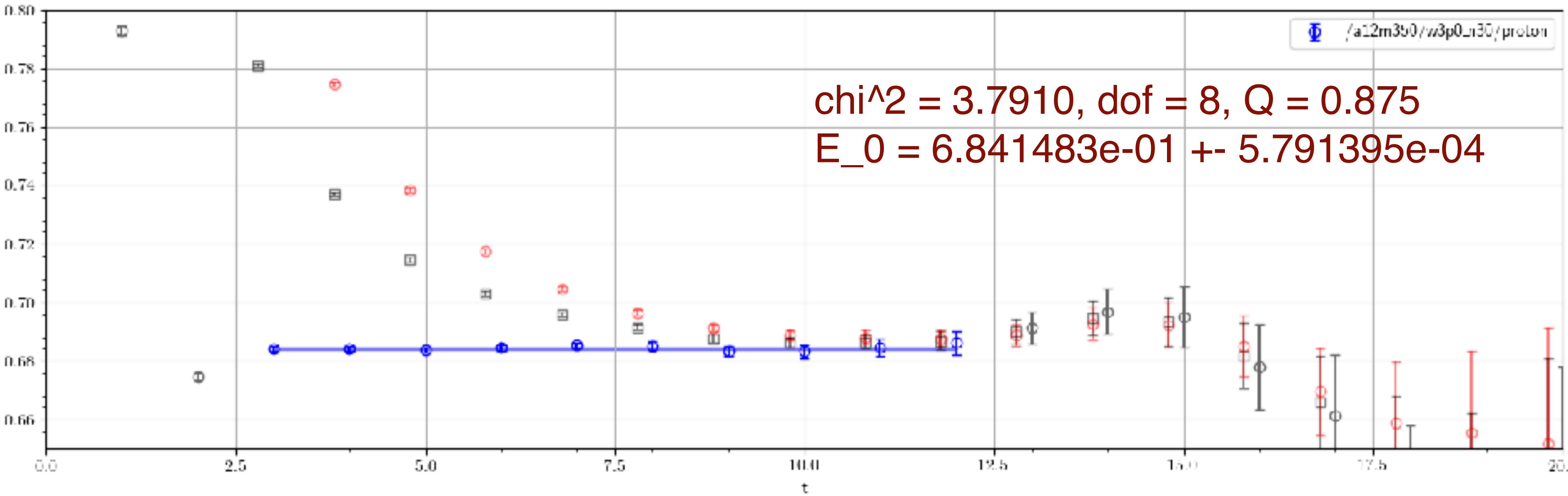

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NPLQCD [arXiv:0903.2990] $m\pi$~400 MeV

$$a_t m_N = 0.20693(33)$$

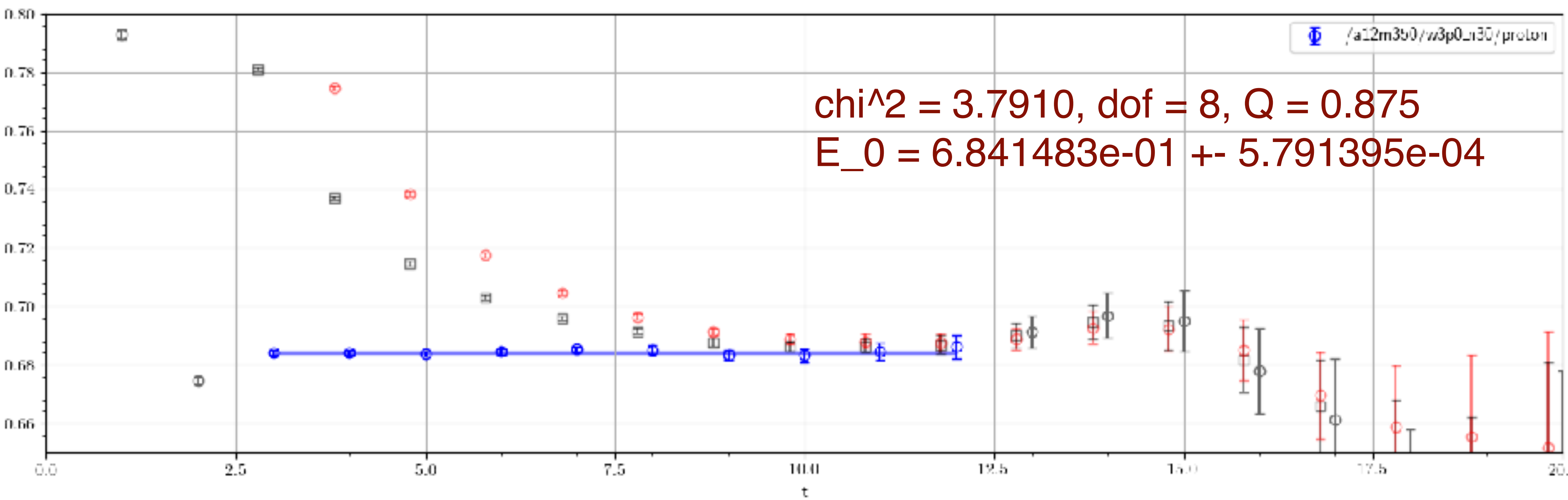
to achieve 0.16% precision with aniso-clover, needed 300K srcs

We are very optimistic this idea will allow for a good LQCD calculations of NN at this interesting pion mass!

Matrix Prony: Improved NN

- How well does it work with an interesting pion mass?
  - Application with MDWF on gradient-flowed HISQ

    $m\pi$~350 MeV, Nsrc = 20,000 (2 srcs/cfg, 10K cfgs)



$$am_N = 0.68417(58)$$ ~ 0.085%, g.s. pulled in 8 time slices ~ 0.96 fm

These calculations are so expensive - it is imperative to extract as much information from them as possible, which is optimally achieved early in Euclidean time where we have a clear theoretical understanding of the correlation functions and they are clean - before the noise sets in

Summary

- Applications of Lattice QCD to Nuclear Physics is Difficult
- With current generation of computers - we have finally made our first “nuclear physics” post diction of a benchmark quantity g_A - with a clear path to sub-percent precision
- The next generation of computers (appearing now at ORNL and LLNL) - plus new ideas - will enable us to begin computing *real* nuclear physics quantities (A=2 (3? 4?)), including $\Delta I=2$ Hadronic Parity Nonconservation
- What do we need?
  - people! (students, postdocs, …) we are personnel-power limited
  - more computing time! tell your friends to review our proposals positively and support computational NP

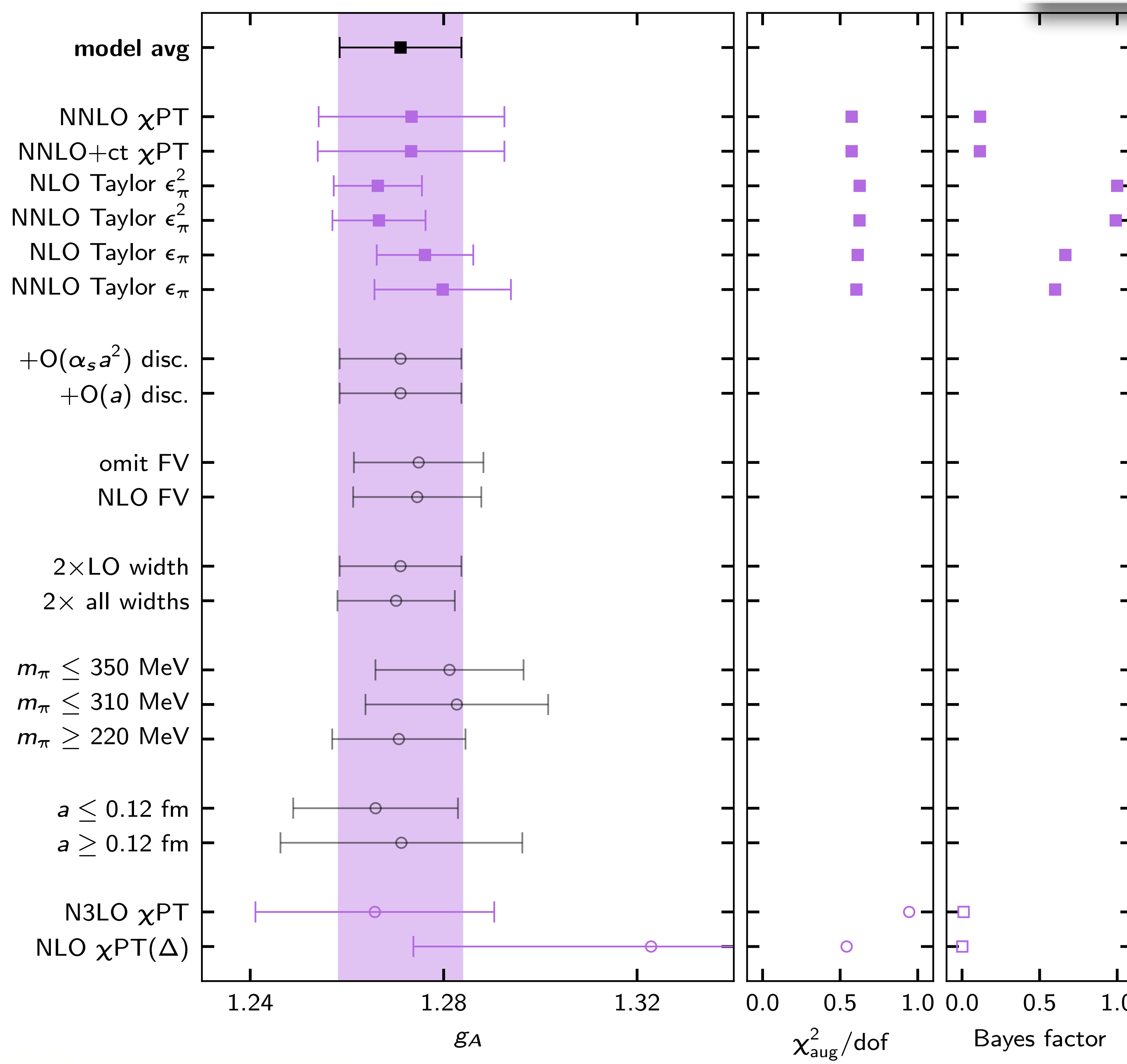
Thank You

Lattice QCD Team

red = postdoc
blue = grad student

Glasgow: Chris Bouchard
INT: Chris Monahan
JLab: Balint Jóo
Jülich: Evan Berkowitz
LBL/UCB: David Brantley, Chia Cheng (Jason) Chang, T. Kurth (NERSC), Henry Monge-Camacho, AWL
LLNL: Pavlos Vranas
Liverpool: Nicolas Garron
NVIDIA: Kate Clark
RIKEN/BNL: Enrico Rinaldi
UNC: Amy Nicholson
William and Mary: Kostas Orginos

plus a few others



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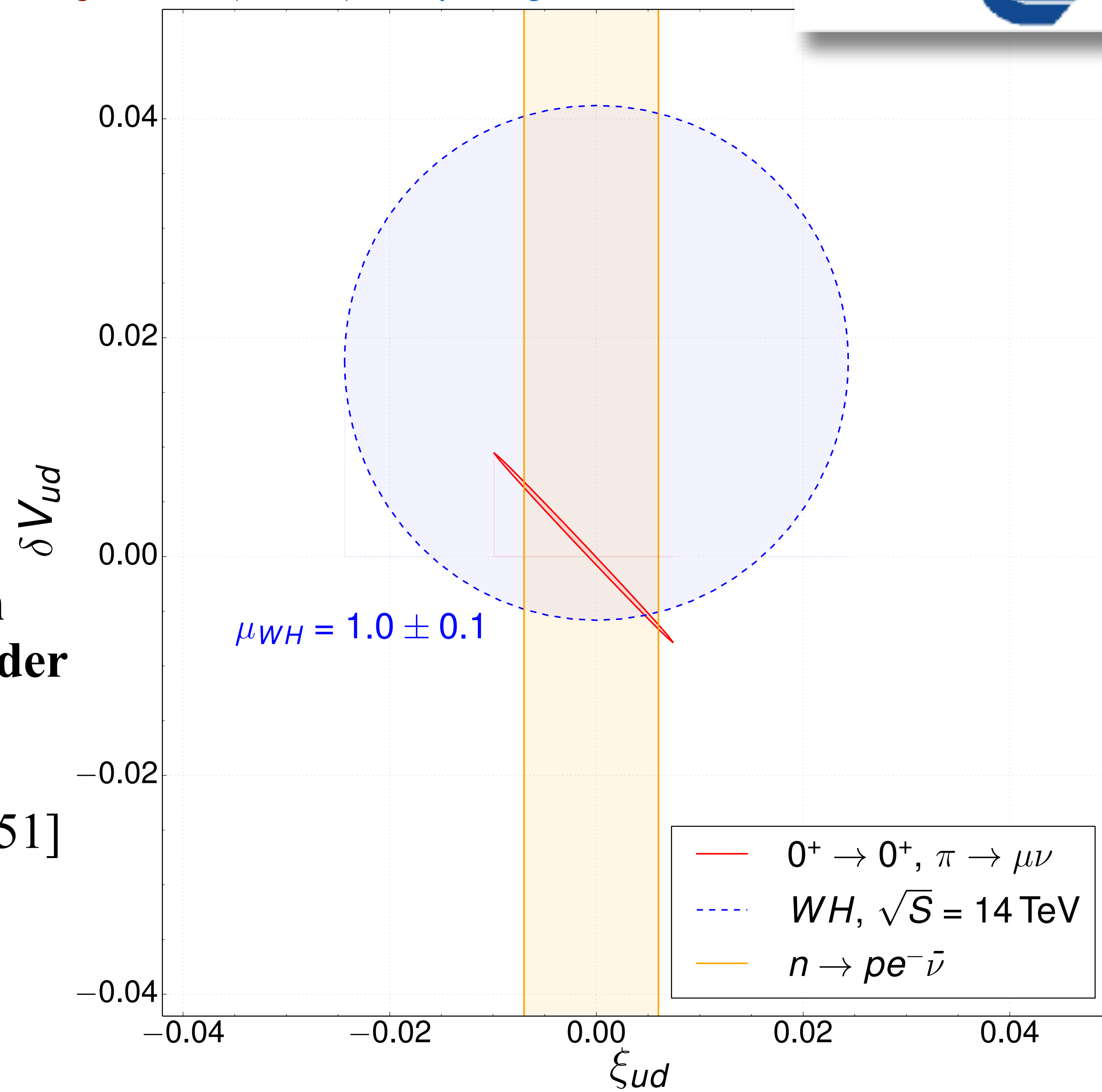
updated figure from
Right-handed charged currents in the era of the Large Hadron Collider
Alioli, Cirigliano, Dekens, de Vries and Mereghetti
JHEP 1705 (2017) [arXiv:1703.04751]



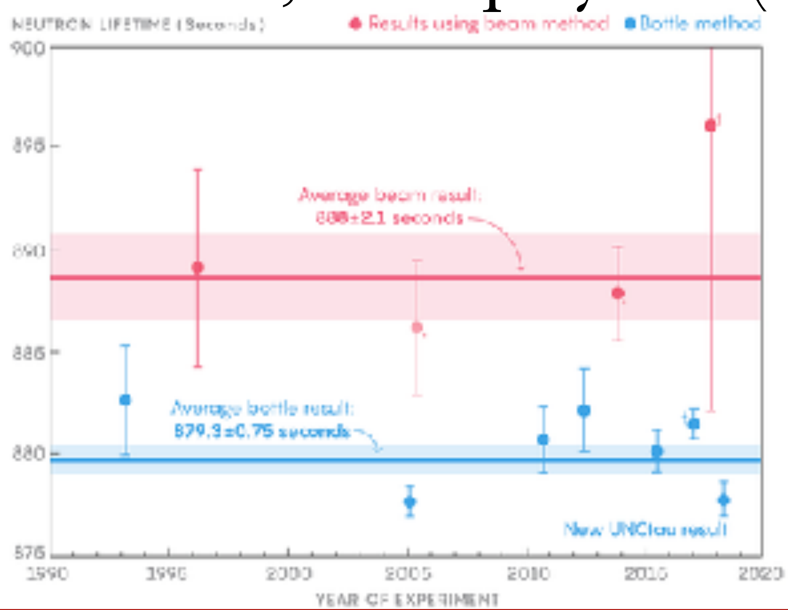
U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

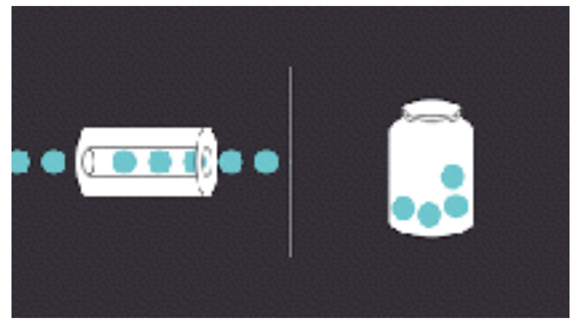
OLCF Oak Ridge Leadership Computing Facility

SciDAC Scientific Discovery through Advanced Computing

Neutron Lifetime…

- there is a 4-sigma discrepancy: beam $\tau_n^{\text{beam}} = 888.0(2.0)s$ and bottle $\tau_n^{\text{bottle}} = 879.4(0.6)s$ measurements of the neutron lifetime, new physics (dark matter) or unknown systematic?





Czarnecki, Marciano, Sirlin
arXiv:1802.01804

$$\tau_n = \frac{5172.0(1.0)\,s}{1 + 3g_A^2}$$

arXiv.org > hep-ph > arXiv:1802.01804

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High Energy Physics – Phenomenology

The Neutron Lifetime and Axial Coupling Connection

Andrzej Czarnecki, William J. Marciano, Alberto Sirlin

(Submitted on 6 Feb 2018 (v1), last revised 22 Feb 2018 (this version, v2))

Experimental studies of neutron decay, $n \to pe\bar{\nu}$, exhibit two anomalies. The first is a 8.6(2.1)s, roughly 4σ difference between the average beam measured neutron lifetime, $\tau_n^{\text{beam}} = 888.0(2.0)$s, and the more precise average trapped ultra cold neutron determination, $\tau_n^{\text{trap}} = 879.4(6)$s. The second is a 5σ difference between the pre2002 average axial coupling, g_A, as measured in neutron decay asymmetries $g_A^{\text{pre2002}} = 1.2637(21)$, and the more recent, post2002, average $g_A^{\text{post2002}} = 1.2755(11)$, where, following the UCNA collaboration division, experiments are classified by the date of their most recent result. In this study, we correlate those τ_n and g_A values using a (slightly) updated relation $\tau_n(1+3g_A^2) = 5172.0(1.1)$s. Consistency with that relation and better precision suggest $\tau_n^{\text{favored}} = 879.4(6)$s and $g_A^{\text{favored}} = 1.2755(11)$ as preferred values for those parameters. Comparisons of g_A^{favored} with recent lattice QCD and muonic hydrogen capture results are made. A general constraint on exotic neutron decay branching ratios is discussed and applied to a recently proposed solution to the neutron lifetime puzzle.