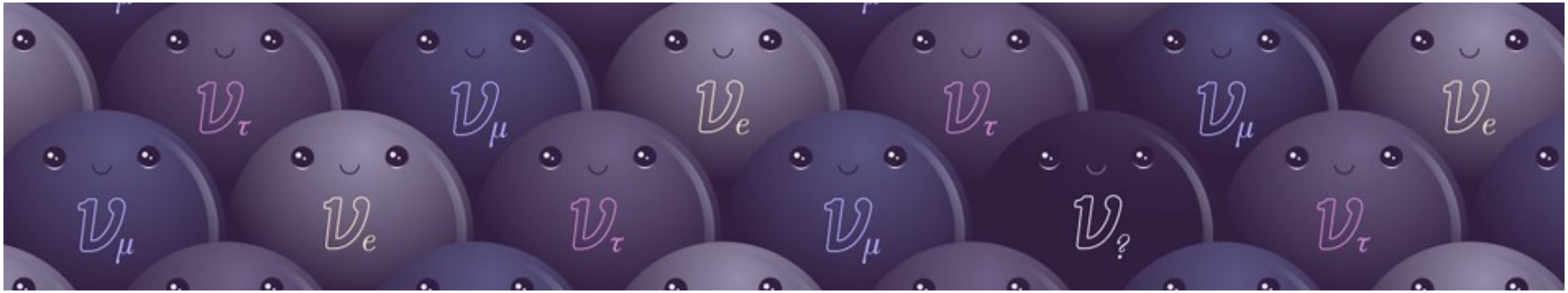

How Lattice QCD Modeling and Uncertainties Work

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Fermilab

Theoretical Physics Uncertainties to Empower Neutrino Experiments
Institute for Nuclear Theory, Seattle, Washington, USA
30 October–3 November 2023

“*ab initio*” Paradigm

- Targets in neutrino experiments are nuclei like ^{12}C, ^{16}O, or ^{40}Ar.
- In Standard Model (particle physics), nuclei emerge from QCD, so just:
  - calculate $\nu A \to lA'X$ scattering amplitude, just like decay $D \to Kl\nu$;
  - alas, beyond humankind’s capabilities in 2023.
- “*ab initio*” paradigm is to treat nuclei as a collection of nucleons with
  - two-, three-, more-body interactions (scattering, EFT);
  - obtain nucleon amplitudes from QCD ← this talk.

Nucleon Amplitudes from QCD

- Nucleon-level matrix elements are feasible:
  - quasielastic and DIS regions now/soon;
  - resonance and SIS regions maybe not so far away.
- Tool of choice is lattice QCD:
  - *The neutrino nucleus cross section problem is complex and has many moving pieces…. Knowing the axial form factor will stop one piece from moving and thus facilitates addressing the other moving pieces…. [N]ucleon transition form factors to the Δ and other low-mass baryon resonances would be similarly valuable.*

Lattice Field Theory

- Everything in QFT can be expressed as

$$\langle \phi(x_1)\phi(x_2)\cdots\phi(x_n)\rangle = \frac{1}{Z}\int \prod_{\phi}\prod_{x} \mathrm{d}\phi_x \, \phi(x_1)\phi(x_2)\cdots\phi(x_n)\mathrm{e}^{-S(\phi)}$$

gluons, quarks, antiquarks

uncountably many spacetime points

- Replace continuous, infinite spacetime by
  - discrete lattice (countably many degrees of freedom)…
  - … in a finite spacetime volume (finitely many degrees of freedom).

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Rigorous definition of QFT.

- discrete lattice (countably many degrees of freedom)…
- … in a finite spacetime volume (finitely many degrees of freedom).

Computational Lattice Gauge Theory

- Finite # degrees of freedom makes the problem computable:
  - $10^{9\text{–}10}$ variables of integration ⇒ Monte Carlo with importance sampling

$$\langle\phi(x_1)\phi(x_2)\cdots\phi(x_n)\rangle = \frac{1}{C}\sum_{c=1}^{C}\phi^{(c)}(x_1)\phi^{(c)}(x_2)\cdots\phi^{(c)}(x_n)$$

$$\phi^{(c)}(x) \sim \mathrm{e}^{-S(\phi)}$$

- Quarks (fermions) are Grassmann variables but can be integrated "by hand", replacing $\psi(x_1)\bar{\psi}(x_2)$ with $G(x_1{-}x_2)$ in all combinations:

$$U_\mu^{(c)}(x) \sim \mathrm{Det}(\not{D} + m)\mathrm{e}^{-S(U)}$$

- K. Wilson showed how to make lattice field theory gauge invariant (1974).

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sea-quark loops, very demanding

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No Modeling, but Uncertainties

- QCD is the theory of the strong interactions; no physics left out:
  - historical caveat of “quenched” approximation.
- Computational science inevitably has uncertainties:
  - “make lattice finer” ↔ “take continuum limit” ↔ “remove UV cutoff”;
  - “make volume larger” ↔ “remove IR cutoff”;
  - adjust $1+n_f$ free parameters to match $1+n_f$ measurements;
  - fitting correlation functions to get physical information.

QCD Lagrangian

- SU(3) gauge symmetry and $1 + n_f + 1$ parameters:

$$
\begin{aligned}
\mathcal{L}_{\mathrm{QCD}} &= \frac{1}{g_0^2}\,\mathrm{tr}[F_{\mu\nu}F^{\mu\nu}] \\
&- \sum_f \bar{\psi}_f (\not{D} + m_f)\psi_f \\
&+ \frac{i\theta}{32\pi^2}\,\varepsilon^{\mu\nu\rho\sigma}\,\mathrm{tr}[F_{\mu\nu}F_{\rho\sigma}]
\end{aligned}
$$

- Gauge coupling g_0 and quarks masses m_f are not directly measurable:
  - each free parameter set by a hadronic property, e.g., mass;
  - coupling equivalent to a scale, hence use a hadron mass here too.

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$$
\begin{aligned}
\mathcal{L}_{\mathrm{QCD}} &= \frac{1}{g_0^2}\,\mathrm{tr}[F_{\mu\nu}F^{\mu\nu}] && M_\Omega \text{ or similar;} \\
&- \sum_f \bar{\psi}_f(\not{D} + m_f)\psi_f && M_\pi,\ M_K,\ M_{J/\psi},\ M_\Upsilon,\ \ldots; \\
&+ \frac{i\theta}{32\pi^2}\,\varepsilon^{\mu\nu\rho\sigma}\,\mathrm{tr}[F_{\mu\nu}F_{\rho\sigma}] && \theta = 0.
\end{aligned}
$$

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Uncertainty Budget

Source	%
Statistics	
Excited-state contamination, correlator fitting choices	
Chiral-continuum extrapolation (continuum) (chiral)	
Lattice spacing: w_0/a, w_0 (fm)	
Quark mass tuning	
Finite volume: exponential topology freezing	
Total (after model averaging)	

Source	%
Statistics	
Excited-state contamination; correlator fitting choices	
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Lattice spacing: w_0/a, w_0 (fm)	

Statistics for Correlation Functions

- Nucleon two-point correlation function:

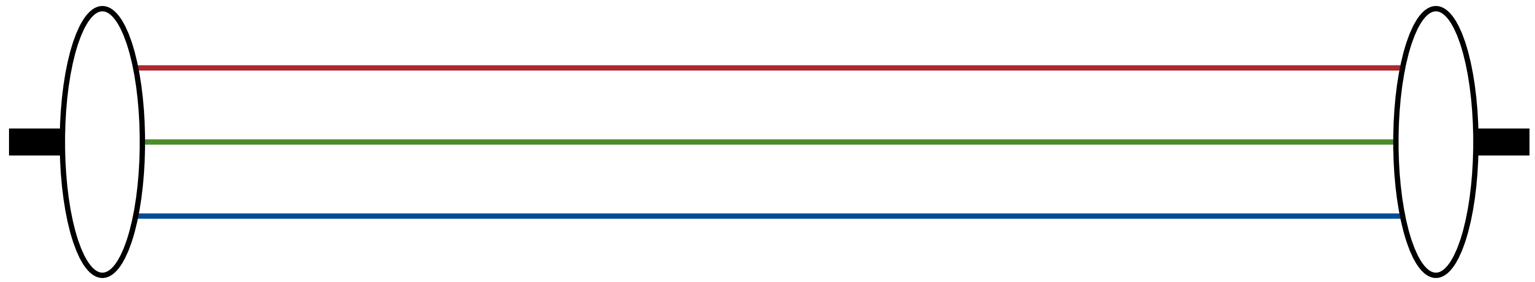
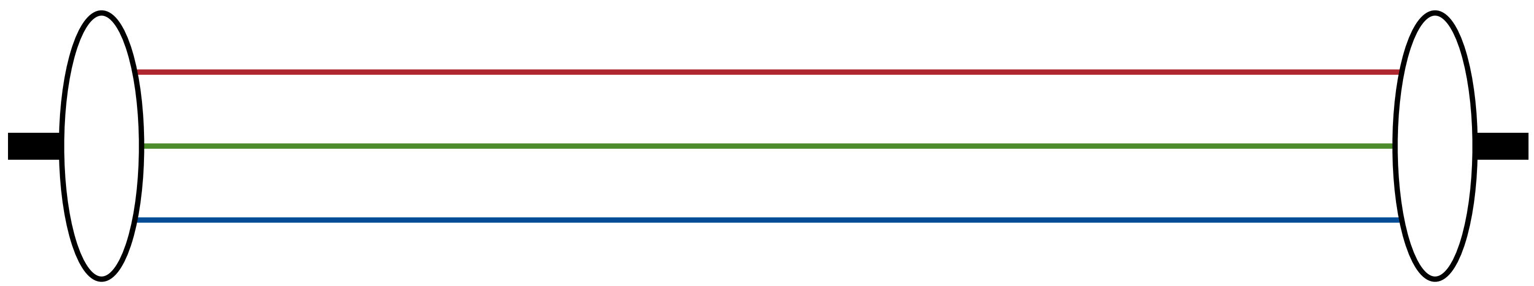
$$\sum_{\boldsymbol{x}} \langle N(t,\boldsymbol{x})\bar{N}(0,\boldsymbol{0})\rangle = \frac{1}{C}\sum_{c=1}^{C} G_u^{(c)}(t,\boldsymbol{x};0,\boldsymbol{0})G_u^{(c)}(t,\boldsymbol{x};0,\boldsymbol{0})G_d^{(c)}(t,\boldsymbol{x};0,\boldsymbol{0})$$
$$= \sum_{n=1}^{\infty} \langle 0|\hat{N}|n\rangle \mathrm{e}^{-M_{N,n}t} \langle n|\hat{N}^{\dagger}|0\rangle$$

where $M_{N,1}$ is nucleon mass and others (n>1) are excited nucleons.

- Statistical uncertainty of LHS estimated from the samples in the usual way (average of square minus square of average).

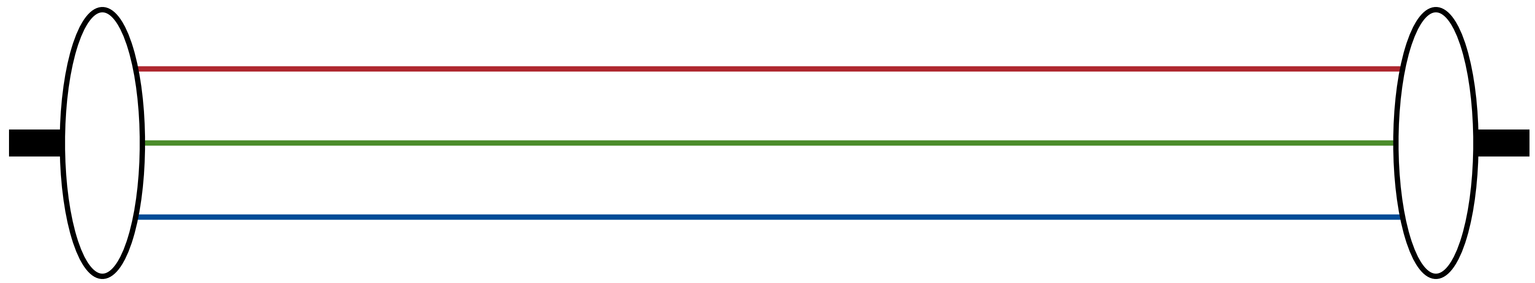
- Obtain (first few) $|\langle 0|\hat{N}|n\rangle|^2$ and $M_{N,n}$ from fitting: can use Hessian error estimate here.

Signal-to-Noise

- Obstacle to statistical precision with nucleons:
  - signal  $\sim \mathrm{e}^{-M_N t}$
  - noise^2 
  - ratio $\sim \mathrm{e}^{-(M_N - 3M_\pi/2)t}$
- Have to try to find the signal at small t; cf., next section.

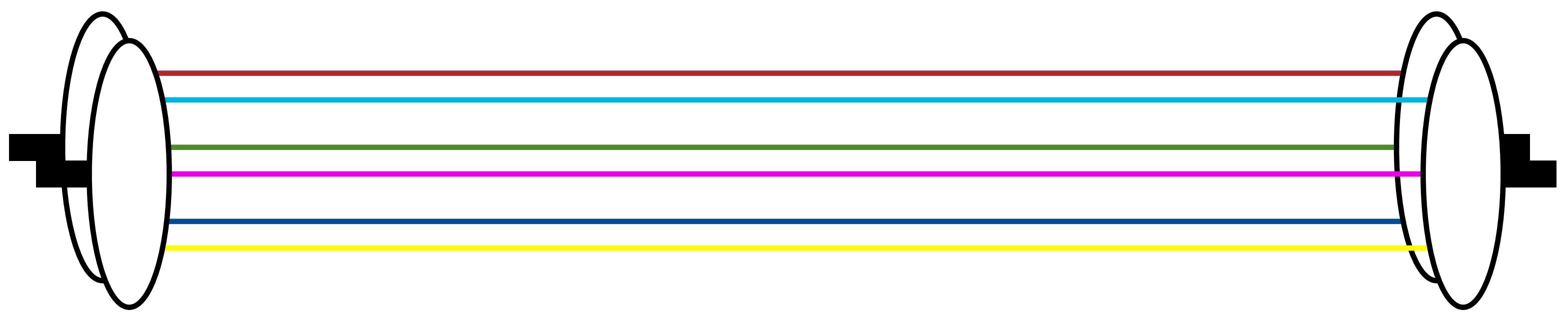
Signal-to-Noise

- Obstacle to statistical precision with nucleons:
  - signal



$\sim \mathrm{e}^{-M_N t}$

  - noise^2



$\sim \mathrm{e}^{-3M_\pi t}$

  - ratio $\sim \mathrm{e}^{-(M_N - 3M_\pi/2)t}$

- Have to try to find the signal at small t; cf., next section.

Statistics for Ensemble Quantities

- Nucleon three-point correlation function:

$$\sum_{\boldsymbol{x}_1,\boldsymbol{x}_2} \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}_2} \langle N(t_2,\boldsymbol{x}_2) A_\mu(t_1,\boldsymbol{x}_1) \bar{N}(0,\boldsymbol{0})\rangle = \sum_{n,m=1}^{\infty} \langle 0|\hat{N}|n\rangle \mathrm{e}^{-E_{N,n}(t_2-t_1)} \langle n|\hat{A}_\mu|m\rangle \mathrm{e}^{-M_{N,m}t_1} \langle m|\hat{N}^\dagger|0\rangle$$

axial form factors

- Matrix element from more fitting with output of previous step.
- Propagate statistical uncertainties and correlations of ensemble quantities (e.g., mass ratios) with resampling, aka “pseudoensembles”:
  - jackknife (Quenouille)—eliminate J adjacent samples, average over C–J;
  - bootstrap (Efron, 1979)—choose samples at random, allowing repeats.

Correlated Statistical Uncertainties

- Related quantities (e.g., form factors at nearby $\boldsymbol{p}$) fluctuate together, so covariance matrix is not close to being diagonal.
- Sample estimate of covariance has well-known problems once the number of (nonzero) entries approaches number of samples.
- "Shrinkage" of spectrum of covariance matrix:
    - linear, e.g., arXiv:1901.07519;
    - nonlinear, e.g., arXiv:2212.12648;
    - used by economists at banks to make money.

Source	%
Statistics	
Excited-state contamination, correlator fitting choices	
Chiral-continuum extrapolation (continuum) (chiral)	
Quark mass tuning	
Lattice spacing: w_0/a, w_0 (fm)	
Finite volume: exponential topology freezing	

Fitting Correlation Functions

- Nucleon two-point correlation function again:

$$\sum_{\boldsymbol{x}} \langle N_i(t, \boldsymbol{x}) \bar{N}_j(0, \mathbf{0}) \rangle = \sum_{n=1}^{\infty} \langle 0|\hat{N}_i|n\rangle \mathrm{e}^{-M_{N,n} t} \langle n|\hat{N}_j^\dagger|0\rangle$$

- Could take t very large, but better to fit time dependence to several states; for nucleons, excited states = special concern.

- Bayesian view natural: priors on mass splittings & weights $A_{i,n} = \langle 0|\hat{N}_i|n\rangle$:

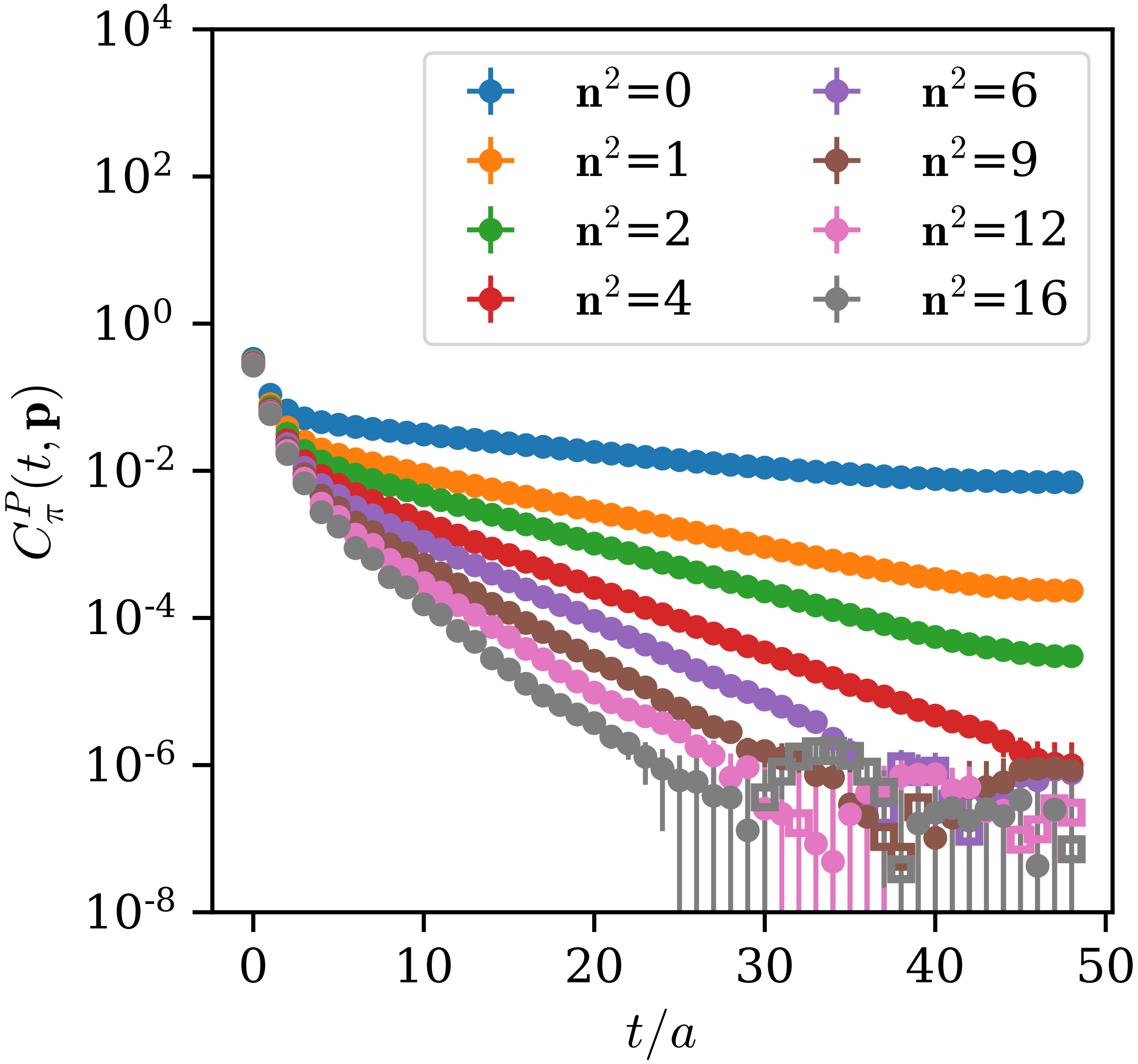
    - truncating is the same as a prior $A \sim \delta(A)$.

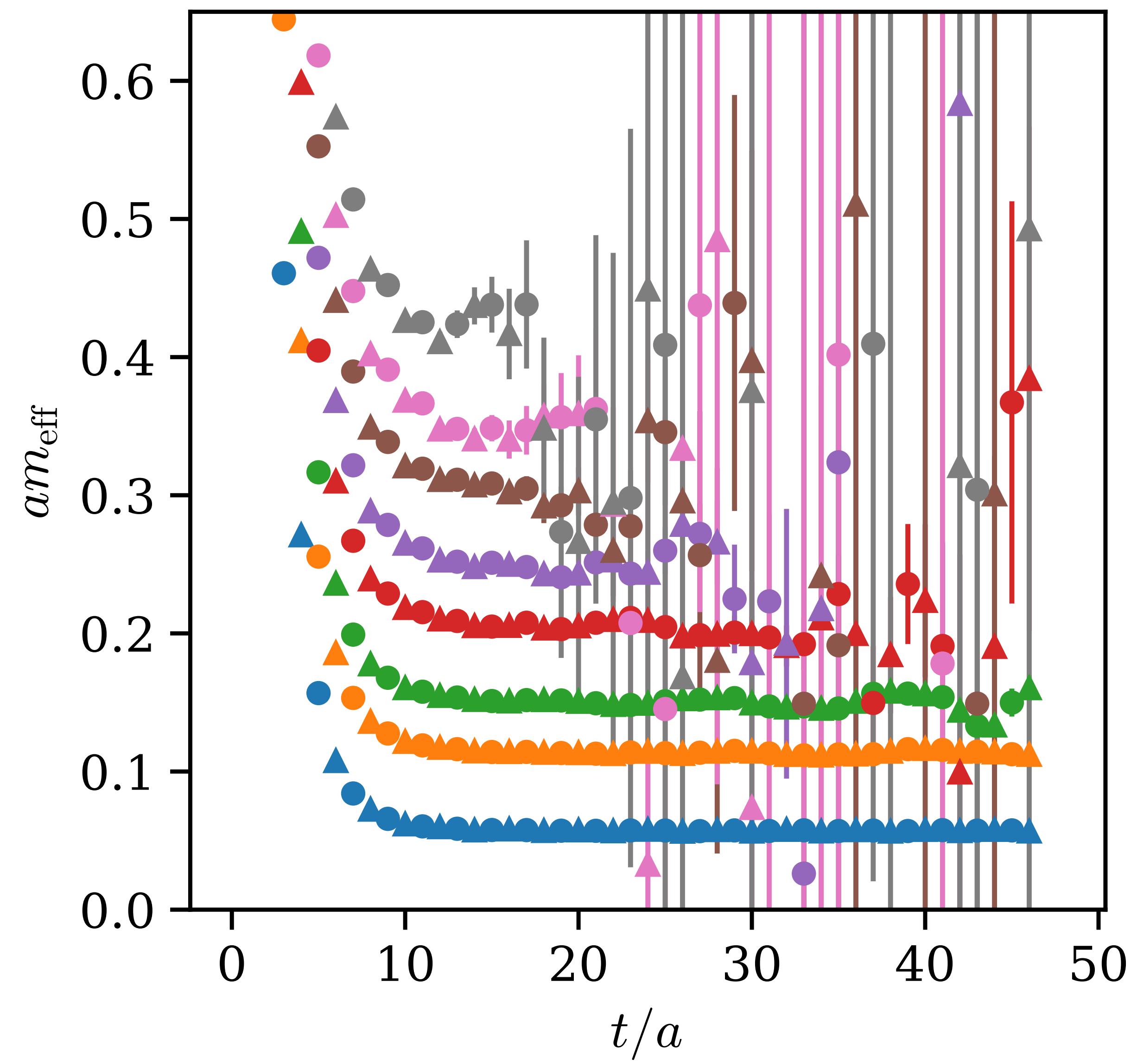
- Matrix correlation: “generalized eigenvalue problem”:

    - yields optimal operator $w_i N_i$ for use in three-point functions.

Pion

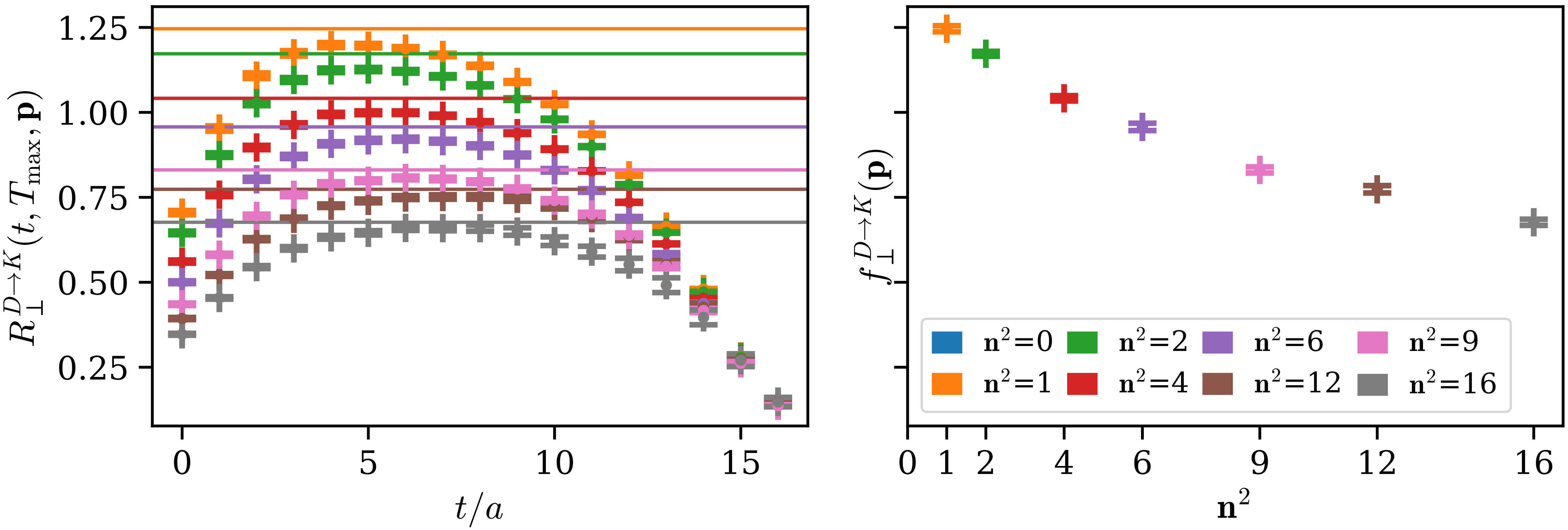
Fermilab Lattice and MILC, arXiv:2212.12648





D → K

Fermilab Lattice and MILC, arXiv:2212.12648



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Symanzik EFT

- Discretization effects can be described as

$$\mathscr{L}_{\text{LGT}} \doteq \mathscr{L}_{\text{Sym}} = \mathscr{L}_{\text{QCD}} + \sum_i a^{d_i} \mathscr{K}_i \mathscr{L}_i$$

  which guides the extrapolation in lattice spacing.

- On same foundation as operator-product expansion, factorization, etc., in perturbative QCD:
  - established in perturbation theory, structure expected to hold nonperturbatively.
- Leading power is usually a^2 or $\alpha_s a^2$, but with several (3–6) different lattice spacings, fit leading⊕subleading.

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Chiral EFT

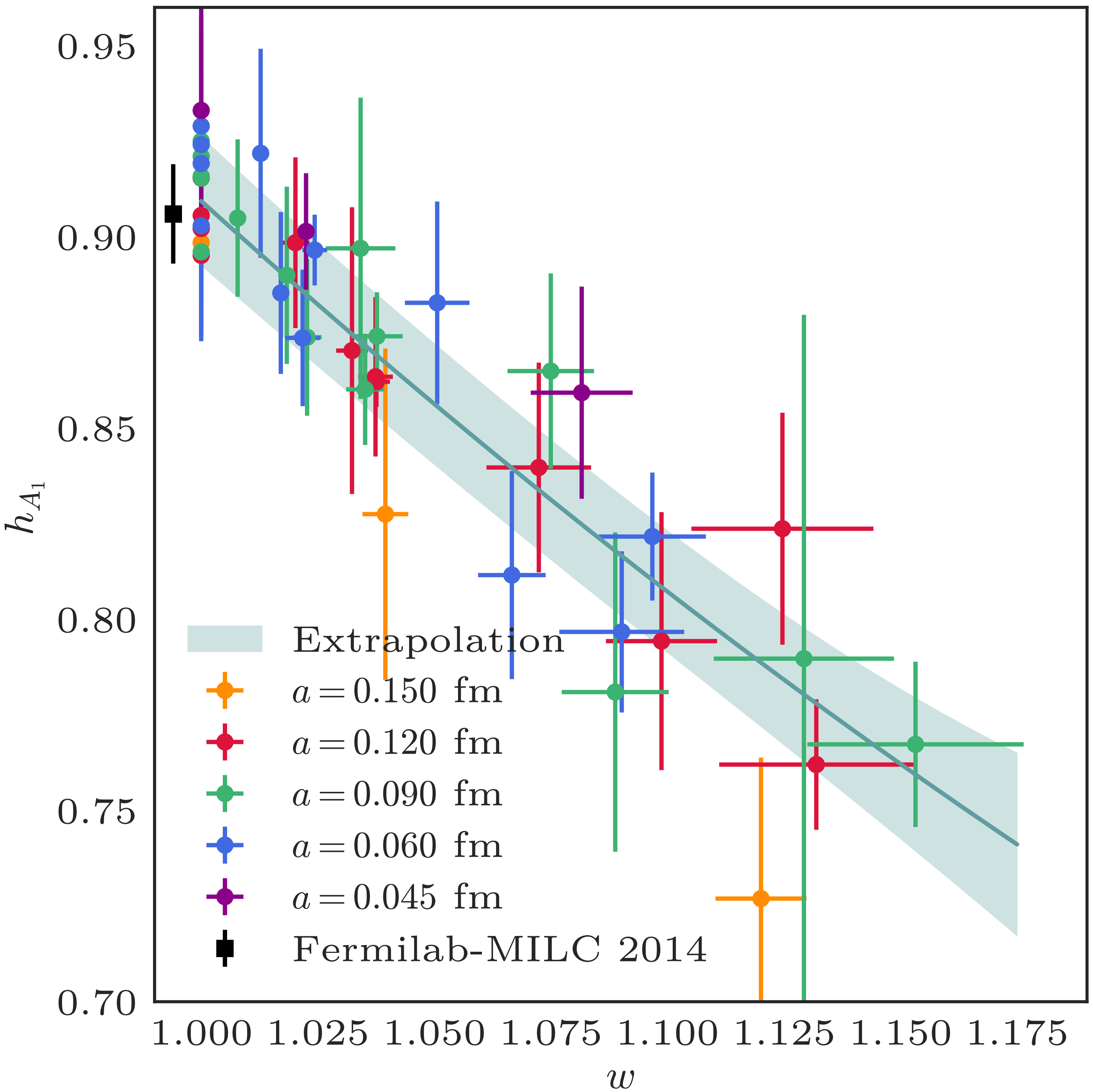
- Making the quark masses as small as down and up is computationally demanding: take somewhere in $\frac{1}{2}(m_u + m_d) \leq m_l < m_s$ and extrapolate.
- That means the pion in the computer has a mass larger than that in Nature. Pion interactions described by chiral Lagrangian

$$\mathscr{L}_{\text{QCD}} \doteq \mathscr{L}_{\chi\text{PT}} = \sum_i \Lambda_\chi^{-d_i} L_i \mathscr{O}_i$$

  coupled to other particles, e.g., nucleon.

- There are many ensembles on disk with physical light-quark mass:
  - very desirable for nucleon because chiral extrapolation less persuasive (empirically) than for kaon, D-meson, B-meson.

- Often, Symanzik EFT and chiral EFT steps combined into a grand fit of quark-mass and lattice-spacing dependence:



- $B \to D^* l\nu$

- arXiv:2105.14019

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Convert from Lattice Units to MeV

- Actually, convert from natural QCD units to SI (electro-atomic) units.
- Vary bare gauge coupling, compute various masses, aM_π, aM_K, aM_Ω, etc. Factor a is fictitious albeit mnemonic that all change in proportion:

$$aM_\Omega \propto \mathrm{e}^{-1/2\beta_0 g_0^2}$$

- Form dimensionless ratios with aM_Ω in denominator, vary am_l & am_s to adjust aM_π/aM_Ω & aM_K/aM_Ω to PDG values for M_π/M_Ω & M_K/M_Ω.
- Compute continuum limit of aM_N/aM_Ω to get M_N/M_Ω; multiply by PDG M_Ω.
- Alternatively, use w_0/a instead of $1/aM_\Omega$ and look up w_0 (fm) in FLAG.

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Uncertainties in aM_π/aM_Ω & aM_K/aM_Ω propagate to am_l & am_s and, hence, everything else.

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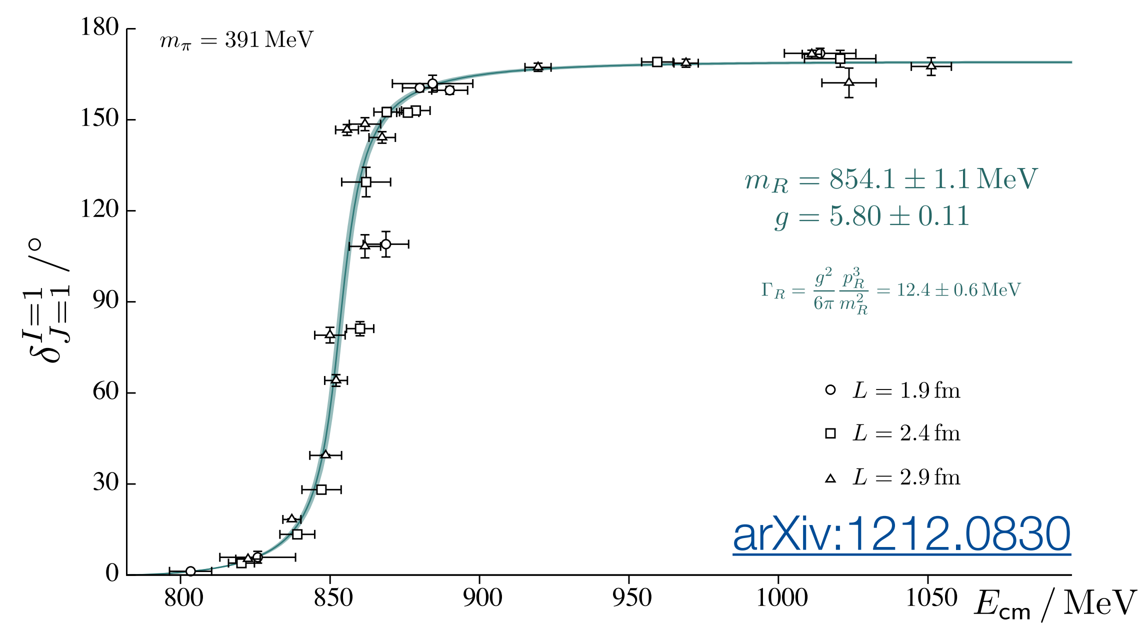
Exponential Finite Volume

- Virtual particle exchange “around the world” are suppressed exponentially:
    - FLAG’s rule of thumb $M_\pi L > 4$; check by having more than one L.
- Resonances are more interesting:
    - ϱ meson (Δ baryon) not really a particle but a feature in the $\pi\pi$ ($N\pi$) scattering amplitude;
    - resonant properties obtained from detailed study of L dependence of two-particle states;
    - path to rigorous $N \to \Delta$ form factors.



arXiv:1212.0830

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Huge literature on theoretical formalism.

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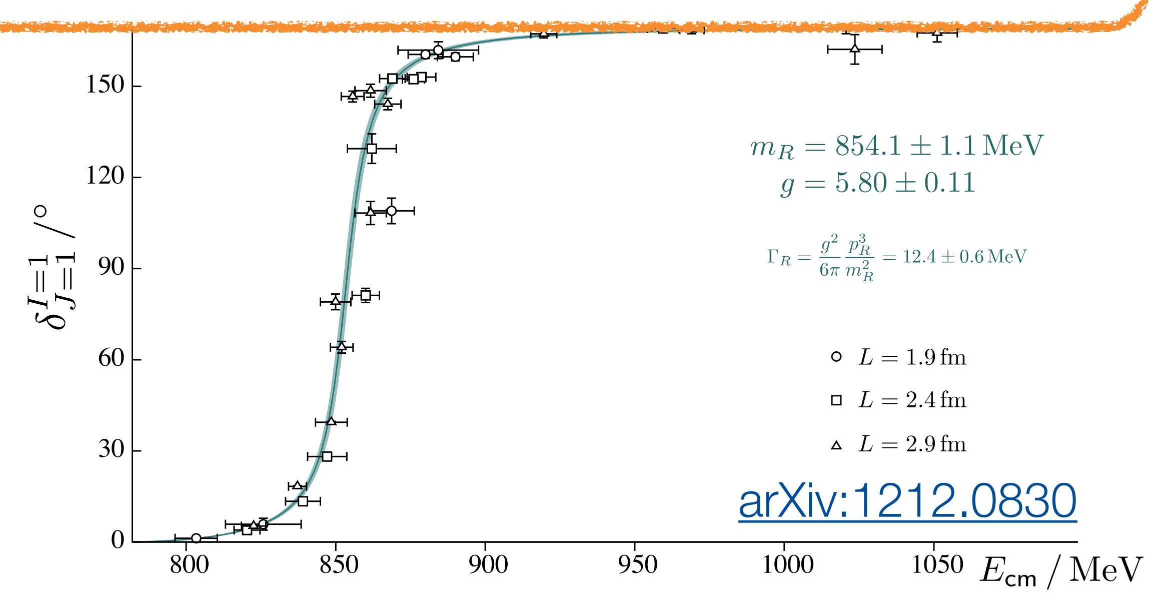

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Topology in Gauge Theories

- QCD states possess a quantum number $e^{i\theta}$ having to do with topology—can't change θ with any local operation.
- In 4-d functional integral, θ is introduced via a term $e^{i\theta Q}$, where Q is the spacetime integral of $\boldsymbol{E}^a \cdot \boldsymbol{B}^a$, which is (close to) an integer:
  - need big change in gauge field, but Markov chain makes small ones.
- Poor sampling of Q is usually just a finite-volume effect:

$$\frac{1}{2\chi_T}\frac{1}{V}\left(1-\frac{Q^2}{\langle Q^2\rangle}\right)$$

(I think) not a big concern in νA, but of course disastrous for neutron EDM.

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Q^2: average of Q^2 in the simulation

$\langle Q^2\rangle$: vev of Q^2 in $\theta = 0$ vacuum

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Total (after model averaging)	

Total Uncertainty

- Choices plus quadrature sum:
  - requires judgment whether a “test” is a cross-check or something that inflates a systematic.
- Bayesian model averaging:
  - introduce an “information criterion” (IC) depending on amount of data, number of fit parameters, quality of resulting fit, etc., which then yields a weight for each discrete set of choices;
  - early usage of Akaike IC by BMW [arXiv1406.4088]; more recent work starting from Bayes’s theorem: Jay & Neil arXiv:2008.01069; Neil & Sitison arXiv:2208.14983, arXiv:2305.19417.