Introduction to Lattice QCD and Hadron Structure – Numerical Methods



Slides available at http://tiny.cc/ggi-lqcd

intervention of the second sec

{20,21}/02/25 - Galileo Galilei Institute

Lattice QCD Calculations in a Nutshell

$$\langle \mathcal{O}
angle_{a,V,ec{\mu}_f} = rac{1}{\mathcal{Z}}\int \mathrm{D}[U]^V \mathrm{D}[\psi ar{\psi}]^{Vn_f} \mathcal{O}(U,\psi,ar{\psi}) \, e^{-S(a,ec{\mu}_f;\,U,\psi,ar{\psi})}$$



Simulation

• <u>Markov chain Monte Carlo</u> to generate ensembles of gluon-field configurations via importance sampling

$$\langle \mathcal{O}
angle = rac{1}{N} \sum_{i}^{N} O(U_i)$$
 with $p(U) = rac{1}{\mathcal{Z}} \exp(-S(U))$

Production – quantity-specific

<u>Construction of hadron correlation functions</u> on background 2 field configurations:

$$\langle N(p',s')|A_{\mu}|N(p,s)
angle$$

Data analysis – post-processing

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



Part 3

Part 1: Simulations summary

In Lattice Gauge Theories, the expectation value of an observable is defined as

$$\langle \mathcal{O}
angle = rac{1}{\mathcal{Z}} \int \mathrm{D}[U] \, \mathcal{O}(U) \, \exp(-S(U))$$

Computed via importance sampling and using Markov-chain Monte Carlo (MCMC) methods

$$|\mathcal{O}
angle = rac{1}{N}\sum_{i}^{N}O(U_{i})$$
 with $p(U) = rac{1}{\mathcal{Z}} ext{exp}(-S(U))$

- Requires independent and identically distributed (IID) samples
- State-of-the-art: Hybrid Monte Carlo (HMC) algorithm

$$\langle \mathcal{O}
angle = rac{1}{\mathcal{Z}} \int \mathrm{D}[U] \, \mathrm{D}[p] \, \mathcal{O}(U) \, \exp(-p^2/2 - S(U))$$

10000

1000

100

 au_Q^{int}

• HMC

3

Importance Sampling



1. Uniformly sampling is effective for approximately constant functions...



3. Importance sampling measures more frequently the regions that give more contribution to the integral, achieving faster convergence



2. ... for more complicated functions it requires a **huge number** of samples to reach high precision and accuracy



4. ... **however**, when the sampling distribution and the function to integrate have little overlap, it may introduce bias!

Markov-Chain Monte Carlo

A Markov-chain is a sequence of samples $\phi^{(0)} \rightarrow \phi^{(1)} \rightarrow \cdots \rightarrow \phi^{(t)} \rightarrow \cdots \rightarrow \phi^{(N)}$ $\phi(t) \in \Omega \leftarrow \text{state space}$ whose probability of extraction is given by a transition probability $T(\phi \rightarrow \phi')$

Properties:

- Markovian: $T(\phi \rightarrow \phi')$ only depends on the current (ϕ) and future (ϕ') state
- Time-homogeneous: $T(\phi \rightarrow \phi')$ is constant along the chain, i.e. t-independent
- **Probability density:** $\int D\phi' T(\phi \to \phi') = 1$ and $T(\phi \to \phi') \ge 0$
- Ergodic & Irreducible: $T(\phi \rightarrow \phi') > 0 \quad \forall \phi, \phi' \in \Omega$

A chain is completely specified by the starting distribution $P_0(\phi^{(0)})$ and the transition probability $T(\phi \rightarrow \phi')$

Equilibrium distribution and detailed balance

Theorem: Given an ergodic Markov chain with transition probability **T**, the limit

$$\lim_{t \to \infty} P^{(t)} = \lim_{t \to \infty} T^t P^{(0)} = \Pi \in P_{\Omega}$$

exists, is unique, and is independent on $P^{(0)}$. Moreover, Π is the unique fixed point of the chain,

i.e.
$$(TP) = P \Leftrightarrow P = \Pi$$

Detailed Balance:

A sufficient (but not necessary) condition to define *T* is detailed balance

$$\Pi(\phi')T(\phi' \to \phi) = \Pi(\phi)T(\phi \to \phi')$$

Proof: Integrate on both sides over $\phi \implies \Pi(\phi') = (T\Pi)(\phi')$, which is the fixed point!

A simple way to satisfy detailed balance is

$$T(\phi \to \phi') = P_C(\phi \to \phi')P_A(\phi \to \phi') \quad \text{with} \quad P_A(\phi \to \phi') = \min\left[1, \frac{\Pi(\phi')P_C(\phi' \to \phi)}{\Pi(\phi)P_C(\phi \to \phi')}\right]$$

Algorithm:

- 1. A candidate ϕ' is proposed from ϕ with probability P_C
- 2. ϕ' is accepted as the next step in the chain with probability P_A
- 3. If ϕ' is rejected, then ϕ remains the next element, i.e. it is repeated in the chain
- 4. Repeat 1.-3. for all points in the configuration (sweep) and iterate.

Note: if
$$P_C(\phi \to \phi') = P_C(\phi' \to \phi)$$
 (symmetrical proposal), then $P_A(\phi \to \phi') = \min\left[1, \frac{\Pi(\phi')}{\Pi(\phi)}\right]$

Remarks & Challenges

- Only the relative probabilities $\frac{\Pi(\phi')}{\Pi(\phi)}$ are needed to construct *T*. No need to know the partition function.
- Similarly, Markov chain can be used to compute integrals of ratios only, e.g.

$$\left< \Box \right> = \frac{\int D\phi \ \Pi(\phi) \Box(\phi)}{\int D\phi \ \Pi(\phi)}$$

- The key challenge is to ensure ergodicity.
 - A **T** not ergodic can lead to wrong results and biases!
- can we get here? $x^{(2)} x^{(1)} x^{(4)} x^{(3)}$ and here?

• Autocorrelation...

Autocorrelation

Subsequent states in a Markov chain are correlated (autocorrelation)

$$\sigma^{2}(\overline{\Box}) = \langle \langle (\overline{\Box} - \langle \Box \rangle)^{2} \rangle \rangle = \frac{1}{N^{2}} \sum_{k,l=1}^{N} \langle \langle \Box^{(k)} \Box^{(l)} \rangle \rangle - \langle \Box \rangle^{2} \qquad [\langle \langle \Box^{(k)} \rangle \rangle = \langle \Box \rangle]$$

and this can be rewritten by introducing the *autocorrelation time* τ

$$\sigma^{2}(\overline{\Box}) = \frac{2\tau^{int,\Box} \operatorname{var}(\Box)}{N} \quad \text{with} \quad \operatorname{var}(\Box) = \langle \Box^{2} \rangle - \langle \Box \rangle^{2} ,$$
$$\tau^{int,\Box} = \frac{1}{2} \left[1 + 2\sum_{t=1}^{N-1} \frac{\Gamma^{(\Box)}(t)}{\Gamma^{(\Box)}(0)} \right] \quad \text{, and} \quad \Gamma^{(\Box(t))} = \langle \langle \Box^{(t+i)} \Box^{(i)} \rangle \rangle - \langle \Box \rangle^{2} ,$$





We now do a tutorial on Markov-chain Monte Carlo simulations of a 1-dimensional harmonic oscillator.

The continuum action of the theory is
$$S[x]=\int_0^T dt\left[rac{1}{2}m\dot{x}^2+rac{1}{2}m\omega^2x^2
ight]$$
A possible discretization is $S[x]=\sum_{i=0}^{N-1}\left[rac{m}{2dt}(x_{i+1}-x_i)^2+rac{m\omega^2dt}{2}x_i^2
ight]$

Our goal is to compute the expectation value of the correlator $C(t)=\langle x(t)x(0)
angle$

whose continuum limit is the well known result
$$C(t)=rac{1}{2m\omega}e^{-\omega|t|}$$
 .

For this, we will use the Jupyter Notebook you find at

http://tiny.cc/ggi-lqcd-nb

year of Lattice QCD



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.

$$C(t) \equiv \left\langle \psi(t)\psi^{\dagger}(0) \right\rangle = \left\langle \psi \right| T^{t} \left| \psi \right\rangle + \dots$$

$$e^{-H}$$

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

Correlation Functions



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:

 $\langle n|\psi
angle=0$, 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* \leftrightarrow *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:

$$\psi_{ ext{meson}}(x) = \sum_{a,lpha,eta} ar{q}_1 \ (x)^a_lpha \ \Gamma_{lpha,eta} \ q_2 \ (x)^a_eta$$

- 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:

$$\circ\,\Gamma=\gamma_5~$$
 gives a pseudoscalar meson (like the pion), with $J^P=0^-$

 $\circ \Gamma = \gamma_{\mu}$ gives a vector meson (like the ho-meson), with $J^P = 1^-$

$$\circ \Gamma = 1$$
 gives a scalar meson, with $J^P = 0^+$.

 $\circ \Gamma = \gamma_5 \gamma_\mu$ 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.

Baryon Interpolating Fields

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

$$\psi_{ ext{baryon}}(x) = \epsilon_{abc} \; P_{\pm} \; \Gamma_A \; q_1(x)^a \left(q_2{}^T\!(x)^b \Gamma_B \; q_3(x)^c
ight)$$

• Spin selection:

This gives more precise results

$$J = \frac{1}{2} \rightarrow (\Gamma^A, \Gamma^B) = (\mathbb{1}, C\gamma_5), (\gamma_5, C), \text{ or } (\mathbb{1}, i\gamma_4 C\gamma_5)$$

$$J = \frac{3}{2} \rightarrow (\Gamma^A, \Gamma^B) = (\mathbb{1}, C\gamma_j)$$

- Parity selection: positive and negative parity selected using $P_{\pm} = \frac{1}{2} \left(\mathbbm{1} \pm \gamma_4 \right)$
- Other symmetries:
 - \circ C is the charge conjugation matrix, ensuring the antisymmetry
 - $\circ \epsilon_{abc}$ 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	Ι	I_z		
p	uud	$\epsilon_{abc}\left(u_{a}^{T}C\gamma_{5}d_{b} ight)u_{c}$	1/2	+1/2		
n	udd	$\epsilon_{abc}\left(d_a^T C \gamma_5 u_b ight) d_c$	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 -		Odd under exchange of u \leftrightarrow d
Σ^+	uus	$\epsilon_{abc} \left(u_a^T C \gamma_5 s_b ight) u_c$	1	+1		
Σ^0	uds	$rac{1}{\sqrt{2}}\epsilon_{abc}\left[\left(u_a^T C\gamma_5 s_b ight)d_c+\left(d_a^T C\gamma_5 s_b ight)u_c ight]$	1	0	>	Even under exchange of $u \leftrightarrow d$
Σ^{-}	dds	$\epsilon_{abc}\left(d_a^T C \gamma_5 s_b ight)d_c$	1	-1	J	
Ξ^0	uss	$\epsilon_{abc}\left(s_{a}^{T}C\gamma_{5}u_{b} ight)s_{c}$	1/2	+1/2	-	
Ξ_	dss	$\epsilon_{abc}\left(s_{a}^{T}C\gamma_{5}d_{b} ight)s_{c}$	1/2	-1/2	-)	
Δ^{++}	uuu	$\epsilon_{abc}\left(u_{a}^{T}C\gamma_{\mu}u_{b} ight)u_{c}$	3/2	+3/2		
Δ^+	uud	$rac{1}{\sqrt{3}}\epsilon_{abc}\left[2\left(u_{a}^{T}C\gamma_{\mu}d_{b} ight)u_{c}+\left(u_{a}^{T}C\gamma_{\mu}u_{b} ight)d_{c} ight]$	3/2	+1/2		Example of chin 3/2
Δ^0	udd	$rac{1}{\sqrt{3}}\epsilon_{abc}\left[2\left(d_a^T C\gamma_\mu u_b ight)d_c+\left(d_a^T C\gamma_\mu d_b ight)u_c ight]$	3/2	-1/2		CAMPIE OF SPIRE STE
Δ^{-}	ddd	$\epsilon_{abc}\left(d_a^T C \gamma_\mu d_b ight) d_c$	3/2	-3/2	J	

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 <u>Wick contractions</u>. Example for the pion:

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

- $= (\gamma_5)_{\alpha\beta}(\gamma_5)_{\alpha'\beta'} \langle \bar{d}(y)^a_{\alpha} u(y)^a_{\beta} \bar{u}(x)^b_{\alpha'} d(x)^b_{\beta'} \rangle$
- $= -(\gamma_5)_{\alpha\beta}(\gamma_5)_{\alpha'\beta'} \langle d(x)^b_{\beta'} \bar{d}(y)^a_{\alpha} \rangle \langle u(y)^a_{\beta} \bar{u}(x)^b_{\alpha'} \rangle$
- $= -(\gamma_5)_{\alpha\beta}(\gamma_5)_{\alpha'\beta'}G_d(x;y)^{ba}_{\beta'\alpha}G_u(y;x)^{ab}_{\beta\alpha'}$



Steps in Wick contractions:

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

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



Steps in Wick contractions:

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

Now, follow the same example for the pion two-point function and compute the Wick contractions for the nucleon two-point functions.

The starting point is

$$\left\langle O_{N_{\pm}}(n)_{\alpha} \,\overline{O}_{N_{\pm}}(m)_{\alpha} \right\rangle = - \left\langle \overline{O}_{N_{\pm}}(m)_{\alpha} \,O_{N_{\pm}}(n)_{\alpha} \right\rangle_{F} = - \left\langle \epsilon_{abc} \,\epsilon_{a'b'c'} \left(\overline{u}(m)_{a} \,C\gamma_{5} \,\overline{d}(m)_{b}^{T} \right) \,\overline{u}(m)_{c} \,P_{\pm} \,u(n)_{c'} \left(u(n)_{a'}^{T} \,C\gamma_{5} \,d(n)_{b'} \right) \right\rangle$$

The final result you should arrive to is

= G

Part 3: Fermions on the Lattice

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

- Many possible discretizations of the Dirac operator
 - Wilson, **Twisted-Mass**, Domain-Wall, Overlap, etc.
- The Dirac operator is a **sparse matrix** (first-neighbors only)
 - \circ Krylov methods are used to solve: $Dec{x}=ec{b}$

$$\circ$$
 e.g. $Dec{x}=ec{e}_i \implies x_j=D_{ji}^{-1}$

$$\circ$$
 e.g. $Dec{x}=ec{\eta} \implies ec{\eta}^\daggerec{x}pprox {
m Tr}(D^{-1})$

with
$$D\equiv D(U,\mu_f) \mathop{\longrightarrow}\limits_{a
ightarrow 0} (i\gamma^\mu D_\mu - m_f)$$

 $4_{
m spin} imes 3_{
m col} imes V$
 $Only first$
neighbours

Fermions on the Lattice

$$\langle \psi_j \bar{\psi}_i
angle = rac{1}{Z} \int \mathcal{D}[U] \mathcal{D}[\psi \bar{\psi}] \psi_j \bar{\psi}_i e^{-S_{YM}(U) - \psi D \psi}$$

 $G = rac{1}{Z} \int \mathcal{D}[U] D_{ji}^{-1} \det D e^{-S_{YM}(U)}$

• Dirac operator is singular at $\mu=0$

- Critical slowing down, e.g.
- Light quark masses 100x more expensive than strange mass
- Common to all discretizations
- Simulations at larger pion mass



Fermions on the Lattice

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

with
$$D\equiv D(U,\mu_f)\mathop{\longrightarrow}\limits_{a
ightarrow 0}(i\gamma^\mu D_\mu-m_f)$$

- Dirac operator is singular at $\mu=0$
 - Critical slowing down, e.g.
 - Light quark masses 100x more expensive than strange mass
 - Common to all discretizations
- Resolved by multigrid methods



Stochastic propagators

Hutchinson Trace Estimator:

Let $A \in \mathbb{C}^{D \times D}$ and $v \in \mathbb{C}^{D}$ be a random vector such that $\langle vv^{\dagger} \rangle = I \implies \operatorname{Tr}(A) = \langle v^{\dagger}Av \rangle$

• Example 1: Quark Loop

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

$$Dec{x} = ec{\eta} \implies ec{\eta}^\dagger ec{x} pprox {
m Tr}(D^{-1})$$

• Example 2: Pion two-point functions $\langle \psi_{\pi^+}(y)\psi_{\pi^+}^{\dagger}(x)\rangle = \langle \bar{d}(y)\gamma_5 u(y)\bar{u}(x)\gamma_5 d(x)\rangle =$ $= -\mathrm{Tr}\left[\gamma_5 G_d(x;y)\gamma_5 G_u(y;x)\right]$

 $\circ ~~~ \gamma_5^{}$ - hermiticity: $~~ \gamma_5 D \gamma_5 = D^\dagger$ (holds also for the inverse

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

• 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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• Example 1: Quark Loop

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

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

$$Dec{x} = ec{\eta} \implies ec{\eta}^\dagger ec{x} pprox \mathrm{Tr}(D^{-1})$$

- Example 2: Pion two-point functions $\langle \psi_{\pi^+}(y)\psi_{\pi^+}^{\dagger}(x)\rangle = \langle \bar{d}(y)\gamma_5 u(y)\bar{u}(x)\gamma_5 d(x)\rangle =$ $= -\mathrm{Tr}\Big[\gamma_5 G_d(x;y)\gamma_5 G_u(y;x)\Big]$
 - $\circ ~~\gamma_{\rm 5}$ hermiticity: $~\gamma_5 D \gamma_5 = D^\dagger$ (holds also for the inverse)

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

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

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

Point-to-all propagators

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!

$$\begin{split} \langle N(\vec{p}',t_s)N(\vec{p},t_0)\rangle &= \sum_{x_0,x_s} e^{i\vec{p}'\vec{x}_s} e^{i\vec{p}\cdot\vec{x}_0} \langle N(\vec{x}_s,t_s)N(\vec{x}_0,t_0)\rangle \\ \text{if } N(\vec{x}_0,t_0) \text{ only} &= e^{i\vec{p}\cdot\vec{x}_0} \sum_{x_s} e^{i\vec{p}'\cdot\vec{x}_s} \langle N(\vec{x}_s,t_s)N(\vec{x}_0,t_0)\rangle \\ \text{defined in } \vec{x}_0 &= e^{i\vec{p}\cdot\vec{x}_0} \langle N(\vec{p}',t_s)N(\vec{0},t_0)\rangle \end{split}$$





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



Two-point functions

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

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



The effects of periodicity

The correlator propagating forward is

 $c_f(t) = c_f^0 e^{-mt}$

Enough for large enough masses

The correlator propagating backward is $c_b(t) = c_b^0 e^{-m(T-t)}$

And accounting for all contributions we get

ntributions we get $c_f(t) = c_f^0 \left(e^{-mt} + e^{-m(T+t)} + ... \right)$ Enough for large $= c_f^0 e^{-mt} \times \sum_{n=0}^{\infty} e^{-nmT}$ enough time extent T $= c_f^0 e^{-mt} \frac{1}{1 - e^{-mT}}$ Required for finite temperature simulations

Pion and Nucleon effective masses



Exponential growth of the error

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

• Parisi-Lapage argument:

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

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

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

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

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Exponential growth of the error

• Parisi-Lapage argument:

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

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

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

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

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

$$\begin{aligned} \frac{\sigma_C(t)}{C(t)} \propto \ e^{t(E_{0,C} \ -\frac{1}{2}E_{0,C^2})} \\ \text{Relative error [in most cases]} \\ \text{increases exponentially in t since} \\ \frac{E_{0,C^2} \leq 2E_{0,C} }{ \end{aligned} } \end{aligned}$$



$$\left[\operatorname{Var}(X) = E[X^2] - E[X]^2\right]$$

$$\begin{split} & \left(\frac{\sigma_C(t)}{C(t)} \propto e^{t(E_{0,C} - \frac{1}{2}E_{0,C^2})} \right) \\ & \quad Relative \; error \; [in \; most \; cases] \\ & \quad increases \; exponentially \; in \; t \; since \\ & \quad E_{0,C^2} \leq 2E_{0,C} \end{split} \end{split}$$

35

Exponential growth of the error

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

- **Parisi-Lapage argument:**
 - $C(t) = \langle \psi^{\dagger}(t)\psi(0) \rangle$

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

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

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

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:

- <u>Smearing of interpolating fields</u>
- Low-mode averaging (LMA)

See e.g.	
"Path integral contour deformations"	
[<u>arXiv:2101.12668]</u> [<u>arXiv:2304.03229</u>]	

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
$$q^{sm}(\vec{x},t) = \sum_{\vec{y}} \left(\mathbbm{1} + \alpha H(\vec{x},\vec{y};U(t)) \right)^n q(\vec{y},t) \stackrel{\stackrel{\stackrel{\stackrel{\stackrel{\stackrel{\stackrel}{\rightarrow}}{\rightarrow}}{=}}}{\underset{k=1}{\overset{\stackrel{\stackrel}{\rightarrow}}{=}}} \left(U_k(\vec{x},t)\delta_{\vec{x},\vec{y}-\hat{k}} + U^{\dagger}_k(\vec{x}-\hat{k},t)\delta_{\vec{x},\vec{y}+\hat{k}} \right)$$
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!



UV-dominated

20

30

t/a

40

50

10

 10^{-9}

0

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

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

60

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Tutorial 2: Pion and Nucleon effective masses

Now we will work on Part 2 of the Jupyter Notebook: http://tiny.cc/ggi-lqcd-nb

But first, let's see how we compute and propagate errors via Jackknife resampling.

Tutorial 2: Data analysis

Jackknife Resampling

Given N correlated measurements $X = \{x_1, x_2, \dots, x_N\}$, we construct **jackknife samples** by systematically **removing one data point at a time** and computing the statistic of interest on the reduced dataset.

Step-by-Step Algorithm:

1. Construct jackknife samples, where each sample excludes one data point:

$${ar X}^{(i)} = \{ {ar x}^{(1)}, {ar x}^{(2)}, \dots, {ar x}^{(N)} \}$$

The jackknife estimate of the mean is then:

$$ar{x}^{(i)} = rac{1}{N-1}\sum_{j
eq i} x_j$$

Part 4: E.g. inputs to 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.



The weak axial-vector matrix element

The transition matrix element of the neutron β -decay is

$$\begin{aligned} \mathcal{M}(n \to p \, e^- \bar{\nu}_e) &= \frac{G_F}{\sqrt{2}} \, V_{ud} \sum_{\mu} \langle p(p') | W_{\mu} | n(p) \rangle \, L_{\mu} \\ \end{aligned} \\ \text{with} \quad \begin{aligned} W_{\mu} &= V_{\mu} - A_{\mu} & \text{Vector contributions are well} \\ V_{\mu} &= \bar{u} \gamma_{\mu} d & \text{determined experimentally from} \\ A_{\mu} &= \bar{u} \gamma_{\mu} \gamma_5 d & \text{lepton-nucleon scattering} \end{aligned} \\ \begin{array}{c} \mathbf{M} & \mathbf{M} \\ \mathbf{M} & \mathbf{M} \\ \mathbf{M}$$

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

Nucleon matrix elements

Nucleon matrix elements relate to moments of PDFs

$$d \qquad \mathcal{O}_{\underline{V}}^{\mu\mu_{1}\mu_{2}...\mu_{n}} = \bar{\psi}\gamma^{\{\mu}iD^{\mu_{1}}iD^{\mu_{2}}...iD^{\mu_{n}\}}\psi$$
et. $\langle 1 \rangle_{u-d} = g_{V}, \ \langle x \rangle_{u-d}, \ ...$

$$(\vec{x}_{s}, t_{s})$$

$$(\vec{x}_{s}, t_{s})$$

$$(\vec{x}_{ins}, t_{ins})$$

$$(\vec{x}_{0}, t_{0})$$

`

Helicity
$$\mathcal{O}_{\underline{A}}^{\mu\mu_{1}\mu_{2}...\mu_{n}} = \bar{\psi}\gamma_{5}\gamma^{\{\mu}iD^{\mu_{1}}iD^{\mu_{2}}...iD^{\mu_{n}}\}\psi$$

ial struct. $\langle 1 \rangle_{\Delta u - \Delta d} = g_{A}, \ \langle x \rangle_{\Delta u - \Delta d}, \ ...$

Transverse = Tensor struct.

$$\mathcal{O}_{\mathbf{T}}^{\nu\mu\mu_{1}\mu_{2}...\mu_{n}} = \bar{\psi}\boldsymbol{\sigma}^{\nu\{\mu}iD^{\mu_{1}}iD^{\mu_{2}}...iD^{\mu_{n}\}}\psi$$

$$\langle 1\rangle_{\delta u-\delta d} = g_{T}, \ \langle x\rangle_{\delta u-\delta d}, \ ...$$



From three-point functions to matrix elements



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

$$\langle N(\vec{p}') | \mathcal{O} | N(\vec{p}) \rangle = \lim_{\substack{t_{\rm s} - t_{\rm ins} \to \infty \\ t_{\rm ins} \to \infty}} \frac{C_{\rm 3pt}(\vec{p}', \vec{p}; t_{\rm s}, t_{\rm ins})}{\sqrt{C_{\rm 2pt}(\vec{p}'; t_{\rm s})C_{\rm 2pt}(\vec{p}; t_{\rm s})}} \sqrt{\frac{C_{\rm 2pt}(\vec{p}'; t_{\rm s} - t_{\rm ins})C_{\rm 2pt}(\vec{p}; t_{\rm ins})}{C_{\rm 2pt}(\vec{p}; t_{\rm s} - t_{\rm ins})C_{\rm 2pt}(\vec{p}'; t_{\rm ins})}}$$

$$Cancels the overlaps \qquad Cancels the residual exponential$$

From three-point functions to matrix elements



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

$$\langle N(\vec{p}') | \mathcal{O} | N(\vec{p}) \rangle = \lim_{\substack{t_{\rm s} - t_{\rm ins} \to \infty \\ t_{\rm ins} \to \infty}} \frac{C_{\rm 3pt}(\vec{p}', \vec{p}; t_{\rm s}, t_{\rm ins})}{\sqrt{C_{\rm 2pt}(\vec{p}'; t_{\rm s})C_{\rm 2pt}(\vec{p}; t_{\rm s})}} \sqrt{\frac{C_{\rm 2pt}(\vec{p}'; t_{\rm s} - t_{\rm ins})C_{\rm 2pt}(\vec{p}; t_{\rm ins})}{C_{\rm 2pt}(\vec{p}'; t_{\rm ins})C_{\rm 2pt}(\vec{p}'; t_{\rm ins})}}$$

$$Cancels the overlaps \qquad Cancels the residual exponential$$

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*'
- $\circ~$ Fix sink interp. field
- $\circ~$ Get any ins. operator
- $\circ~$ Get any ins. mom.
- Get any source mom. (pt. source)
- Get multiple source interp. fields





- Fixed-insertion:
- Fix ins. time t_{ins}
- Fix ins. mom. q
- Fix ins. operator
- $\circ~$ Get any sink interp. field current
- $\circ~$ Get any source interp. fields
- Get any sink time t_{s}
- Get any sink mom.
- $\circ~$ 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"
 - Isovector *u-d*, *u+d-2s* and *u+d+s-3c* axial charges of <u>40 baryons</u>
 - One in a kind study:
 - Computed using fixed-insertion
 - i.e. fixed current and momentum transfer
 - Got g_A for any possible baryon!





[arXiv:1606.01650]

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 $Q^2=0 \rightarrow$ charges/couplings



Nucleon two-point functions

$$G(t_s) = \sum_{ec x} P_0^{lphaeta} \langle ar{\chi}_N^eta (ec{x}_{ ext{s}}, t_{ ext{s}}) | \chi_N^lpha (ec{0}, 0)
angle = \sum_k c_k e^{-t_s E_k}$$

- Two-point functions
 - \circ Ground state dominance at large-time limit $\left. G(t_s) = c_0^{-t_s m_N}
 ight|_{t_s o \infty}$

with $\chi^lpha_N(x)=\epsilon^{abc}u^a_lpha(x)[u^b(x)C\gamma_5d^c(x)]$

- \circ Error increases exponentially with t
- Density of excited states increases with volume







Nucleon three-point functions

$$\begin{array}{l} G_{\Gamma}(P;\vec{q};t_{\mathrm{s}},t_{\mathrm{ins}}) = \sum_{\vec{x}_{\mathrm{s}},\vec{x}_{\mathrm{ins}}} e^{-i\vec{q}\cdot\vec{x}_{\mathrm{ins}}} P^{\alpha\beta} \langle \bar{\chi}_{N}^{\beta}(\vec{x}_{\mathrm{s}},t_{\mathrm{s}}) | \mathcal{O}_{\Gamma}(\vec{x}_{\mathrm{ins}},t_{\mathrm{ins}}) | \chi_{N}^{\alpha}(\vec{0},0) \rangle \\ \bullet \quad \text{Three-point functions} e.g. \ \mathcal{O}_{A}(x) = \bar{\psi}(x)\gamma_{5}\gamma^{\mu}\psi(x) \end{array}$$

- \circ Ground state at $t_{
 m s}
 ightarrow \infty, \ (t_s t_{
 m ins})
 ightarrow \infty$
- \circ Error increases exponentially with $t_{
 m s}$
- Statistics increased to keep errors constant





$\times 750$ 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							
Nucl	eon 2pt	477							

~30M inversions!

Nucleon three-point functions

$$G_{\Gamma}(P;ec{q};t_{
m s},t_{
m ins})=\sum_{ec{x}_{
m s},ec{x}_{
m ins}}e^{-iec{q}\cdotec{x}_{
m ins}}P^{lphaeta}\langle ar{\chi}_N^eta(ec{x}_{
m s},t_{
m s})|\mathcal{O}_{\Gamma}(ec{x}_{
m ins},t_{
m ins})|\chi_N^lpha(ec{0},0)
angle$$

$$egin{pmatrix} G_{\Gamma}(t_{
m s},t_{
m ins})\simeq A_{00}e^{-m_{N}t_{
m s}}+A_{01}ig(e^{-E_{1}t_{
m ins}}+e^{-E_{1}t_{
m s}+(E_{1}-m_{N})t_{
m ins}}ig)+A_{11}e^{-E_{1}t_{
m s}}\ G(t)\simeq c_{0}e^{-m_{N}t_{
m s}}+c_{1}e^{-E_{1}t_{
m s}} & { extstyle exts$$





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



~30M inversions!

The three ensembles and model averaging



Continuum limit and comparison with other studies



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

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

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

$$egin{aligned} &\langle p(p')|A_\mu|n(p)
angle \ &A_\mu = ar{u}\gamma_\mu\gamma_5 d \end{aligned} egin{aligned} &\langle N(p')|A^{
m isov}_\mu|N(p)
angle \ &A^{
m isov}_\mu = ar{u}\gamma_\mu\gamma_5 u - ar{d}\,\gamma_\mu\gamma_5 d \end{aligned}$$

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

... and at finite momentum transfer



$$\Pi_{\mu}(\Gamma_k;ec{q}) = rac{\mathcal{A}^{0,0}_{\mu}(\Gamma_k,ec{q})}{\sqrt{c_0(ec{0})c_0(ec{q})}}$$
 Three-point ground state

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

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

$$\Pi_0(\Gamma_k,ec q) = -rac{q_k {\cal K}}{2m_N} \Big[G_A(Q^2) + rac{(m_N-E_N)}{2m_N} G_P(Q^2) \Big]$$

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

Dipole vs z-expansion





Comparison with other studies



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

