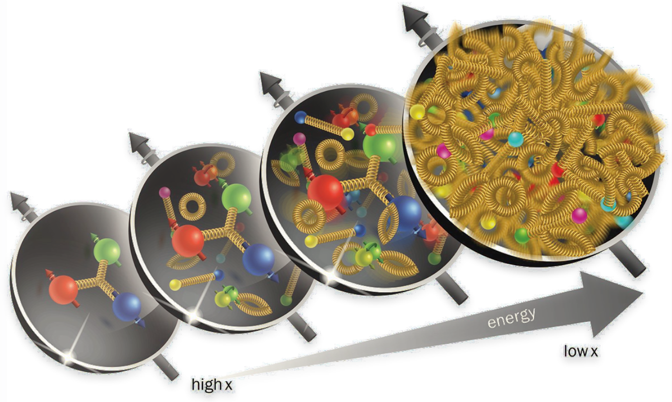
Hadron Structure

High-Performance Computing

Theoretical Physics

Applied Mathematics



Dr. Simone Bacchio

Associate Research Scientist

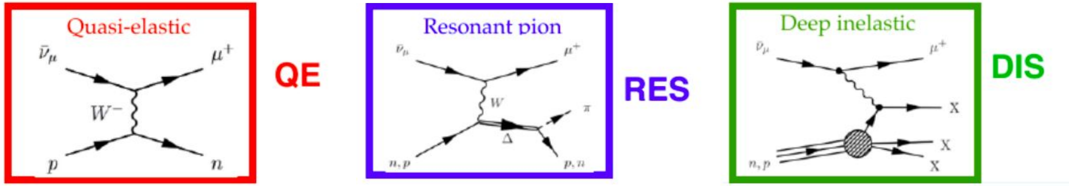
CaSToRC, The Cyprus Institute

Ph.D. & Dr. Rer. Nat. (MSC Fellow, UCY & BUW)

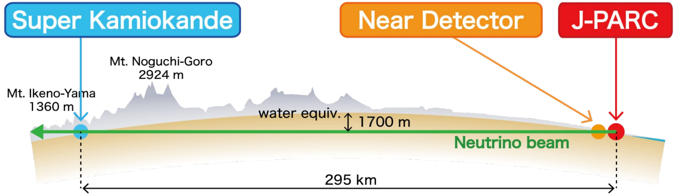
09/09/24 - The Cyprus Institute

Motivation: Neutrino oscillation experiments

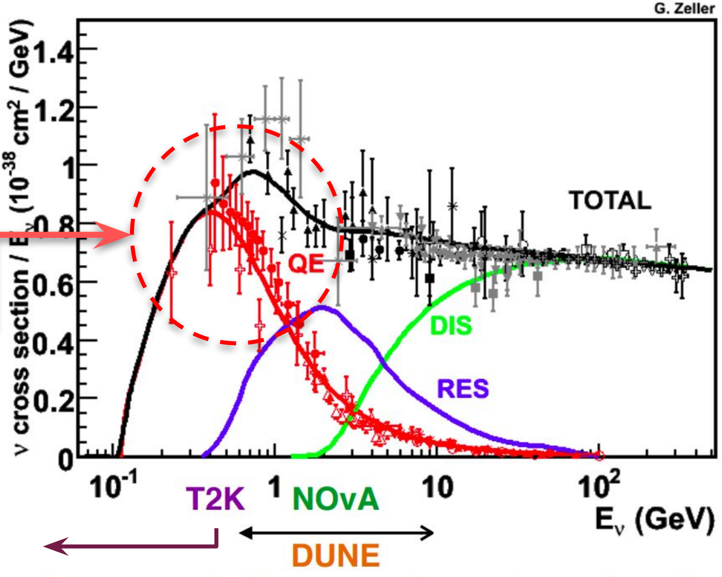
Monte-Carlo simulation needs input on the differential cross section to reconstruct the energy of the neutrino from the momentum of the detected charged lepton.



We focus on quasi-elastic scattering providing first-principle predictions on axial form factors



T2K: Tokai to Super-Kamiokande
E = 0.6 GeV, L/E ≈ 500 km/GeV.



J.A. Formaggio, G. Zeller, Reviews of Modern Physics, 84 (2012)

The weak axial-vector matrix element

The transition matrix element of the neutron β-decay is

$$\mathcal{M}(n \to p\, e^-\, \bar{\nu}_e) = \frac{G_F}{\sqrt{2}}\, V_{ud}\, \sum_\mu \underbrace{\langle p(p') | W_\mu | n(p) \rangle}\, L_\mu$$

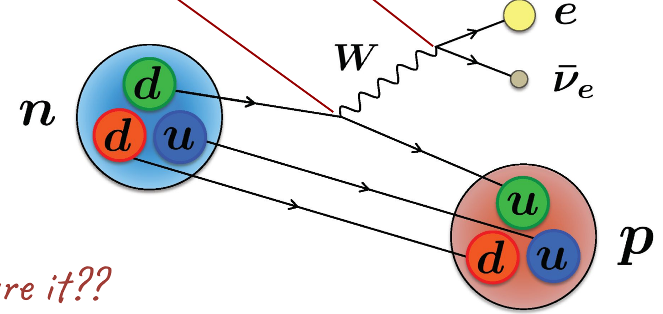
with
$$W_\mu = V_\mu - A_\mu$$
$$V_\mu = \bar{u}\gamma_\mu d$$
$$A_\mu = \bar{u}\gamma_\mu\gamma_5 d$$

Vector contributions are well determined experimentally from lepton-nucleon scattering

Axial-vector matrix element

$$\langle p(p') | A_\mu | n(p) \rangle$$

How to measure it??



Neutrino-nucleon scattering processes are related to matrix elements at finite momentum transfer.

How to? Lattice QCD Simulations

$$\langle \mathcal{O} \rangle_{a,V,\vec{\mu}_f} = \frac{1}{\mathcal{Z}} \int \mathrm{D}[U]^V \, \mathrm{D}[\psi\bar{\psi}]^{V n_f} \, \mathcal{O}(U,\psi,\bar{\psi}) \, e^{-S(a,\vec{\mu}_f;\, U,\psi,\bar{\psi})}$$

Simulation

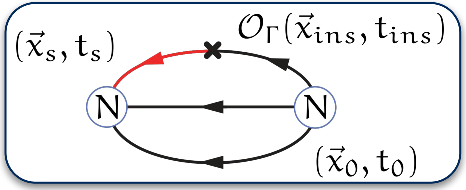
- Markov chain Monte Carlo to generate ensembles of gluon-field configurations via importance sampling [Jacob Finkenrath, Wed.- Thur.]

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i^N O(U_i) \quad \textit{with} \quad p(U) = \frac{1}{\mathcal{Z}} \exp(-S(U))$$

Analysis

- Construction of hadron correlation functions on background field configurations:

$$\langle N(p', s') | A_\mu | N(p, s) \rangle$$

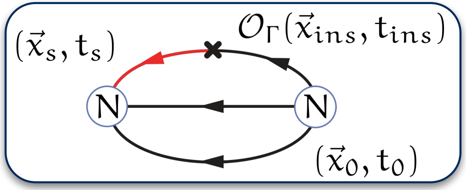


Data analysis – post-processing

- Statistical analysis, resampling, derived quantities
- Excited state contamination and stochastic errors
- Continuum and infinite volume extrapolation

Topics covered in this talk

- Basic concepts:
  - Correlation functions
  - Interpolating fields
  - Wick contractions



- Implementation:
  - Fermions on the Lattice
  - Stochastic and point sources
  - Two-point functions
  - Noise-reduction techniques

[GPUs: Mathias Wagner, Tue.- Thu.]

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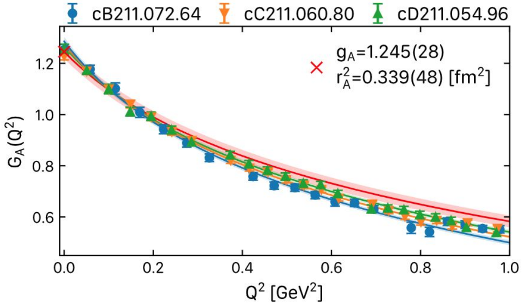


Correlation Functions

The correlation function between two states ψ is equivalent to the matrix elements of the transport operator up to exponentially-suppressed thermal effects, due to the finite size.

$$C(t) \equiv \langle \psi(t)\psi^\dagger(0) \rangle = \left\langle \psi \middle| \underbrace{T}_{e^{-H}}{}^{t} \middle| \psi \right\rangle + \ldots$$

By inserting a complete set of eigenstates of the transfer matrix $\sum_n |n\rangle \langle n|$, we obtain

$$C(t) = \sum_n \underbrace{\lambda_n^t}_{\langle n| T |n\rangle} \langle \psi|n\rangle \langle n|\psi\rangle \underbrace{=}_{T = e^{-H}} \sum_{n=0}^{\infty} |\underbrace{Z_n}_{\langle n|\psi\rangle}|^2 e^{-E_n t} \longrightarrow$$

Exponential suppression!

Correlation Functions

The correlation function between two states ψ is equivalent to the matrix elements of the transport c… size.

In Lattice QCD we can easily extract ground-state matrix elements:

$$\lim_{t\to\infty} C(t) = |Z_0|^2 \; e^{-E_0 t}$$

By inserting a complete set of eigenstates of the transfer matrix $\sum_n |n\rangle\langle n|$, we obtain

$$C(t) = \sum_n \lambda_n^t \langle\psi|n\rangle\langle n|\psi\rangle = \sum_{n=0}^{\infty} |Z_n|^2 e^{-E_n t} \longrightarrow$$

Exponential suppression!

$\lambda_n = \langle n| T |n\rangle$

$T = e^{-H}$

$Z_n = \langle n|\psi\rangle$

Interpolating Fields: How to measure properties of hadrons?

Our goal is then to construct an interpolating field ψ, whose ground state is the desired hadron.

To achieve this we can exploit quantum numbers and other properties: $\langle n|\psi\rangle = 0$, *if wrong quantum numbers*

- **Flavor structure:** Use the correct combination of quark fields to represent the desired flavor quantum numbers.
- **Spin and parity selection:** Choose the appropriate Dirac structure (Γ) to match the desired spin J and parity P.
- **Other symmetries:** Certain hadrons are e.g. *even under exchange of u↔d*. Implement these symmetries correctly.
- **Momentum projection:** Sum the interpolating operator over spatial points with a phase factor to project onto definite momentum states.

Additionally the interpolating field should preserve:

- **Gauge invariance:** Ensure the interpolating operator is gauge-invariant, using color indices and Wilson lines (if necessary).
- **Symmetry under the cubic group:** Since the lattice breaks continuous rotational symmetry, operators must transform according to irreps of the cubic group.

Meson Interpolating Fields

For **mesons**, the simplest interpolating operator is a bilinear quark-antiquark field of the form:

$$\psi_{\text{meson}}(x) = \sum_{a,\alpha,\beta} \bar{q}_1(x)^a_\alpha \, \Gamma_{\alpha,\beta} \, q_2(x)^a_\beta$$

- **Flavor structure:** The specific quarks q_1 and q_2 determine the flavor quantum numbers of the meson.
- **Spin and parity selection:** The choice of Γ determines the spin and parity of the meson. For example:
  - $\Gamma = \gamma_5$ gives a pseudoscalar meson (like the pion), with $J^P = 0^-$.
  - $\Gamma = \gamma_\mu$ gives a vector meson (like the ρ-meson), with $J^P = 1^-$.
  - $\Gamma = 1$ gives a scalar meson, with $J^P = 0^+$.
  - $\Gamma = \gamma_5\gamma_\mu$ gives an axial-vector meson (like the a_1-meson), with $J^P = 1^+$.
- **Gauge invariance:** The quark fields are in the same location *x* and color indices are traced.

- **Momentum projection:**

$$\psi(\vec{p}, t) = \sum_{\vec{x}} e^{i\vec{p}\vec{x}} \psi(\vec{x}, t)$$

Baryon Interpolating Fields

For **baryons**, there are various options to construct the interpolating field

$$\psi_{\text{baryon}}(x) = \epsilon_{abc}\, P_{\pm}\, \Gamma_A\, q_1(x)^a \left({q_2}^T(x)^b \Gamma_B\, q_3(x)^c \right)$$

This gives more precise results

- **Spin selection:**
  - $J = {}^1\!/_2 \rightarrow \ (\Gamma^A, \Gamma^B) = (\mathbb{1}, C\gamma_5),\ (\gamma_5, C),\ \text{or}\ (\mathbb{1}, \mathrm{i}\gamma_4 C\gamma_5)$
  - $J = {}^3\!/_2 \rightarrow \ (\Gamma^A, \Gamma^B) = (\mathbb{1}, C\gamma_j)$
- **Parity selection:** positive and negative parity selected using $P_{\pm} = \frac{1}{2}(\mathbb{1} \pm \gamma_4)$
- **Other symmetries:**
  - C is the charge conjugation matrix, ensuring the antisymmetry
  - ϵ_{abc} ensures antisymmetry in the color indices (so that the wavefunction is antisymmetric overall, respecting the Pauli exclusion principle).

Examples of Baryon Interpolating Fields

Baryon	Quark content	Interpolating field	I	I_z
p	uud	$\epsilon_{abc}\left(u_a^T C\gamma_5 d_b\right) u_c$	1/2	+1/2
n	udd	$\epsilon_{abc}\left(d_a^T C\gamma_5 u_b\right) d_c$	1/2	-1/2
Λ	uds	$\frac{1}{\sqrt{6}}\epsilon_{abc}\left[2\left(u_a^T C\gamma_5 d_b\right) s_c + \left(u_a^T C\gamma_5 s_b\right) d_c - \left(d_a^T C\gamma_5 s_b\right) u_c\right]$	0	0
Σ^+	uus	$\epsilon_{abc}\left(u_a^T C\gamma_5 s_b\right) u_c$	1	+1
Σ^0	uds	$\frac{1}{\sqrt{2}}\epsilon_{abc}\left[\left(u_a^T C\gamma_5 s_b\right) d_c + \left(d_a^T C\gamma_5 s_b\right) u_c\right]$	1	0
Σ^-	dds	$\epsilon_{abc}\left(d_a^T C\gamma_5 s_b\right) d_c$	1	-1
Ξ^0	uss	$\epsilon_{abc}\left(s_a^T C\gamma_5 u_b\right) s_c$	1/2	+1/2
Ξ^-	dss	$\epsilon_{abc}\left(s_a^T C\gamma_5 d_b\right) s_c$	1/2	-1/2
Δ^{++}	uuu	$\epsilon_{abc}\left(u_a^T C\gamma_\mu u_b\right) u_c$	3/2	+3/2
Δ^+	uud	$\frac{1}{\sqrt{3}}\epsilon_{abc}\left[2\left(u_a^T C\gamma_\mu d_b\right) u_c + \left(u_a^T C\gamma_\mu u_b\right) d_c\right]$	3/2	+1/2
Δ^0	udd	$\frac{1}{\sqrt{3}}\epsilon_{abc}\left[2\left(d_a^T C\gamma_\mu u_b\right) d_c + \left(d_a^T C\gamma_\mu d_b\right) u_c\right]$	3/2	-1/2
Δ^-	ddd	$\epsilon_{abc}\left(d_a^T C\gamma_\mu d_b\right) d_c$	3/2	-3/2

Odd under exchange of $u \leftrightarrow d$

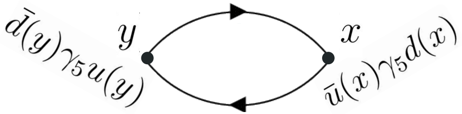
Even under exchange of $u \leftrightarrow d$

Example of spin 3/2

Wick Contractions

Now we need to construct correlation functions $C(t) \equiv \langle \psi(t)\psi^\dagger(0) \rangle$ of interpolating fields

We do this via Wick contractions. Example for the pion:



$$\langle \psi_{\pi^+}(y)\psi^\dagger_{\pi^+}(x)\rangle = \langle \bar{d}(y)\gamma_5 u(y)\bar{u}(x)\gamma_5 d(x)\rangle =$$

$$= \quad (\gamma_5)_{\alpha\beta}(\gamma_5)_{\alpha'\beta'}\langle \bar{d}(y)^a_\alpha u(y)^a_\beta \bar{u}(x)^b_{\alpha'} d(x)^b_{\beta'}\rangle$$

$$= \quad -(\gamma_5)_{\alpha\beta}(\gamma_5)_{\alpha'\beta'}\langle d(x)^b_{\beta'}\bar{d}(y)^a_\alpha\rangle\langle u(y)^a_\beta \bar{u}(x)^b_{\alpha'}\rangle$$

$$= \quad -(\gamma_5)_{\alpha\beta}(\gamma_5)_{\alpha'\beta'} G_d(x;y)^{ba}_{\beta'\alpha} G_u(y;x)^{ab}_{\beta\alpha'}$$

Quark propagator

$$= \quad -\mathrm{Tr}\left[\gamma_5 G_d(x;y)\gamma_5 G_u(y;x)\right]$$

Steps in Wick contractions:

1. Explicitly write position, spin and color indices.
2. Construct all possible pairs of quark-antiquark and multiply by -1 for every commutation of quarks.
3. Write in terms of propagators and recombine indices, if possible.

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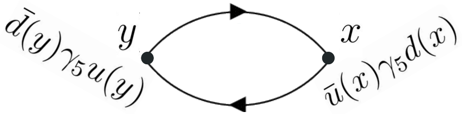

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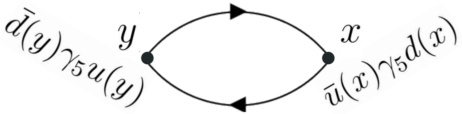

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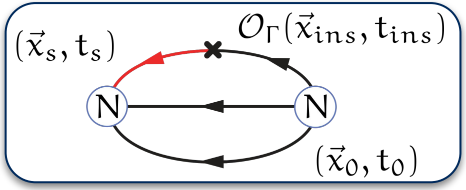

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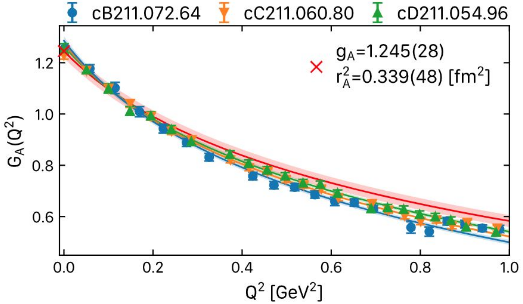


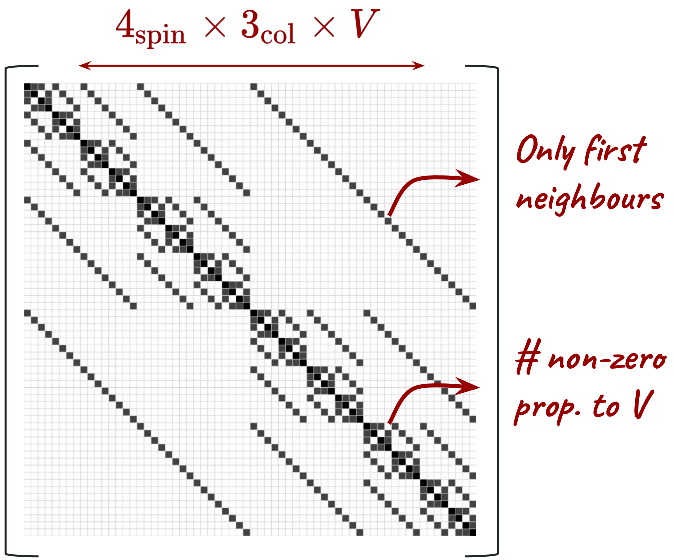
Fermions on the Lattice

$$\underbrace{\langle \psi_j \bar\psi_i \rangle}_{G} = \frac{1}{Z}\int \mathcal{D}[U]\mathcal{D}[\psi\bar\psi]\, \psi_j\bar\psi_i\, e^{-S_{YM}(U)-\bar\psi D\psi}$$

$$= \frac{1}{Z}\int \mathcal{D}[U]\, D^{-1}_{ji}\, \det D\, e^{-S_{YM}(U)}$$

with $\quad D \equiv D(U,\mu_f) \xrightarrow[a\to 0]{} (i\gamma^\mu D_\mu - m_f)$

- Many possible discretizations of the Dirac operator
    - *Wilson, **Twisted-Mass**, Domain-Wall, Overlap, etc.*
- The Dirac operator is a **sparse matrix** (first-neighbors only)
    - *Krylov methods are used to solve:* $\quad D\vec{x} = \vec{b}$
    - e.g. $\quad D\vec{x} = \vec{e}_i \implies x_j = D^{-1}_{ji}$
    - e.g. $\quad D\vec{x} = \vec{\eta} \implies \vec{\eta}^\dagger\vec{x} \approx \mathrm{Tr}(D^{-1})$



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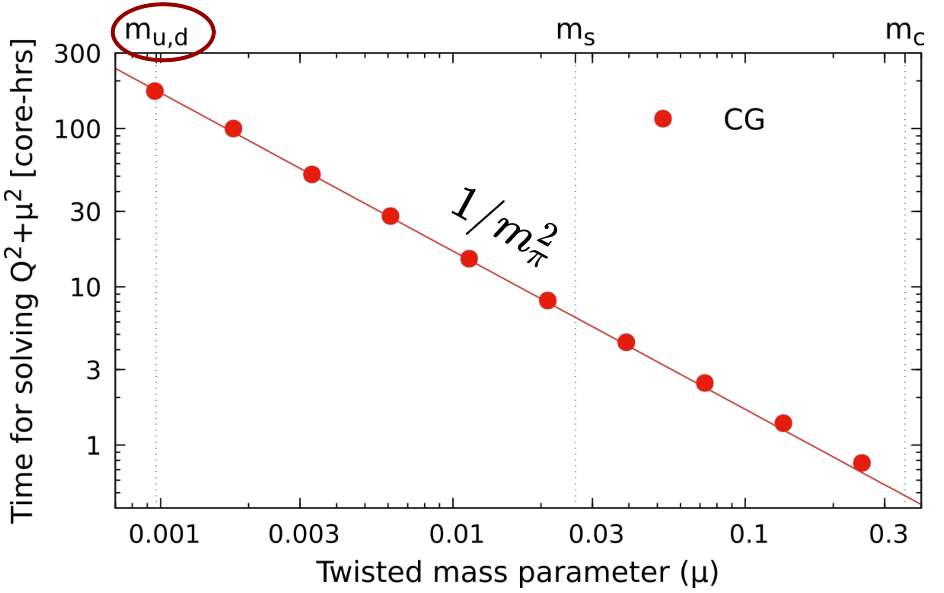
- Dirac operator is singular at *μ=0*
  - *Critical slowing down, e.g.*
  - *Light quark masses 100x more expensive than strange mass*
  - *Common to all discretizations*

~ **Simulations at larger pion mass**

[Solvers: Gustavo Ramirez, Wed.- Fri.]



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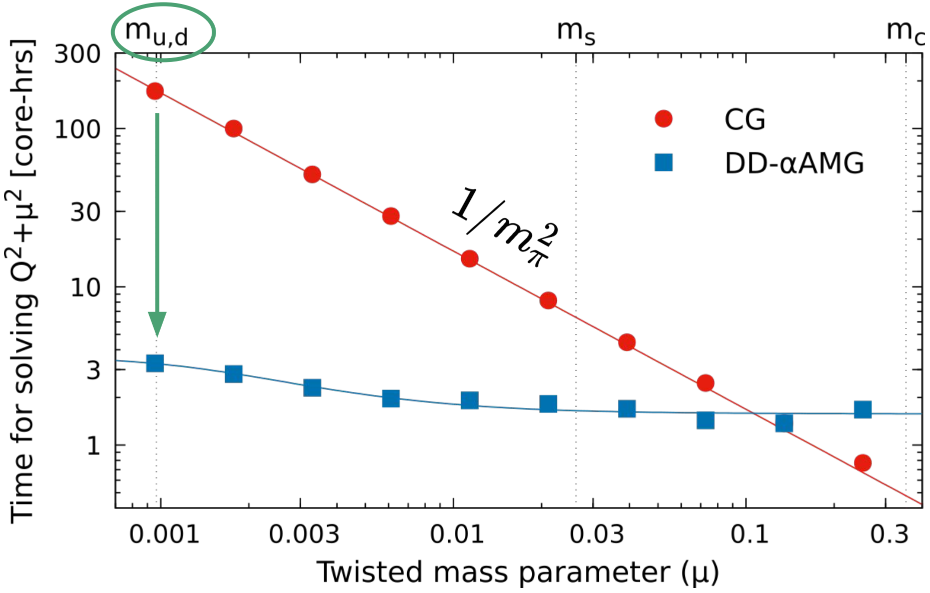
✓ **Resolved by multigrid methods**

[Solvers: Gustavo Ramirez, Wed.- Fri.]



Stochastic propagators

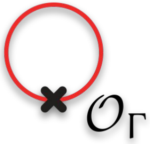
$$\boldsymbol{D\vec{x} = \vec{\eta} \implies \vec{\eta}^\dagger \vec{x} \approx \mathrm{Tr}(D^{-1})}$$

- <u>Hutchinson Trace Estimator:</u>

Let $A \in \mathbb{C}^{D\times D}$ and $v \in \mathbb{C}^D$ be a random vector such that

$$\langle v v^\dagger \rangle = I \quad \Rightarrow \quad \mathrm{Tr}(A) = \langle v^\dagger A v \rangle$$

- Example 1: Quark Loop



$$\Gamma_{\mu\nu}\langle \psi_\nu(x)\bar{\psi}_\mu(x)\rangle = \langle \mathrm{Tr}(\Gamma D^{-1})\rangle_U = \langle \eta^\dagger \Gamma D^{-1}\eta\rangle_{U,\eta}$$
$$= \langle \eta^\dagger \Gamma x\rangle_{U,\eta} \quad \text{with} \quad Dx = \eta$$

  - Usually time-slice stochastic sources for allowing correlation in time

- Example 2: Pion two-point functions

$$\langle \psi_{\pi^+}(y)\psi^\dagger_{\pi^+}(x)\rangle = \langle \bar{d}(y)\gamma_5 u(y)\bar{u}(x)\gamma_5 d(x)\rangle =$$
$$= -\mathrm{Tr}\left[\gamma_5 G_d(x;y)\gamma_5 G_u(y;x)\right]$$

  - γ_5 - hermiticity: $\gamma_5 D \gamma_5 = D^\dagger$ (holds also for the inverse)

$$= -\mathrm{Tr}\left[G_u^\dagger(y;x) G_u(y;x)\right]$$

  - and using time-slice stochastic source in *t="0"*:

$$C(t) = \langle \psi_{\pi^+}(t)\psi_{\pi^+}(0)\rangle = \langle x^\dagger(t)x(t)\rangle_{U,\eta(0)}$$

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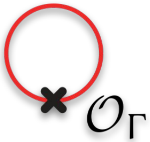

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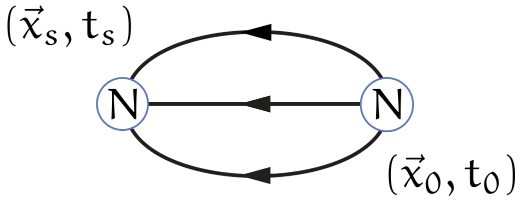
Point-to-all propagators

$$D\vec{x} = \vec{e}_i \implies x_j = D^{-1}_{ji}$$

Or we can just propagate from a single point to all.



- **Disadvantage:** compared to stochastic sources we do not exploit volume-average over the spatial volume, but use only one point.
- **Advantage:** any momentum can be inserted at the source!

$$\langle N(\vec{p}\,', t_s) N(\vec{p}, t_0)\rangle = \sum_{x_0, x_s} e^{i\vec{p}\,'\vec{x}_s} e^{i\vec{p}\vec{x}_0} \langle N(\vec{x}_s, t_s) N(\vec{x}_0, t_0)\rangle$$

if $N(\vec{x}_0, t_0)$ *only defined in* $\vec{x}_0$

$$= e^{i\vec{p}\vec{x}_0} \sum_{x_s} e^{i\vec{p}\,'\vec{x}_s} \langle N(\vec{x}_s, t_s) N(\vec{x}_0, t_0)\rangle$$

$$= e^{i\vec{p}\vec{x}_0} \langle N(\vec{p}\,', t_s) N(\vec{0}, t_0)\rangle$$

Note on stochastic sources:

while for mesons we use:

$$\langle \xi(\vec{x}) \xi^\dagger(\vec{y})\rangle = \delta_{\vec{x},\vec{y}}$$

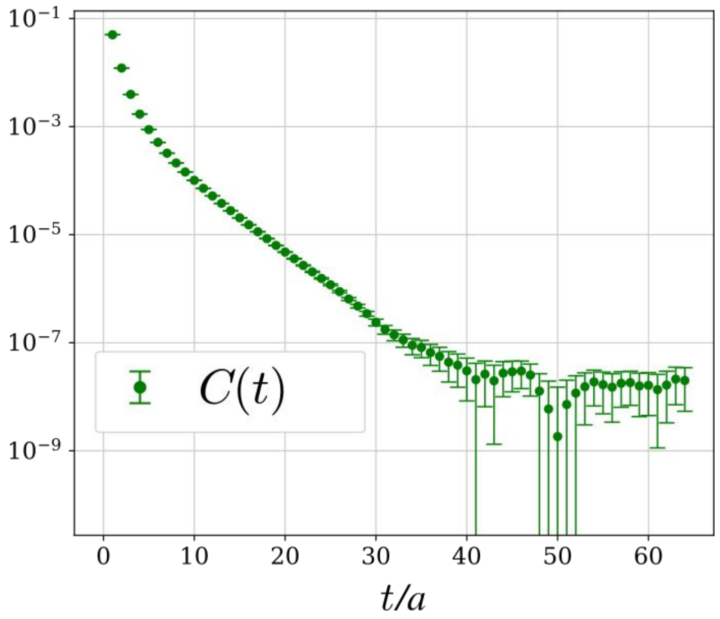
for baryons we should use:

$$\langle \xi(\vec{y}) \xi(\vec{y}\,') \xi(\vec{y}\,'')\rangle = \delta_{\vec{y},\vec{y}\,'} \delta_{\vec{y}\,',\vec{y}\,''}$$

Two-point functions

Let's consider now the case of hadron two-point functions

$$C(t) \equiv \left\langle \psi(t)\psi^\dagger(0) \right\rangle = \sum_{n=0}^{\infty} |\underbrace{Z_n}_{\langle n|\psi\rangle}|^2 e^{-E_n t}$$



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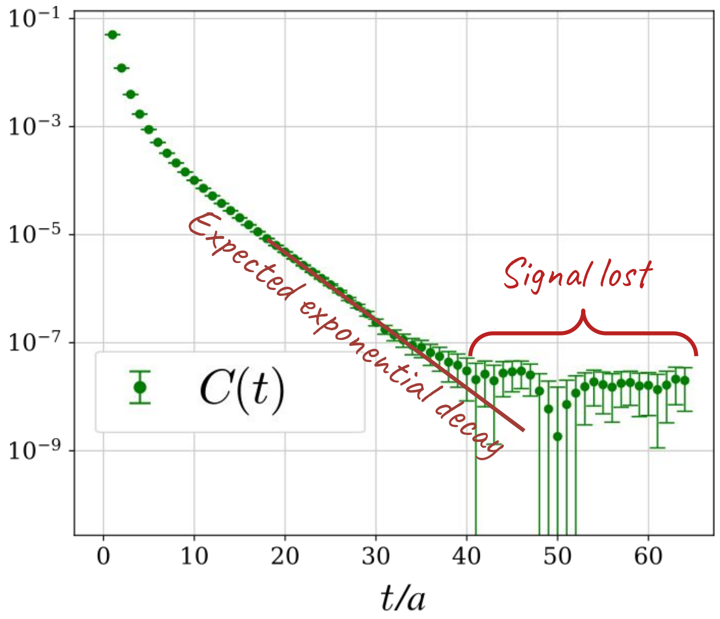
$\langle n|\psi\rangle$

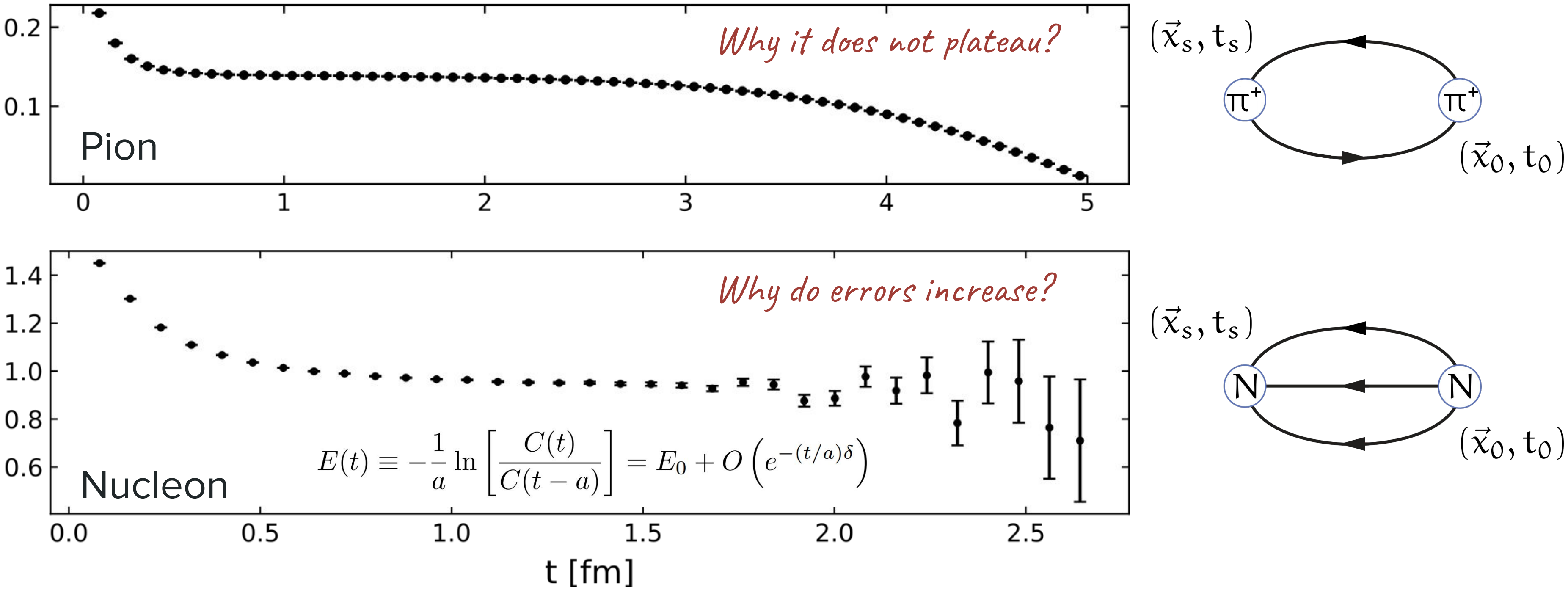
A main use of hadron two-point functions is to extract the energy spectrum of interpolating fields

$$E(t) \equiv -\frac{1}{a}\ln\left[\frac{C(t)}{C(t-a)}\right] = E_0 + O\left(e^{-(t/a)\delta}\right)$$

Effective mass



Pion and Nucleon effective masses



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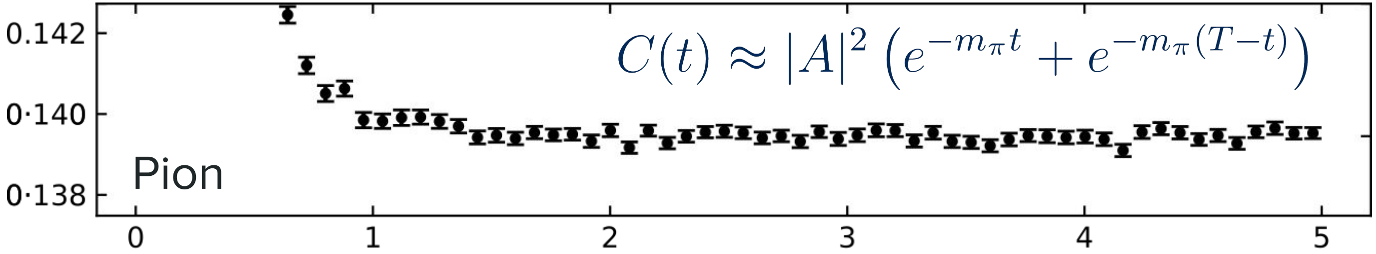

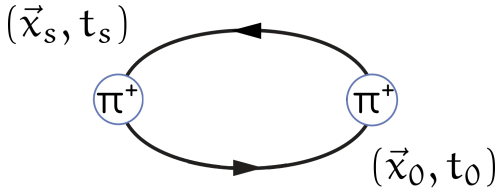

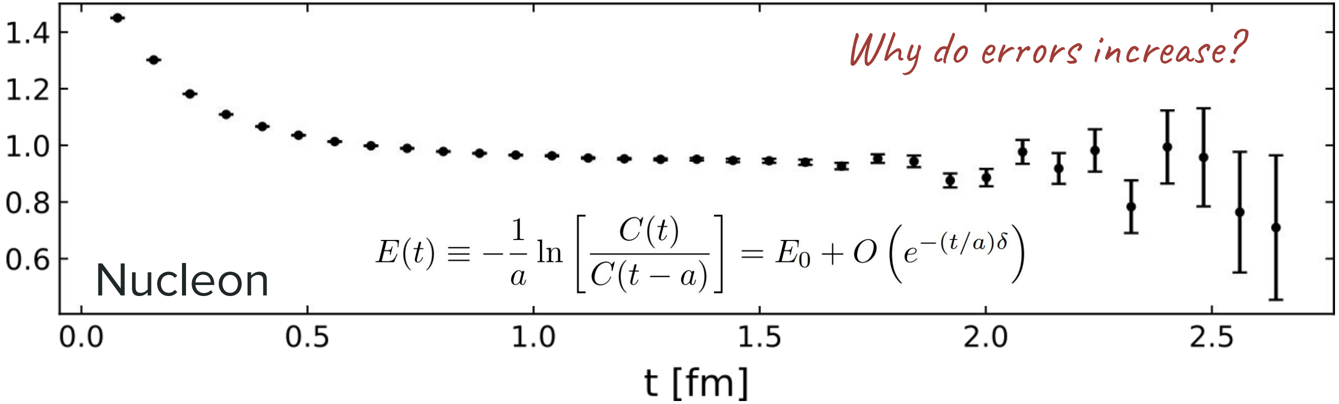

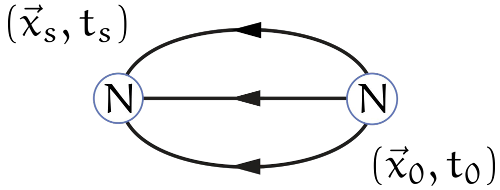

Exponential growth of the error

Why do errors grow exponentially for the nucleon and not for the pion?

- **Parisi-Lapage argument:**

$$\mathrm{Var}(X) = E[X^2] - E[X]^2$$

$$C(t) = \langle \psi^\dagger(t)\psi(0)\rangle$$

$$\sigma_C^2(t) = \langle \psi^\dagger(0)\psi(t)\psi^\dagger(t)\psi(0)\rangle - \langle \psi^\dagger(t)\psi(0)\rangle^2$$

$$\frac{\sigma_C(t)}{C(t)} = \sqrt{\frac{\langle \psi^\dagger(0)\psi(t)\psi^\dagger(t)\psi(0)\rangle}{\langle \psi^\dagger(t)\psi(0)\rangle^2} - 1}$$

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at large t

$$\approx \sqrt{\frac{|B|^2 e^{-tE_{0,C^2}}}{|A|^4 e^{-2tE_{0,C}}} - 1}$$

$$\frac{\sigma_C(t)}{C(t)} \propto e^{t(E_{0,C} - \frac{1}{2}E_{0,C^2})}$$

Relative error [in most cases] increases exponentially in t since

$$E_{0,C^2} \leq 2E_{0,C}$$

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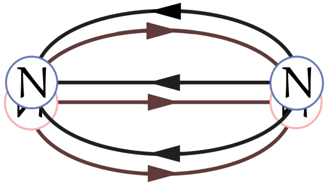
- **Pion:** $\frac{\sigma_C(t)}{C(t)} \propto e^{t\left(m_\pi - \frac{2}{2}m_\pi\right)} = \underline{\text{const.}}$

- **Nucleon:** $\frac{\sigma_C(t)}{C(t)} \propto e^{t\left(m_N - \frac{3}{2}m_\pi\right)}$



Same quantum numbers of 3 pions!

$$\frac{\sigma_C(t)}{C(t)} \propto e^{t\left(E_{0,C} - \frac{1}{2}E_{0,C^2}\right)}$$

Relative error [in most cases] increases exponentially in t since

$$E_{0,C^2} \leq 2E_{0,C}$$

Noise-reduction techniques

How to tackle the exponential-growth of the noise?

by developing noise-reduction techniques!

There is a vast literature on this techniques for the signal-to-noise problem, including many experimental / exploratory / innovative approaches.

Here we will focus on two production-ready techniques:

- Smearing of interpolating fields
- Low-mode averaging (LMA)

See e.g.

"Path integral contour deformations"

[arXiv:2101.12668]
[arXiv:2304.03229]

1st technique: Smearing of interpolating fields

The interpolating fields we have considered are all local, but extended ones would still have the same quantum numbers, e.g.

Added a link to preserve gauge invariance

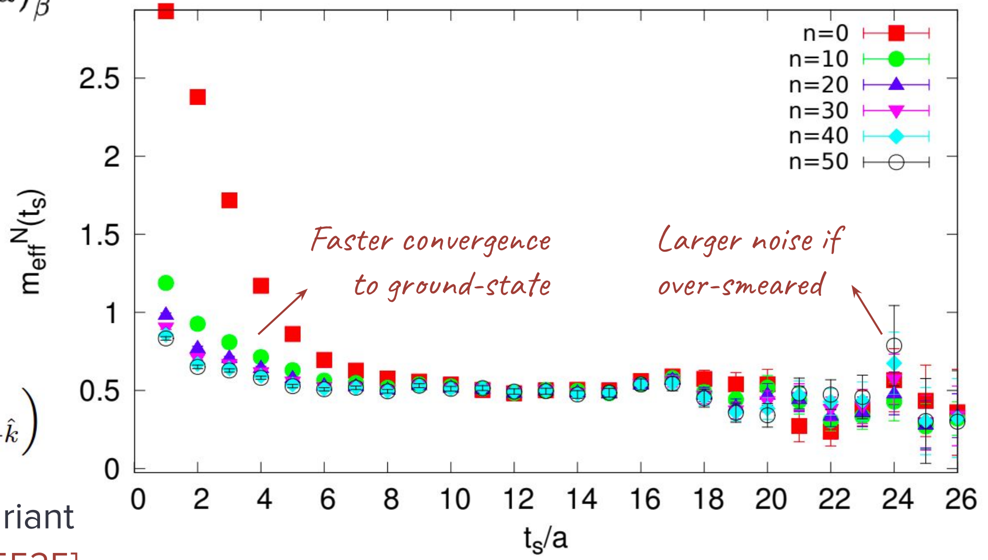
$$\psi_{\text{meson}}(x) = \sum_{a,b,\alpha,\beta} \bar{q}_1\,(x)^a_\alpha\;\Gamma_{\alpha,\beta}\;U^{ab}_\mu(x)\;q_2\,(x+\mu)^b_\beta$$

Wuppertal / Gaussian smearing

Parameters

$$q^{sm}(\vec{x},t) = \sum_{\vec{y}} \Big(\mathbb{1} + \alpha H(\vec{x},\vec{y};U(t))\Big)^n q(\vec{y},t)$$

$$H(\vec{x},\vec{y};U(t)) = \sum_{k=1}^{3}\Big(U_k(\vec{x},t)\delta_{\vec{x},\vec{y}-\hat{k}} + U_k^\dagger(\vec{x}-\hat{k},t)\delta_{\vec{x},\vec{y}+\hat{k}}\Big)$$



In case of boost, momentum smearing is a better variant [arXiv:1602.05525]

2nd technique: Low-Mode Averaging (LMA)

Concept: Low-modes dominate at large distance in correlation functions!

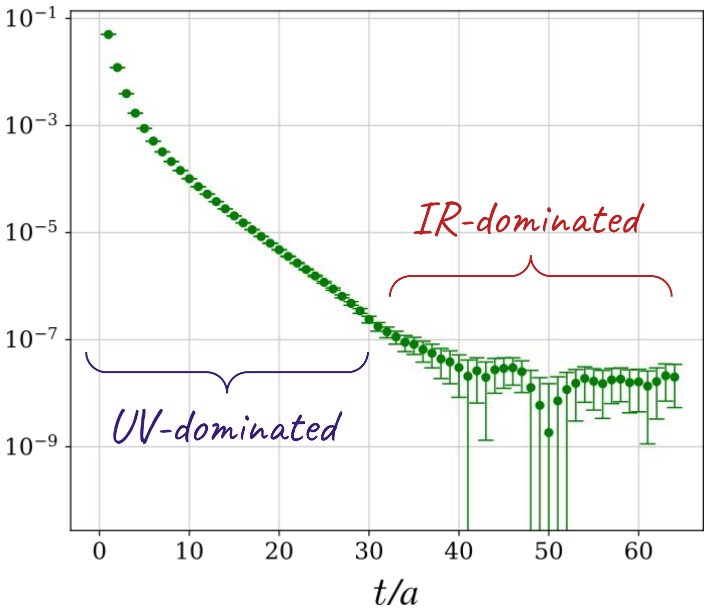
$$S_r(x,y) = \overbrace{|P_{\mathrm{IR}} Q_r^{-1} P_{\mathrm{IR}} \eta(x)\rangle \langle \eta(y)| \gamma_5}^{\text{IR contribution}} + \overbrace{|P_{\mathrm{UV}} Q_r^{-1} P_{\mathrm{UV}} \eta(x)\rangle \langle \eta(y)| \gamma_5}^{\text{UV contribution}}$$

Quark Propagator

$$= \underbrace{\sum_{j=1}^{K} \frac{|v_j(x)\rangle \langle v_j(y)| \gamma_5}{\lambda_j + ir\mu}}_{\text{Computed Exactly}} + \underbrace{\frac{1}{N} \sum_{\eta} |\widetilde{\phi}_r^{\eta}(x)\rangle \langle \eta(y)| \gamma_5 \Big|_{N \gg 1}}_{\text{Computed Stochastically}},$$

- In the correlation function computed stochastically, we replace the IR part with an **exact** knowledge of it

$$C_{\mathrm{LMA}}(t) = C_{\mathrm{stoch.}}(t) - C^{\mathrm{IR}}_{\mathrm{stoch.}}(t) + C^{\mathrm{IR}}_{\mathrm{exact.}}(t)$$



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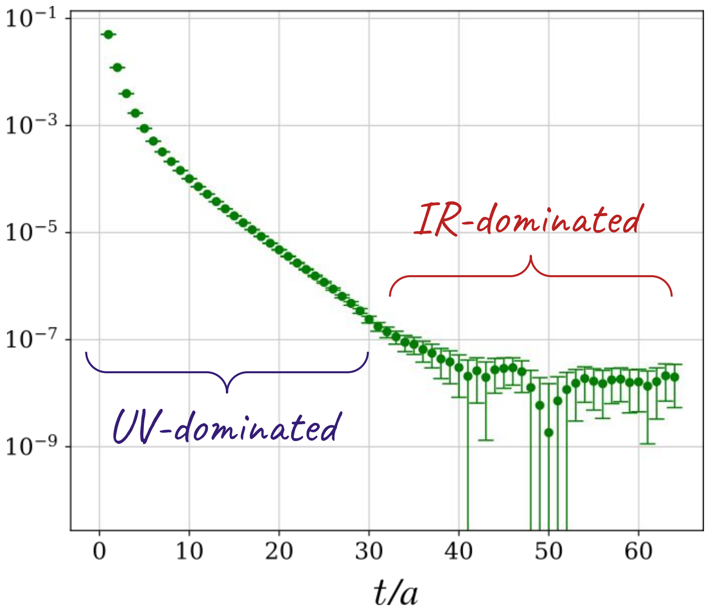

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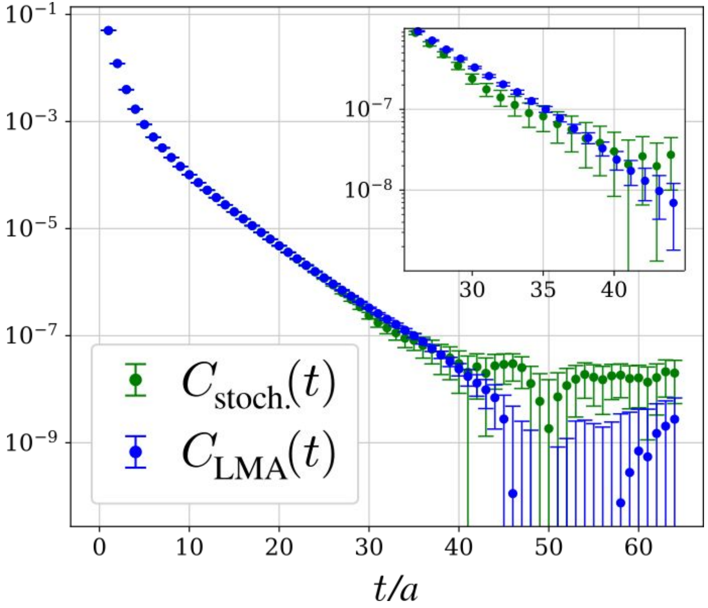
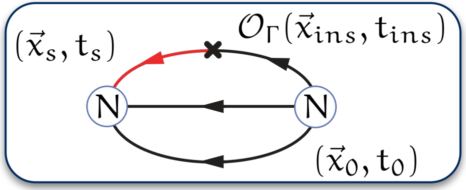


Topics covered in this talk

- Basic concepts:
  - ✔ Correlation functions
  - ✔ Interpolating fields
  - ✔ Wick contractions



- Implementation:
  - ✔ Fermions on the Lattice
  - ✔ Stochastic and point sources
  - ✔ Two-point functions
  - ✔ Noise-reduction techniques

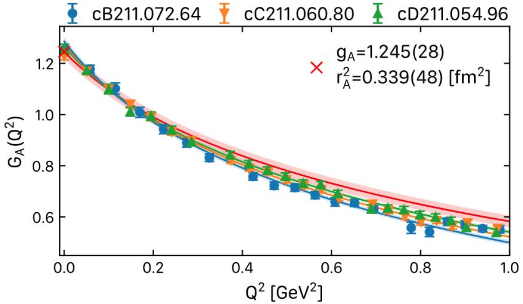
[GPUs: Mathias Wagner, Tue.- Thu.]

[Solvers: Gustavo Ramirez, Wed.- Fri.]

- Nucleon structure:
  - ○ Three-point functions
  - ○ Excited State Contaminations
  - ○ Extraction of Matrix elements

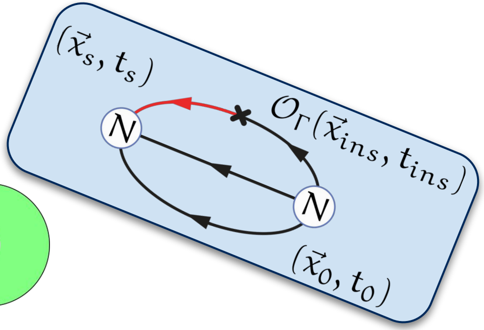
[Data analysis:
Christian Hoelbling, Mon.- Tue.]

[Scattering and resonances:
Fernando Romero-López, Fri.]



Nucleon matrix elements

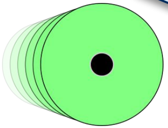
Nucleon matrix elements relate to moments of PDFs



Unpolarized = Vector struct.

$$\mathcal{O}_V^{\mu\mu_1\mu_2\ldots\mu_n} = \bar{\psi}\gamma^{\{\mu}iD^{\mu_1}iD^{\mu_2}\ldots iD^{\mu_n\}}\psi$$

$$\langle 1\rangle_{u-d} = g_V\,, \quad \langle x\rangle_{u-d}, \quad \ldots$$



Helicity = Axial struct.

$$\mathcal{O}_A^{\mu\mu_1\mu_2\ldots\mu_n} = \bar{\psi}\gamma_5\gamma^{\{\mu}iD^{\mu_1}iD^{\mu_2}\ldots iD^{\mu_n\}}\psi$$

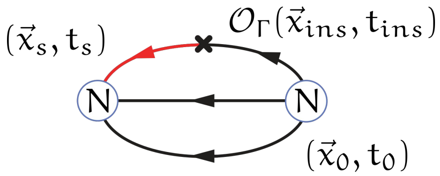
$$\langle 1\rangle_{\Delta u-\Delta d} = g_A, \quad \langle x\rangle_{\Delta u-\Delta d}, \quad \ldots$$

Transverse = Tensor struct.

$$\mathcal{O}_T^{\nu\mu\mu_1\mu_2\ldots\mu_n} = \bar{\psi}\sigma^{\nu\{\mu}iD^{\mu_1}iD^{\mu_2}\ldots iD^{\mu_n\}}\psi$$

$$\langle 1\rangle_{\delta u-\delta d} = g_T, \quad \langle x\rangle_{\delta u-\delta d}, \quad \ldots$$

From three-point functions to matrix elements



Three-point function *Matrix element*

How to go from $\langle \psi_N(\vec{p}\,', t_\mathrm{s}) | \mathcal{O}(t_\mathrm{ins}) | \psi_N(\vec{p}, 0)\rangle$ to $\langle N(\vec{p}\,') | \mathcal{O} | N(\vec{p})\rangle$?

We focus on the ground-state only:

$$C_\mathrm{3pt}(\vec{p}\,', \vec{p}; t_\mathrm{s}, t_\mathrm{ins}) \approx \langle \psi_N(\vec{p}\,', t_\mathrm{s}) | N(\vec{p}\,', t_\mathrm{s})\rangle e^{-E_N(p')(t_\mathrm{s}-t_\mathrm{ins})} \langle N(\vec{p}\,', t_\mathrm{ins}) | \mathcal{O}(t_\mathrm{ins}) | N(\vec{p}, t_\mathrm{ins})\rangle e^{-E_N(p)\,t_\mathrm{ins}} \langle N(\vec{p}, 0) | \psi_N(\vec{p}, 0)\rangle$$

$$= \langle \psi_N(\vec{p}\,') | N(\vec{p}\,')\rangle \langle N(\vec{p}\,') | \mathcal{O} | N(\vec{p})\rangle \langle N(\vec{p}) | \psi_N(\vec{p})\rangle \; e^{-E_N(p')(t_\mathrm{s}-t_\mathrm{ins}) - E_N(p)\,t_\mathrm{ins}}$$

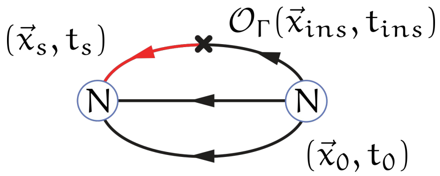
$$C_\mathrm{2pt}(\vec{p}; t_\mathrm{s}) \approx \langle \psi_N(\vec{p}) | N(\vec{p})\rangle \langle N(\vec{p}) | \psi_N(\vec{p})\rangle \; e^{-E_N(p)\,t_\mathrm{s}}$$

$$\langle N(\vec{p}\,') | \mathcal{O} | N(\vec{p})\rangle = \lim_{\substack{t_\mathrm{s}-t_\mathrm{ins}\to\infty \\ t_\mathrm{ins}\to\infty}} \underbrace{\frac{C_\mathrm{3pt}(\vec{p}\,', \vec{p}; t_\mathrm{s}, t_\mathrm{ins})}{\sqrt{C_\mathrm{2pt}(\vec{p}\,'; t_\mathrm{s}) C_\mathrm{2pt}(\vec{p}; t_\mathrm{s})}}_{\text{Cancels the overlaps}} \underbrace{\sqrt{\frac{C_\mathrm{2pt}(\vec{p}\,'; t_\mathrm{s}-t_\mathrm{ins}) C_\mathrm{2pt}(\vec{p}; t_\mathrm{ins})}{C_\mathrm{2pt}(\vec{p}; t_\mathrm{s}-t_\mathrm{ins}) C_\mathrm{2pt}(\vec{p}\,'; t_\mathrm{ins})}}}_{\text{Cancels the residual exponential}}$$

From three-point functions to matrix elements

Three-point function *Matrix element*

How to go from $\langle \psi_N(\vec{p}\,', t_s)|\mathcal{O}(t_{ins})|\psi_N(\vec{p}, 0)\rangle$ to $\langle N(\vec{p}\,')|\mathcal{O}|N(\vec{p})\rangle$?



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$$C_{3pt}(\vec{p}\,', \vec{p}; t_s, t_{ins}) \approx \langle \psi_N(\vec{p}\,', t_s)|\overbrace{N(\vec{p}\,', t_s)\rangle e^{-E_N(p')(t_s - t_{ins})}\langle N(\vec{p}\,', t_{ins})}|\mathcal{O}(t_{ins})|\overbrace{N(\vec{p}, t_{ins})\rangle e^{-E_N(p)\,t_{ins}}\langle N(\vec{p}, 0)}|\psi_N(\vec{p}, 0)\rangle$$

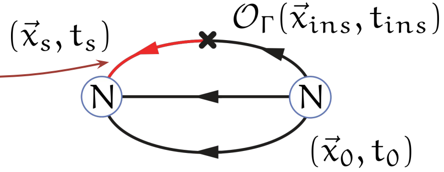
$$= \langle \psi_N(\vec{p}\,')|N(\vec{p}\,')\rangle\langle N(\vec{p}\,')|\mathcal{O}|N(\vec{p})\rangle\langle N(\vec{p})|\psi_N(\vec{p})\rangle\ e^{-E_N(p')(t_s - t_{ins}) - E_N(p)\,t_{ins}}$$

$$C_{2pt}(\vec{p}; t_s) \approx \langle \psi_N(\vec{p})|N(\vec{p})\rangle\langle N(\vec{p})|\psi_N(\vec{p})\rangle\ e^{-E_N(p)\,t_s}$$

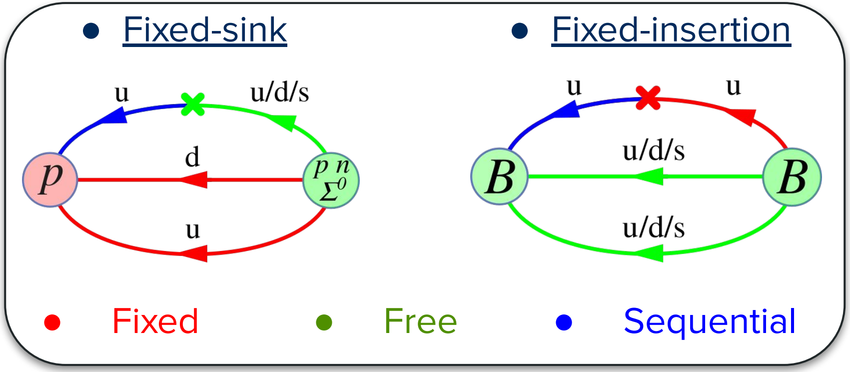
$$\boxed{\langle N(\vec{p}\,')|\mathcal{O}|N(\vec{p})\rangle = \lim_{\substack{t_s - t_{ins}\to\infty \\ t_{ins}\to\infty}} \underbrace{\frac{C_{3pt}(\vec{p}\,', \vec{p}; t_s, t_{ins})}{\sqrt{C_{2pt}(\vec{p}\,'; t_s)C_{2pt}(\vec{p}; t_s)}}}_{\text{Cancels the overlaps}} \underbrace{\sqrt{\frac{C_{2pt}(\vec{p}\,'; t_s - t_{ins})C_{2pt}(\vec{p}; t_{ins})}{C_{2pt}(\vec{p}; t_s - t_{ins})C_{2pt}(\vec{p}\,'; t_{ins})}}}_{\text{Cancels the residual exponential}}}$$

How to compute three-point functions?

Three-point functions require computing a *sequential propagator*.



It can be done in two ways:



- Fixed-sink:
  - Fix sink time t_s
  - Fix sink mom. p'
  - Fix sink interp. field

- Fixed-insertion:
  - Fix ins. time t_{ins}
  - Fix ins. mom. q
  - Fix ins. operator

Fixed-sink:
  - Get any ins. operator
  - Get any ins. mom.
  - Get any source mom. (pt. source)
  - Get multiple source interp. fields

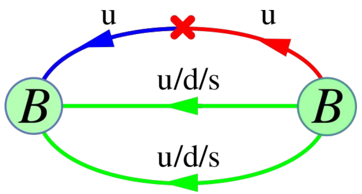
Fixed-insertion:
  - Get any sink interp. field current
  - Get any source interp. fields
  - Get any sink time t_s
  - Get any sink mom.
  - Get any source mom. (pt. source)

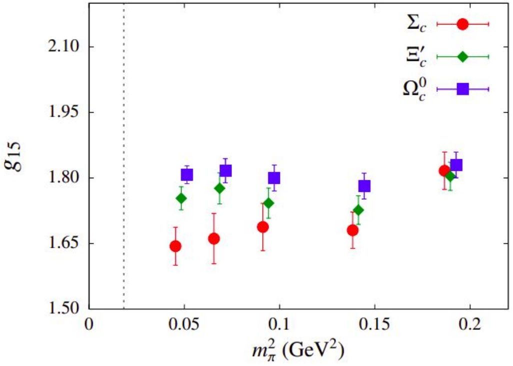
Example of fixed-insertion results

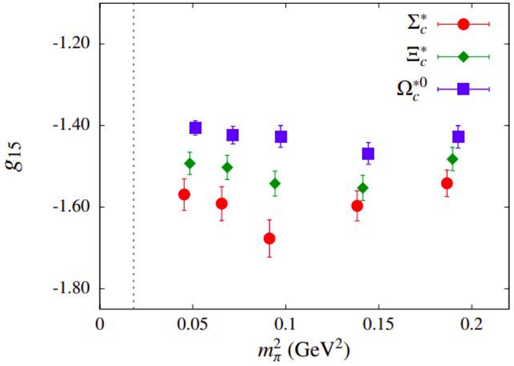
- “Axial charges of hyperons and charmed baryons using N_f=2+1+1 twisted mass fermions”

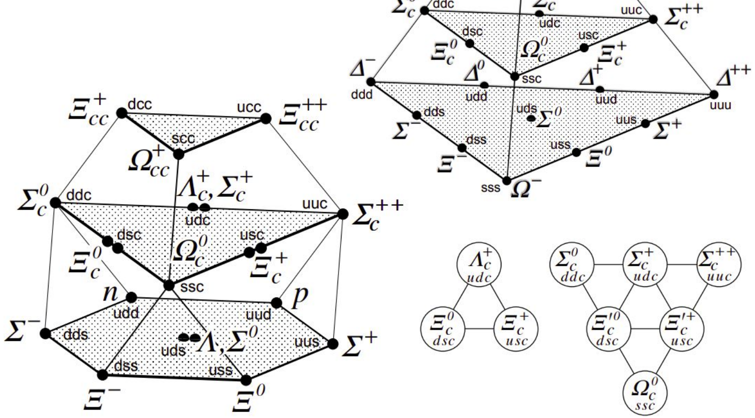
  [arXiv:1606.01650]

  - Isovector *u-d*, *u+d-2s* and *u+d+s-3c* axial charges of 40 baryons
  - One in a kind study:
    - Computed using fixed-insertion
    - i.e. fixed current and momentum transfer
    - Got g_A for any possible baryon!





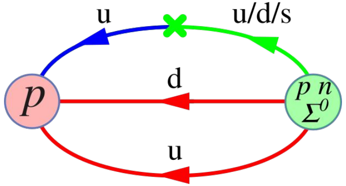


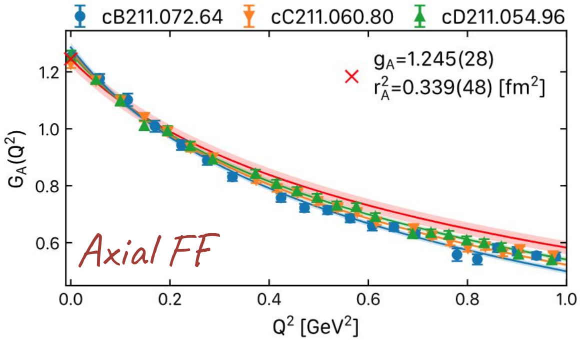


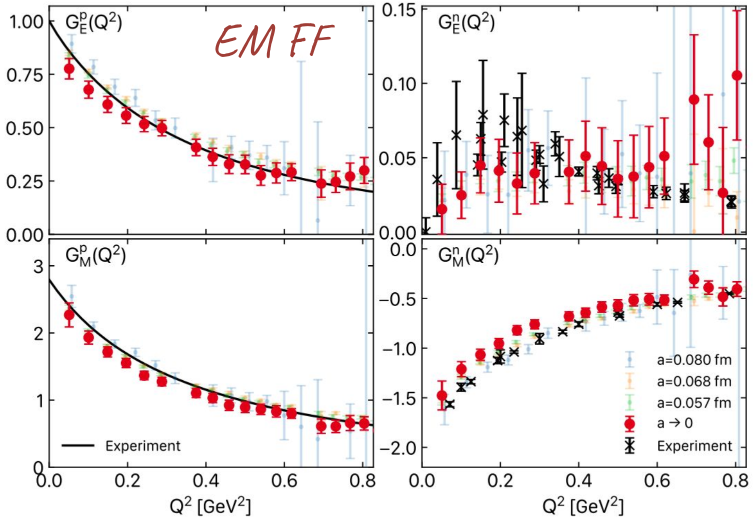
Example of fixed-sink results

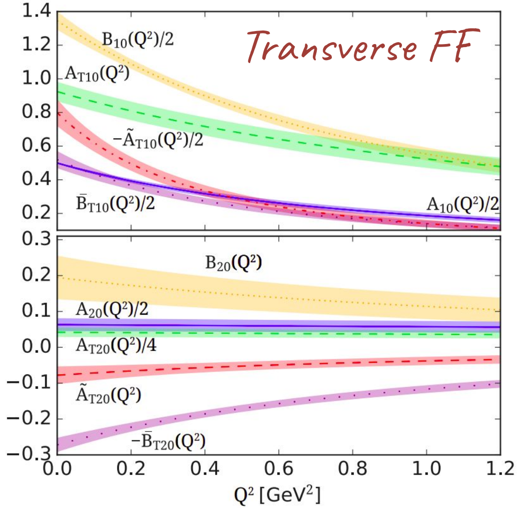
Most studies on nucleon structure uses fixed-sink since allows for a very reach programme.

- <u>Any ins. current/operator:</u> axial, vector, tensor, first and second Mellin moments, etc.
- <u>Any momentum transfer:</u> Form Factors (Q^2-dependence), extrapolation to Q^2=0 ➜ charges/couplings







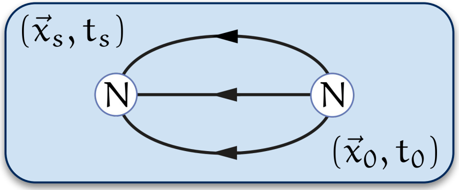


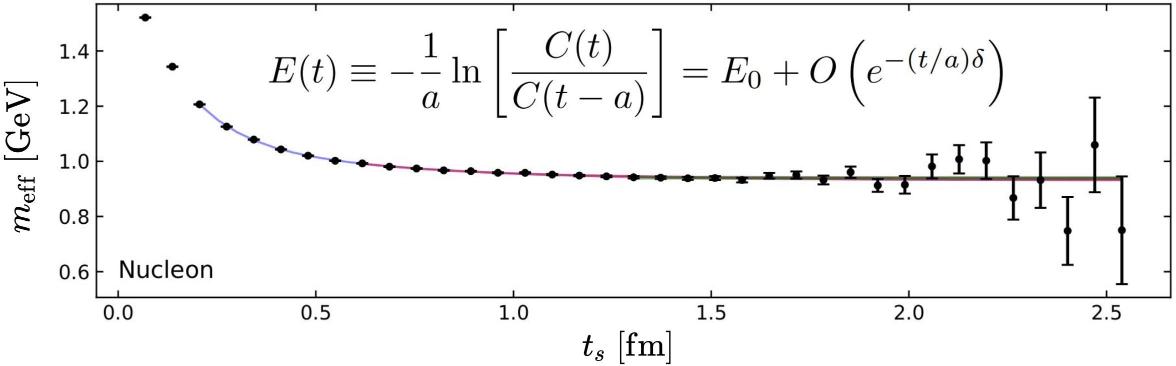
Nucleon two-point functions

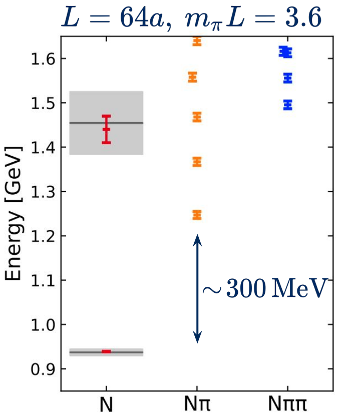
$$G(t_s) = \sum_{\vec{x}} P_0^{\alpha\beta} \langle \bar{\chi}_N^{\beta}(\vec{x}_s, t_s) | \chi_N^{\alpha}(\vec{0}, 0) \rangle = \sum_k c_k e^{-t_s E_k}$$

with $\chi_N^{\alpha}(x) = \epsilon^{abc} u_{\alpha}^{a}(x)[u^b(x) C\gamma_5 d^c(x)]$

- Two-point functions
  - Ground state dominance at large-time limit $G(t_s) = c_0^{-t_s m_N}\Big|_{t_s \to \infty}$
  - Error increases exponentially with t
  - Density of excited states increases with volume







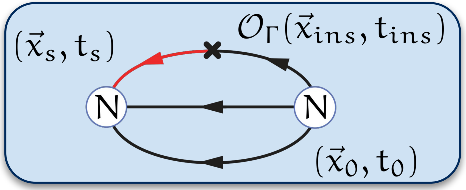
Nucleon three-point functions

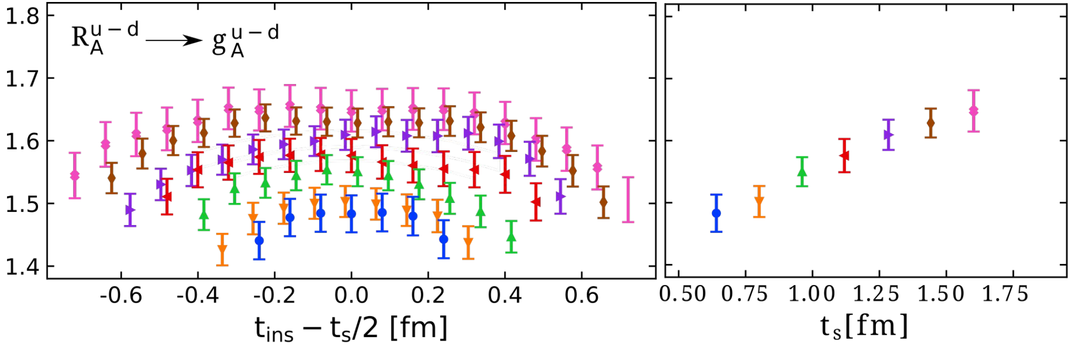
$$G_\Gamma(P;\vec{q};t_s,t_{ins}) = \sum_{\vec{x}_s,\vec{x}_{ins}} e^{-i\vec{q}\cdot\vec{x}_{ins}} P^{\alpha\beta} \langle \bar{\chi}^\beta_N(\vec{x}_s,t_s)|\mathcal{O}_\Gamma(\vec{x}_{ins},t_{ins})|\chi^\alpha_N(\vec{0},0)\rangle$$

suitable projector

e.g. $\mathcal{O}_A(x) = \bar{\psi}(x)\gamma_5\gamma^\mu\psi(x)$

- Three-point functions
  - Ground state at $t_s \to \infty$, $(t_s - t_{ins}) \to \infty$
  - Error increases exponentially with t_s
  - Statistics increased to keep errors constant





×750 configurations

t_s/a	t_s[fm]	n_{src}
8	0.64	1
10	0.80	2
12	0.96	5
14	1.12	10
16	1.28	32
18	1.44	112
20	1.60	128
Nucleon 2pt		477

~30M inversions!

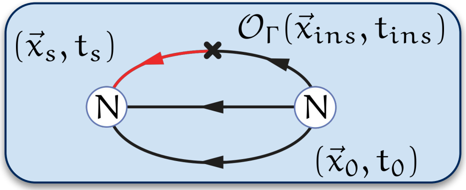
Nucleon three-point functions

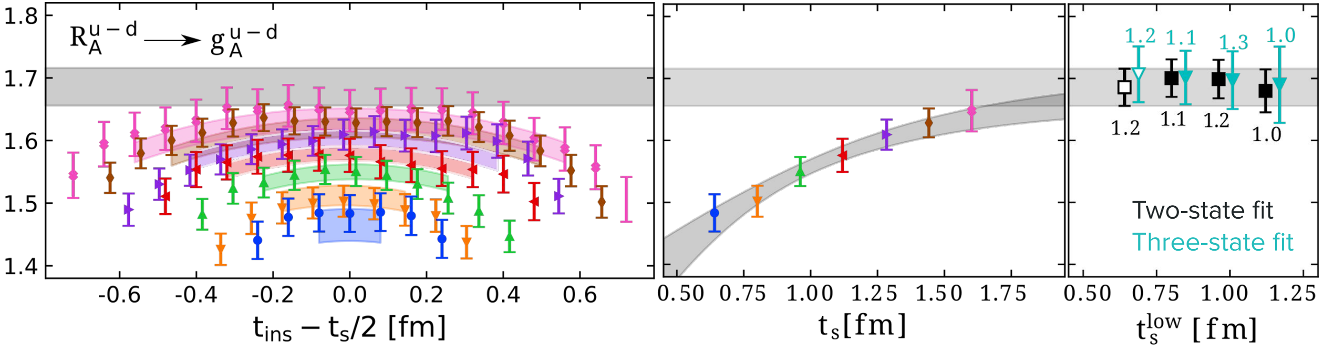
$$G_\Gamma(P;\vec{q};t_s,t_{ins}) = \sum_{\vec{x}_s,\vec{x}_{ins}} e^{-i\vec{q}\cdot\vec{x}_{ins}} P^{\alpha\beta} \langle \bar{\chi}^{\beta}_N(\vec{x}_s,t_s) | \mathcal{O}_\Gamma(\vec{x}_{ins},t_{ins}) | \chi^{\alpha}_N(\vec{0},0) \rangle$$

$$G_\Gamma(t_s,t_{ins}) \simeq A_{00}e^{-m_N t_s} + A_{01}\left(e^{-E_1 t_{ins}} + e^{-E_1 t_s + (E_1 - m_N)t_{ins}}\right) + A_{11}e^{-E_1 t_s}$$

$$G(t) \simeq c_0 e^{-m_N t_s} + c_1 e^{-E_1 t_s}$$

Desired matrix element: $\mathcal{M} = \dfrac{A_{00}}{c_0}$





$\times 750$ configurations

t_s/a	t_s[fm]	n_{src}
8	0.64	1
10	0.80	2
12	0.96	5
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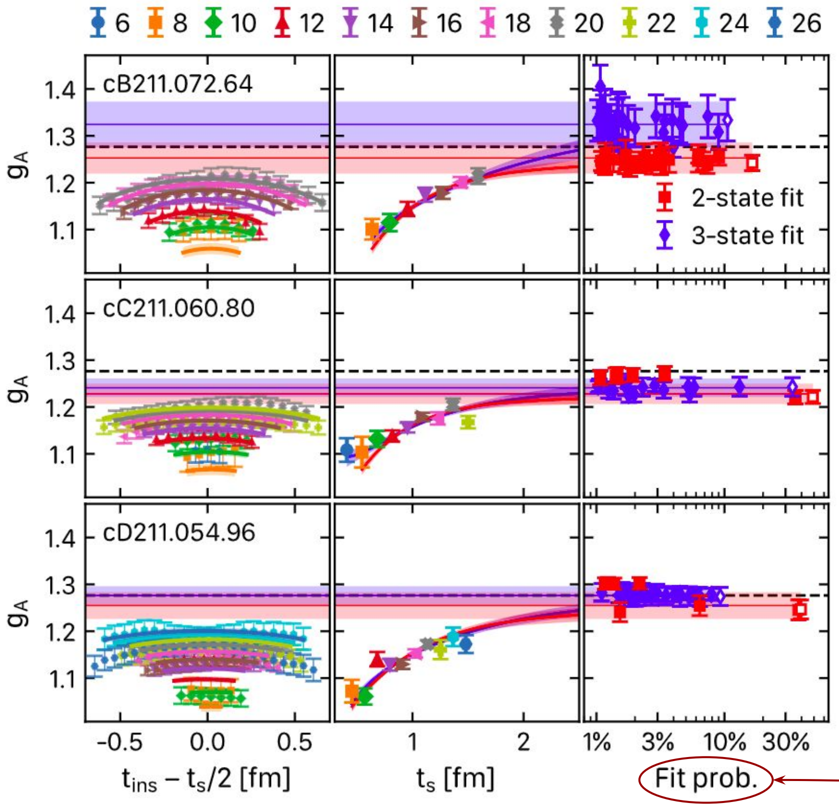
20	1.60	128
Nucleon 2pt		477

~30M inversions!

[C. Alexandrou, S. B., et al. “Nucleon axial, tensor, and scalar charges and σ-terms in lattice QCD”. Phys. Rev., D102(5):054517, 2020]

The three ensembles and model averaging



Ensemble	V/a^4	β	a [fm]	m_π [MeV]	$m_\pi L$
cB211.072.64	$64^3 \times 128$	1.778	0.07957(13)	140.2(2)	3.62
cC211.060.80	$80^3 \times 160$	1.836	0.06821(13)	136.7(2)	3.78
cD211.054.96	$96^3 \times 192$	1.900	0.05692(12)	140.8(2)	3.90

cB211.072.64		
750 configurations		
t_s/a	t_s[fm]	n_{src}
8	0.64	1
10	0.80	2
12	0.96	5
14	1.12	10
16	1.28	32
18	1.44	112
20	1.60	128
Nucleon 2pt		477

cC211.060.80		
400 configurations		
t_s/a	t_s[fm]	n_{src}
6	0.41	1
8	0.55	2
10	0.69	4
12	0.82	10
14	0.96	22
16	1.10	48
18	1.24	45
20	1.37	116
22	1.51	246
Nucleon 2pt		650

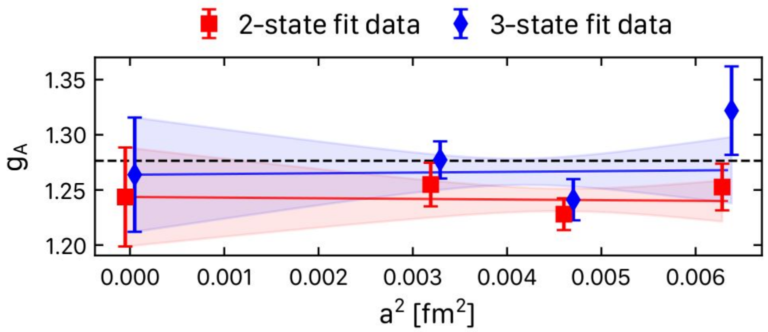
cD211.054.96		
500 configurations		
t_s/a	t_s[fm]	n_{src}
8	0.46	1
10	0.57	2
12	0.68	4
14	0.80	8
16	0.91	16
18	1.03	32
20	1.14	64
22	1.25	16
24	1.37	32
26	1.48	64
Nucleon 2pt		480

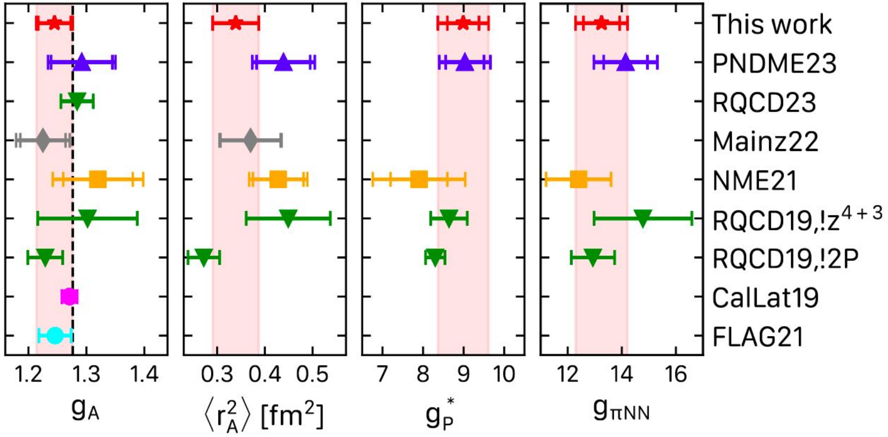
Up to 1.5fm for all ensembles

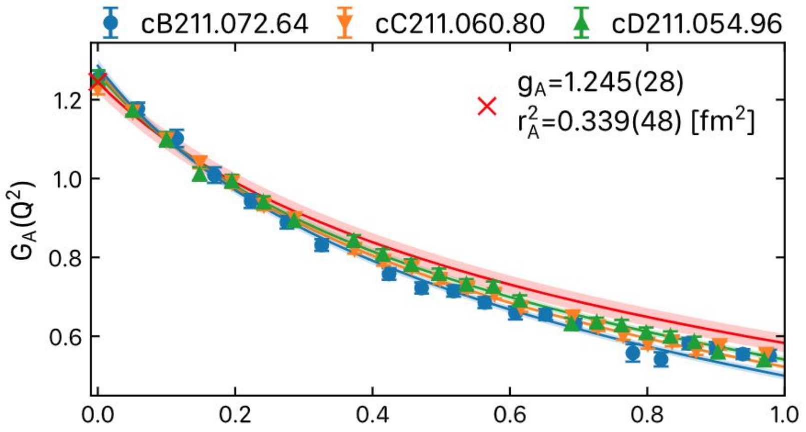
Model average over thousands of fits: $\log(w_i) = -\frac{\chi_i^2}{2} + N_{\mathrm{dof},i}$

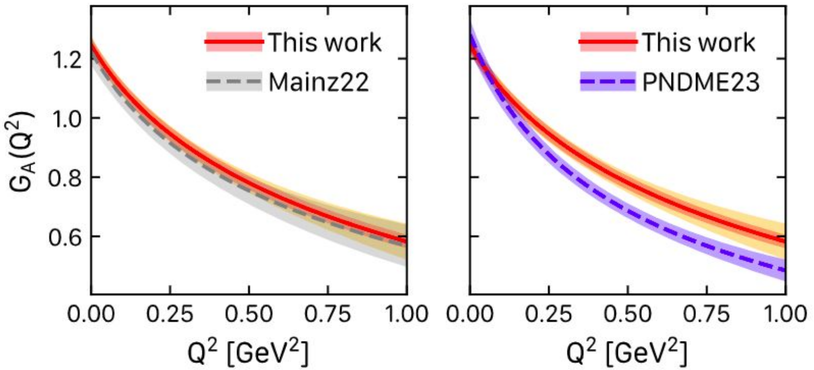
$p_i = \frac{w_i}{Z}$ with $Z = \sum_i w_i$. [E. T. Neil, J. W. Sitison, arXiv:2208.14983]

Continuum limit and comparison with other studies



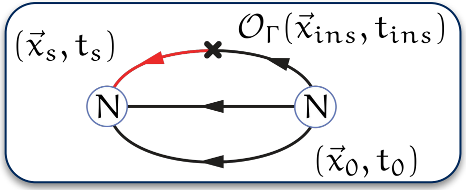






Thank you for your attention!

- Basic concepts:
  - ✔ Correlation functions
  - ✔ Interpolating fields
  - ✔ Wick contractions



- Implementation:
  - ✔ Fermions on the Lattice
  - ✔ Stochastic and point sources
  - ✔ Two-point functions
  - ✔ Noise-reduction techniques

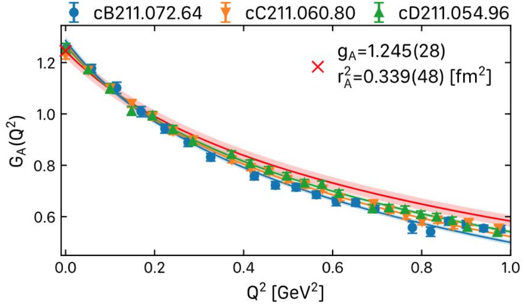
[GPUs: Mathias Wagner, Tue.- Thu.]

[Solvers: Gustavo Ramirez, Wed.- Fri.]

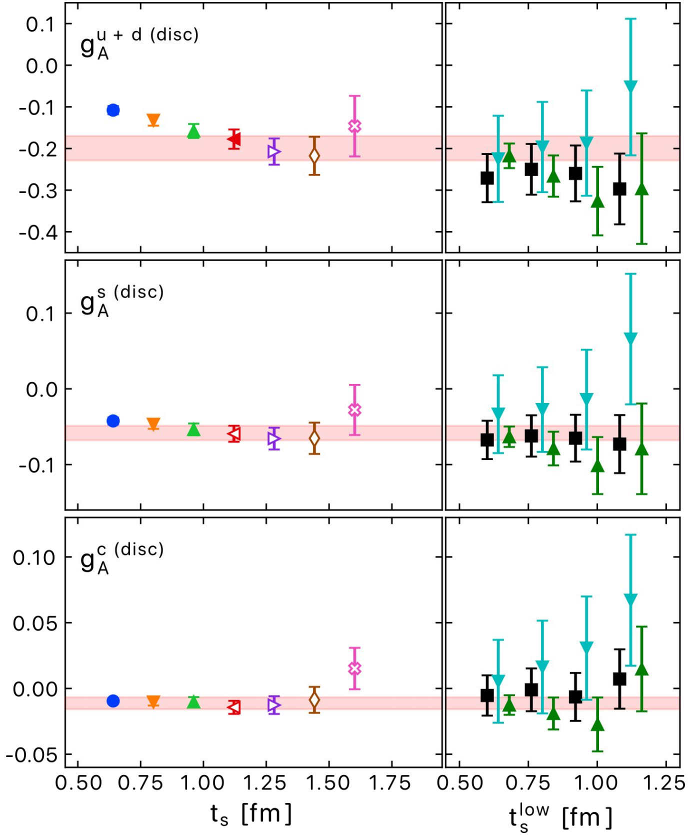
- Nucleon structure:
  - ✔ Three-point functions
  - ✔ Excited State Contaminations
  - ✔ Extraction of Matrix elements

[Data analysis: Christian Hoelbling, Mon.- Tue.]

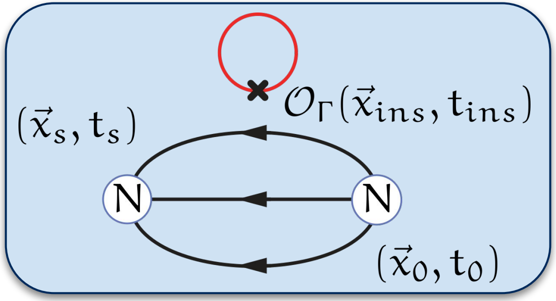
[Scattering and resonances: Fernando Romero-López, Fri.]



Disconnected contributions



- Loop calculations
  - Stochastic sources
  - Hierarchical probing
  - Low-mode deflation
- Disconnected contributions
  - Correlation between loops and two-point



The weak axial-vector matrix element

The transition matrix element of the neutron β-decay is

$$\mathcal{M}(n \to p\, e^- \bar{\nu}_e) = \frac{G_F}{\sqrt{2}} V_{ud} \sum_\mu \underbrace{\langle p(p') | W_\mu | n(p) \rangle}\, L_\mu$$

with

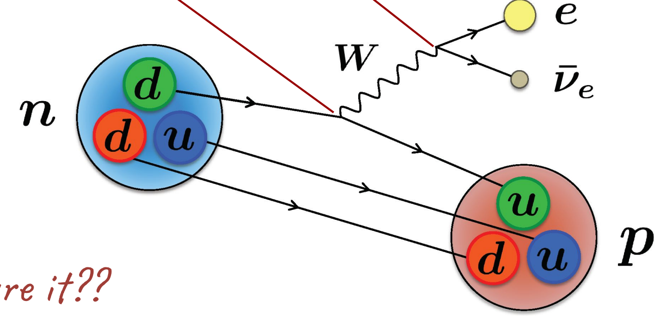
$$W_\mu = V_\mu - A_\mu$$
$$V_\mu = \bar{u}\gamma_\mu d$$
$$A_\mu = \bar{u}\gamma_\mu \gamma_5 d$$

Vector contributions are well determined experimentally from lepton-nucleon scattering

Axial-vector matrix element

$$\langle p(p') | A_\mu | n(p) \rangle$$

How to measure it??



Neutrino-nucleon scattering processes are related to matrix elements at finite momentum transfer.

The axial and induced pseudoscalar FF

Neglecting isospin-breaking effects, transition FFs are equivalent to isovector FFs

$$\langle p(p')|A_\mu|n(p)\rangle \qquad \xrightarrow{u=d} \qquad \langle N(p')|A_\mu^{\text{isov}}|N(p)\rangle$$

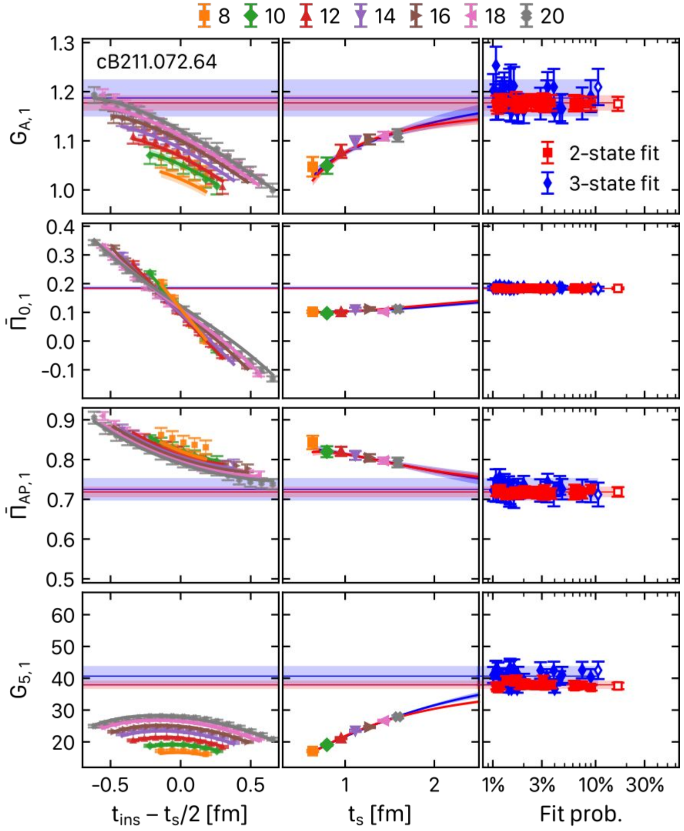
$$A_\mu = \bar{u}\gamma_\mu\gamma_5 d \qquad\qquad A_\mu^{\text{isov}} = \bar{u}\gamma_\mu\gamma_5 u - \bar{d}\gamma_\mu\gamma_5 d$$

Matrix elements are decomposed into Lorentz-invariant form factors (FF)

$$\langle N(p',s')|A_\mu|N(p,s)\rangle = \bar{u}_N(p',s')\left[\gamma_\mu G_A(Q^2) - \frac{Q_\mu}{2m_N}G_P(Q^2)\right]\gamma_5 u_N(p,s),$$

Axial FF *Induced pseudoscalar FF*

… and at finite momentum transfer



$$\Pi_\mu(\Gamma_k;\vec{q}) = \frac{\mathcal{A}^{0,0}_\mu(\Gamma_k,\vec{q})}{\sqrt{c_0(\vec{0})c_0(\vec{q})}}$$

Three-point ground state

Two-point ground state

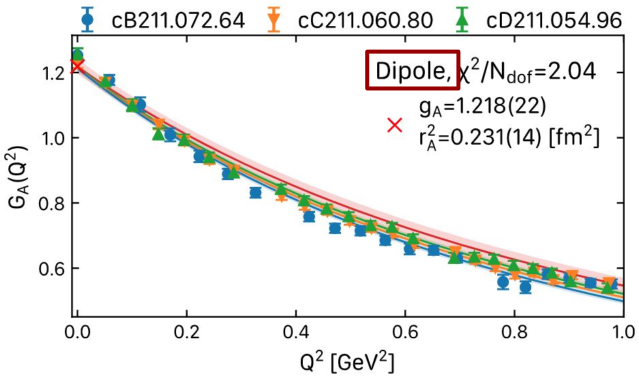
Combined fit of all three-point functions at the same Q^2

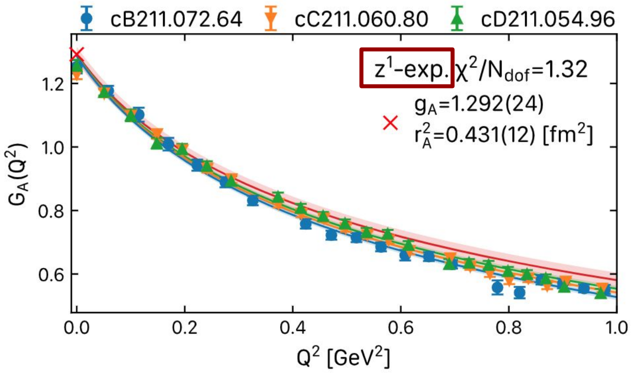
$$\Pi_i(\Gamma_k,\vec{q}) = \frac{i\mathcal{K}}{4m_N}\left[\frac{q_k q_i}{2m_N}G_P(Q^2) - \delta_{i,k}(m_N+E_N)G_A(Q^2)\right]$$

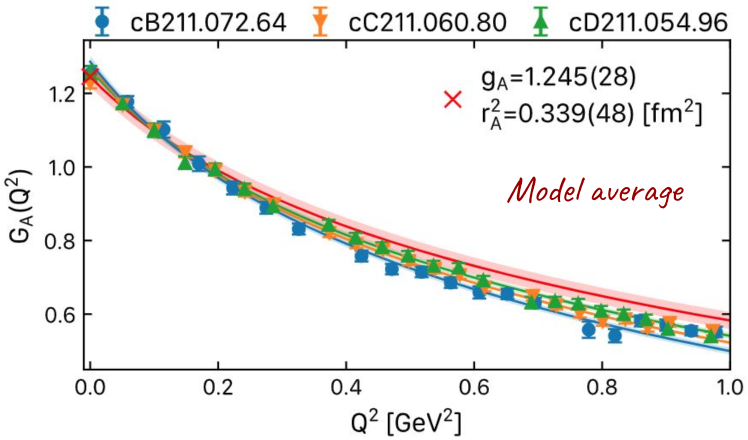
$$\Pi_0(\Gamma_k,\vec{q}) = -\frac{q_k\mathcal{K}}{2m_N}\left[G_A(Q^2) + \frac{(m_N-E_N)}{2m_N}G_P(Q^2)\right]$$

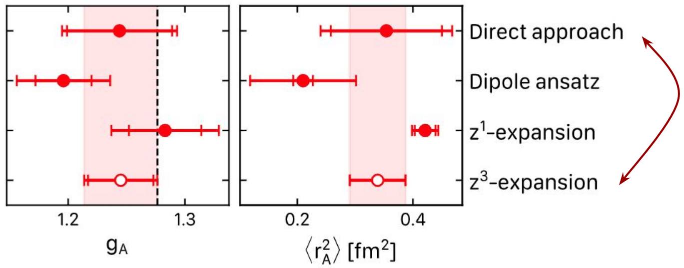
$$\Pi_5(\Gamma_k,\vec{q}) = -\frac{iq_k\mathcal{K}}{2m_N}G_5(Q^2) \longrightarrow \textit{Pseudoscalar FF}$$

Dipole vs z-expansion



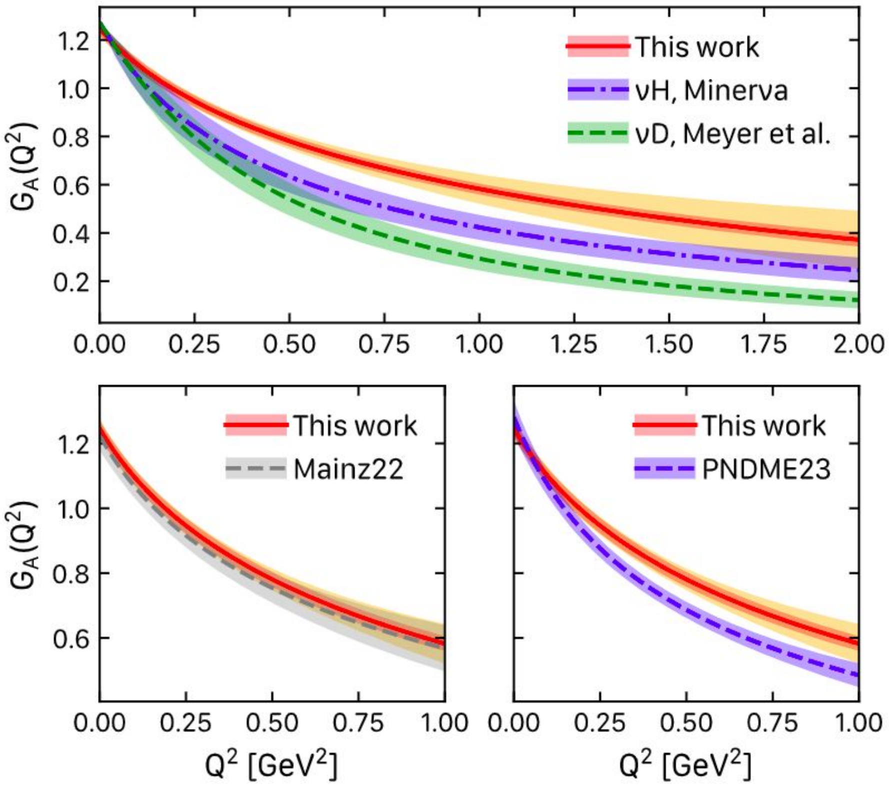






Compatible with the direct approach but smaller error because all information used

Comparison with other studies



- Overall good agreement between recent lattice results and better agreement with the very recent results from Minerva