Pion mass dependence of the nucleon mass and the pion-nucleon sigma term from lattice QCD and EFT

INT Workshop:
Origin of the Visible Universe: Unraveling the Proton Mass
June 13-17

André Walker-Loud

Outline

- Who?
- What?
- Where?
- When?
- Why?

Outline

- ❑ Who? CalLat Collaboration
- ❑ What? $\langle N|m_u\bar{u}u + m_d\bar{d}d|N\rangle \ \left[\langle N|m_s\bar{s}s|N\rangle\,, \langle N|m_c\bar{c}c|N\rangle\right]$
- ❑ Why Why not?
- ❑ Where? Summit at OakRidge Leadership Computing Facility and Lassen at LLNL
- ❑ When? The last few years
- ❑ How? Lattice QCD
  - ❑ Lattice QCD brief intro
  - ❑ Feynman-Hellmann Method versus Direct Method
  - ❑ Our results

Who?

California Lattice Collaboration

*Not all in California

(postdoc, grad student)

This project

Nolan Miller	UNC → Mainz
Grant Bradley	UNC → Brown
Malcolm Lazarow	UC Berkeley
Zack Hall	UNC
Chris Körber	Bochum University
Aaron Meyer	UC Berkeley / LBNL
Henry Monge-Camacho	ORNL
Chris Bouchard	Glasgow U.
Kate Clark	NVIDIA
Nicolas Garron	Liverpool Hope
Ben Hörz	LBNL → Intel
Dean Howarth	LBNL
Bálint Joó	ORNL
Amy Nicholson	UNC
Enrico Rinaldi	U. Michigan / RIKEN
Pavlos Vranas	LLNL
André Walker-Loud	LBNL

What?

- We are computing the scalar quark condensation in the nucleon

$$\sigma_{\pi N} = \langle N | m_u \bar{u} u + m_d \bar{d} d | N \rangle = \langle N | \hat{m} (\bar{u} u + \bar{d} d) | N \rangle \qquad \hat{m} = \frac{m_u + m_d}{2}$$

- We are also interested in the strange and charm scalar condensation in the nucleon

$$\langle N | m_s \bar{s} s | N \rangle \,, \quad \langle N | m_c \bar{c} c | N \rangle$$

- I will focus on the light-quark matrix elements in this talk

Why?

- This workshop — how does the proton mass emerge from QCD?

$$m_N = \frac{\beta}{2g}\langle N|G^2|N\rangle + \sum_q \langle N|(1+\gamma_m)m_q\bar{\psi}_q\psi_q|N\rangle$$

$$= \underline{\langle N|\frac{\beta}{2g}G^2 + \gamma_m \sum_q m_q\bar{\psi}_q\psi_q|N\rangle} + \underline{\sum_q \langle N|m_q\bar{\psi}_q\psi_q|N\rangle}$$

RG Invariant
Unambiguous
How do I define this term
non-perturbatively?

RG Invariant
Unambiguous

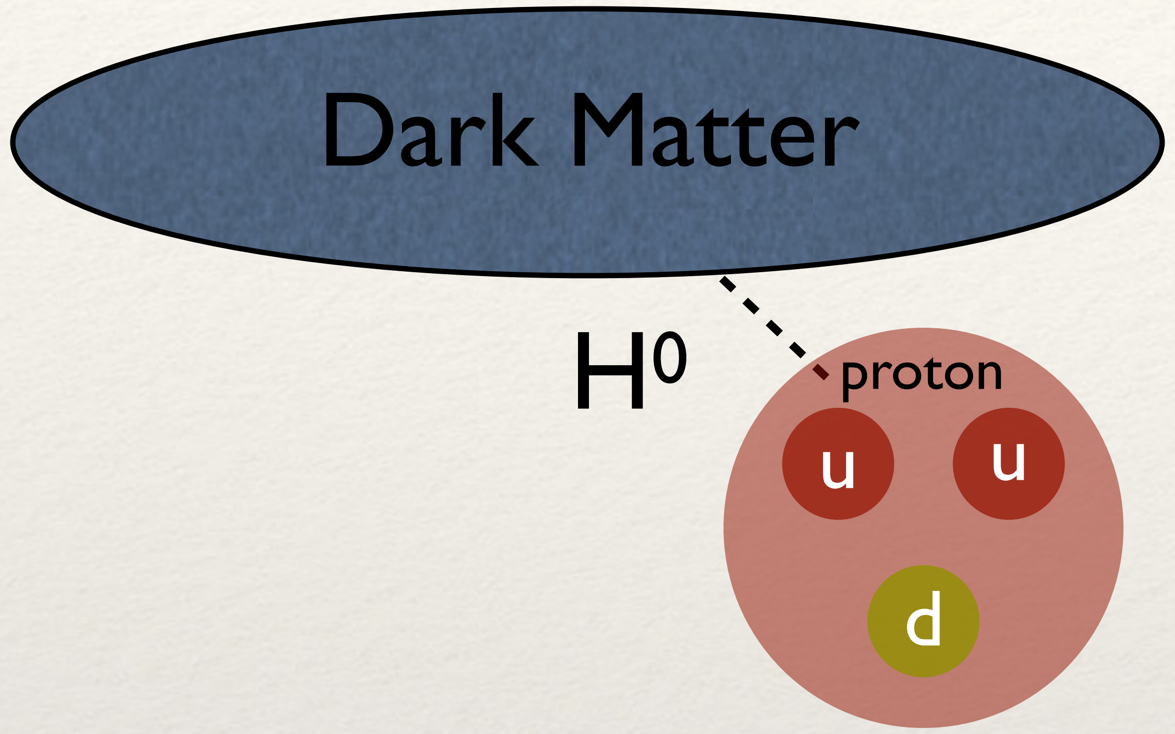
- NOTE: I have not specified what quark flavors I am summing over…

  certainly, we have no hope to compute the light and strange matrix elements w/o LQCD

  the charm content is well estimated by pQCD — but — we might be hyper-sensitive to it

Why?

- Prospective scattering of Dark Matter off matter is sensitive to these matrix elements



$$\sigma \propto |f|^2 \qquad f = \frac{2}{9} + \frac{7}{9} \sum_{q=u,d,s} f_q \qquad f_q \equiv \frac{\langle N | m_q \bar{q} q | N \rangle}{m_N}$$

see eg. Cheung, Hall, Pinner, Ruderman JHEP 05 (2013) 100 [arXiv:1211.4873]

- These scalar current matrix elements are difficult to measure experimentally
  $f_{u,d}$: can be estimated from pion-nucleon scattering
  f_s : no good way to estimate (it turns out) - SU(3) Baryon XPT does not converge

- "Perfect" problem for LQCD

Why?

- Uncertainty was dominated by strange content
  value was estimated using SU(3) baryon Chiral Perturbation Theory (XPT)

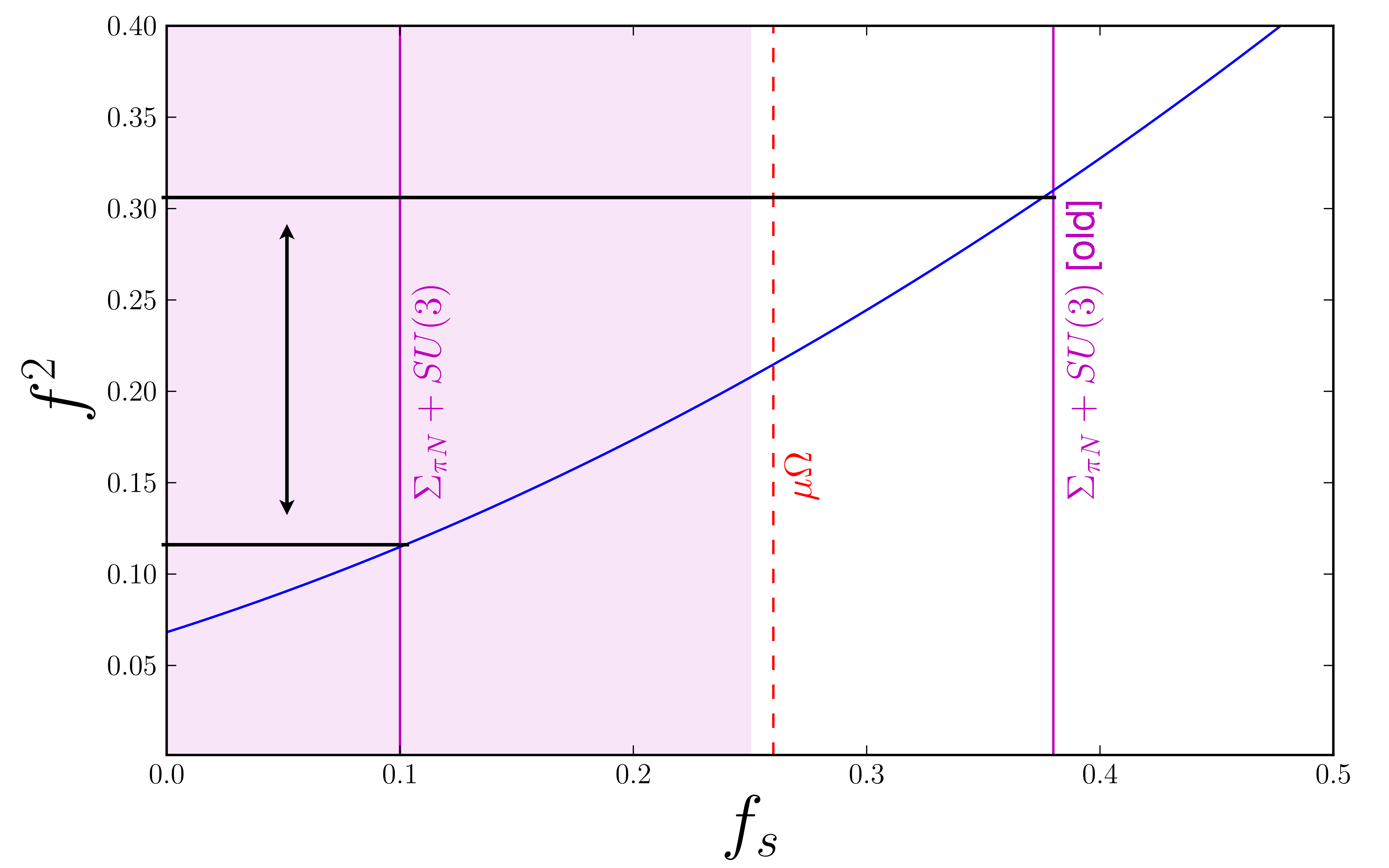


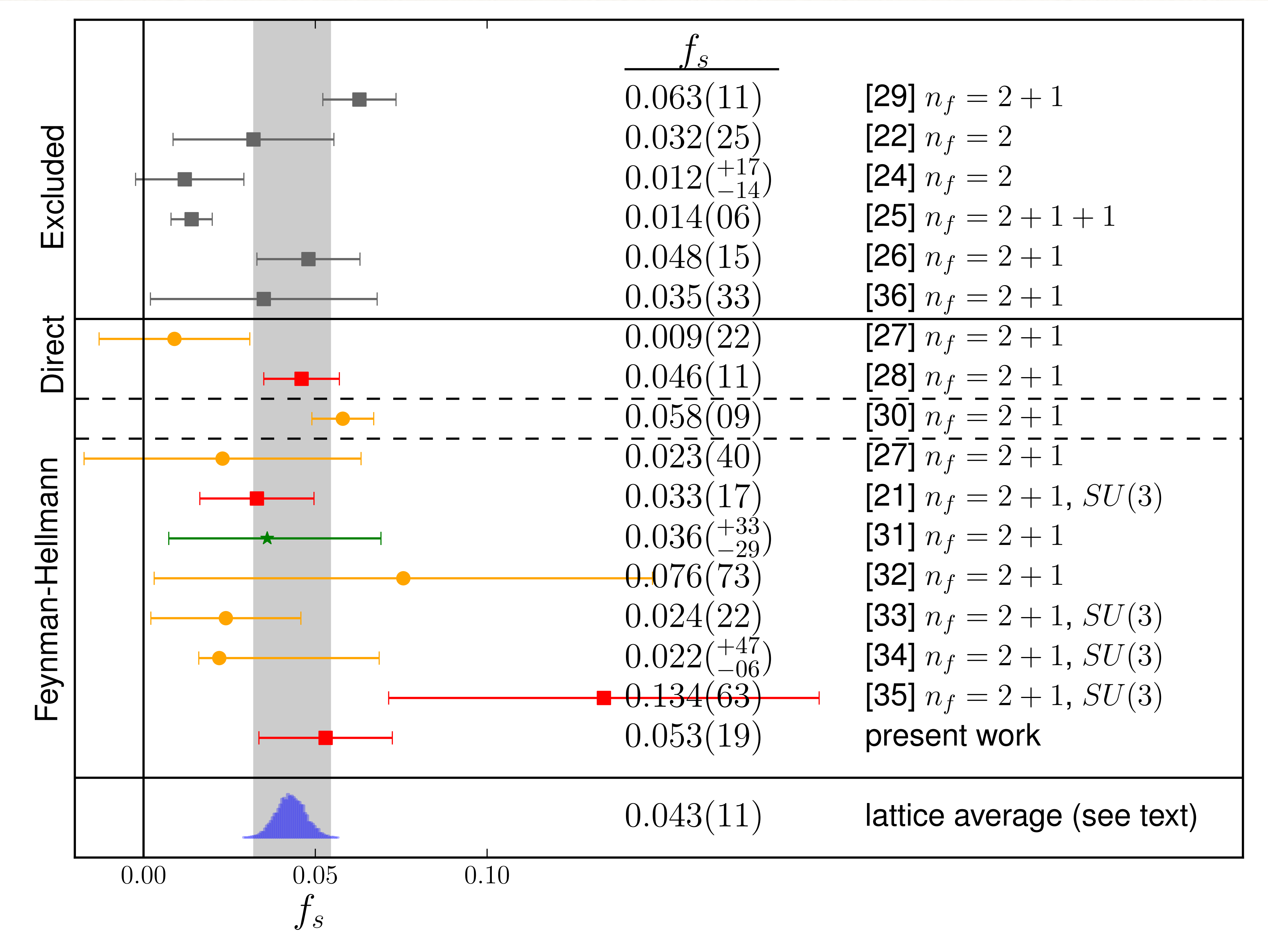
figure adapted from Cheung, Hall, Pinner, Ruderman
JHEP 05 (2013) 100 [arXiv:1211.4873]

Why?

- LQCD $f_s = \frac{\langle N|m_s\bar{s}s|N\rangle}{m_N} = \frac{\sigma_s}{m_N} = \frac{40 \pm 10\ \text{MeV}}{m_N}$

$$\sigma_s = \begin{cases} 52.9 \pm 7.0\ \text{MeV} & N_f = 2+1 \\ 41.0 \pm 8.8\ \text{MeV} & N_f = 2+1+1 \end{cases}$$

Junnarkar & Walker-Loud
PRD 87 (2013) [arXiv:1301.1114]



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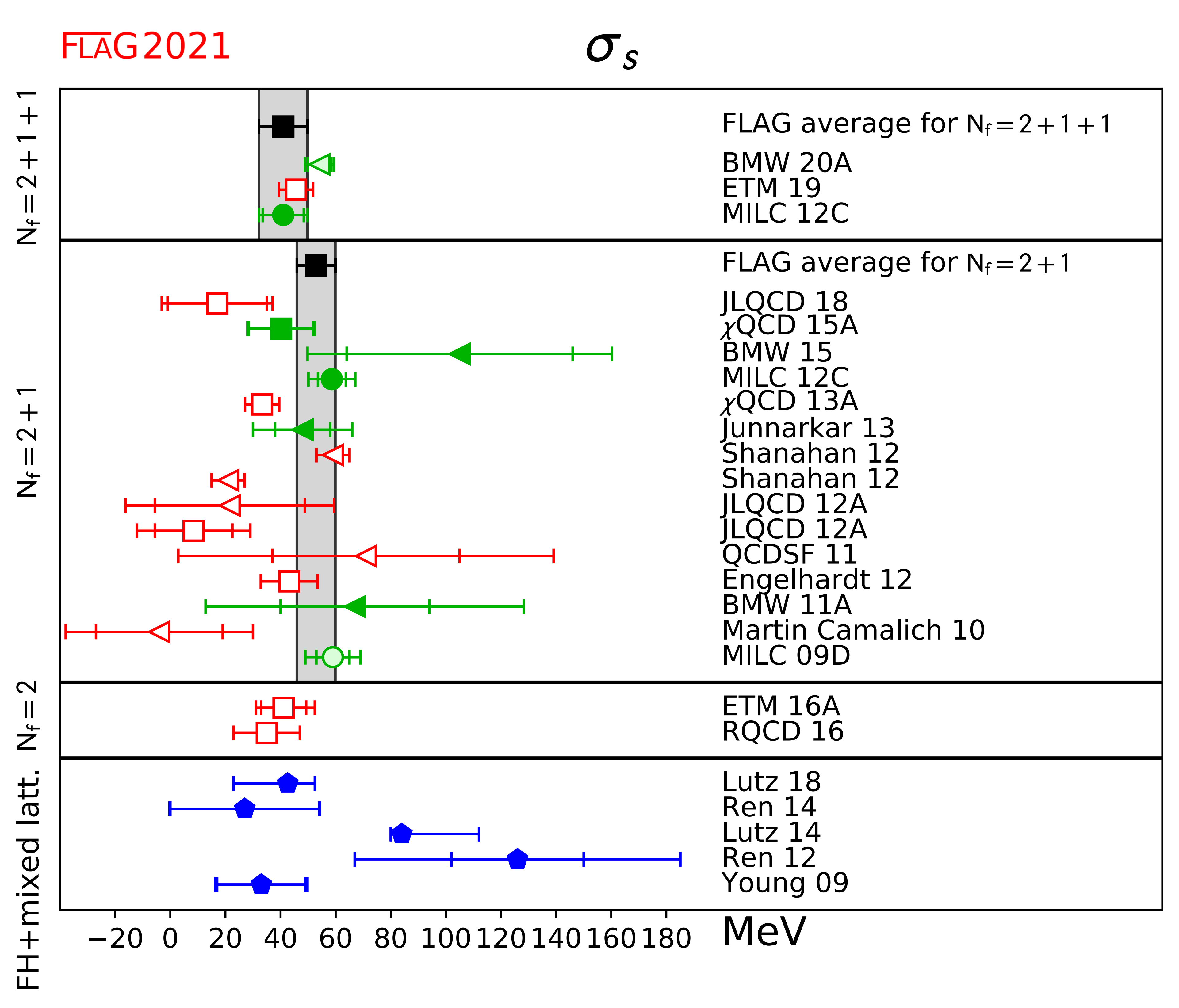
[arXiv:2111.09849]



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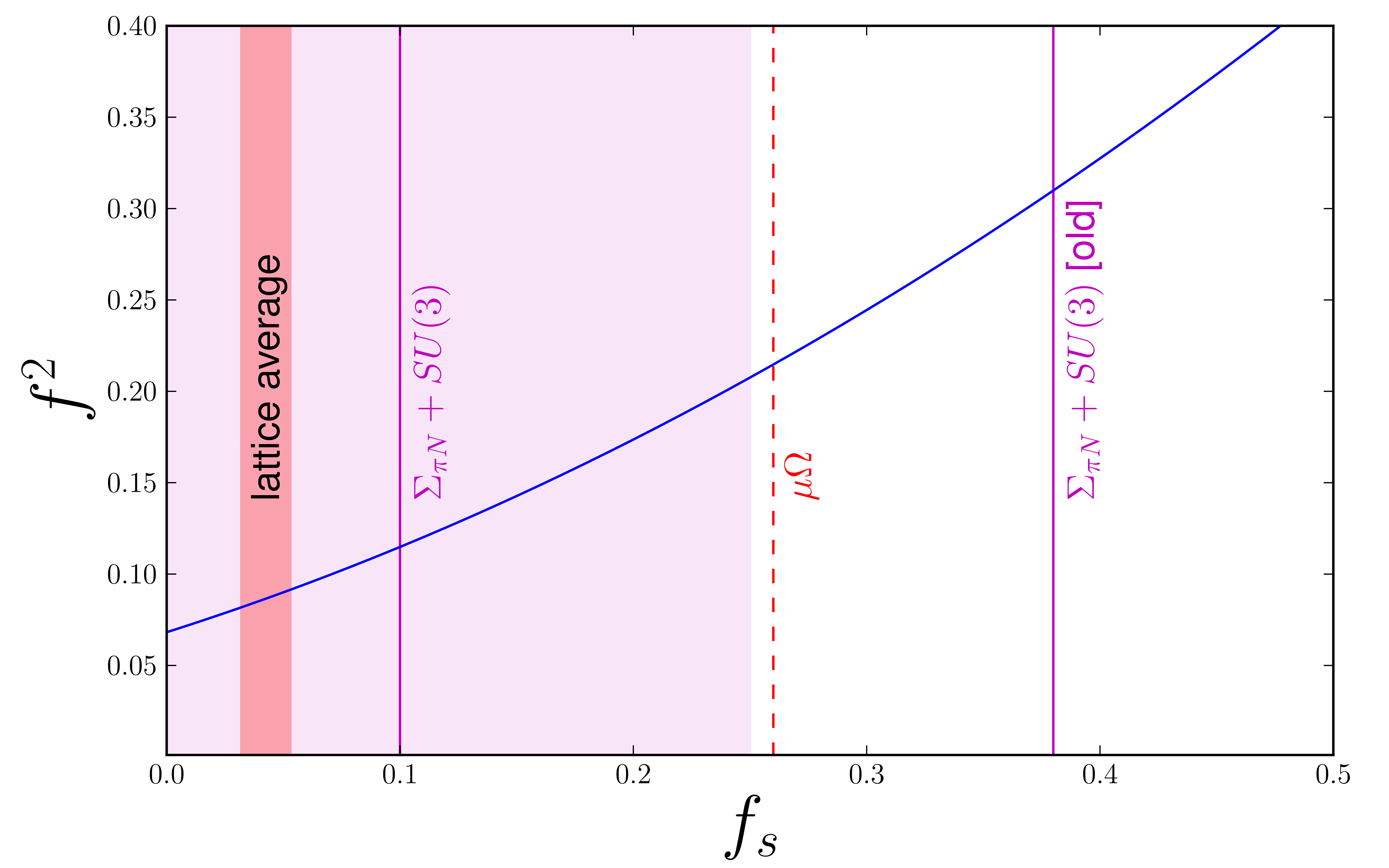


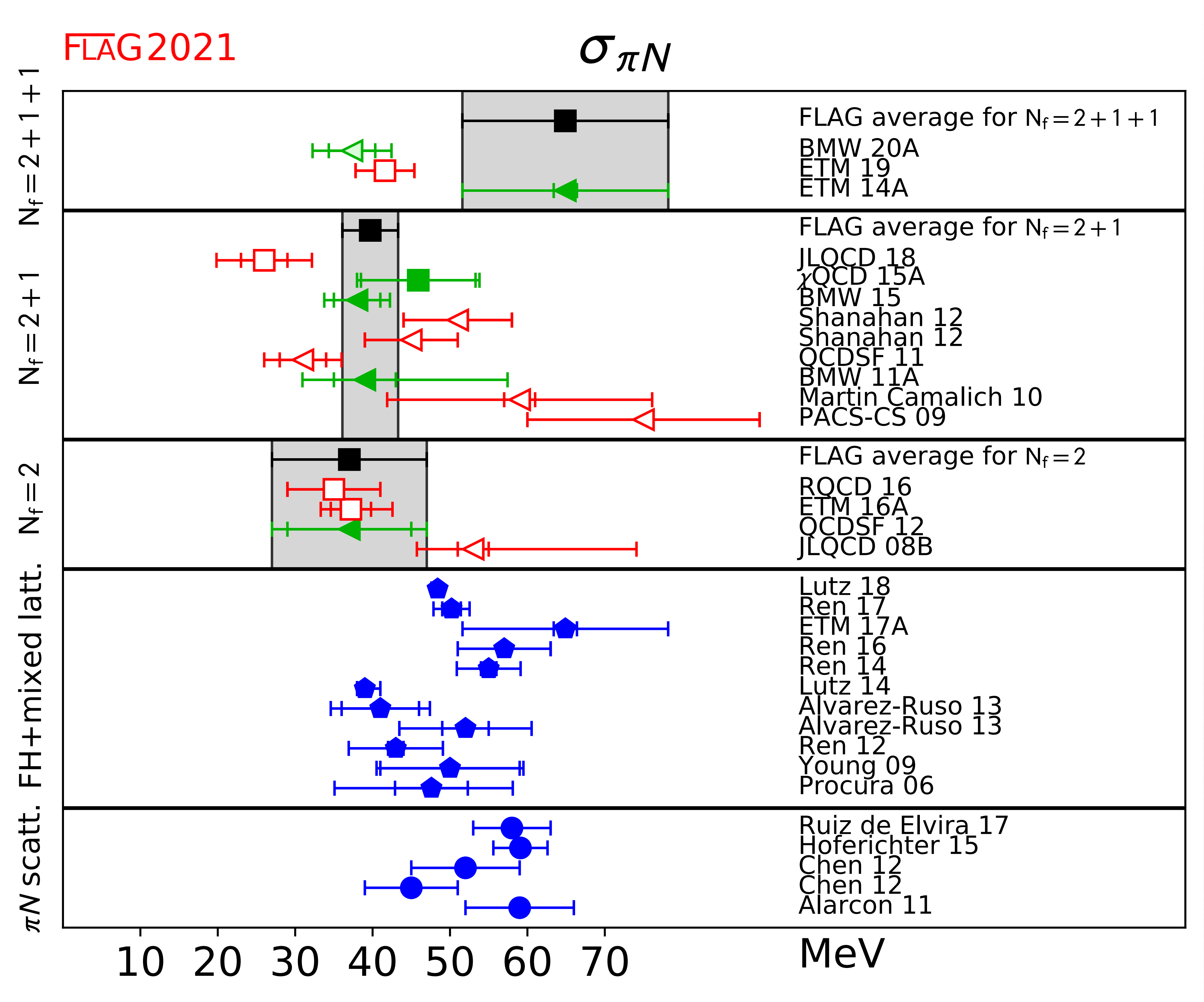
figure adapted from Cheung, Hall, Pinner, Ruderman
JHEP 05 (2013) 100 [arXiv:1211.4873]

Uncertainty is now sensitive to light-quark matrix element

and heavy?

Why?

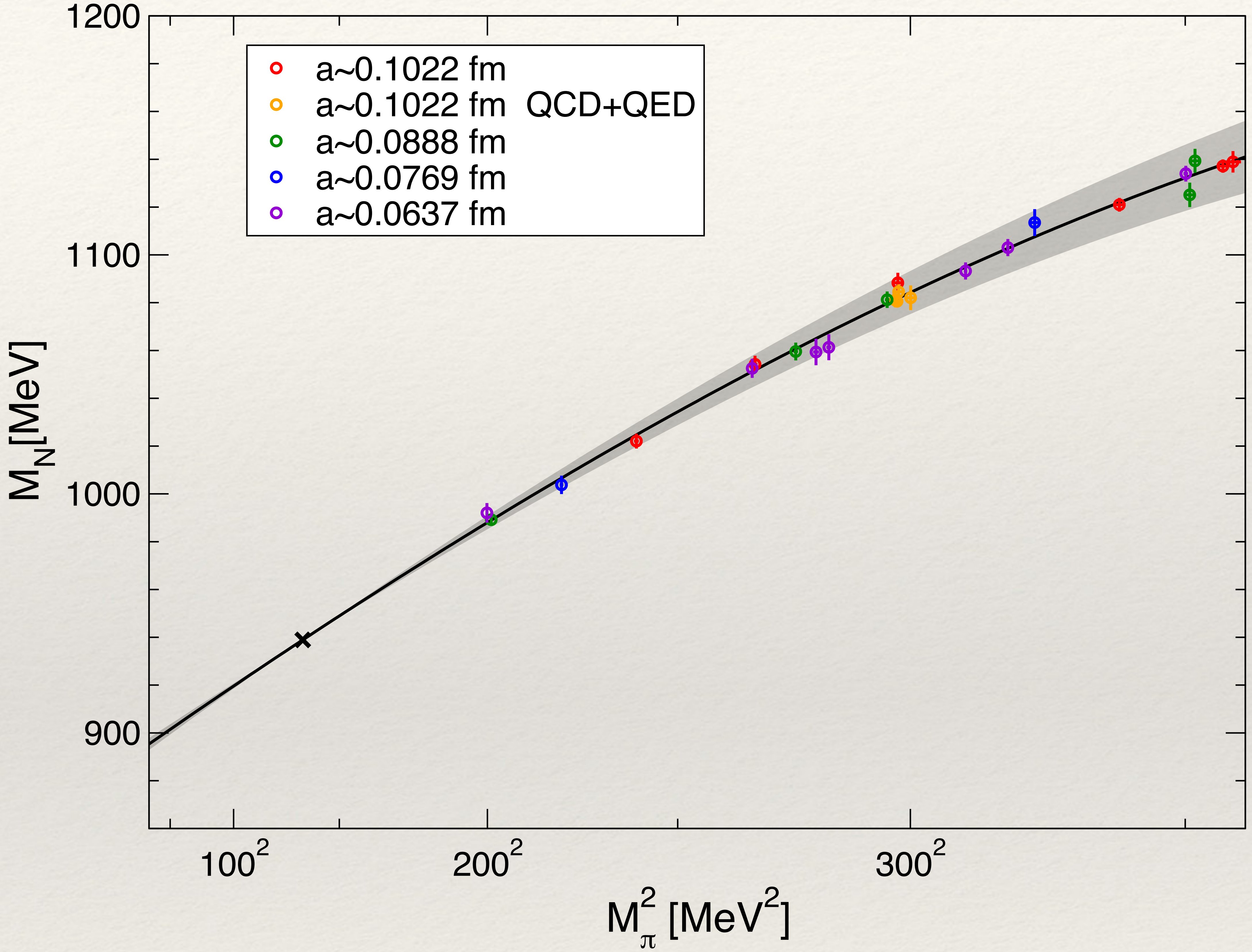
- ❑ Light-quark matrix element



LQCD

PHENO

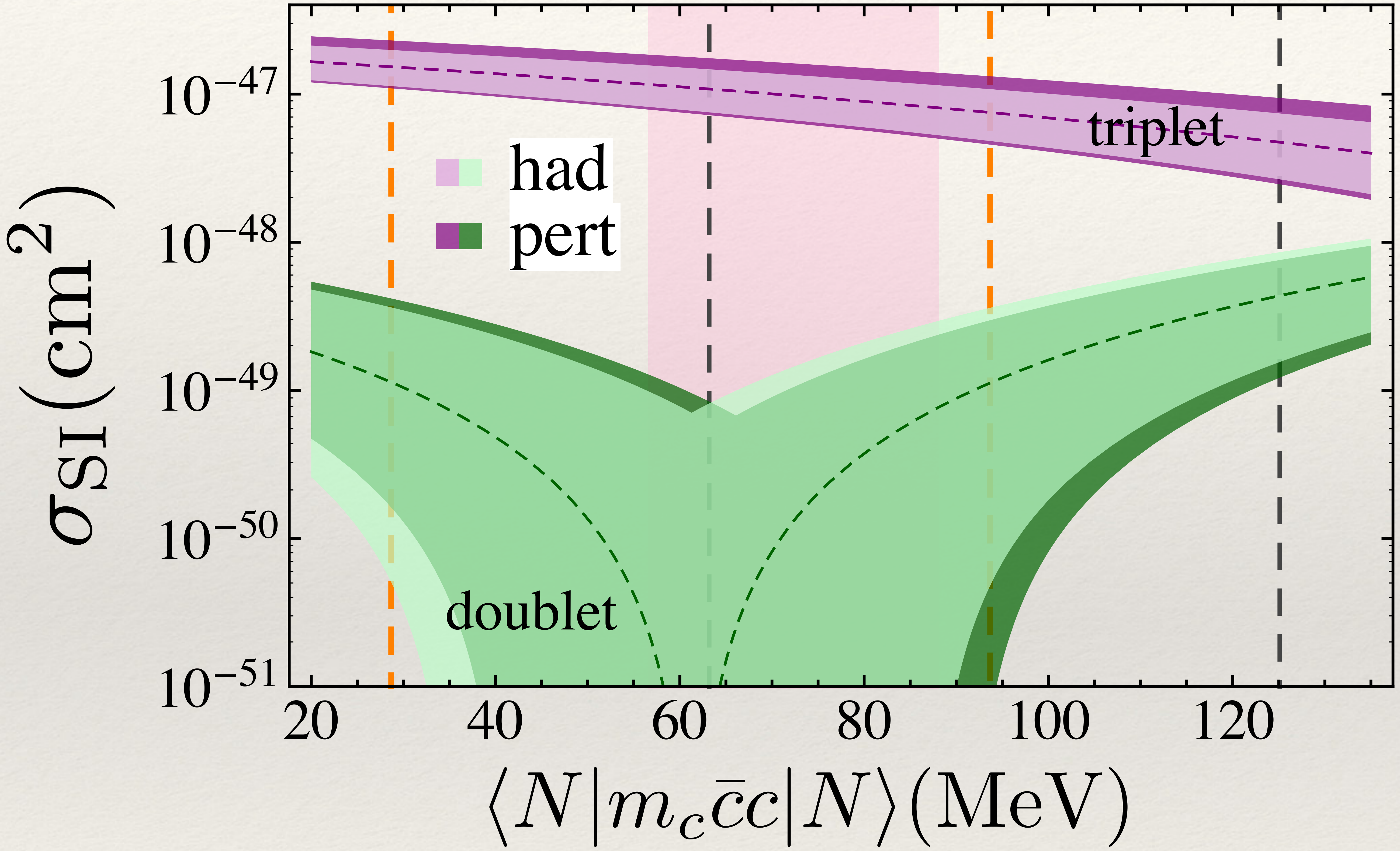
BMWc: Borsanyi et al
[arXiv:2007.03319]



Is the tension due to LQCD systematics?
Mpi extrapolation?
Excited states?

Why?

- The charm content may be particularly interesting



Hill & Solon
PRL 112 (2014) [arXiv:1309.4092]

WIMP Dark Matter scattering through HIGGS portal

- heavy WIMP (integrate out to SMEFT)
- cancellation between spin-0 and spin-2 gluon contributions to spin-independent (SI) cross section
- Normally - one would not need to precisely know a heavy quark matrix element
- Depending upon precise value of charm content, SI cross section can drop below “neutrino-floor”

How?

- Lattice QCD is "perfect" tool to compute these scalar quark matrix elements
- Two ways to perform the calculation
  - Direct method: matrix element
  - Indirect method: Feynman-Hellmann Theorem

Introduction to LQCD

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

$$= \frac{1}{\mathcal{Z}}\int DU \det\left(\mathrm{i}\not{D} - \mathrm{M}\right)\mathcal{O}(\mathrm{t})\mathcal{O}(0)\mathrm{e}^{\mathrm{iS_M}[\bar{\psi},\psi,\mathrm{U}]}$$

Slide adapted from E. Berkowitz

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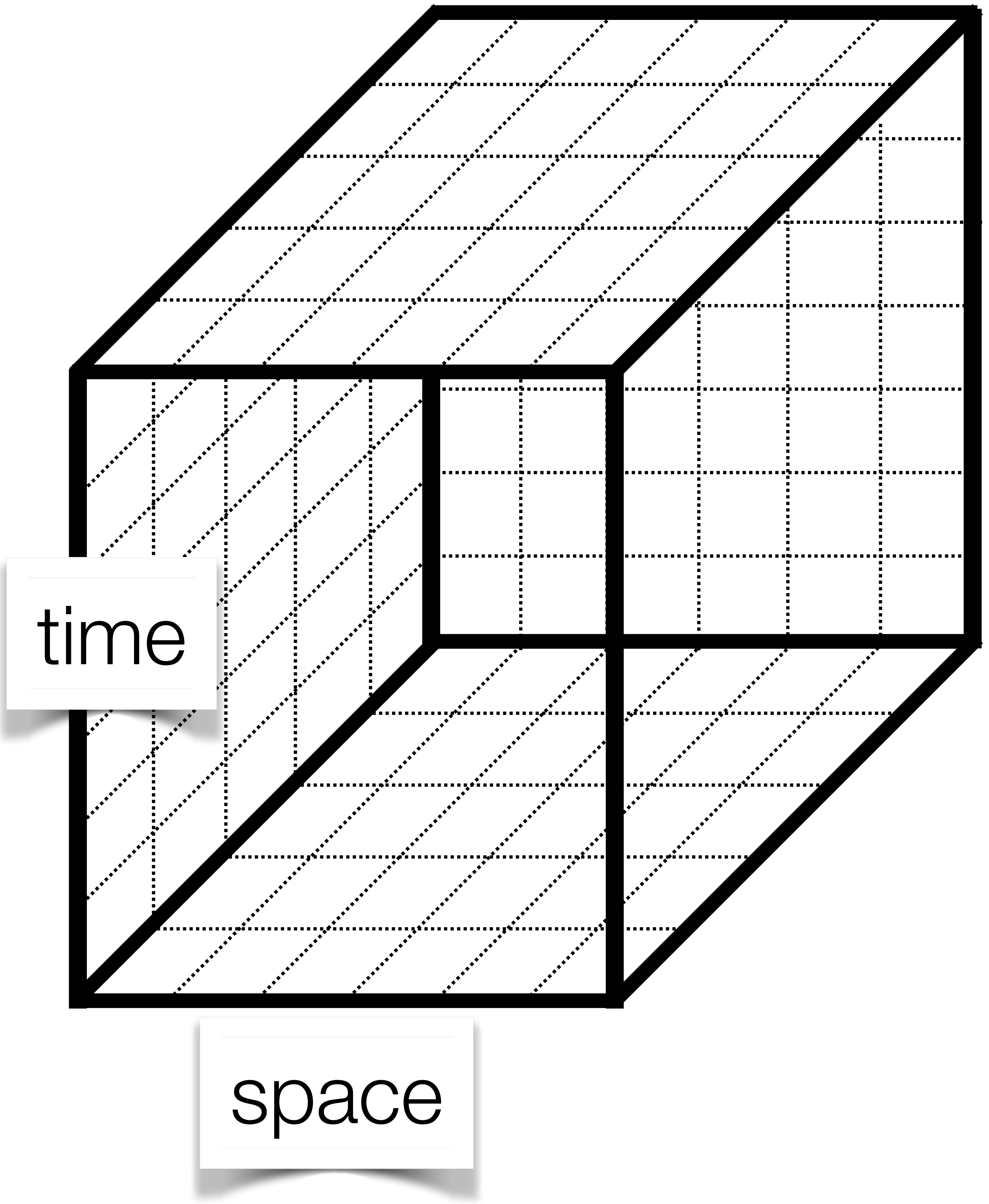
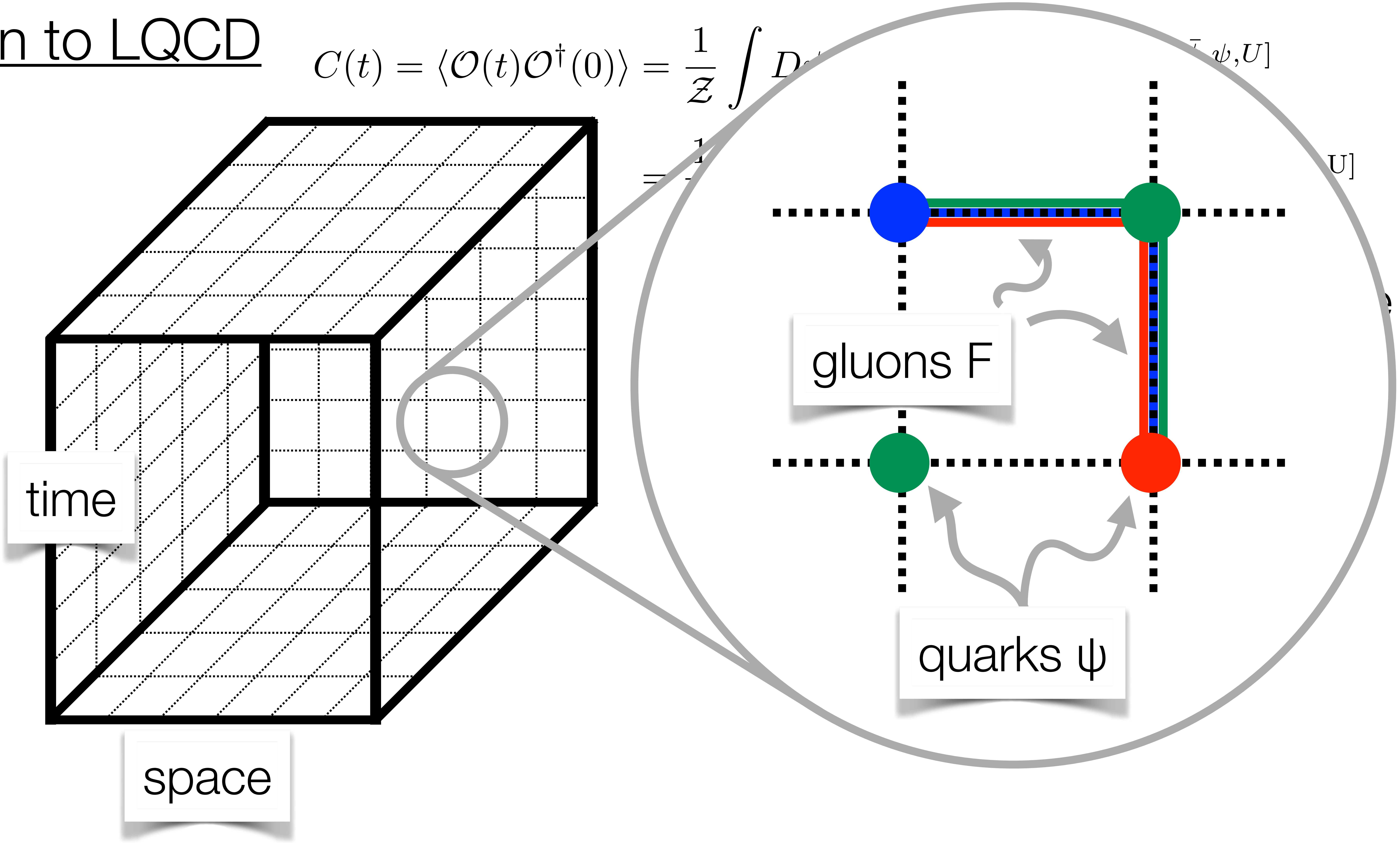


lattice
finite volume

Introduction to LQCD

$$C(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0)\rangle = \frac{1}{\mathcal{Z}}\int D \ldots$$



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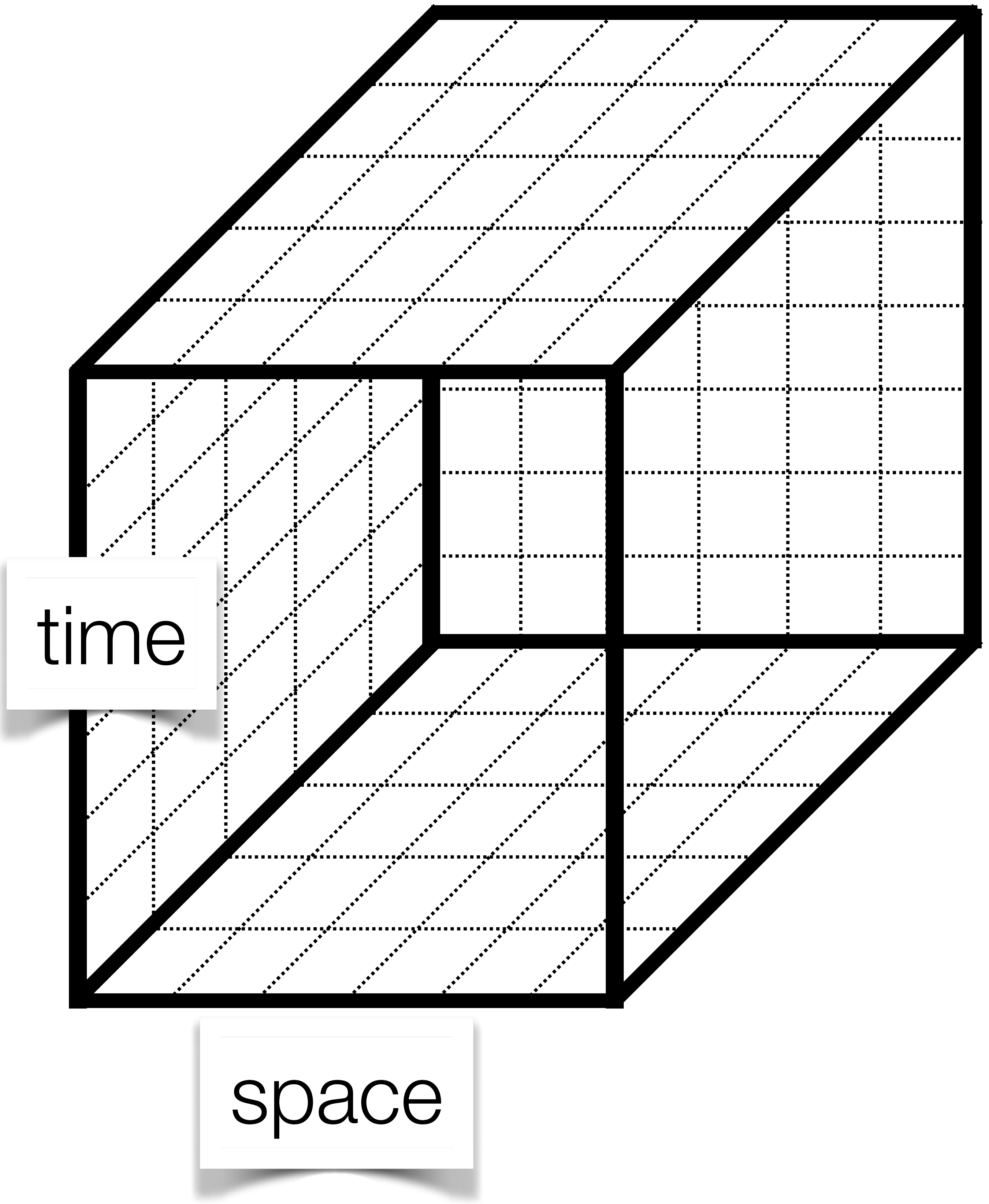

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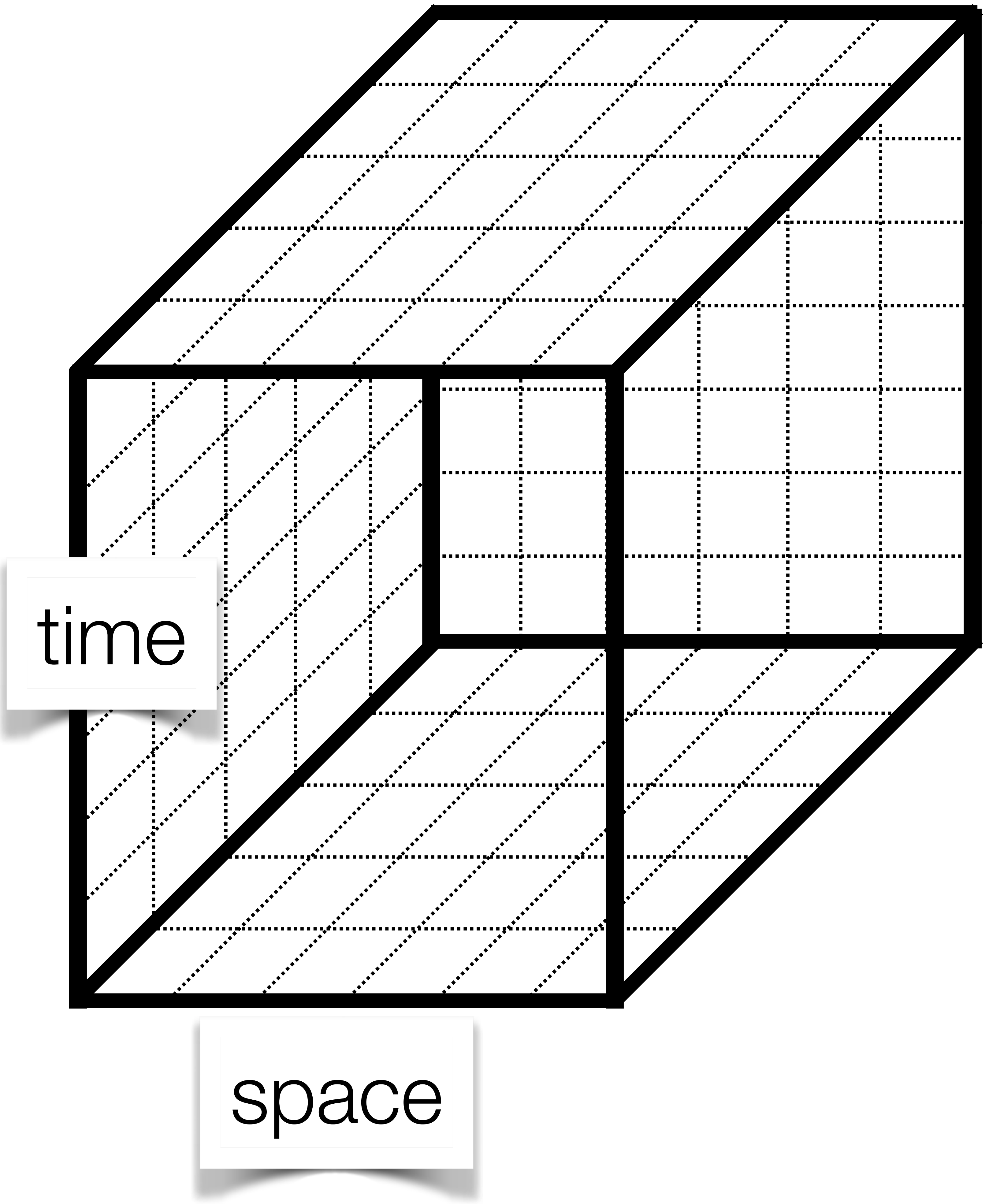

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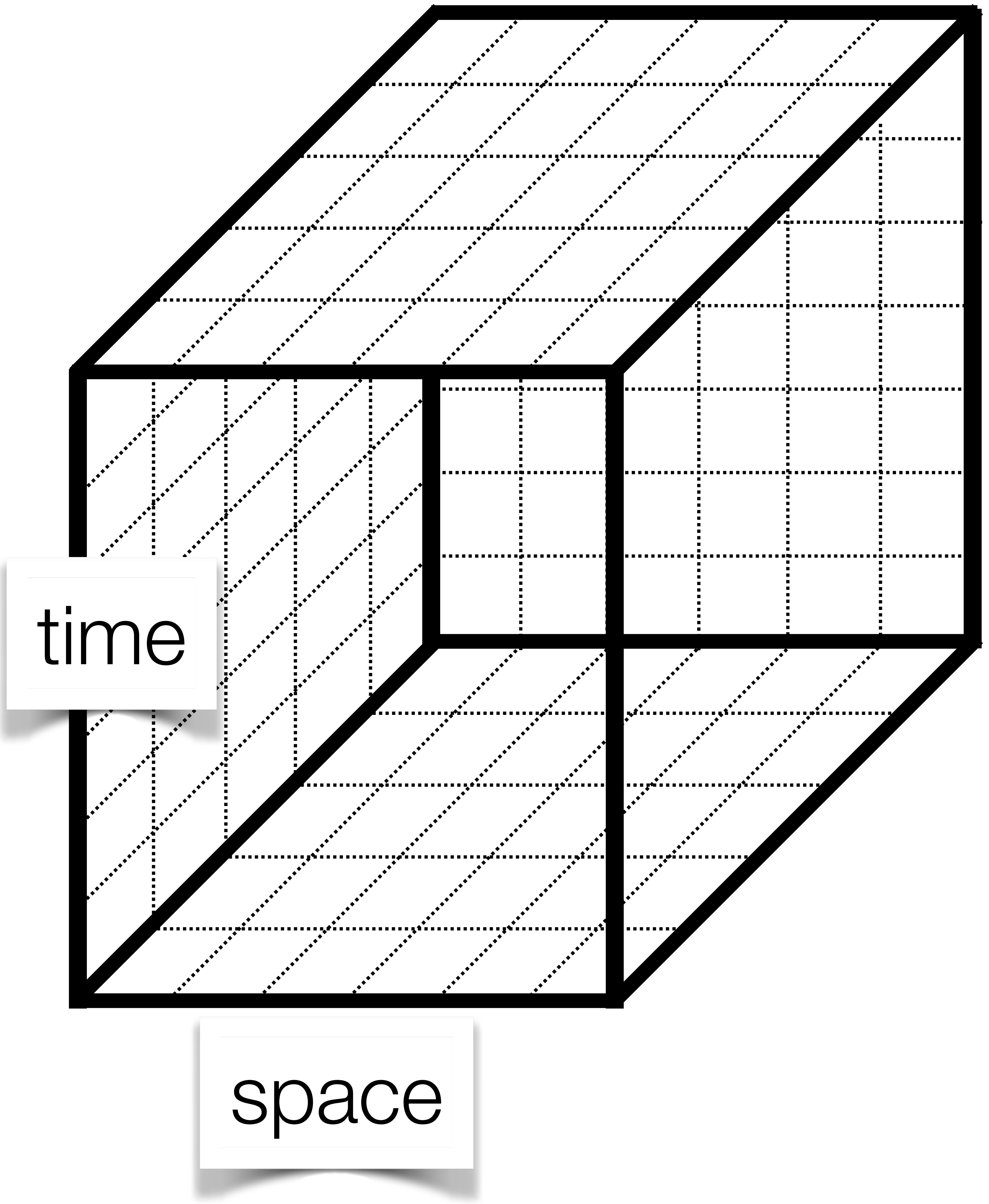

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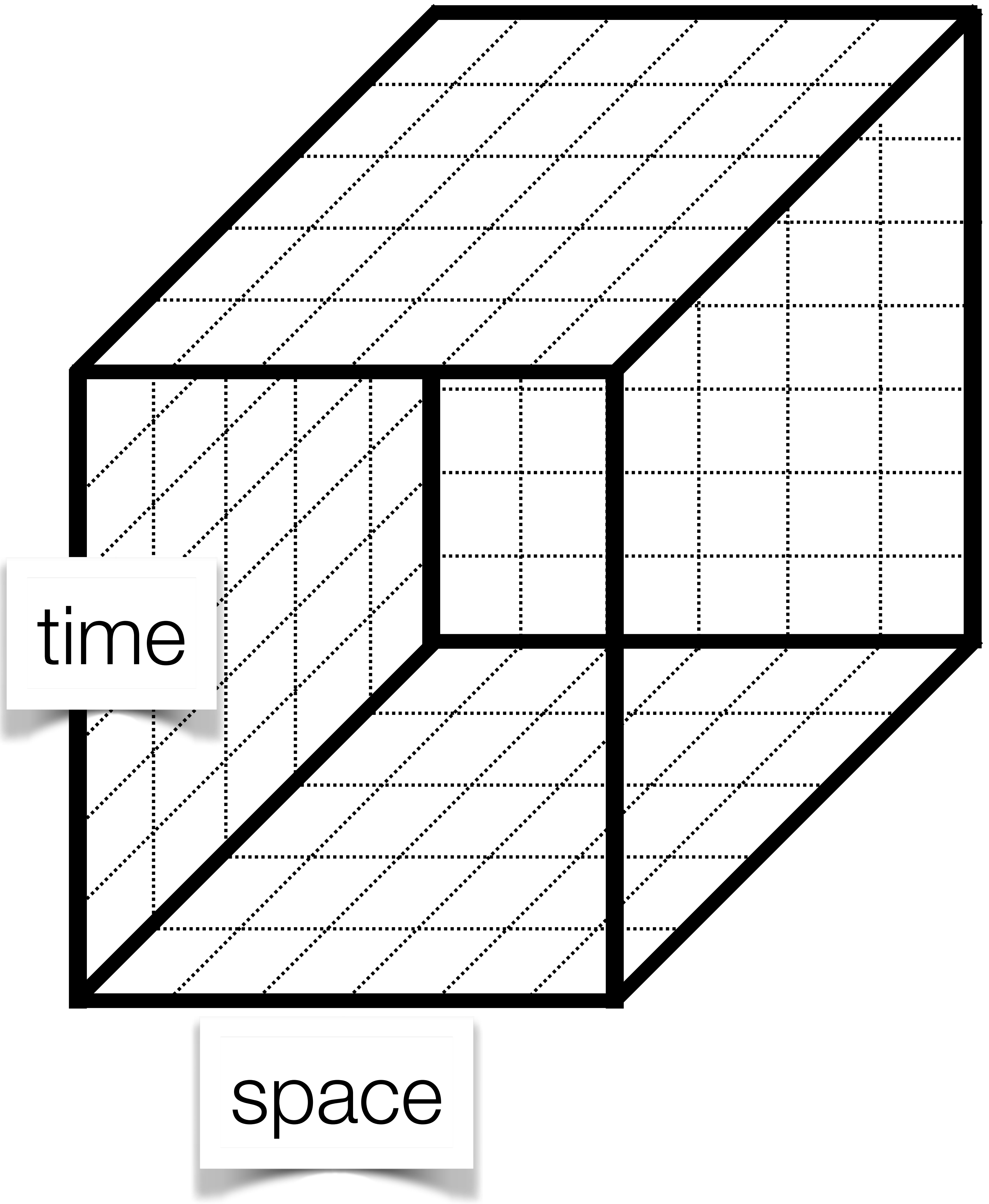

$$\{U_1, U_2, U_3, \ldots, U_N\}$$

Markov Chain Monte Carlo

Introduction to LQCD

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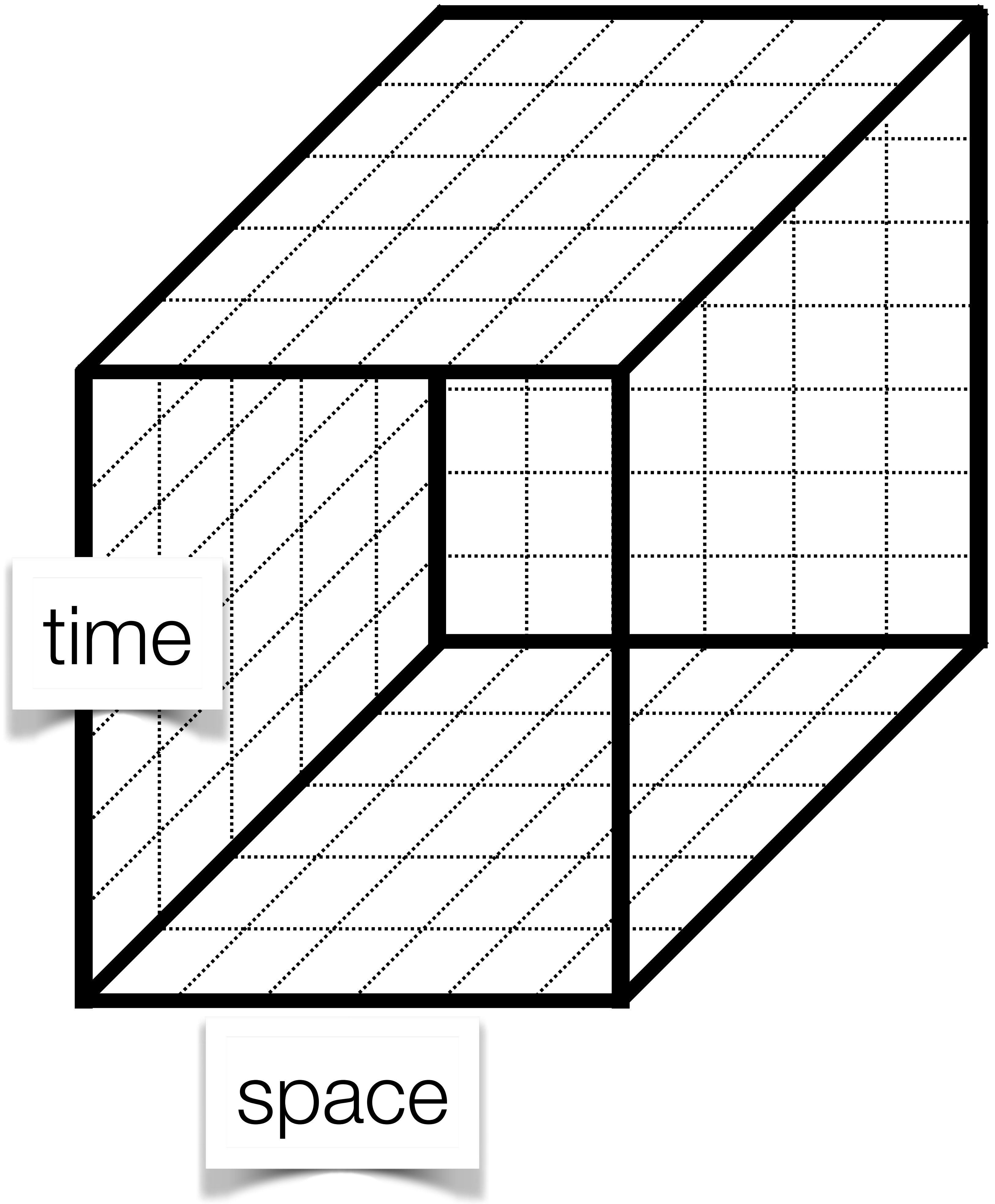

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Markov Chain Monte Carlo

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

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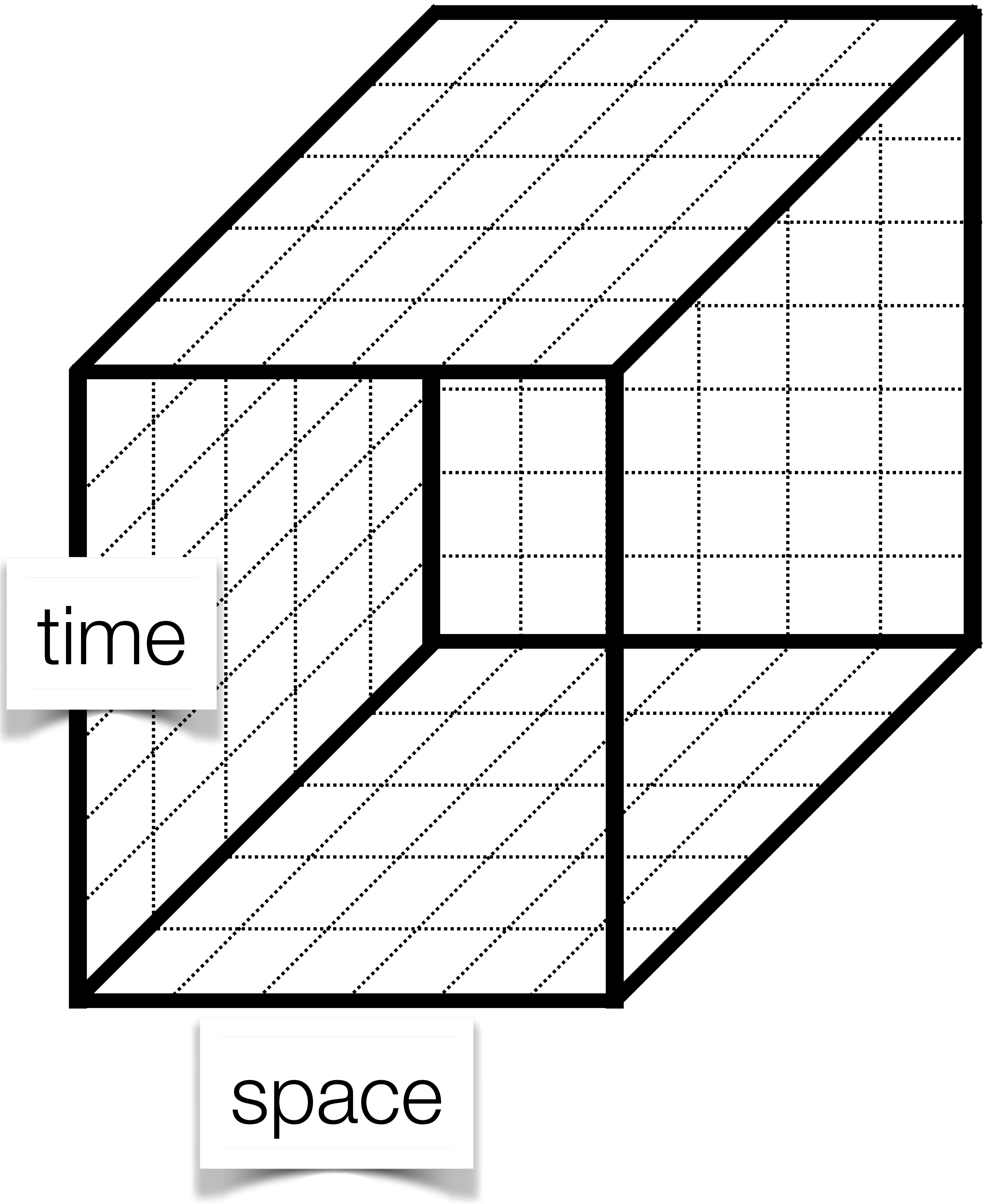
Introduction to LQCD



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Markov Chain Monte Carlo

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

Slide adapted from E. Berkowitz

Introduction to LQCD

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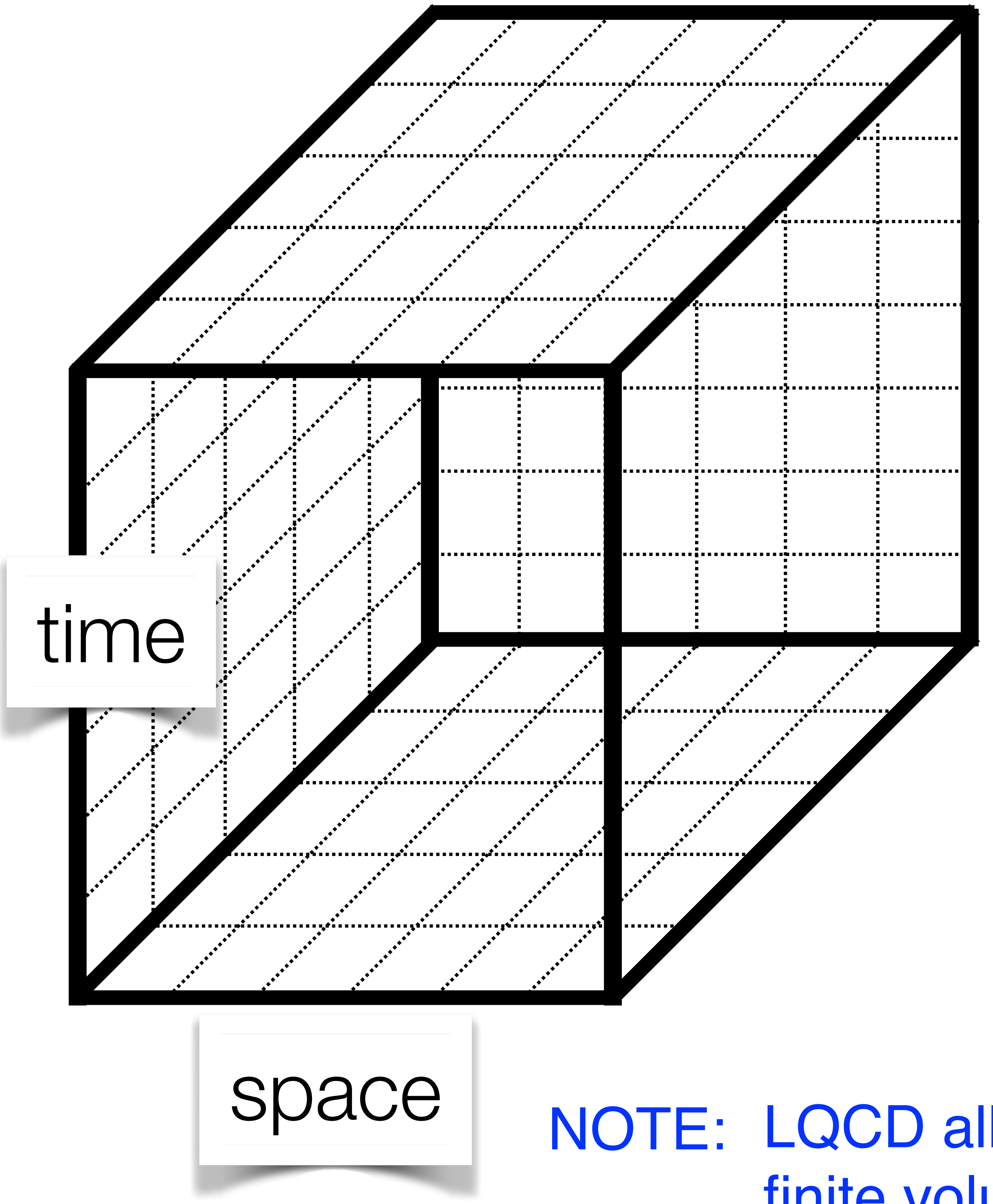

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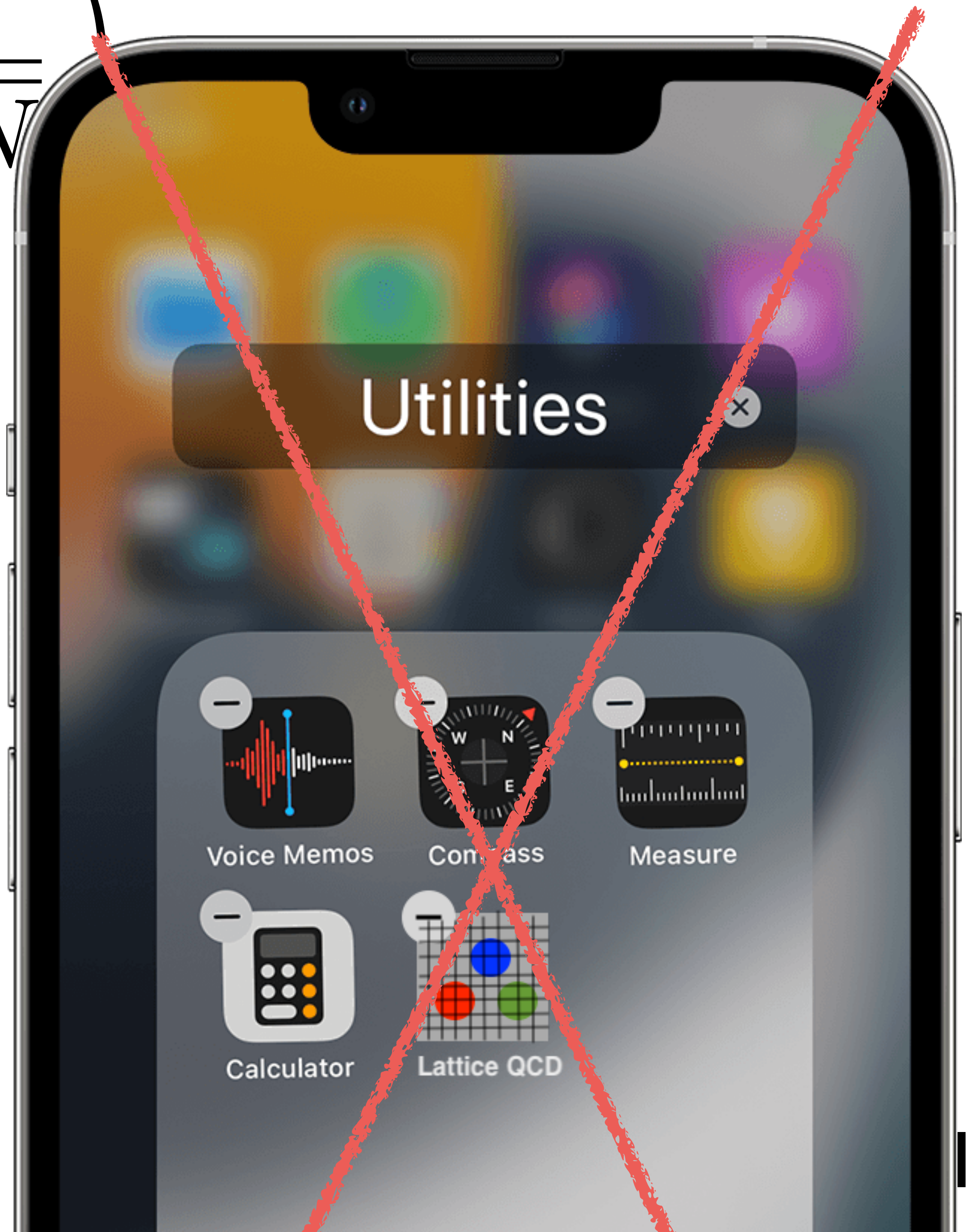
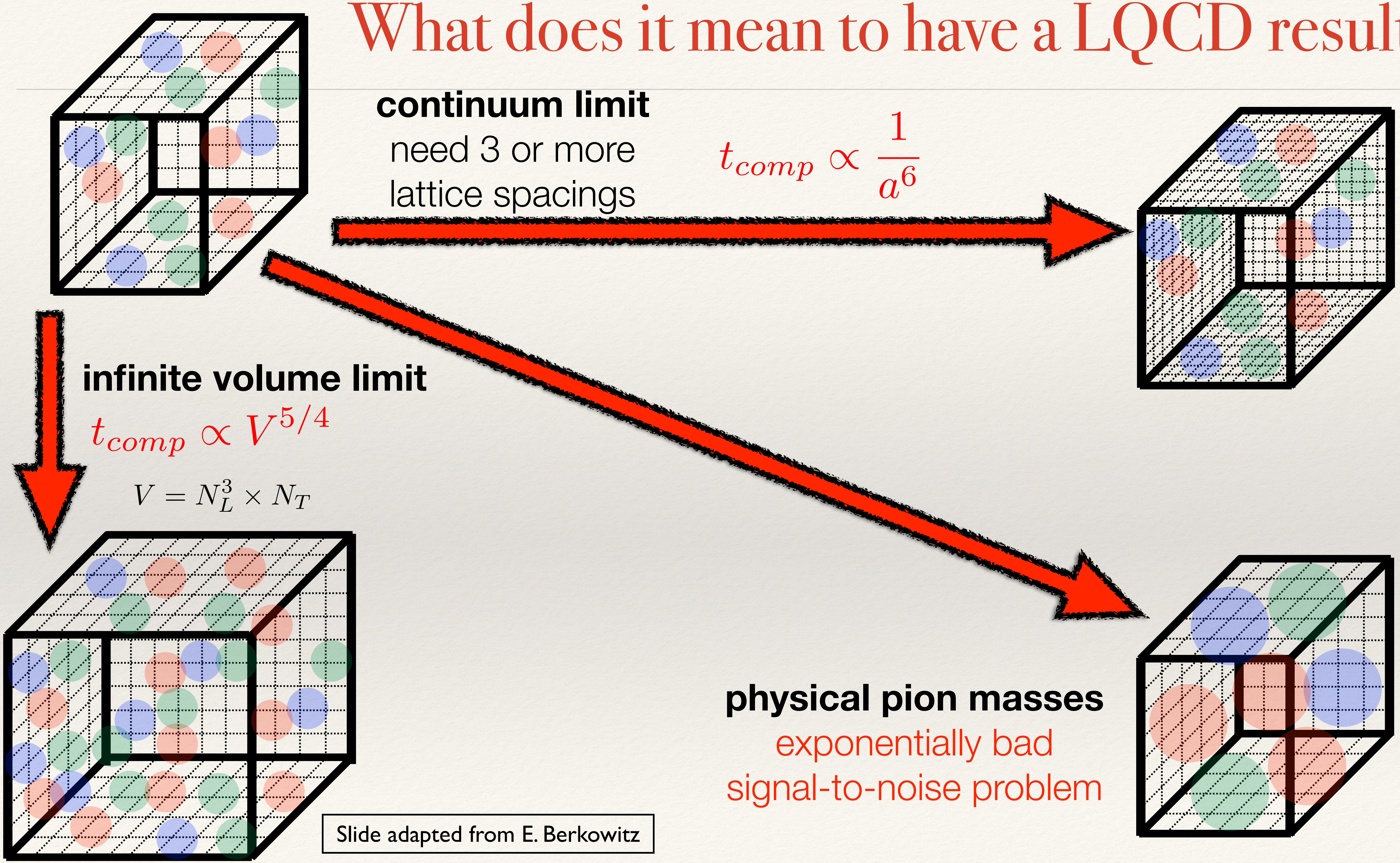


NOTE: LQCD allows us to compute Euclidean space, finite volume, correlation functions

Non-trivial numerical analysis (and sometimes formalism) to extract spectrum, matrix elements, form factors, …

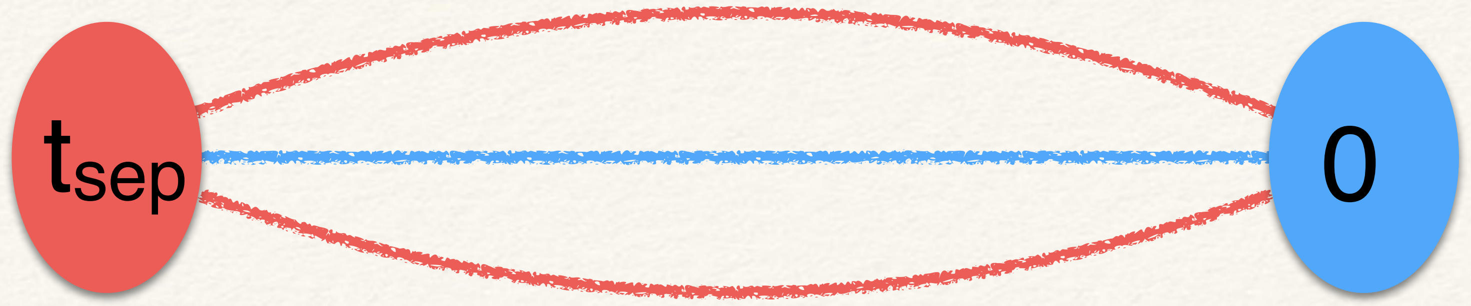
Slide adapted from E. Berkowitz

What does it mean to have a LQCD result?



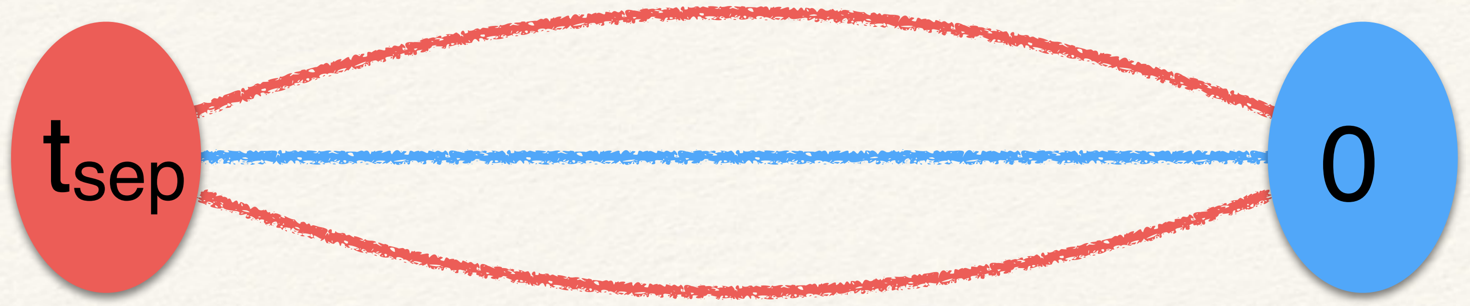
LQCD: 2 point functions

$$C(t, \mathbf{p}) = \sum_{\mathbf{x}} e^{-i\mathbf{p}\cdot\mathbf{x}} \langle \Omega | O(t, \mathbf{x}) O^\dagger(0, \mathbf{0}) | \Omega \rangle$$



$$\begin{aligned}
C(t) &= \sum_{\mathbf{x}} \langle \Omega | O(t, \mathbf{x}) O^\dagger(0, \mathbf{0}) | \Omega \rangle && \text{focus on 0-momentum} \\
&= \sum_{\mathbf{x}} \langle \Omega | e^{\hat{H}t} O(0, \mathbf{x}) e^{-\hat{H}t} O^\dagger(0, \mathbf{0}) | \Omega \rangle && \text{time-evolve operator} \\
&= \sum_n \sum_{\mathbf{x}} \langle \Omega | e^{\hat{H}t} O(0, \mathbf{x}) e^{-\hat{H}t} | n \rangle \langle n | O^\dagger(0, \mathbf{0}) | \Omega \rangle && \text{multiply by 1,} \quad 1 = \sum_n |n\rangle\langle n| \\
&= \sum_n e^{-E_n t} \sum_{\mathbf{x}} \langle \Omega | O(0, \mathbf{x}) | n \rangle \langle n | O^\dagger(0, \mathbf{0}) | \Omega \rangle && \text{define vacuum to have 0-energy} \\
&= \sum_n e^{-E_n(\mathbf{p}=0)t} \langle \Omega | O(0) | n, \mathbf{p} = 0 \rangle \langle n, \mathbf{p} = 0 | O^\dagger(0) | \Omega \rangle \\
&= \sum_n e^{-E_n t} z_n z_n^\dagger && \text{sum of exponentials}
\end{aligned}$$

LQCD: 2 point functions



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

$$= A_0 e^{-E_0 t} \left(1 + \sum_{n>0} r_n e^{-\Delta_{n0} t} \right)$$

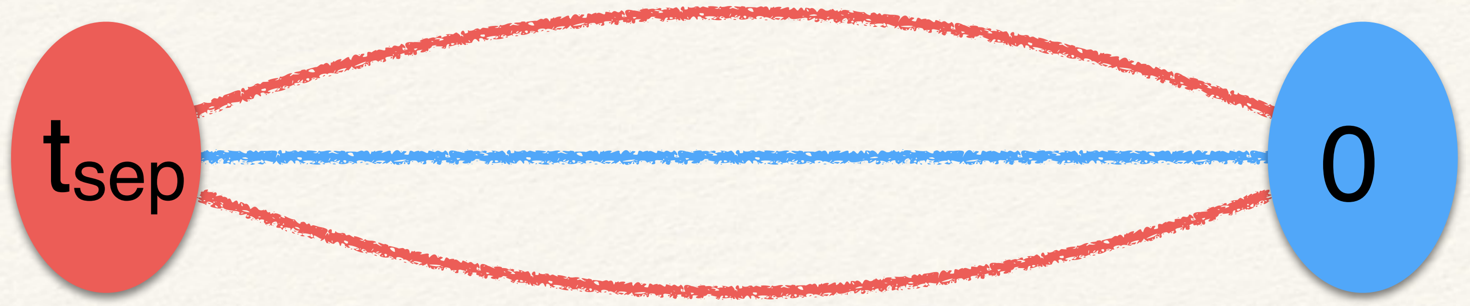
$$\Delta_{n0} = E_n - E_0$$

$$m_{\text{eff}}(t) = \ln \left(\frac{C(t)}{C(t+1)} \right) \underbrace{\longrightarrow}_{\text{large } t} E_0 + \sum_{n>0} r_n \left(e^{-\Delta_{n0} t} - e^{-\Delta_{n0} t + 1} \right)$$

NOTE: if the creation operator is conjugate to the annihilation operator

$$r_n \geq 0$$

LQCD: 2 point functions



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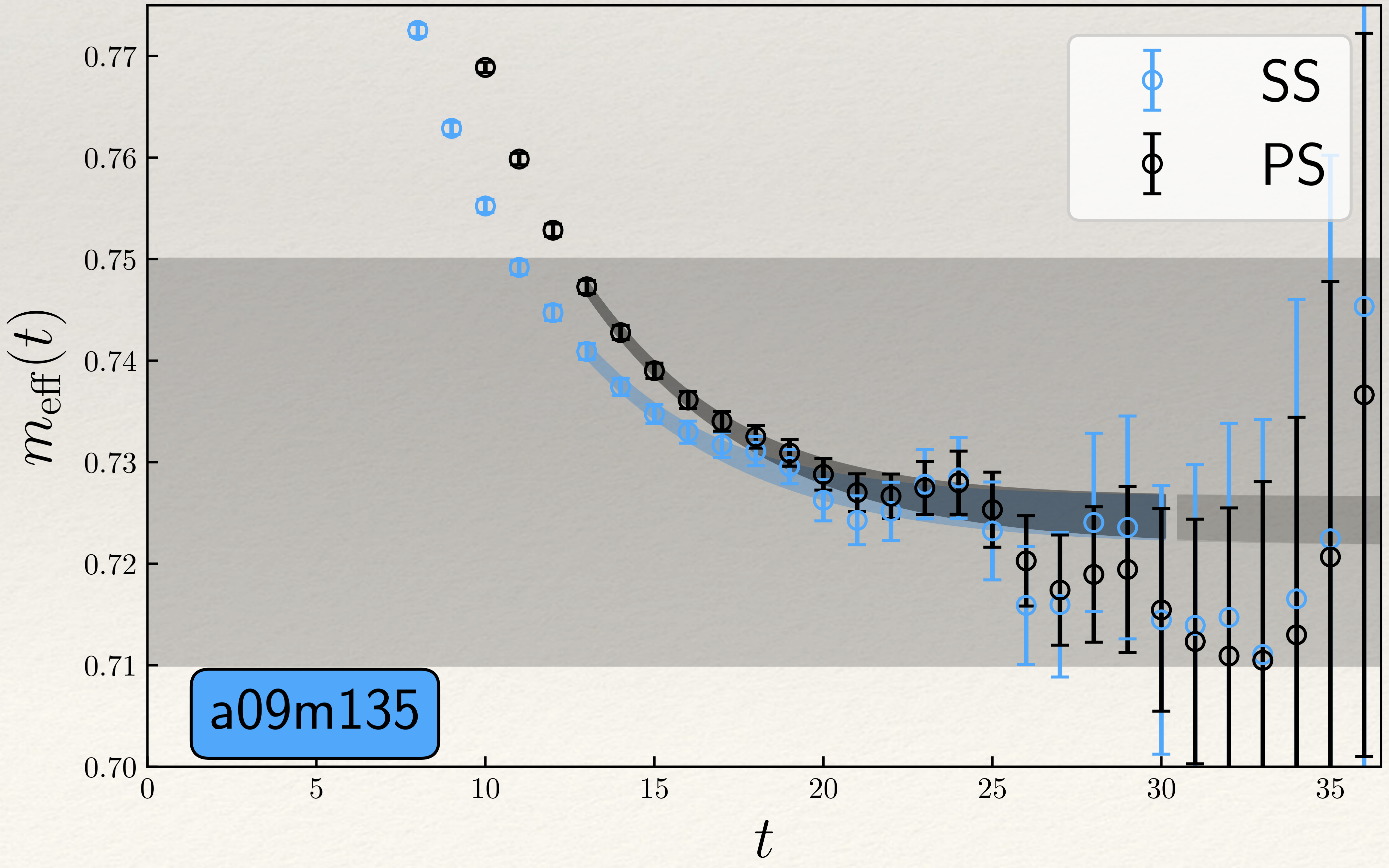
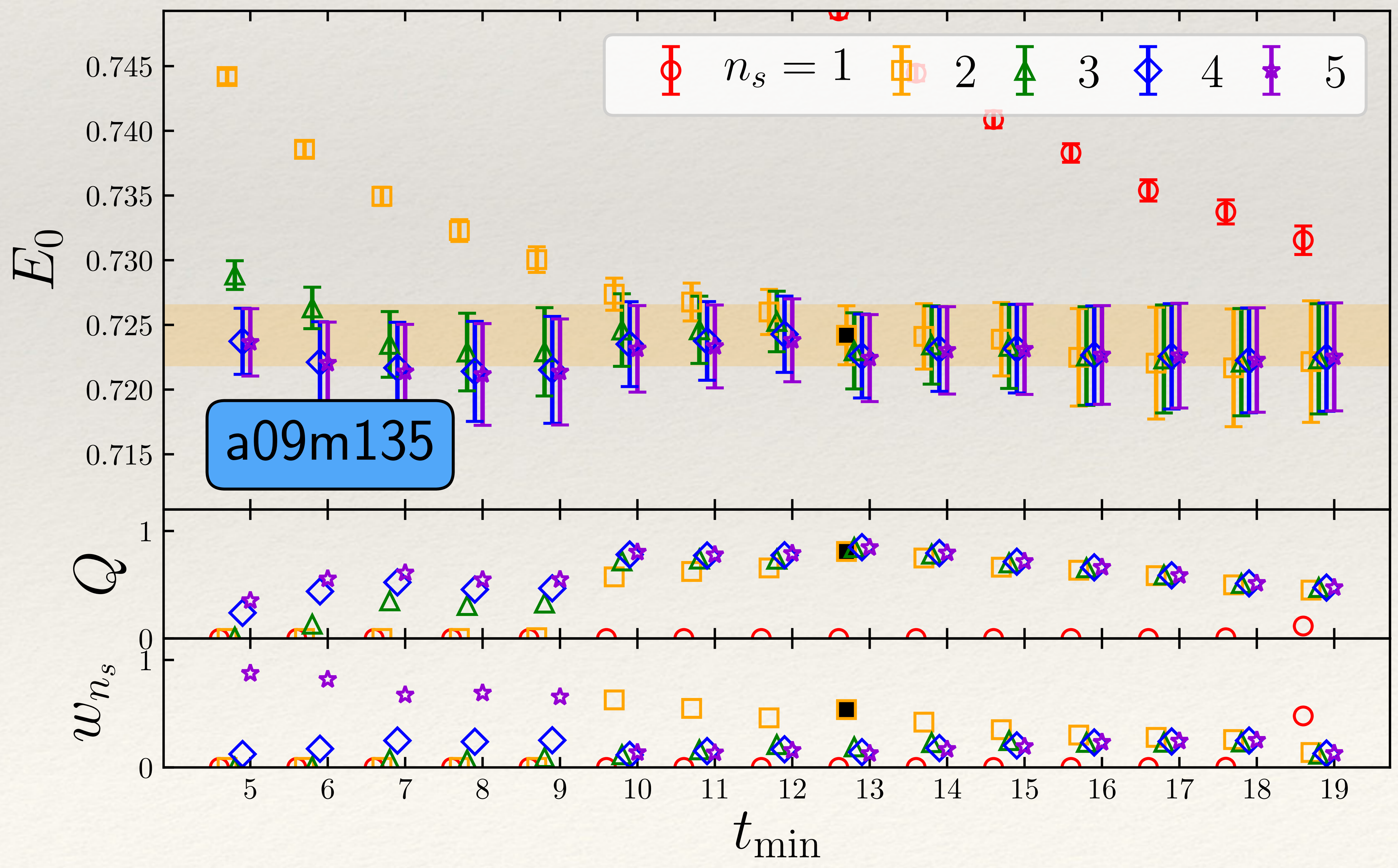
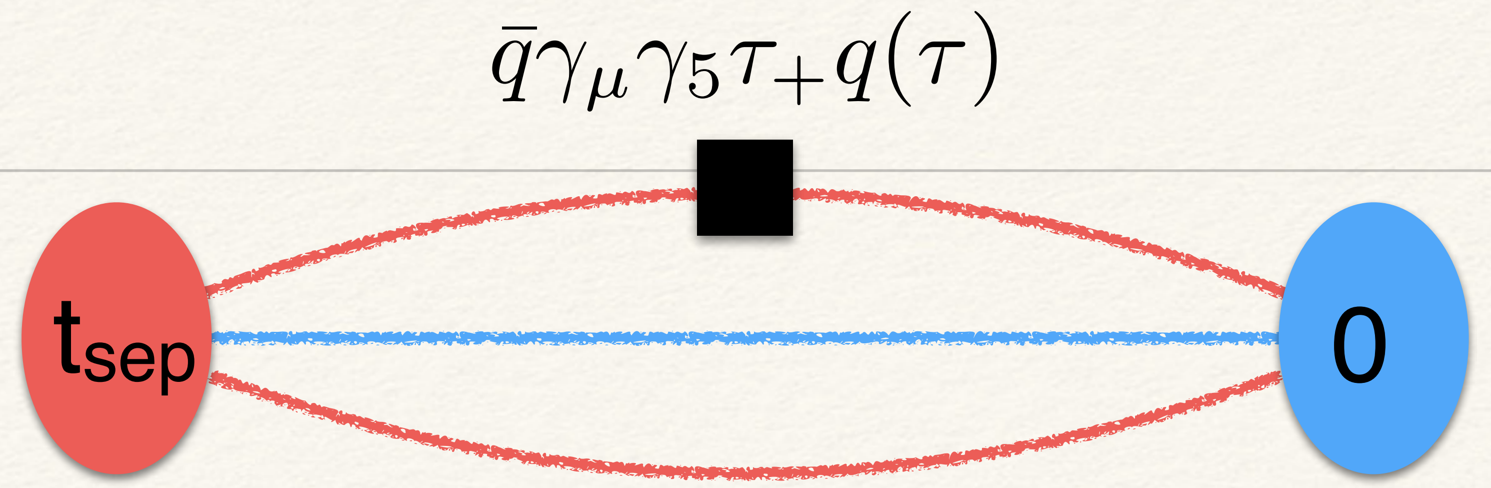
but… signal-to-noise - can not simply "wait till long time" to get ground state (g.s.)





LQCD: 3 point functions

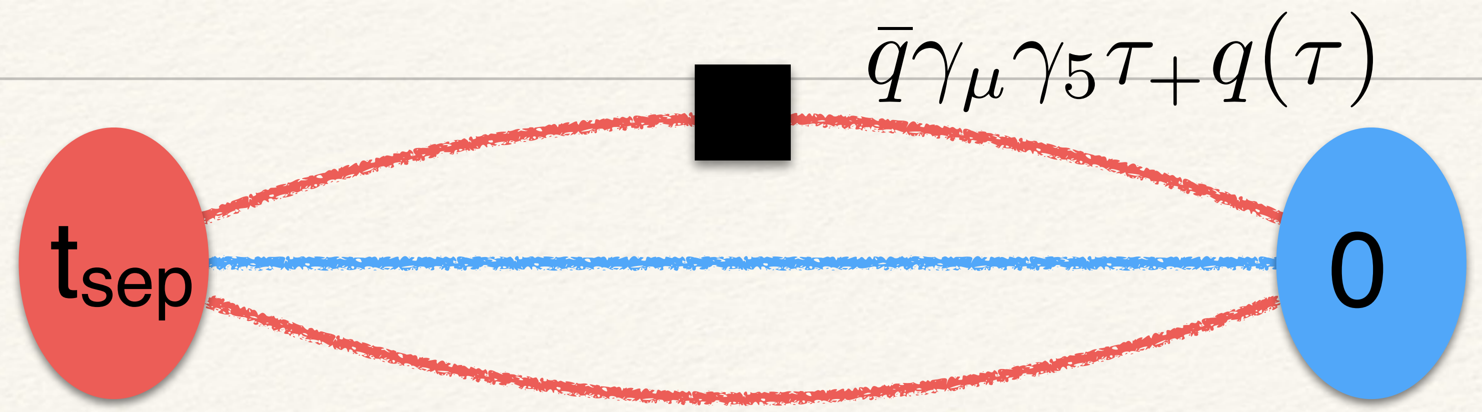


- The most common method (sub-optimal) to compute nucleon matrix elements
  - For a few values of t, compute the 3-point function for all τ

$$C_\Gamma(t,\tau,\mathbf{p},\mathbf{q}) = \sum_{\mathbf{y},\mathbf{x}} e^{-i\mathbf{p}\cdot\mathbf{y}} e^{i\mathbf{q}\cdot\mathbf{x}} \langle\Omega|N(t,\mathbf{y})j_\Gamma(\tau,\mathbf{x})N^\dagger(0,\mathbf{0})|\Omega\rangle$$

  - Each choice of t is a new, expensive computation
  - Ideally, t ~ 2 $t_{2pt\text{-}gs}$, but, S/N prevents that
  - The g.s. matrix-element/form-factor must be determined through an extrapolation in t and τ after numerical analysis

LQCD: 3 point functions



- Consider zero-momentum (p=0) and zero momentum transfer (q=0)

use "multiply by 1" trick

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

$$C_\Gamma(t,\tau) = \sum_{\mathbf{y},\mathbf{x}} \langle \Omega | N(t,\mathbf{y}) j_\Gamma(\tau,\mathbf{x}) N^\dagger(0,\mathbf{0}) | \Omega \rangle$$

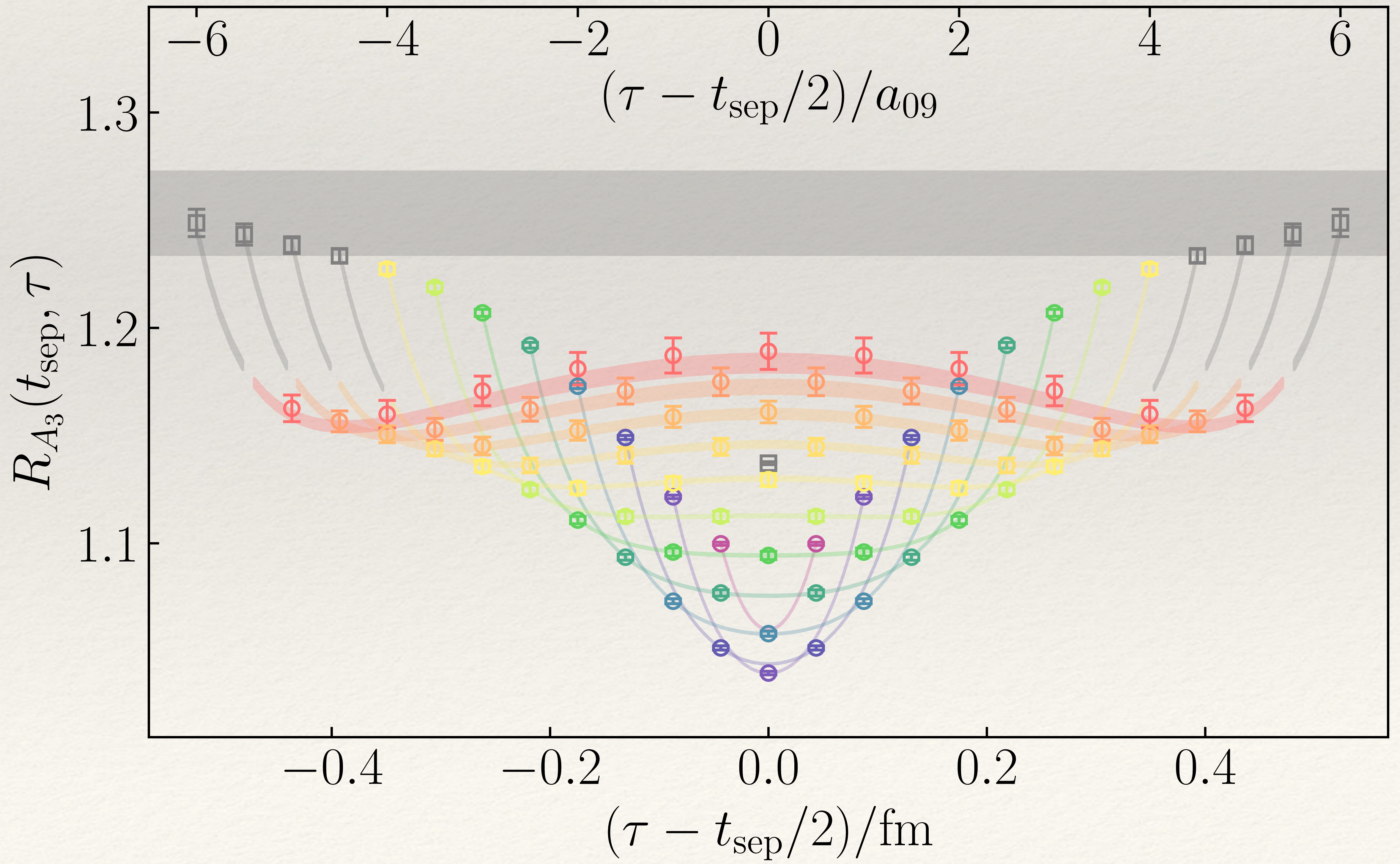
$$= |z_0|^2 g^\Gamma_{00} e^{-E_0 t} + \underbrace{\sum_{n>0} |z_n|^2 g^\Gamma_{nn} e^{-E_n t}}_{} + \underbrace{2\sum_{n<m} z_n z^\dagger_m g^\Gamma_{nm} e^{-(E_n + \frac{\Delta_{mn}}{2} t)} \cosh\left[\Delta_{mn}\left(\tau - \frac{t}{2}\right)\right]}_{}$$

"scattering" (sc) excited states

"transition" (tr) excited states

- scattering excited states only depend on t
- transition excited states depend on t and τ

- NOTE: for intermediate t, there is a conspiracy of excited states that give the appearance of no excited state contamination



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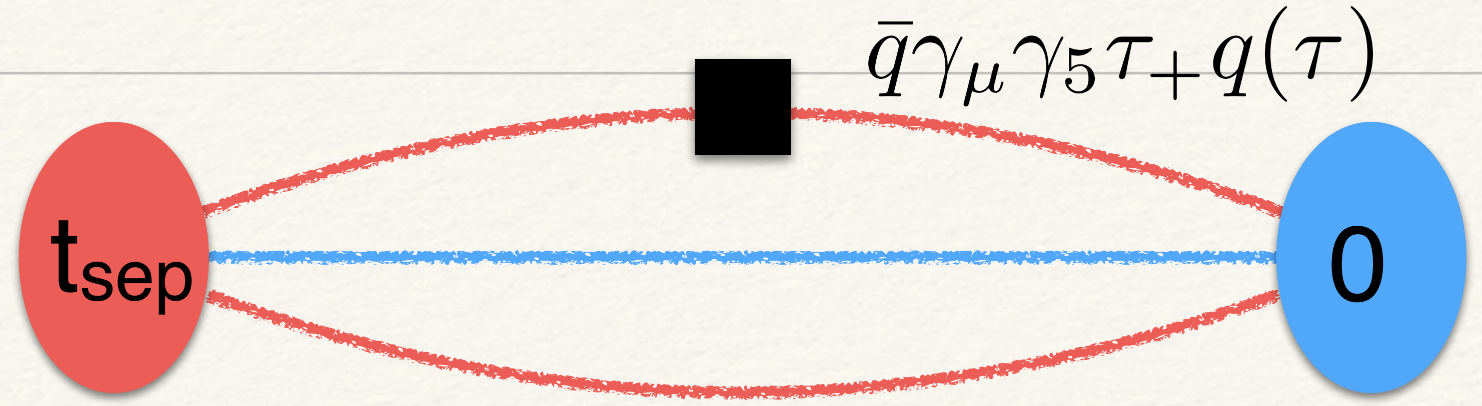
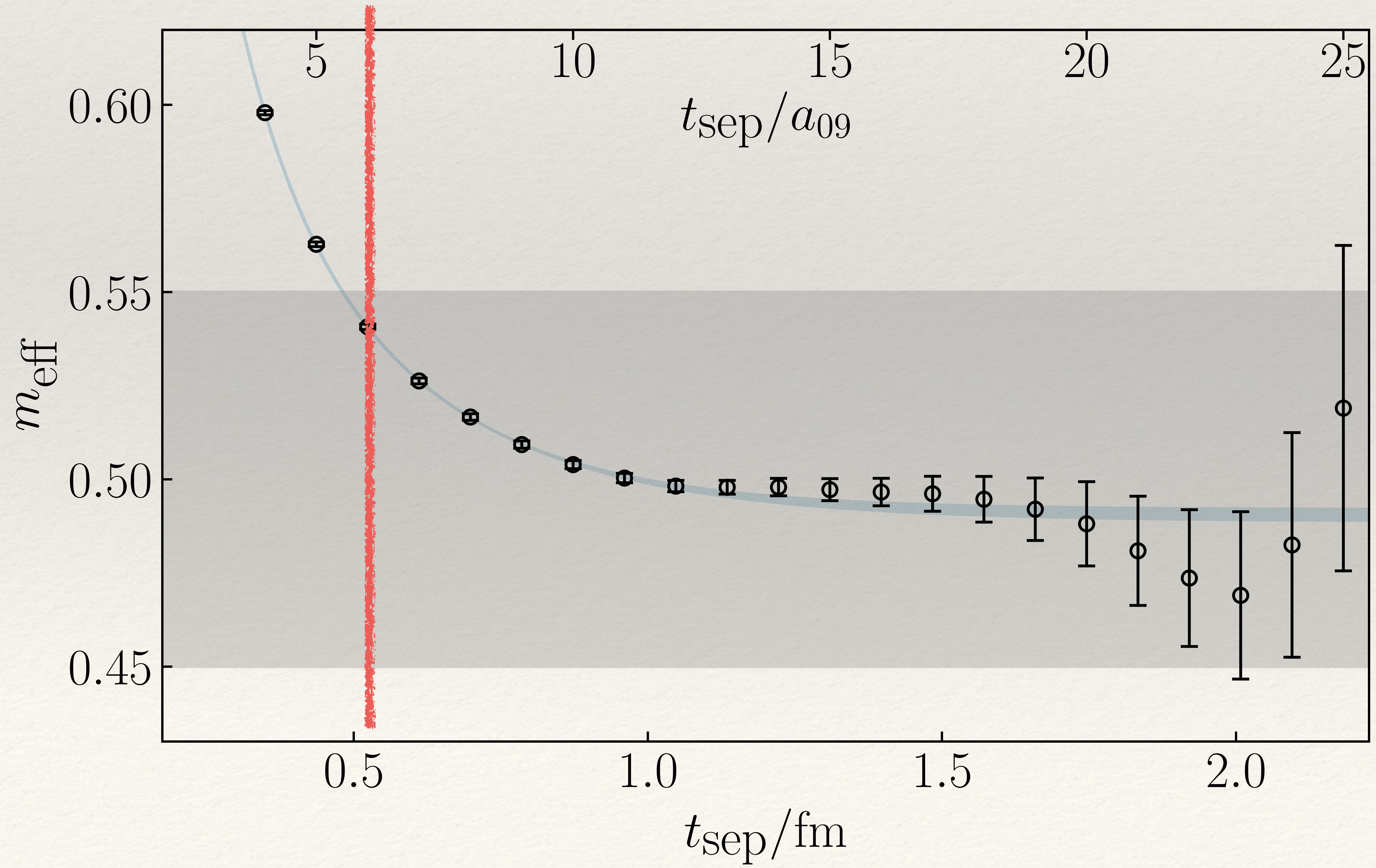
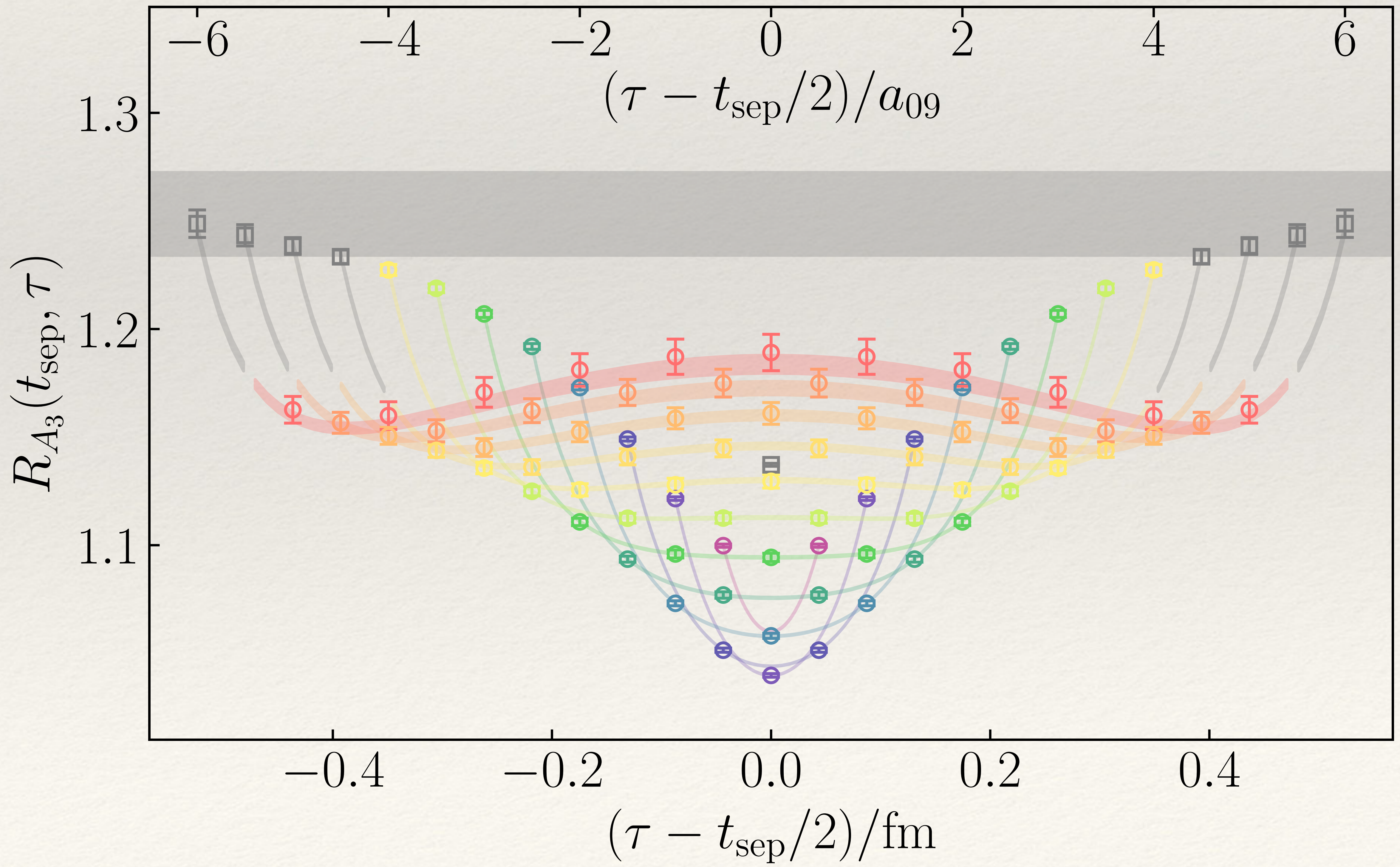


- Consider zero-momentum (p=0) and zero momentum transfer (q=0)
- NOTE: 2pt at t=6 (similar to 3pt with t=12, τ=6) has significant excited state contamination





LQCD: Feynman-Hellmann Method

Bouchard, Chang, Kurth, Orginos, WL
PRD 96 (2017) [arXiv:1612.06963]

$$C(t) = \langle\Omega|O(t)O^\dagger(0)|\Omega\rangle = \frac{1}{Z}\int D\Phi e^{-S_G - \int d^4x \bar{\psi}_q[D+m_q]\psi_q} O(t)O(0)$$

$$-\partial_{m_q} C(t) = \frac{1}{Z}\int D\Phi e^{-S_G - \int d^4x \bar{\psi}_q[D+m_q]\psi_q} O(t)\int d^4z \bar{\psi}_q(z)\psi_q(z)O(0) - C(t)\int d^4z \langle\Omega|\bar{\psi}_q(z)\psi_q(z)|\Omega\rangle$$

$$= \int d^4z \langle\Omega|O(t)\bar{\psi}_q(z)\psi_q(z)O^\dagger(0)|\Omega\rangle + \text{terms to subtract vacuum bubbles}$$

Feynman-Hellmann Theorem
relate spectrum to matrix elements $\quad \partial_\lambda E_n = \langle n|H_\lambda|n\rangle$

in QFT - differentiate effective mass?

$$\partial_{m_q} m_{\text{eff}}(t) = \partial_{m_q}\ln\left(\frac{C(t)}{C(t+1)}\right) = \frac{-\partial_{m_q}C(t+1)}{C(t+1)} - \frac{-\partial_{m_q}C(t)}{C(t)} = \langle N|\bar{q}q|N\rangle + \text{ excited states}$$

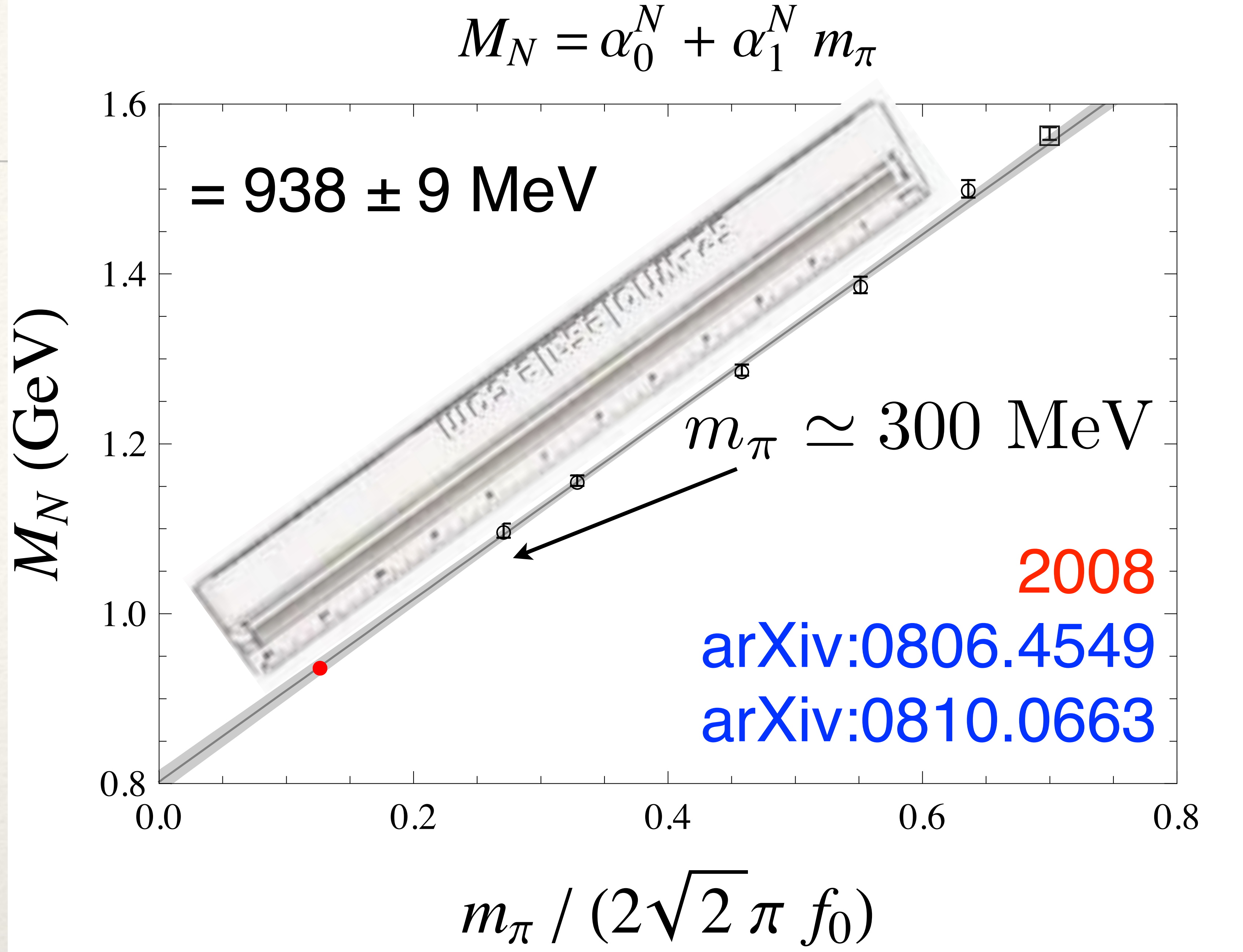
LQCD: Feynman-Hellmann Method

Study nucleon mass versus quark mass to extract light-quark matrix elements

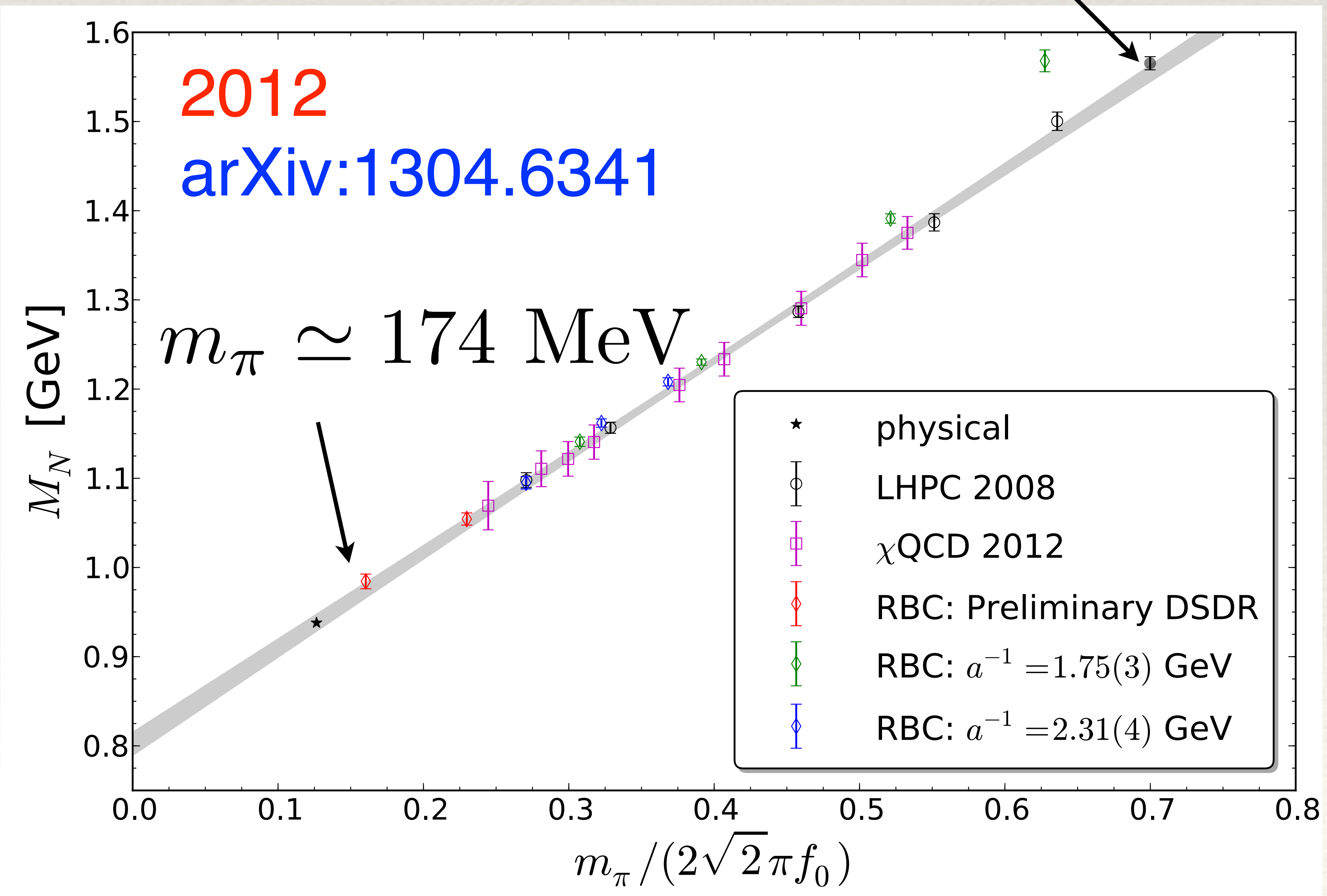
Heavy Baryon XPT: $$M_N = M_0 - 4\bar{c}_1 \frac{M_\pi^2}{4\pi F} - \frac{3\pi g_A^2}{2}\frac{M_\pi^3}{(4\pi F)^2} + \cdots$$

Convergence issues

- NLO predicts a large, negative correction
- M_N increases monotonically with increasing quark/pion mass
- Must include at least NNLO - but also - warning of large cancellations between orders (not healthy for EFT expansion)
- Ignore this issue and proceed (hope convergence is OK for light-enough pion mass)
- Need to convert pion mass dependence to quark-mass dependence will come back to this point



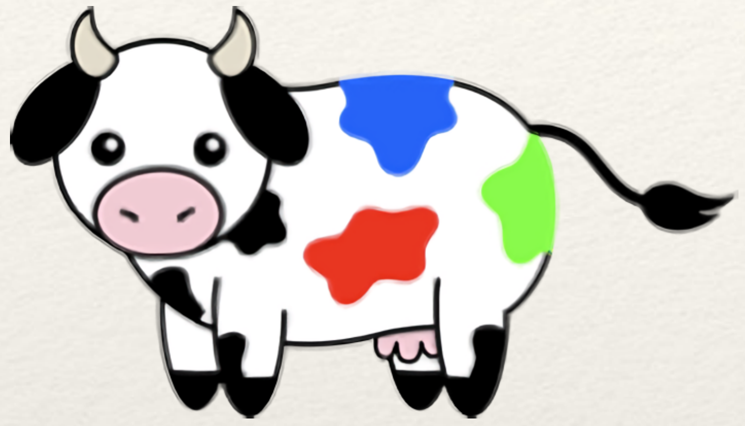
$m_\pi \simeq 758$ MeV



LQCD: Our Results - When and Where and what action

Möbius Domain Wall Fermions on rooted HISQ sea

HISQ ensembles from MILC and CalLat Collaborations

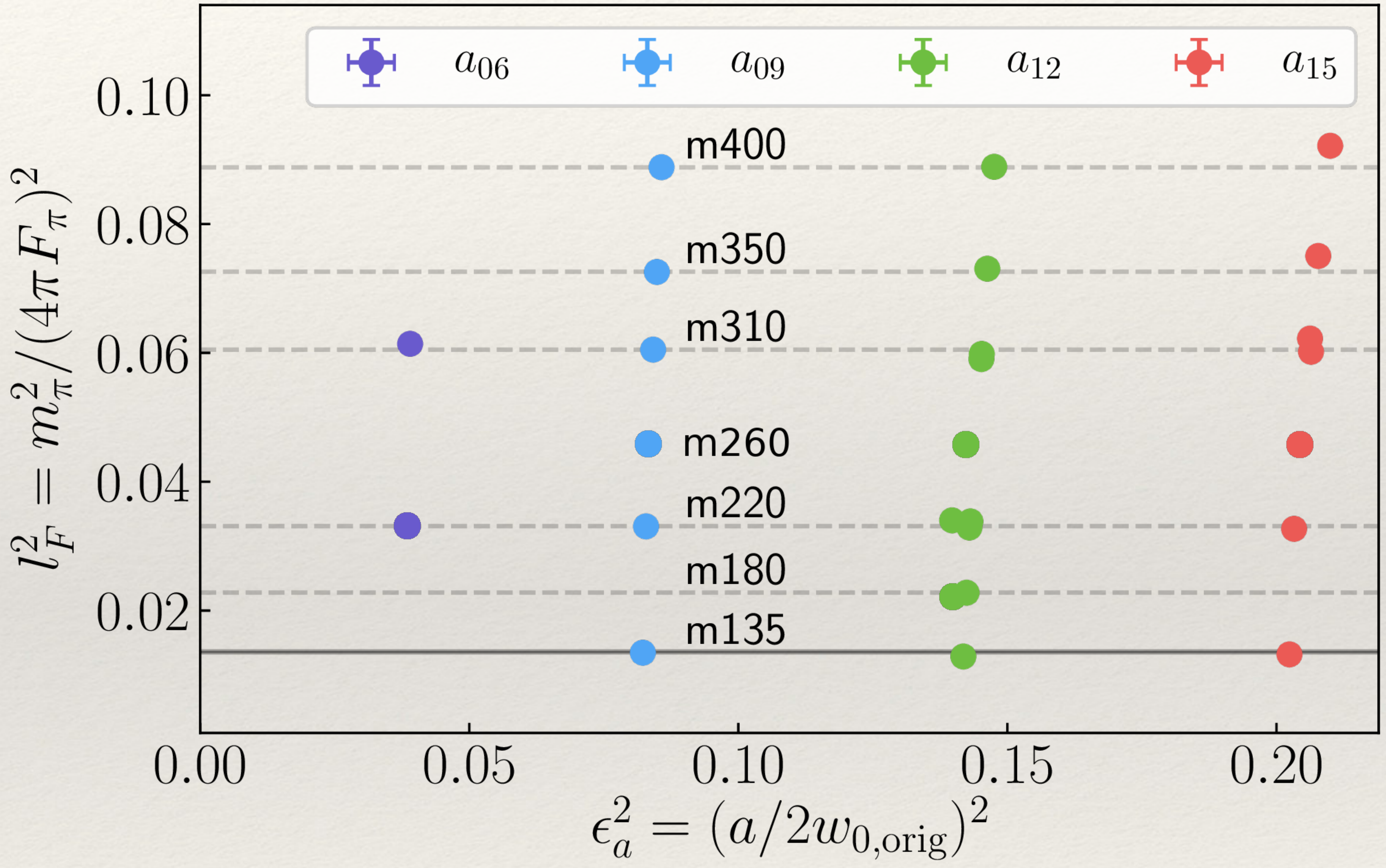


MDWF quarks efficiently solved with QUDA on NVIDIA GPU machines from 2016 — present

Lassen @ LLNL
Grand Challenge

Summit @ OLCF
DOE INCITE

Parameter space in pion mass and lattice spacing



LQCD: Our Results – How to extrapolate to physical point?

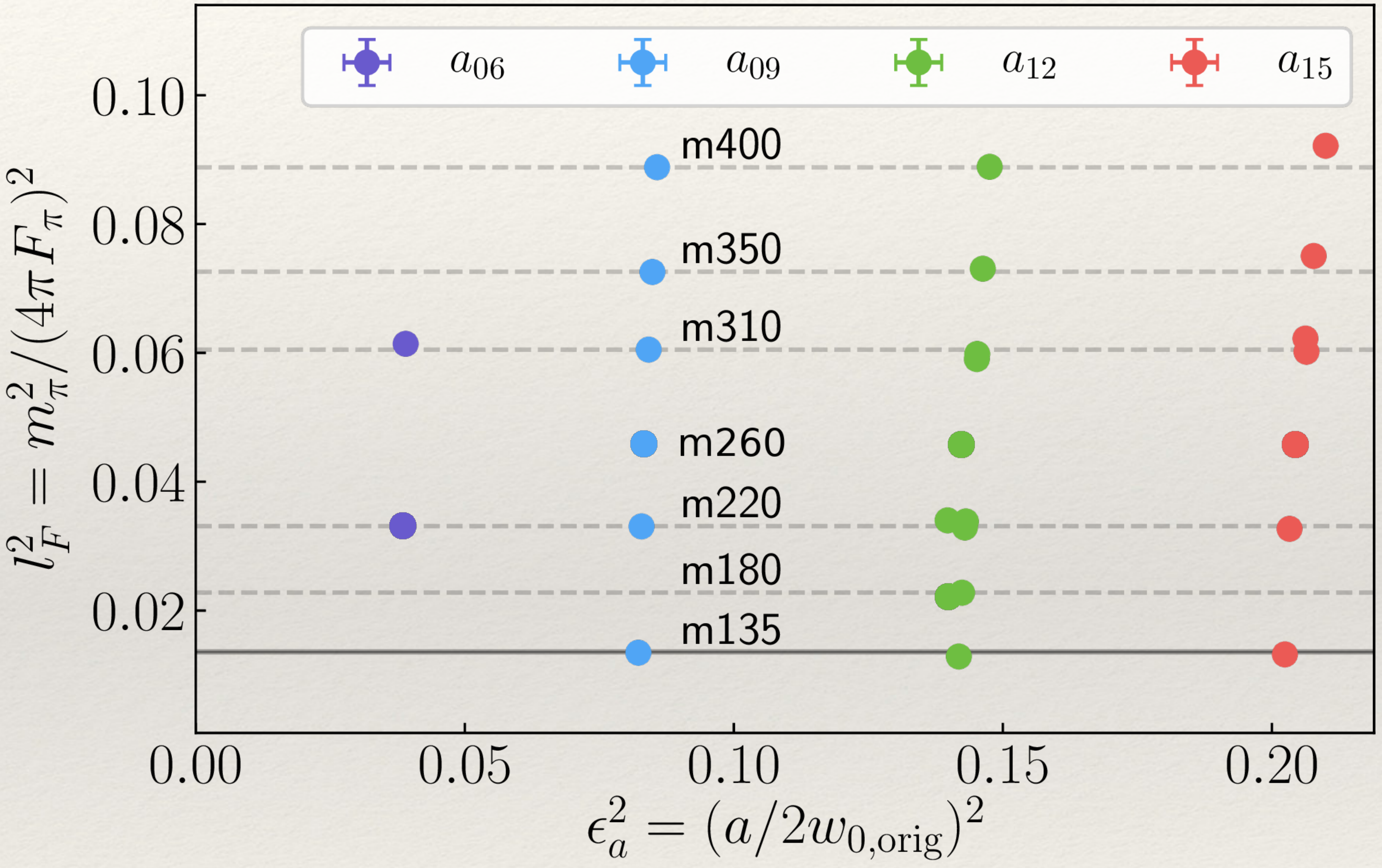
Consider 3 options

- ❑ $M_N(m_q)$
- ❑ $M_N(M_\pi)$
- ❑ $M_N(\varepsilon_\pi)$ / $(4\pi F_\pi)$

There are challenges with each choice.

- ❑ The first 2 require scale setting
- ❑ m_q expansion
  - ❑ bare parameter expansion often converge slower
  - ❑ requires renormalization
- ❑ The second method requires ∂M_π to ∂m_q conversion
- ❑ The last method requires knowledge of $\partial F_\pi/\partial m_q$

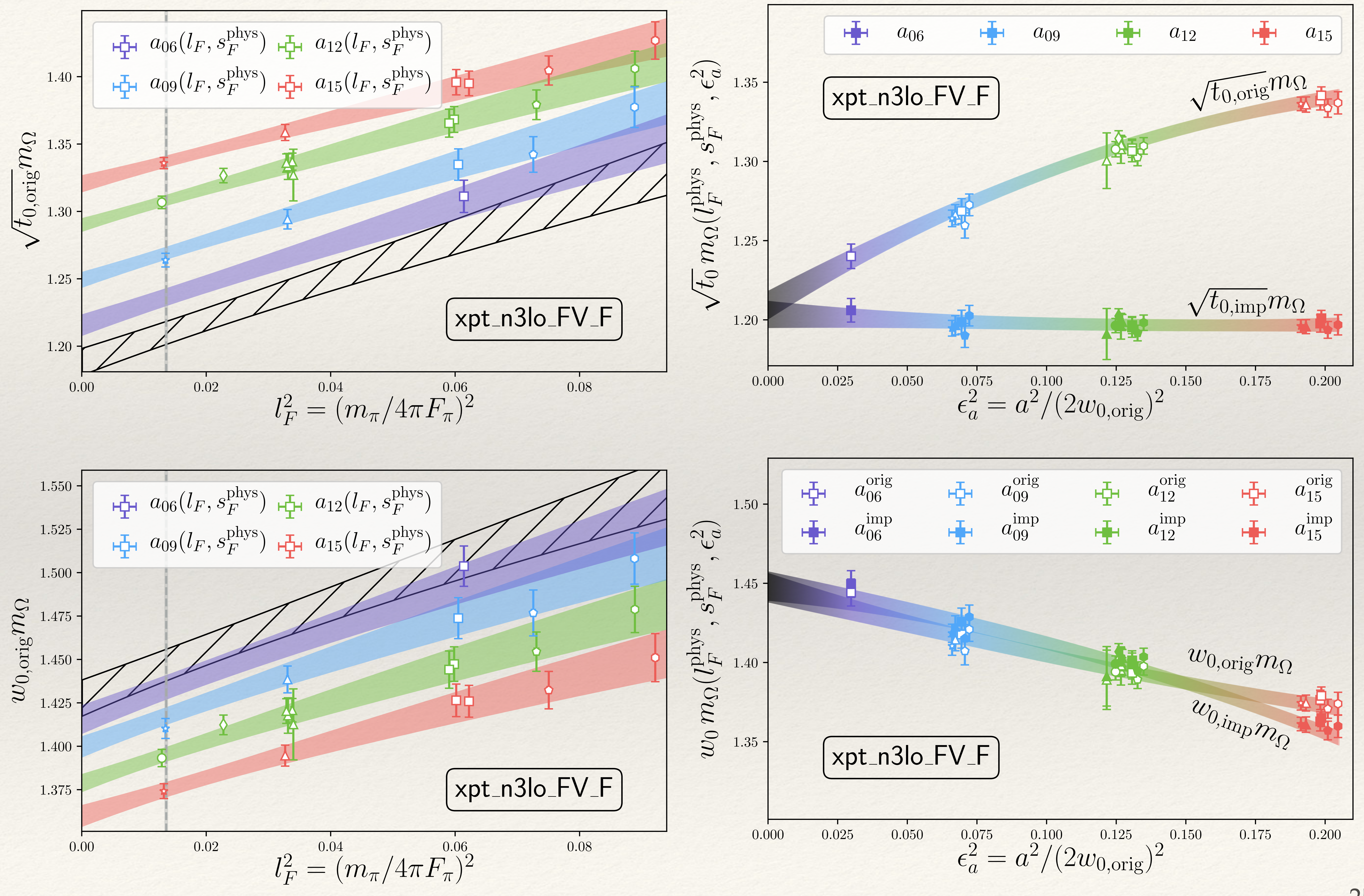
Parameter space in pion mass and lattice spacing



LQCD: Our Results – How to extrapolate to physical point?

Scale Setting: 2011.12166

- Precise scale setting is possible (sub-percent)
- Scale setting induces correlation among all ensembles
- Scale-setting uncertainty can often be dominant for hadron spectrum
- Subsequent extrapolations in MeV can become complicated from the correlation
- Alternatively: form dimensionless ratios and extrapolate $\dfrac{M_N}{4\pi F_\pi}$



LQCD: Our Results – How to extrapolate to physical point?

Extrapolation Options

$$M_N(m_q) = M_0 - \frac{4\bar{c}_1 2B\hat{m}}{4\pi F} - \frac{3\pi g_A^2 (2B\hat{m})^{3/2}}{2(4\pi F)^2} + \cdots$$

$$\begin{aligned} M_N(M_\pi) &= M_0 - \frac{4\bar{c}_1 M_\pi^2}{4\pi F_\pi} - \frac{3\pi g_A^2 M_\pi^3}{2(4\pi F_\pi)^2} + \cdots \\ &= M_0 - (4\pi F_\pi)\frac{4\bar{c}_1 M_\pi^2}{(4\pi F_\pi)^2} - (4\pi F_\pi)\frac{3\pi g_A^2 M_\pi^3}{2(4\pi F_\pi)^3} + \cdots \end{aligned}$$

$$\frac{M_N(\epsilon_\pi)}{4\pi F_\pi} = \frac{M_0}{4\pi F_\pi} - 4\bar{c}_1 \epsilon_\pi^2 - \frac{3\pi g_A^2}{2}\epsilon_\pi^3 + \cdots$$

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

In principle, all methods should yield the same result

Discrepancies are an additional systematic uncertainty we must add to the result (if we are honest)

We are in the process of performing these three analysis methods

LQCD: Our Results – How to extrapolate to physical point?

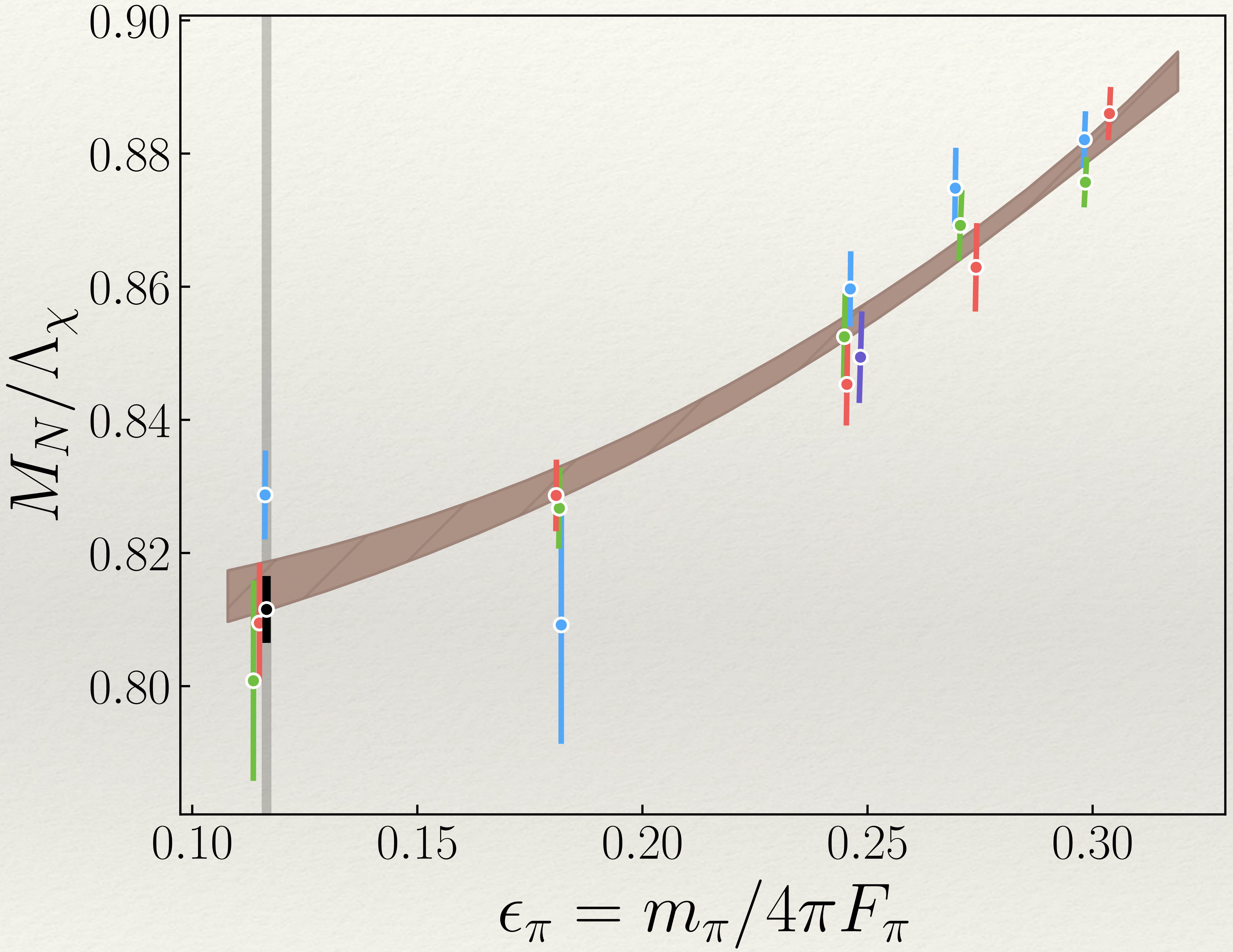
Use XPT to related quark mass derivative to derivative in M_π or ε_π

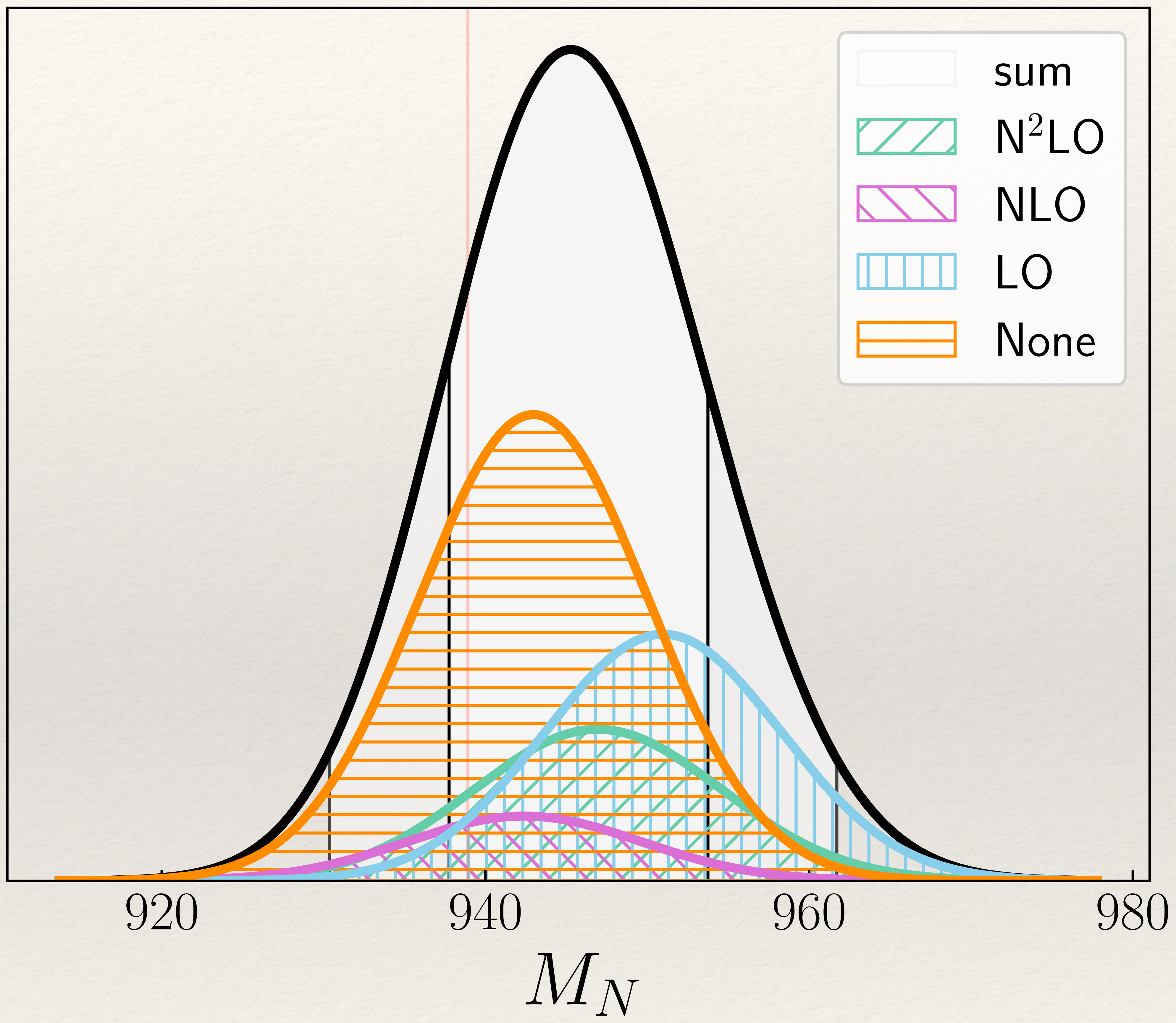
$$
\begin{aligned}
\hat{m}\partial_{\hat{m}} &= \hat{m}\frac{\partial\epsilon_\pi}{\partial_{\hat{m}}}\partial_{\epsilon_\pi} \\
&= \hat{m}\left(\frac{\partial}{\partial_{\hat{m}}}\frac{\sqrt{m_\pi^2}}{4\pi F_\pi}\right)\partial_{\epsilon_\pi} \\
&= \left(\frac{\hat{m}\partial_{\hat{m}}m_\pi^2}{2m_\pi 4\pi F_\pi} - \frac{m_\pi}{4\pi F_\pi}\frac{\hat{m}\partial_{\hat{m}}F_\pi}{F_\pi}\right)\partial_{\epsilon_\pi} \\
&= \left(\frac{\hat{m}\partial_{\hat{m}}m_\pi^2}{m_\pi^2} - 2\frac{\hat{m}\partial_{\hat{m}}F_\pi}{F_\pi}\right)\frac{\epsilon_\pi}{2}\partial_{\epsilon_\pi}\,.
\end{aligned}
$$

$$
\begin{aligned}
\hat{m}\partial_{\hat{m}}M_N &= \Lambda_\chi\hat{m}\partial_{\hat{m}}\left(\frac{M_N}{\Lambda_\chi}\right) + \frac{M_N}{\Lambda_\chi}\hat{m}\partial_{\hat{m}}\Lambda_\chi \\
&= \left(\frac{\hat{m}\partial_{\hat{m}}m_\pi^2}{m_\pi^2} - 2\frac{\hat{m}\partial_{\hat{m}}F_\pi}{F_\pi}\right)\frac{\epsilon_\pi}{2}\left[\Lambda_\chi\partial_{\epsilon_\pi}\left(\frac{M_N}{\Lambda_\chi}\right) + M_N\frac{\partial_{\epsilon_\pi}\Lambda_\chi}{\Lambda_\chi}\right]
\end{aligned}
$$

LQCD: Our Results – How to extrapolate to physical point?

Consistent with PDG at 1-sigma



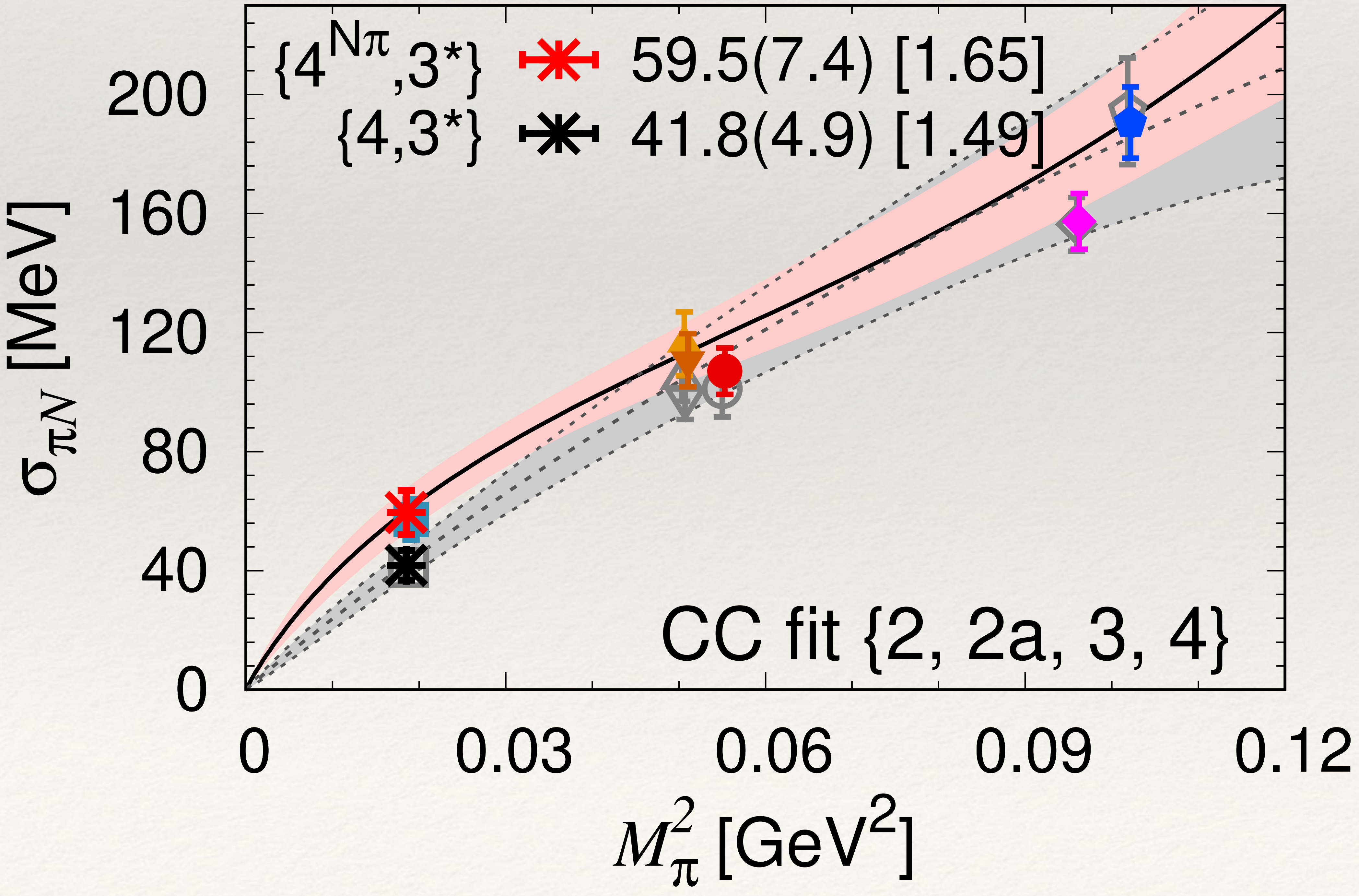


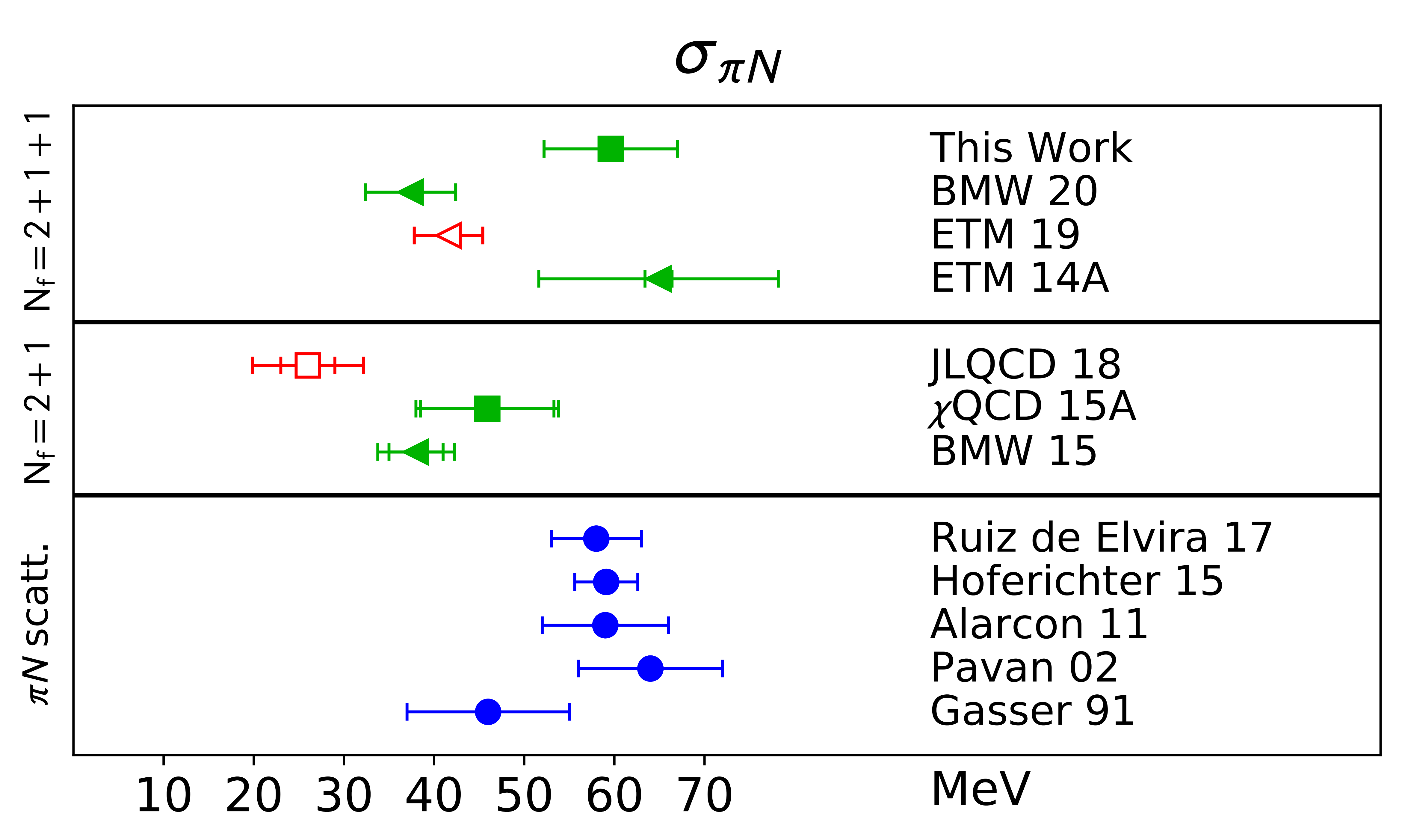
To quote a value of $\sigma_{\pi N}$, we need to finalize our M_π and F_π analysis - results hopefully this fall

LQCD: Our Results – How to extrapolate to physical point?

Interesting new result:
Gupta, Park, Hoferichter, Mereghetti, Yoon, Bhattacharya
PRL 127 (2021) [2105.12095]

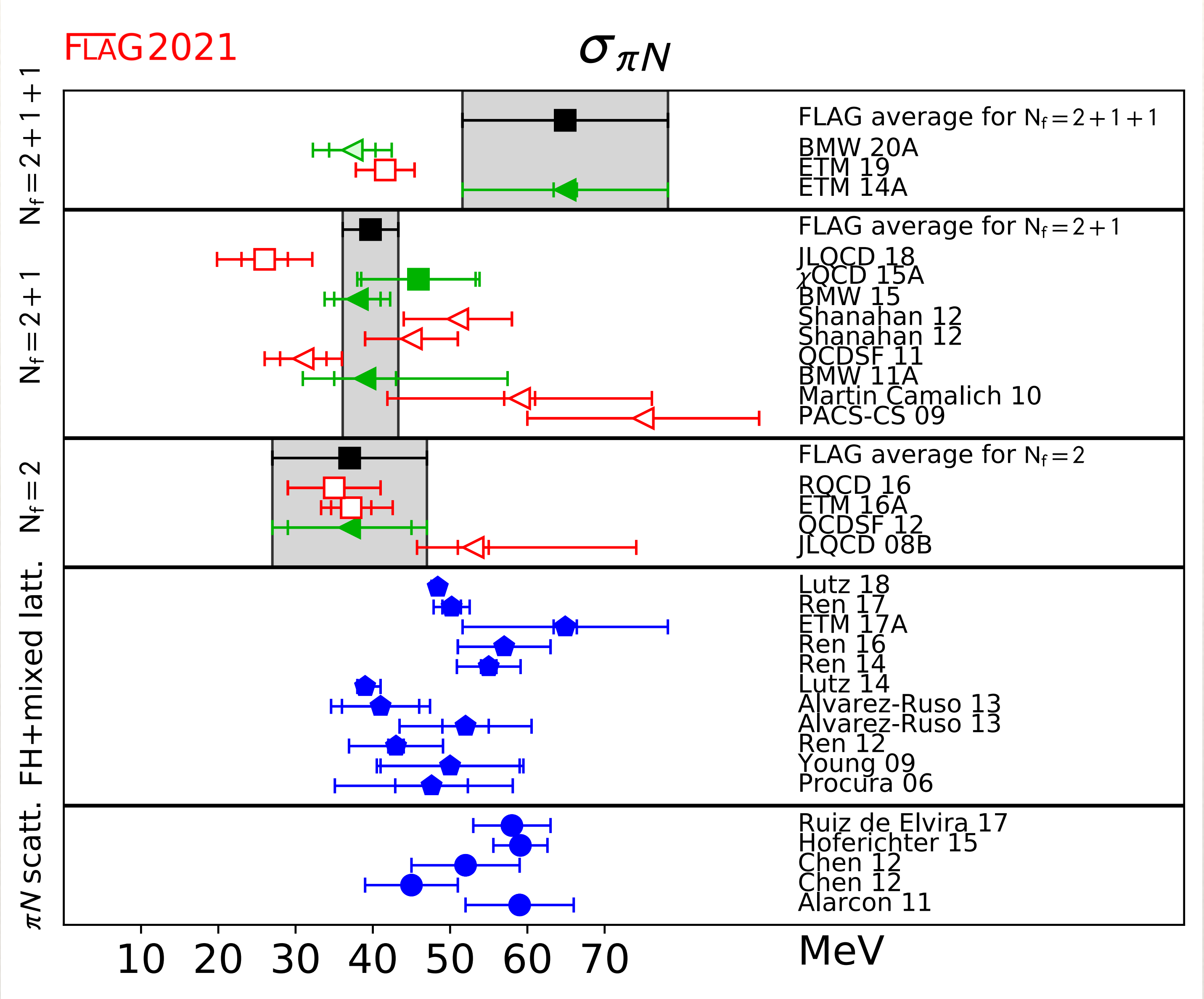
Hypothesize excited states are not fully quantified in other results - when encouraged to be “natural” sigma-term increases to be compatible with pheno

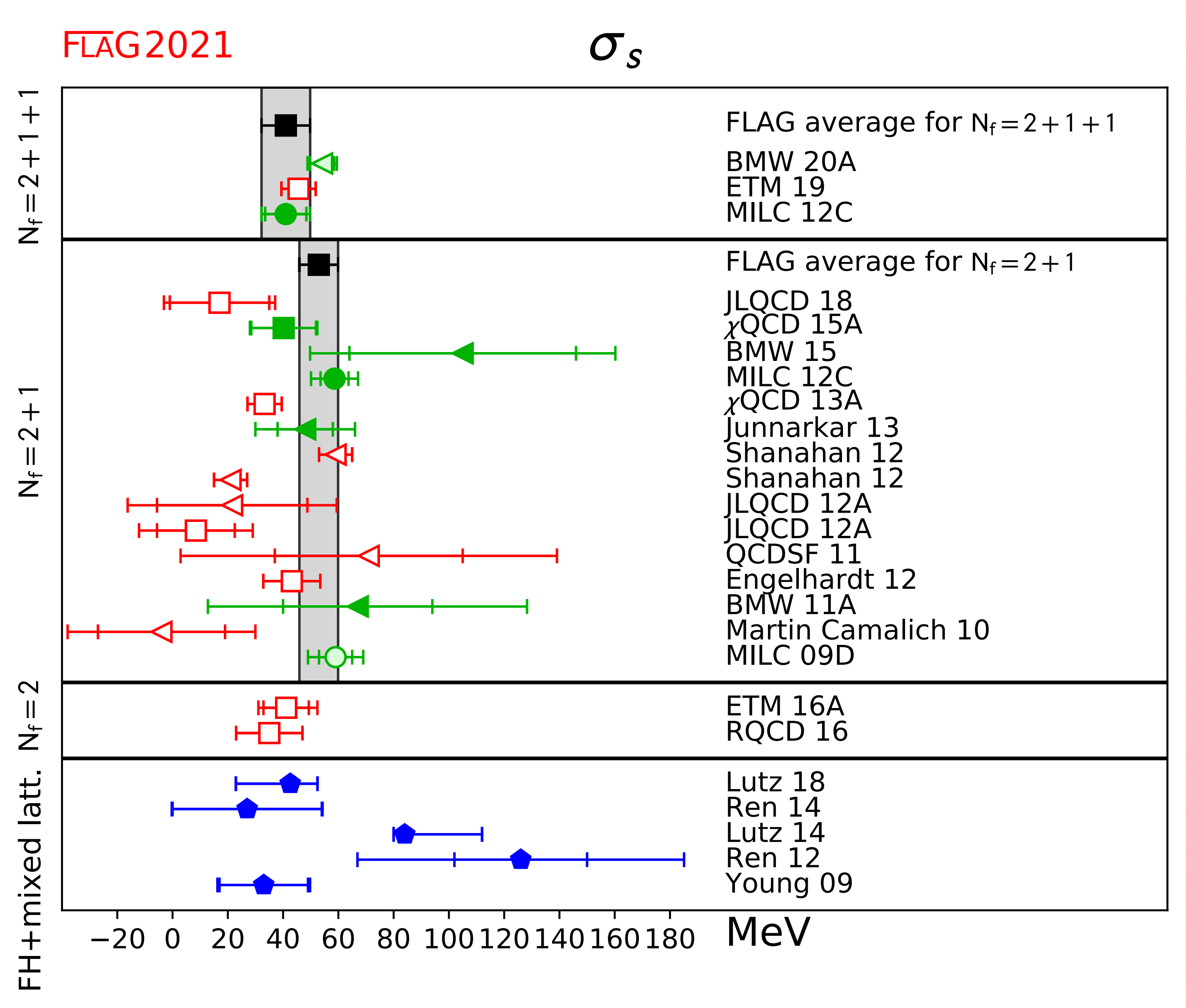


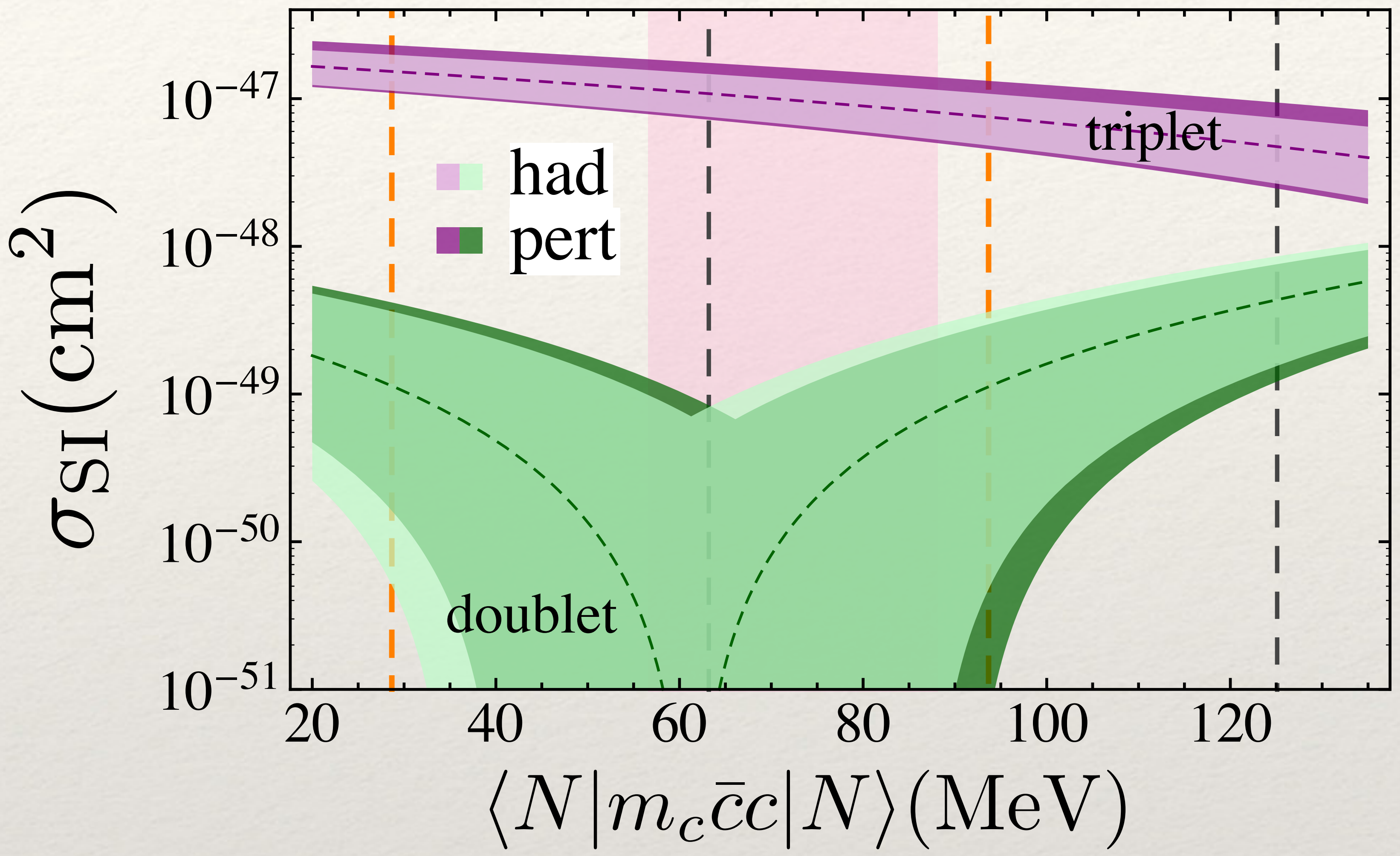


LQCD: Global Average

$$m_N = \langle N|\frac{\beta}{2g}G^2 + \gamma_m \sum_q m_q \bar{\psi}_q \psi_q |N\rangle + \sum_q \langle N| m_q \bar{\psi}_q \psi_q |N\rangle$$







$\sigma_{\pi N} \in [30 - 70]$ MeV

$\sigma_s \in [32 - 60]$ MeV

$$\sigma_c \simeq \begin{cases} 88(29) & \chi\text{QCD [1304.1194]} \\ 107(22) & \text{ETMC [1909.00485]} \\ 69(07) & {}^*\text{BMWc [2007.03319]} \end{cases}$$

bottom and top contributions are well estimated with perturbative QCD
Shifman, Vainstein, Zakharov and many updates from others
PLB78 (1978) 443

$\sigma_b \simeq 66$ MeV

$\sigma_t \simeq 64$ MeV

Conclusions

- Lattice QCD can provide unambiguous values for the light, strange and charm scalar matrix elements of the nucleon
  - But - systematic uncertainties (excited state contamination) remains an issue to obtain more stable and precise values - discrepancy between different results is larger than quoted uncertainties
    please keep this in mind for ALL LQCD results

- I anticipate my collaboration (CalLat) will have a robust determination of $\sigma_{\pi N}$ this fall (next, σ_s & σ_c)
  - ~30 ensembles to control all extrapolations
    - 7 pion masses, 130 ≲ M_π ≲ 400 MeV
    - 4 lattice spacings (3 at the physical pion mass)
    - multiple volumes at 3 different pion masses

- The scalar charm content of the nucleon is particularly important to determine precisely
  - If σ_c ~ 60 ± 5 MeV and Dark Matter is heavy (WIMP),
    natural explanation as to why we have not yet observed dark-matter — nucleus scattering
    Hill & Solon PRL 112 (2014) [arXiv:1309.4092]

- I'm interested to understand if we can find a non-perturbative definition of the the trace-anomaly
  the LQCD user can choose how many quarks to directly compute - how is this reflected in the remaining terms?

$$m_N = \langle N| \frac{\beta}{2g} G^2 + \gamma_m \sum_q m_q \bar{\psi}_q \psi_q |N\rangle + \sum_q \langle N| m_q \bar{\psi}_q \psi_q |N\rangle$$

Thank You