Moments of the Pion Light-Cone Distribution Amplitude from the Heavy-Quark Operator Product Expansion

Fermilab

THE HOPE COLLABORATION

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Outline

Standard Model of Particle Physics

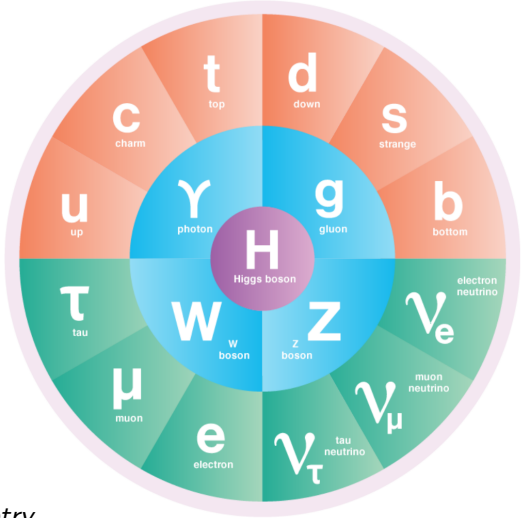


Figure credit: *Symmetry*

CKM Matrix

- Free parameters in the Standard Model
- Control overlap among six quark flavors (and therefore decay rates)
- Complex phase – affects violation of symmetries
- Best experimental measurements of magnitudes

$$\begin{pmatrix} |V_{ud}| & |V_{us}| & |V_{ub}| \\ |V_{cd}| & |V_{cs}| & |V_{cb}| \\ |V_{td}| & |V_{ts}| & |V_{tb}| \end{pmatrix} \approx \begin{pmatrix} 0.97 & 0.23 & 0.004 \\ 0.23 & 0.97 & 0.04 \\ 0.01 & 0.04 & 0.999 \end{pmatrix}$$

Unitarity Triangle

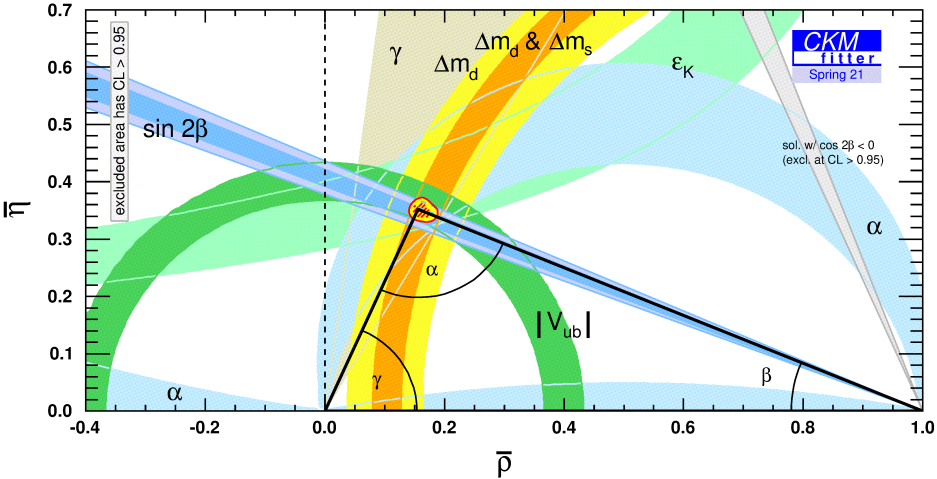


Figure credit: CKMFitter

Pion Decay

$$\Gamma\left(\pi^+ \to \mu^+ \nu_\mu\right) = \frac{G_F f_\pi^2 |V_{ud}|^2}{8\pi} m_\pi m_\mu^2 \left(1 - \frac{m_\mu^2}{m_\pi^2}\right)^2$$

- Decay rate depends on
  - Kinematic factors (m_μ, m_π)
  - CKM matrix element (V_{ud})
  - Pion structure (f_π)
- Need to disentangle pion structure from weak interactions to extract V_{ud} from experimental lifetime $\tau = 1/\Gamma$
- Simple decay – single parameter encodes pion structure

$B \to \pi\pi$ Decay

- Rate depends on CKM matrix elements and terms such as

$$f^+(0)\int_0^1 dx\, T_i^I(x)\varphi_\pi(x) + \int_0^1 d\xi\, dx\, dy\, T_i^{II}(\xi, x, y)\varphi_B(\xi)\varphi_\pi(x)\varphi_\pi(y)$$

  where $T_i^{I,II}$ are known functions and φ_B, φ_π are structure functions
- Complicated decay form (various ways to subdivide quark energies) – require convolution of functions to capture structure
- Sensitive to symmetry violation and thus complex phase of CKM matrix

Light-Cone Distribution Amplitude

$$\langle 0|\bar{\psi}(z)\gamma^{\mu}\gamma^{5}W[z,-z]\psi(-z)|M(\mathbf{p})\rangle = if_M p^{\mu}\int_{-1}^{1} d\xi\, e^{-i\xi p\cdot z}\varphi_M(\xi)$$

- Represents overlap between meson and $q\bar{q}$ pair with momenta $(1 \pm \xi)/2$
- Relates quark-level process (weak interactions) to hadron-level interactions (decay rates)
- Universal (relates to multiple different processes)

Pion Electromagnetic Form Factor

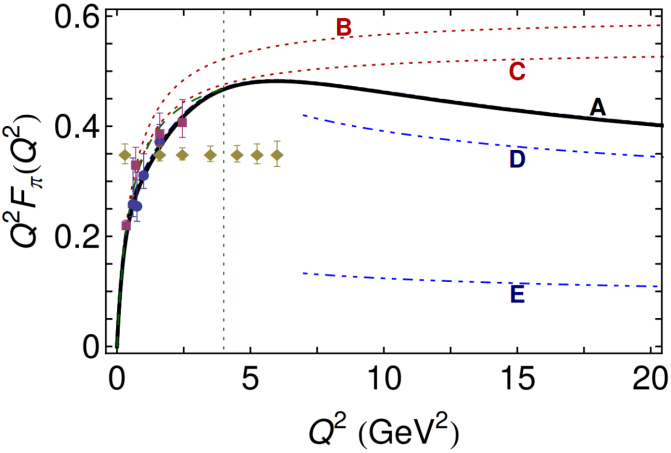


Figure credit: L. Chang et al., nucl-th/1307.0026, PRL **111**, 141802

Running Coupling

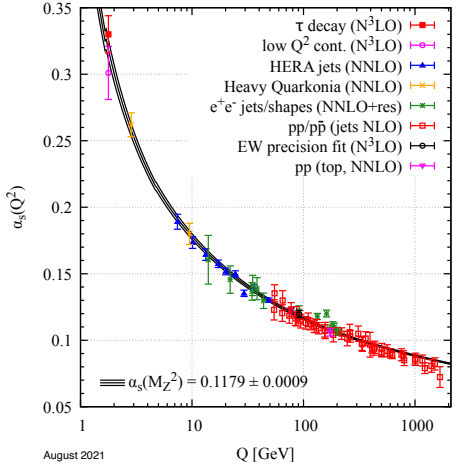


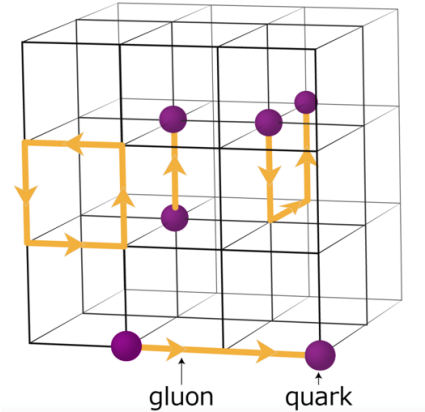
Figure credit: Particle Data Group

What is Lattice QCD?

- Non-perturbative method to perform QCD calculations
- Based on Feynman path integral discretized in 4-D Euclidean space-time

What is Lattice QCD?

- Non-perturbative method to perform QCD calculations
- Based on Feynman path integral discretized in 4-D Euclidean space-time
- Finite lattice spacing a (UV regulator)
- Need to take $a \to 0$ to match to continuum theory



Source: JICFuS, Tsukuba

Monte Carlo Integration

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}A \, e^{-S[A]} \mathcal{O}[A]$$

- A = gluon field (ignore sea quarks for now – *quenched approximation*)
- For a $64^3 \times 128$ lattice, integral is $\sim 10^9$ dimensional
  - Trapezoid rule requires $> 2^{10^9}$ points

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- Generate gauge fields once, use for many observables

Objects Calculable on Lattice

- Quark propagator
  - In free field theory, $S \sim \frac{1}{\not{p}+m}$
  - For interacting theory, replace $\not{p} \to i\not{D}$
  - Determined by inverting Dirac operator $D(m|n)_{ab}^{\alpha\beta} = i\not{D} + m$
  - Here, $D(m|n)_{ab}^{\alpha\beta}$ is finite $(12L^3T \times 12L^3T)$ square matrix

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- Create correlation functions by combining quark propagators

$$
\begin{aligned}
C_2^{\pi}(t) &= \langle \mathcal{O}_{\pi}(t)\mathcal{O}_{\pi}^{\dagger}(0)\rangle \\
&= \langle \left(\bar{\psi}_d\gamma_5\psi_u\right)(t)\left(\bar{\psi}_u\gamma_5\psi_d\right)(0)\rangle \\
&= \mathrm{Tr}[D_u^{-1}(t|0)\gamma_5 D_d^{-1}(0|t)\gamma_5]
\end{aligned}
$$

Figure credit: Gattringer and Lang (2010)

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\end{aligned}
$$

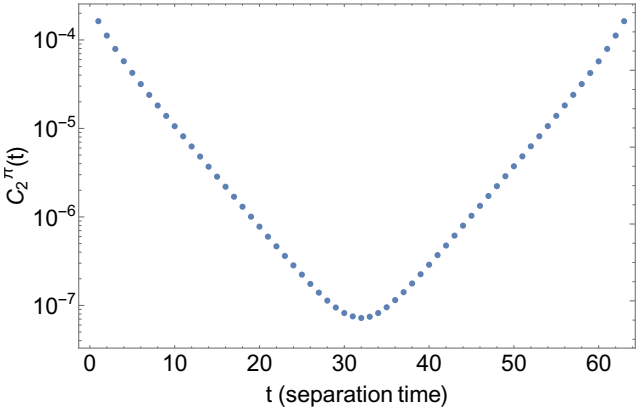
- Can also create 3-point functions

$$
C_3^{\mu}(t,\tau) = \langle \mathcal{O}_{\pi}(t)V^{\mu}(\tau)\mathcal{O}_{\pi}^{\dagger}(0)\rangle
$$

Figure credit: Gattringer and Lang (2010)

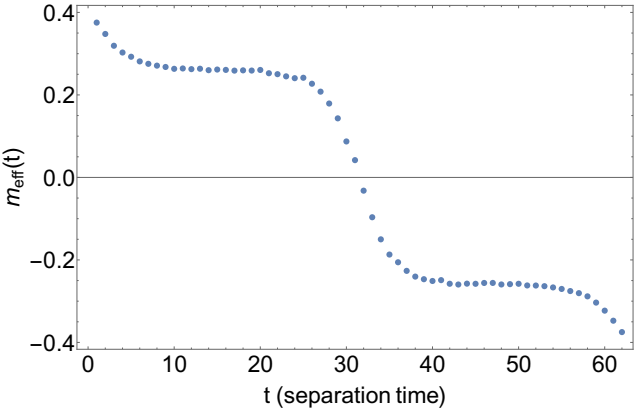
Behavior of Correlators

$$C_2(t) = \sum Z_n e^{-E_n t} \to Z_0 e^{-E_0 t}$$



Effective Mass

$$m_{\text{eff}}(t) = \ln\left(\frac{C_2(t)}{C_2(t+1)}\right) \to E_0$$



Computational Cost

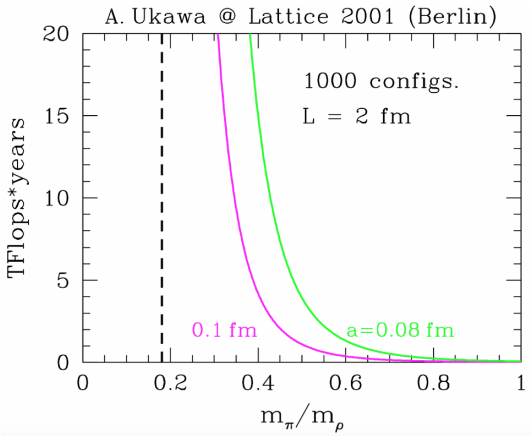


Image credit: Wikimedia Commons

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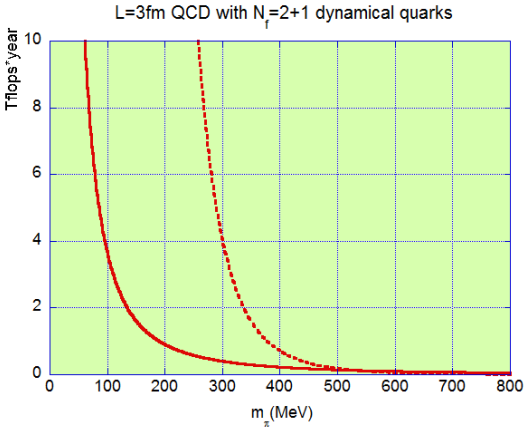

Figure credit: A. Ukawa @ CERN 2010

Image credit: Wikimedia Commons

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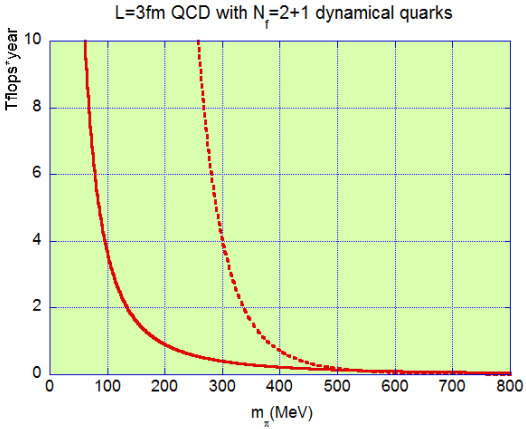

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Lattice Determination of LCDA

$$\langle 0|\bar{d}(-z)\gamma_\mu\gamma_5\mathcal{W}[-z,z]u(z)|\pi^+(p)\rangle = ip_\mu f_\pi \int_{-1}^{1} d\xi\, e^{-i\xi p\cdot z}\varphi_\pi(\xi)$$

- z is light-like separation ($z^2 = 0$)
- Euclidean space $\Rightarrow$ light-cone is single point
- Need indirect methods
  - Quasi-PDF [Ji, 1305.1539, PRL **110**, 262002]
  - Pseudo-PDF [Radyushkin, 1705.01488, PRD **96** 034025; Radyushkin, 1909.08474, PRD **100** 116011]
  - Expansion into moments

Lattice Determination of LCDA

- Expansion of LCDA into Mellin moments

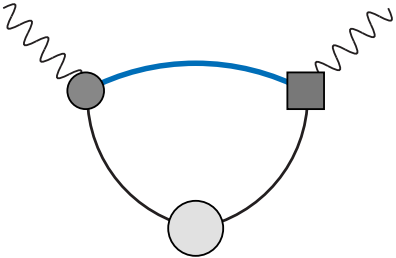
$$\langle \xi^n \rangle = \int_{-1}^{1} d\xi \, \xi^n \varphi_\pi(\xi)$$

- Moments can be written in terms of local derivative operators
- Second moment computed with this approach [Bali et al., 1903.08038, JHEP **2020**, 37]
- For $n > 2$, mix with lower-dimensional lattice operators – diverge instead of converging as $a \to 0$
- Alternative approach to compute moments needed

Hadronic Tensor

$$V^{\mu\nu}(q,p) = \int d^4x\, e^{iq\cdot x} \langle 0| T\left[A^\mu(x/2)A^\nu(-x/2)\right] |\pi^+(p)\rangle$$

- Transition between pion and two axial current insertions
- Amenable to lattice calculations



Source: arXiv:hep-lat/0507007, PRD **73**, 014501

W. Detmold (MIT)

C.-J. D. Lin (NYCU)

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- Transition between pion and two axial current insertions
- Amenable to lattice calculations
- Free to make currents flavor changing (and intermediate quark heavy)

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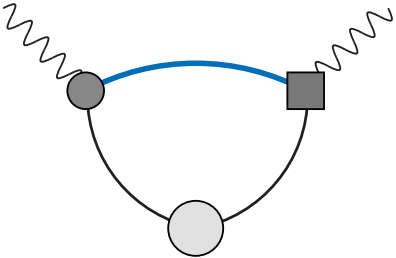

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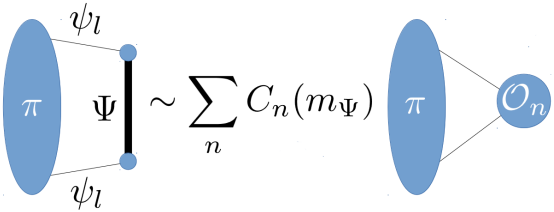
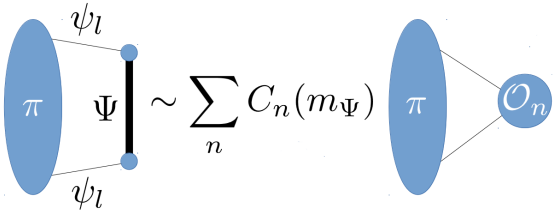
Operator Product Expansion (OPE)



$$\sim \sum_n C_n(m_\Psi) \qquad + \mathcal{O}\left(\frac{1}{m_\Psi^\tau}, \frac{1}{Q^\tau}\right)$$

Operator Product Expansion (OPE)



$$+\mathcal{O}\left(\frac{1}{m_\Psi^\tau}, \frac{1}{Q^\tau}\right)$$

$$\left\langle 0 \left| \gamma^\mu \frac{-i(i\not{D} + \not{q}) + m_\Psi}{(iD+q)^2 + m_\Psi^2} \gamma^\nu \right| \pi^+(\mathbf{p}) \right\rangle = \left\langle 0 \left| \gamma^\mu \frac{i(i\not{D} + \not{q}) + m_\Psi}{q^2 + (iD)^2 + m_\Psi^2} \sum_{n=0}^{\infty} \left(\frac{2iq \cdot D}{q^2 + (iD)^2 + m_\Psi^2} \right)^n \gamma^\nu \right| \pi^+(\mathbf{p}) \right\rangle$$

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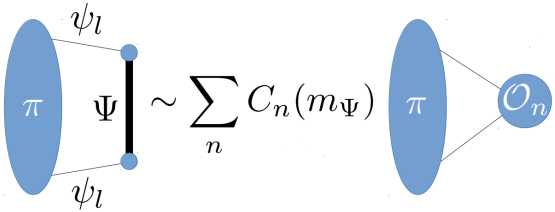

$$+\mathcal{O}\left(\frac{1}{m_\Psi^\tau}, \frac{1}{Q^\tau}\right)$$

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$$= \left\langle 0 \left| \gamma^\mu \frac{i(i\not{D}+\not{q})+m_\Psi}{q^2+m_\Psi^2} \sum_{n=0}^{\infty} \left(\frac{2p\cdot q}{q^2+m_\Psi^2} \right)^n \gamma^\nu \right| \pi^+(\mathbf{p}) \right\rangle \langle \xi^n \rangle + O\left(\frac{\Lambda_{\mathrm{QCD}}}{(q^2+m_\Psi^2)^{1/2}} \right)$$

using $D|\pi^+(\mathbf{p})\rangle \to \xi p|\pi^+(\mathbf{p})\rangle$, $D^2 \sim O(\Lambda_{\mathrm{QCD}}^2)$

Heavy Quark Operator Product Expansion (HOPE)

$$V^{\mu\nu}(p,q) = \frac{2if_\pi \varepsilon^{\mu\nu\rho\sigma} q_\rho p_\sigma}{\tilde{Q}^2} \sum_{\substack{n=0 \\ \text{even}}}^{\infty} \frac{\tilde{\omega}^n}{2^n(n+1)} C_W^{(n)}(\tilde{Q}, m_\Psi, \mu) \langle \xi^n \rangle(\mu) + O\left(\frac{\Lambda_{\text{QCD}}}{\tilde{Q}}\right)$$

$$\tilde{Q}^2 = -q^2 - m_\Psi^2 \,, \qquad \tilde{\omega} = \frac{p \cdot q}{\tilde{Q}^2}$$

- Odd moments vanish by isospin symmetry

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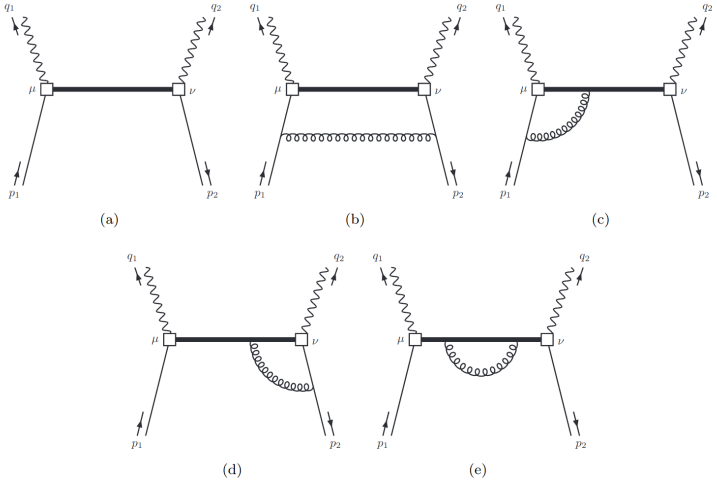
$$\tilde{Q}^2 = -q^2 - m_\Psi^2\,, \qquad \tilde{\omega} = \frac{p \cdot q}{\tilde{Q}^2}$$

- Odd moments vanish by isospin symmetry
- Need to suppress $\Lambda_{\text{QCD}}/\tilde{Q}$ corrections $\Rightarrow$ need either q or m_Ψ large
- Large-q (short-distance) studied in [Braun and Müller, 0709.1348, EPJC **55**, 349; Bali et al., 1807.06671, PRD **98** 094507]
- This talk will discuss large-m_Ψ approach

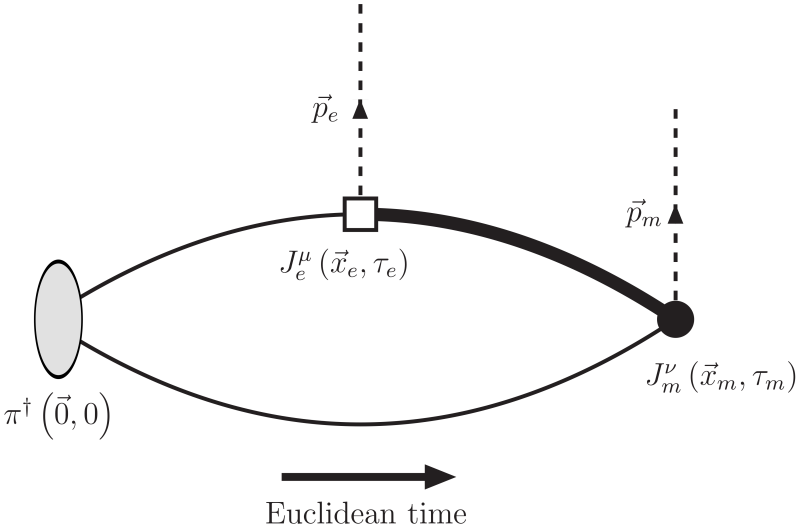
Wilson Coefficients



Y. Zhao (Argonne)

Detmold, AVG, Kanamori, Lin, Perry, Zhao, 2103.09529, PRD **104**, 074511

Heavy-Quark Operator Product Expansion (HOPE)



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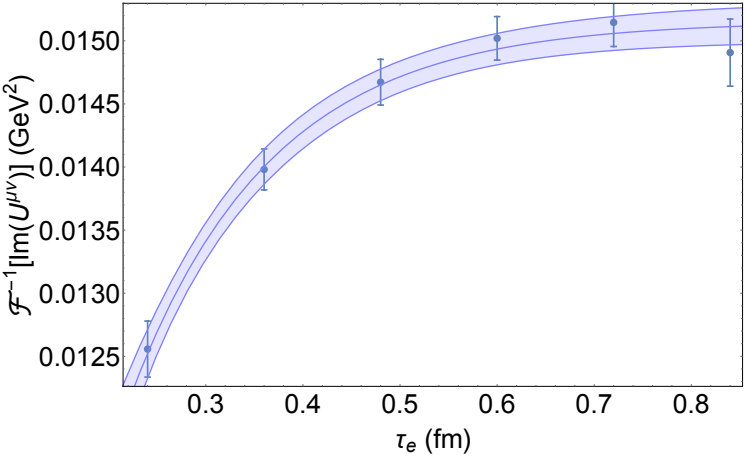
$$\int dq_4 e^{-iq_4\tau} V^{\mu\nu}(q,p) = \int d^3\mathbf{x}\, e^{i\mathbf{q}\cdot\mathbf{x}} \left\langle 0 \left| \mathcal{T}\left[A^\mu\left(\frac{\mathbf{x}}{2},\frac{\tau}{2}\right) A^\nu\left(-\frac{\mathbf{x}}{2},-\frac{\tau}{2}\right)\right] \right| \pi^+(\mathbf{p}) \right\rangle$$

- Inverse FT of $V^{\mu\nu}$ calculable on lattice in terms of 2-point and 3-point functions

$$C_2(\tau) = \langle \mathcal{O}_\pi(\tau)\mathcal{O}_\pi^\dagger(0)\rangle$$
$$C_3(\tau_e,\tau_m) = \langle A^\mu(\tau_e)A^\nu(\tau_m)\mathcal{O}_\pi^\dagger(0)\rangle$$

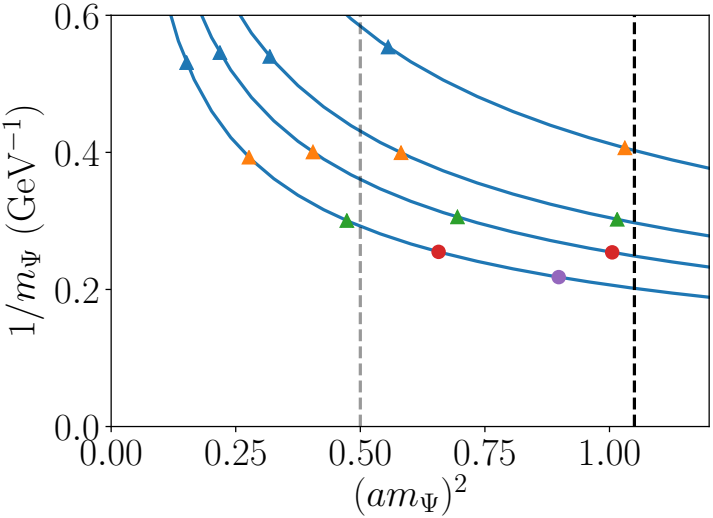
- Isolation of ground state relies on sufficiently large separation between 0 and $\min\{\tau_e,\tau_m\}$

Excited States



- $\tau_m - \tau_e$ fixed at 0.06 fm
- Excited state contamination becomes $\sim 1\%$ by $\tau_e = 0.7$ fm

Ensembles Used



Ensembles Used

$L^3 \times T$	a (fm)	N_{cfg}	N_{src}	N_ψ	N_{prop}
$24^3 \times 48$	0.0813	650	12	2	312,000
$32^3 \times 64$	0.0600	450	10	3	270,000
$40^3 \times 80$	0.0502	250	6	4	120,000
$48^3 \times 96$	0.0407	341	10	5	341,000

- Quenched approximation with $m_\pi = 550$ MeV
  - Fine dynamical ensembles prohibitively expensive
  - Total compute time: $O(10^7)$ CPU-hours
- Wilson-clover fermions with non-perturbatively tuned c_{SW}
- With clover term, results fully $O(a)$ improved
  - Axial current renormalizes multiplicatively: $A^\mu \to A^\mu Z_A(1 + \tilde{b}_A a \tilde{m}_q)$
  - This only affects overall normalization (not $\langle \xi^2 \rangle$)

Software Used

- Calculations performed using Chroma library for lattice QCD
- Accelerated using QPhiX library (with AVX-512 intrinsics)
- Dynamical calculation ported to Bridge++ for use on the supercomputer Fugaku (ARM-based)
- Currently working on custom multi-mass solver for heavy quarks

S. Mondal (MSU)

I. Kanamori (RIKEN)

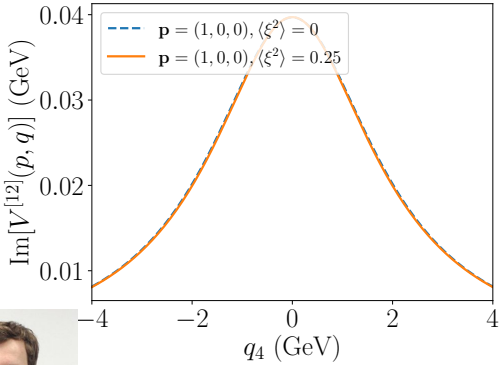
Choice of Kinematics

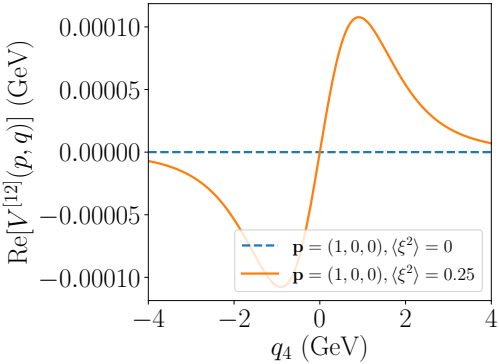
$$V^{\mu\nu}(p,q) = \frac{2i f_\pi \varepsilon^{\mu\nu\rho\sigma} q_\rho p_\sigma}{\tilde{Q}^2} \sum_{\substack{n=0 \\ \text{even}}}^{\infty} \frac{\tilde{\omega}^n}{2^n(n+1)} C_W^{(n)}(\tilde{Q}, m_\Psi, \mu) \langle \xi^n \rangle(\mu) + O\left(\frac{\Lambda_{\text{QCD}}}{\tilde{Q}}\right)$$

- Wilson coefficients $C_W^{(n)}(\mu = 2\text{ GeV})$ calculated to 1-loop
- Fit parameters: f_π, m_Ψ, $\langle \xi^2 \rangle$
- Contribution of second moment $\langle \xi^2 \rangle$ suppressed by

$$\frac{\tilde{\omega}^2}{2^2 \times 3} = \frac{1}{3}\left(\frac{p \cdot q}{\tilde{Q}^2}\right)^2 \lesssim 10^{-2}$$

Choice of Kinematics

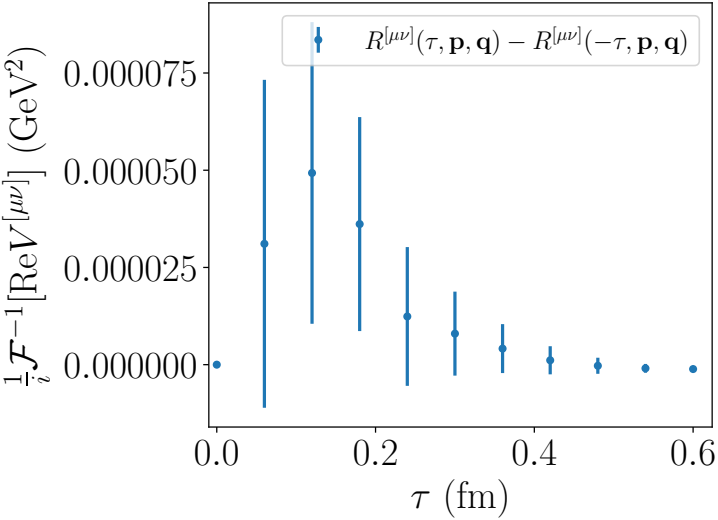




R. Perry (Barcelona)

$$\mathbf{p} = (1,0,0) = (0.64\ \text{GeV}, 0, 0)$$
$$2\mathbf{q} = (1,0,2) = (0.64\ \text{GeV}, 0, 1.28\ \text{GeV})$$

Noise Reduction



Noise Reduction

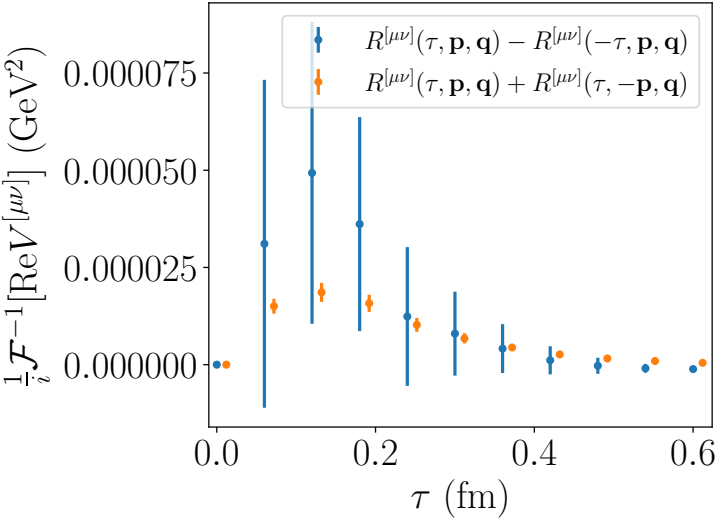
By γ_5-hermiticity of quark propagators,

$$C_3^{\mu\nu}(\tau_e, \tau_m; \mathbf{p}_e, \mathbf{p}_m)^* = C_3^{\nu\mu}(\tau_m, \tau_e; \mathbf{p}_m, \mathbf{p}_e)$$

As a result,

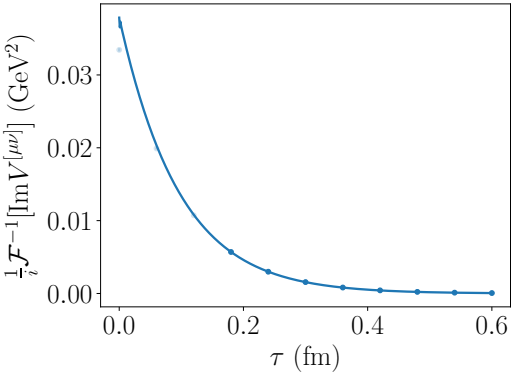
$$\begin{aligned}\mathrm{Re}[V^{\mu\nu}(\mathbf{p}, q)] &= \int_0^\infty d\tau\ [R^{\mu\nu}(\tau; \mathbf{p}, \mathbf{q}) - R^{\mu\nu}(-\tau; \mathbf{p}, \mathbf{q})] \sin(q_4\tau) \\ &= \int_0^\infty d\tau\ [R^{\mu\nu}(\tau; \mathbf{p}, \mathbf{q}) + R^{\mu\nu}(\tau; -\mathbf{p}, \mathbf{q})] \sin(q_4\tau)\end{aligned}$$

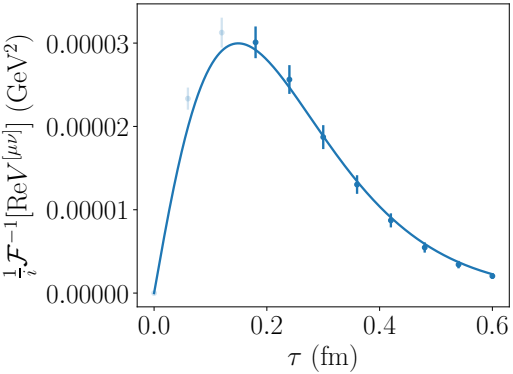
Noise Reduction



Fitting Hadronic Tensor

- Fit ratio of 2- and 3-point correlators to inverse FT of OPE



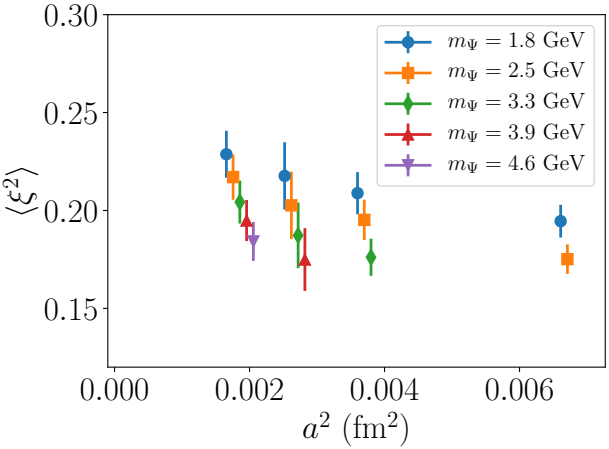


$$f_\pi = 149 \pm 1 \text{ MeV}$$

$$m_\Psi = 1.85 \pm 0.01 \text{ GeV}$$

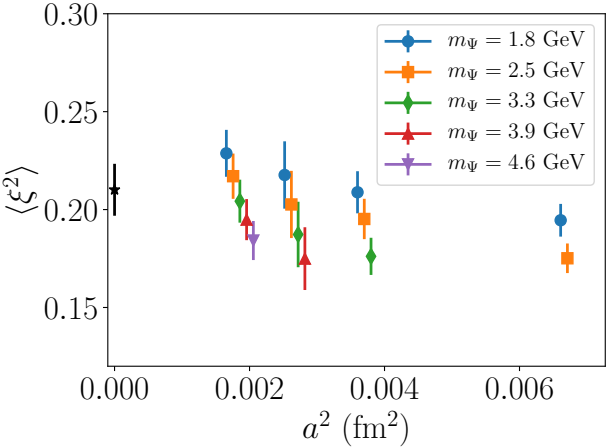
$$\langle \xi^2 \rangle = 0.209 \pm 0.011$$

Fits to Various Ensembles



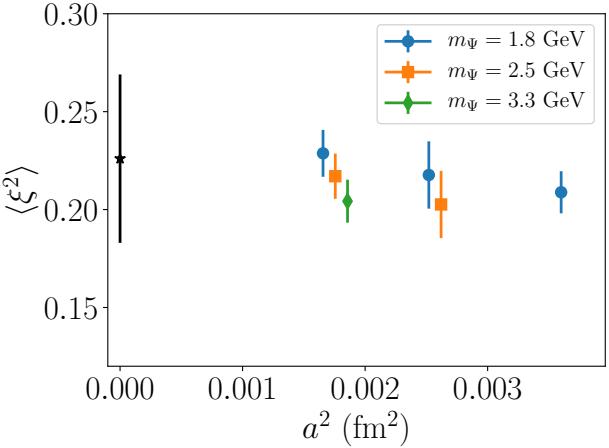
Masses are (left to right) $\{1.8, 2.5, 3.3, 3.9, 4.6\}$ GeV

Continuum Extrapolation



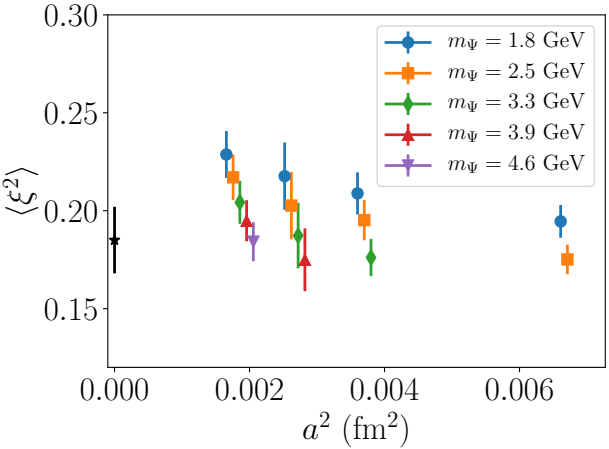
$$\text{data} = \langle \xi^2 \rangle + \frac{A}{m_\Psi} + Ba^2 + Ca^2 m_\Psi + Da^2 m_\Psi^2 \Rightarrow \langle \xi^2 \rangle = 0.210 \pm 0.013 \text{ (stat.)}$$

Uncertainty in Continuum Extrapolation



- Original fit restricted am_Ψ to < 1.05

Uncertainty in Higher-Twist Effects

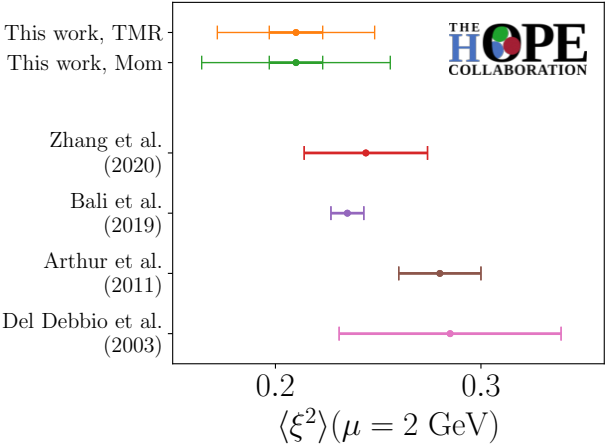


Could add twist-4 term to fit: data $= \langle \xi^2 \rangle + A m_\Psi^{-1} + B m_\Psi^{-2} + C a^2 + D a^2 m_\Psi + E a^2 m_\Psi^2$

Combined Uncertainty

$$
\begin{aligned}
\langle \xi^2 \rangle = 0.210 &\pm 0.013 \text{ (statistical)} \\
&\pm \mathbf{0.016} \text{ (continuum)} \\
&\pm \mathbf{0.025} \text{ (higher twist)} \\
&\pm 0.002 \text{ (excited states)} \\
&\pm 0.0002 \text{ (finite volume)} \\
&\pm 0.014 \text{ (unphysically heavy pion)} \\
&\pm 0.002 \text{ (fit range)} \\
&\pm 0.008 \text{ (running coupling)} \\
\hline
\langle \xi^2 \rangle = 0.210 &\pm 0.036 \text{ (total, exc. quenching)}
\end{aligned}
$$

Comparison to Literature



Detmold, AVG, Kanamori, Lin, Mondal, Perry, Zhao, 2109.15241, PRD **105**, 034506

Quenched Approximation

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}A\, \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\ \exp(-\bar{\psi}\not{D}\psi)\mathcal{O}[A]\exp(-S[A])}{\int \mathcal{D}A\, \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\ \exp(-\bar{\psi}\not{D}\psi)\exp(-S[A])}$$

Quenched Approximation

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}A\, \cancel{\mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, \exp(-\bar{\psi}\not{D}\psi)}\, \mathcal{O}[A] \exp(-S[A])}{\int \mathcal{D}A\, \cancel{\mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, \exp(-\bar{\psi}\not{D}\psi)} \exp(-S[A])}$$

- Neglect of sea quarks in calculation

Quenched Approximation

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}A\, \cancel{\mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, \exp(-\bar{\psi}\not{D}\psi)}\, \mathcal{O}[A] \exp(-S[A])}{\int \mathcal{D}A\, \cancel{\mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, \exp(-\bar{\psi}\not{D}\psi)} \exp(-S[A])}$$

- Neglect of sea quarks in calculation
- Omits sea quark loops (including those in bottom two diagrams)
- Dramatically reduces cost of ensemble generation
- Usually relatively mild effects but formally uncontrolled (breaks unitarity)

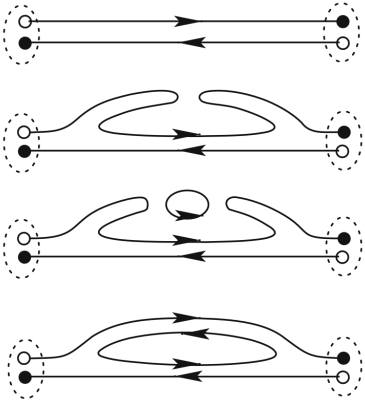


Figure credit: Gattringer and Lang (2010)

Dynamical Ensembles

- Dynamical quarks only affect background gluon fields – factors from rest of calculation
- Configurations reused by different collaborations for different calculations
- Redoing quenched calculations with dynamical ensembles from CLS collaboration

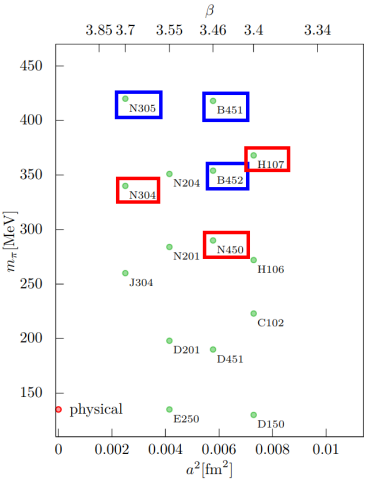
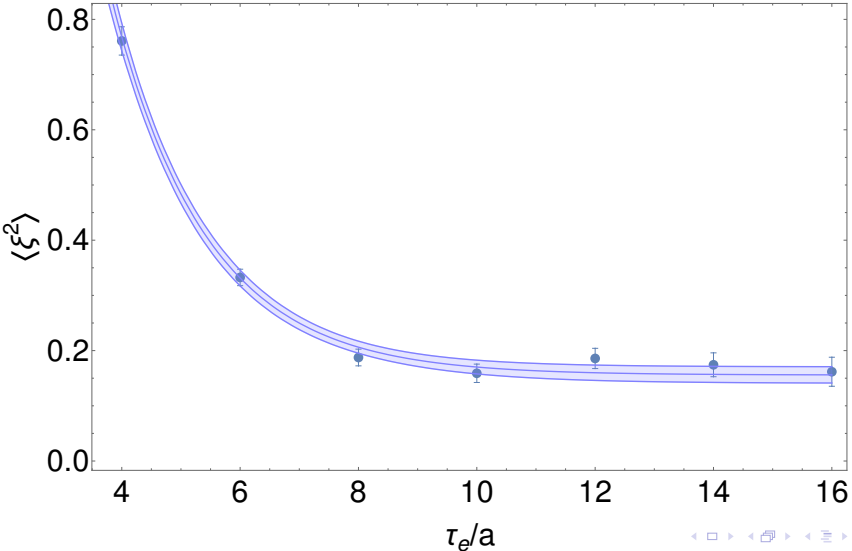
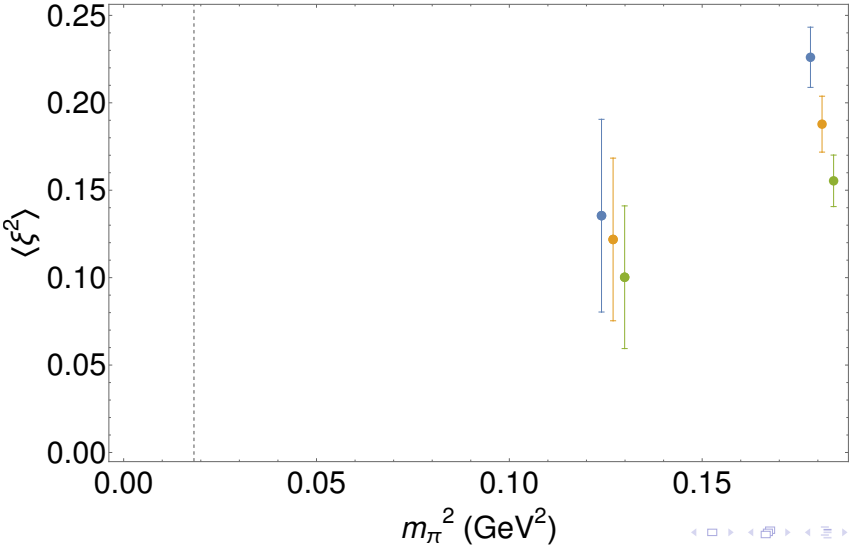


Figure credit: S. Collins @ CERN (2019)

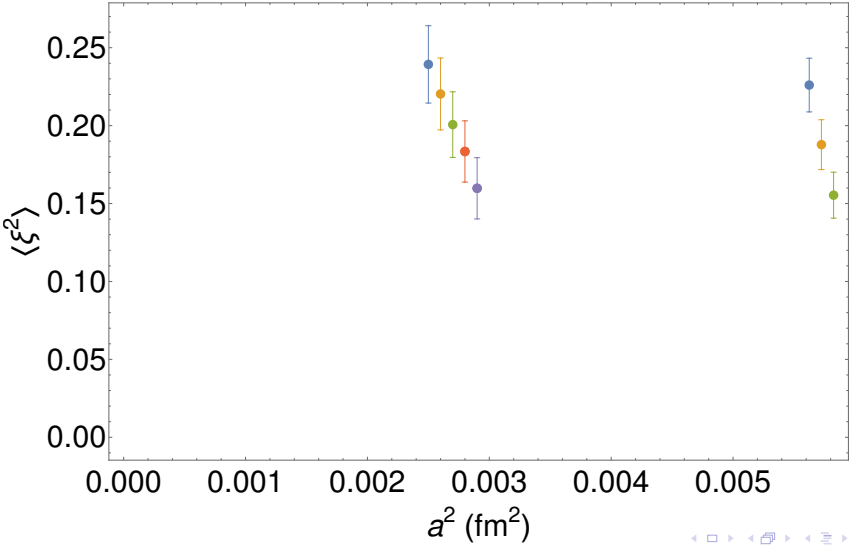
Excited State Contamination



Pion Mass Dependence (Preliminary)



Lattice Spacing Dependence (Very Preliminary)

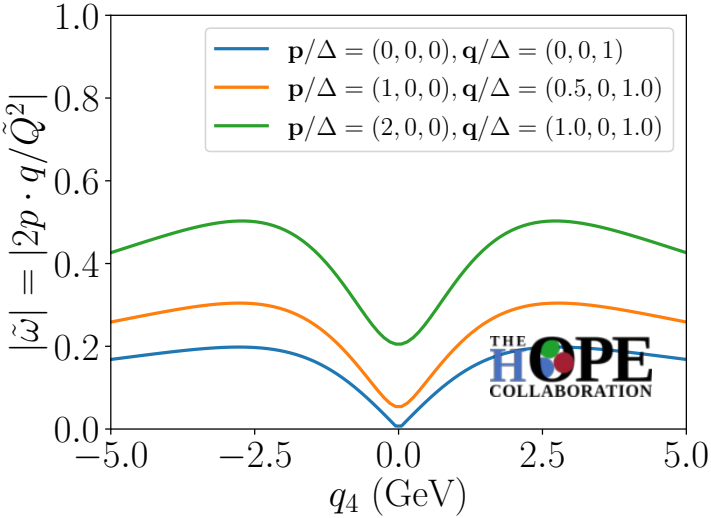


Suppression of Signal

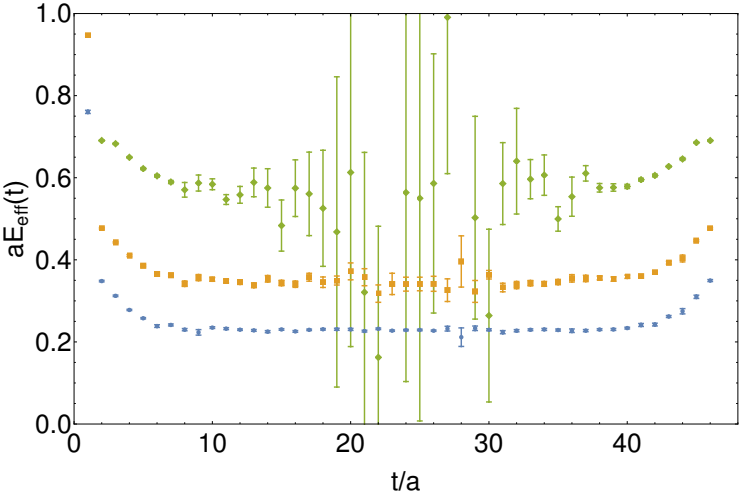
$$V^{\mu\nu}(p,q) = \frac{2if_\pi \varepsilon^{\mu\nu\rho\sigma} q_\rho p_\sigma}{\tilde{Q}^2} \sum_{\substack{n=0 \\ \text{even}}}^{\infty} \frac{\tilde{\omega}^n}{2^n(n+1)} C_W^{(n)}(\tilde{Q}, m_\Psi, \mu) \langle \xi^n \rangle(\mu) + O\left(\frac{\Lambda_{\text{QCD}}}{\tilde{Q}}\right)$$

- $\langle \xi^n \rangle$ suppressed by $(\tilde{\omega}/2)^n \sim 0.1^n$
- Splitting signal into real/imaginary parts facilitates extraction of $\langle \xi^2 \rangle$
- Trick works best for $n = 2$ (only 2 channels available)

Higher Momentum



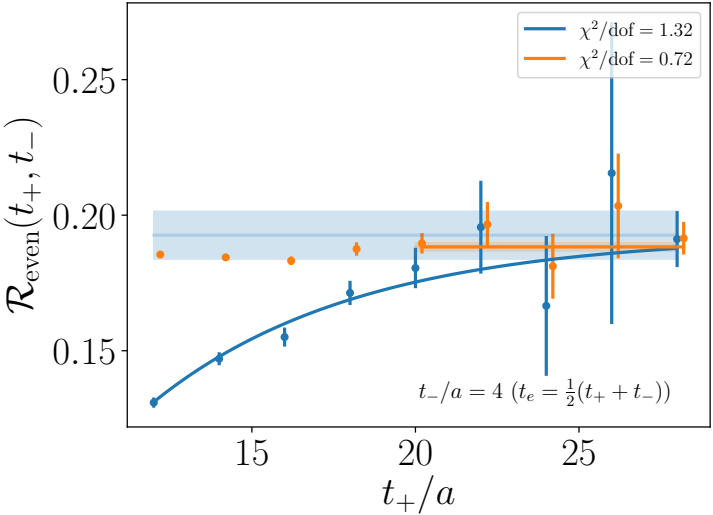
Signal-to-Noise Problem



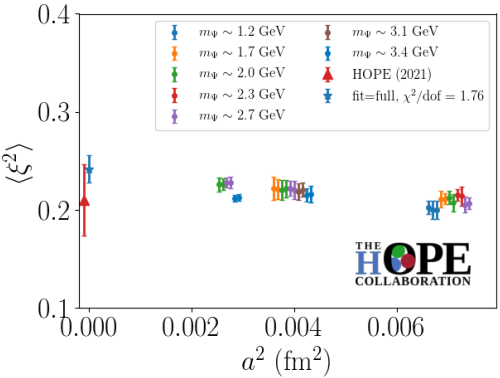
Variational Method

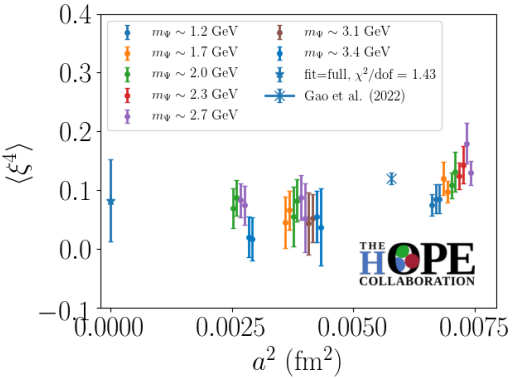
- Excited state contamination more severe at larger **p**
- Also steeper penalty for extending Euclidean time
- Solution – better interpolating operator to create pion
- Pion can be created with $\bar{\psi}\gamma_5\psi$ or $\bar{\psi}\gamma_4\gamma_5\psi$
- Use both and take optimal linear combination to reduce excited state contamination

Variational Method



Preliminary Results





$\langle \xi^2 \rangle = 0.245 \pm 0.014$ (stat.)

$\langle \xi^4 \rangle = 0.075 \pm 0.050$ (stat.)

Conclusion

- Pion LCDA important but challenging – good to have complementary methods
- $\langle \xi^2 \rangle (\mu = 2 \text{ GeV}) = 0.210 \pm 0.036$ (quenched) – compatible with other methods
- Moving to dynamical ensembles with lighter masses
- Preliminary extraction of $\langle \xi^4 \rangle$ – working to increase statistics

Thank you to R. Edwards, B. Joó, S. Ueda and others for software development (Chroma, QPhiX, Bridge++) and to ASRock, Barcelona Supercomputing Center, and RIKEN for computational resources!

Multi-Mass Solver

- Need to invert Dirac operator $D = \not{D} + m$ for quark propagators
- Can write $D = 1 - \kappa H$ with $\kappa = \frac{1}{2(m+4)}$ and

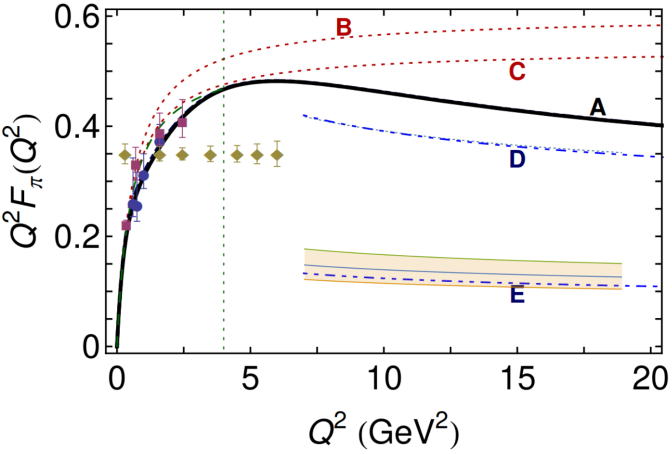
$$H(n|m) = \sum_{\mu} (1 - \gamma_\mu) U_\mu \delta_{n+\hat{\mu},m}$$

- Can expand D^{-1} as *hopping expansion*

$$D^{-1}\psi = \sum_{j=0}^{\infty} \kappa^j H^j \psi$$

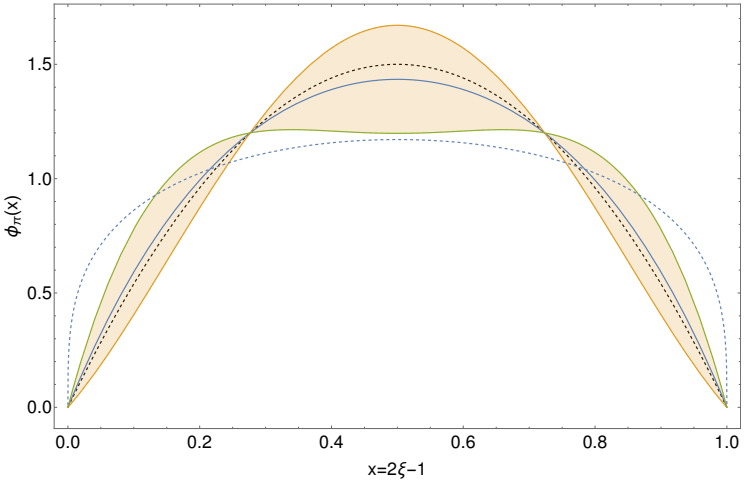
- H is independent of m – can reuse $H^j\psi$ for all masses
- More expensive for single mass but can be competitive with enough masses

Pion Electromagnetic Form Factor



Adapted from L. Chang et al., nucl-th/1307.0026

Reconstruction of LCDA



Comparison of LCDA Models

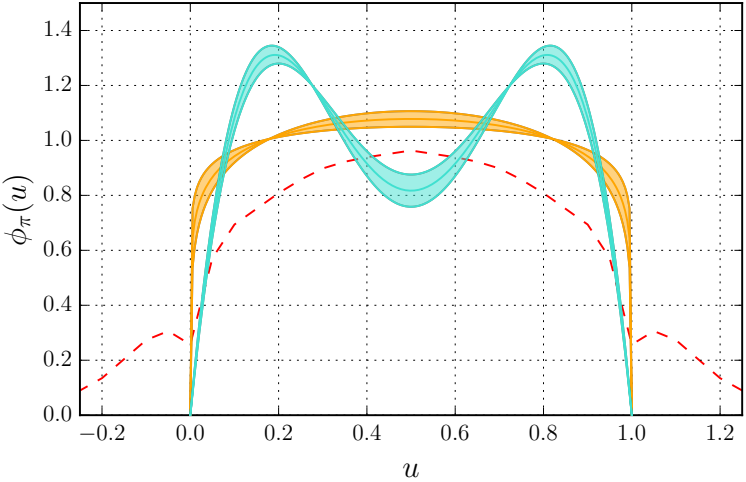


Figure credit: Bali et al., 1807.06671, PRD **98**, 094507