Unlocking higher-order moments of parton distribution functions from lattice QCD

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PDF and Lattice QCD

- Connection between PDFs and hadronic matrix elements, which are calculable in lattice QCD, is established through the moments of the PDFs $<x^n>$

Curci, Furmanski, Petronzio: 1980
Collins, Soper: 1982

- Lattice QCD calculations of the moments of the PDFs, provide, in principle, a means for the complete reconstruction of the PDFs.

Kronfeld, Photiadis: 1985
Martinelli, Sachrajda: 1987 - 1988

- This possibility has remained impractical due to the theoretical and numerical challenges associated with computing high moments

Alternative approaches have been developed to determine the x-dependence of the PDFs

the heavy-quarks OPE	Aglietti et al.: 1998 Detmold, Lin: 2005
the quasi-PDF	Ji: 2013
the psuedo-PDF	Radyushkin: 2017 Karpie, Orginos, Zafeiropoulos: 2018
the OPE-based method	Chambers et al.: 2017
the current-current approach	Braun, Müller: 2008 Ma, Qiu: 2018
and the hadron tensor method	Lian et al.: 2019

- These approaches allow in principle an indirect determination of the moments of PDF of nucleons and pions

Egerer et al.: 2022
Gao et al.: 2020-2023

Method that addresses both the theoretical and numerical challenges faced in the past, which hindered the direct calculation of moments of any order from lattice QCD

Twist-2 operators

$$O_n^{rs}(x) = O^{rs}_{\mu_1\cdots\mu_n}(x) = \overline{\psi}^{r}(x)\gamma_{\{\mu_1}\overset{\leftrightarrow}{D}_{\mu_2}\cdots\overset{\leftrightarrow}{D}_{\mu_n\}}\psi^s(x) \qquad \widehat{O}_n^{rs}(x) = Z_n^{\mathrm{MS}}\widehat{O}^{rs}_{n,\mathrm{B}}(x)$$

- Calculate matrix elements using lattice QCD
  - Rotational group symmetry is broken into the hypercubic group H(4)
- Irreducible representations of O(4) generally become reducible representations of H(4) inducing unwanted mixings under renormalization
  - Irreps of H(4) allow mixing with lower dimensional operators and complicate mixings with operators of the same dimension

Beccarini et al.: 1995
Gockeler et al.: 1996

- Operators with different index combinations belong to different irreps of H(4)

O_3 $\quad \mu_1 = \mu_2 = \mu_3$ → $1/a^2\delta_{\mu_i\mu_j}\cos(ap_{\mu_j})$ Kronfeld, Photiadis: 1985

$\mu_1 \neq \mu_2 = \mu_3$ → $O_{411} - O_{433}$ Martinelli, Sachrajda: 1987

$\mu_1 \neq \mu_2 \neq \mu_3$ → $\left\langle h(p)|\widehat{O}_n|h(p)\right\rangle = p_{\mu_1}\cdots p_{\mu_n}A_n^h(\mu)$

Narayanan,
Neuberger:2006

Gradient flow

Lüscher 2010
Lüscher, Weisz 2011

$x_\mu = (\mathbf{x}, x_4)$ $t \to$ flow-time $[t] = -2$

$A_\mu(x) = A^a_\mu(x) T^a$ $\to$ gluon fields

$$\boxed{\begin{aligned} &\partial_t B_\mu(x,t) = D_\nu G_{\nu\mu}(x,t) \\ &B_\mu(x,t)|_{t=0} = A_\mu(x) \end{aligned}}$$

$$D_\nu = \partial_\nu + [B_\nu(x,t), \cdot]$$

$$G_{\mu\nu}(x,t) = \partial_\mu B_\nu(x,t) - \partial_\nu B_\mu(x,t) + [B_\mu, B_\nu]$$

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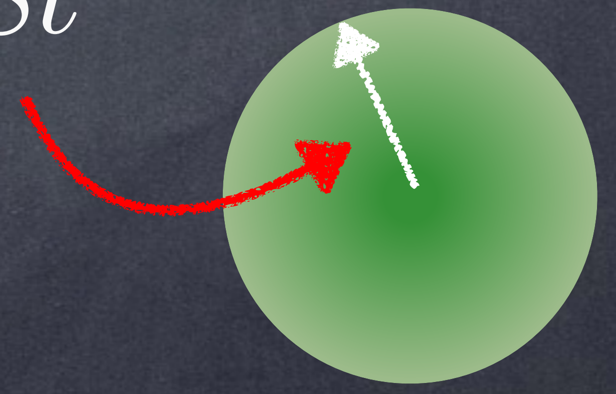
$$\partial_t B_\mu = \partial_\nu \partial_\nu B_\mu$$

$$B_\mu(x,t) = \int d^4y \ K(x-y;t) A_\mu(y)$$

$$K(x;t) = \int \frac{d^4p}{(2\pi)^4} \mathrm{e}^{ipx} \mathrm{e}^{-tp^2} = \frac{\mathrm{e}^{-x^2/4t}}{(4\pi t)^2}$$

- Gaussian damping at large momenta
- Smoothing at short distance over a range $\sqrt{8t}$



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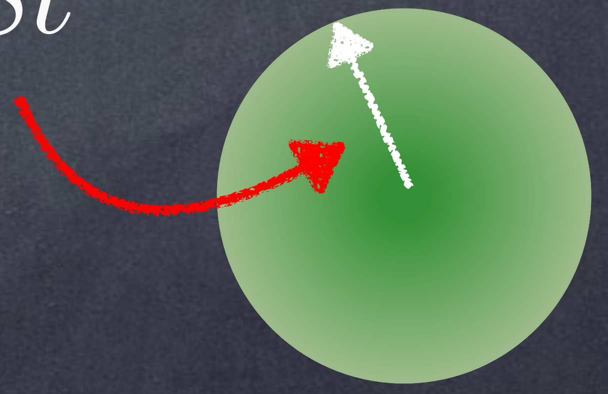


$$\boxed{\begin{array}{c} B_\mu(x,t) \qquad t > 0 \qquad \text{finite} \\ \text{Continuum limit is finite} \end{array}}$$

Lüscher, Weisz: 2011

Gradient flow

Lüscher: 2013

$x_\mu = (\mathbf{x}, x_4) \quad t \to \text{flow-time} \quad [t] = -2$

$$\boxed{\begin{aligned} \partial_t \chi(x,t) &= \Delta \chi(x,t) \\ \partial_t \bar{\chi}(x,t) &= \bar{\chi}(x,t) \overleftarrow{\Delta} \\ \chi(x, t=0) &= \psi(x) \\ \bar{\chi}(x, t=0) &= \bar{\psi}(x) \end{aligned}}$$

$\Delta = D_{\mu,t} D_{\mu,t} \qquad D_{\mu,t} = \partial_\mu + B_{t,\mu}$

Gradient flow

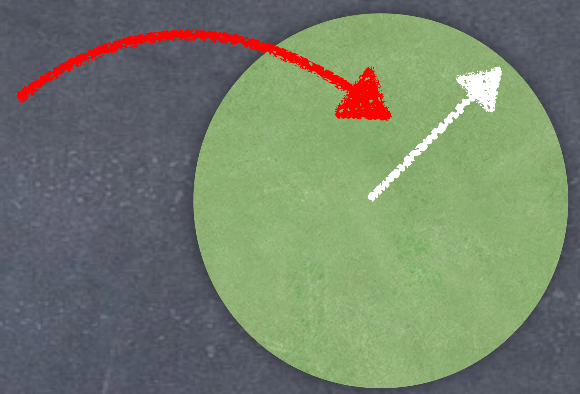
Lüscher: 2013

$x_\mu = (\mathbf{x}, x_4) \quad t \to \text{flow-time} \quad [t] = -2$

$$\chi(x,t) = \int d^4y K(x-y,t)\psi(y) \quad K(x,t) = \frac{1}{4\pi t^2}\mathrm{e}^{-\frac{x^2}{4t}}$$

$$\boxed{\begin{gathered}\partial_t \chi(x,t) = \Delta\chi(x,t) \\ \partial_t \bar{\chi}(x,t) = \bar{\chi}(x,t)\overleftarrow{\Delta} \\ \chi(x,t=0) = \psi(x) \\ \bar{\chi}(x,t=0) = \bar{\psi}(x)\end{gathered}}$$

- Smoothing over a range $\sqrt{8t}$



- Gaussian damping at large momenta

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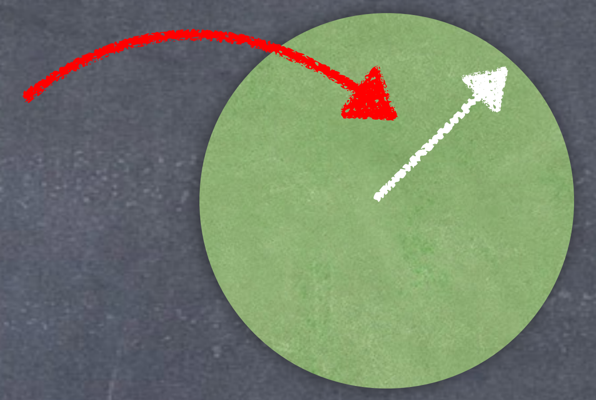

- Gaussian damping at large momenta

$$\Delta = D_{\mu,t}D_{\mu,t} \qquad D_{\mu,t} = \partial_\mu + B_{t,\mu}$$

$$\chi_R(x,t) = Z_\chi^{1/2}\chi(x,t)$$

$$\mathcal{O}(x,t) = \overline{\chi}(x,t)\Gamma(x,t)\chi(x,t) \qquad \mathcal{O}_R = Z_\chi \mathcal{O}$$

$$\Sigma_t = \langle\overline{\chi}(x,t)\chi(x,t)\rangle \qquad \Sigma_{t,R} = Z_\chi \Sigma_t$$

Gradient flow

Lüscher: 2013

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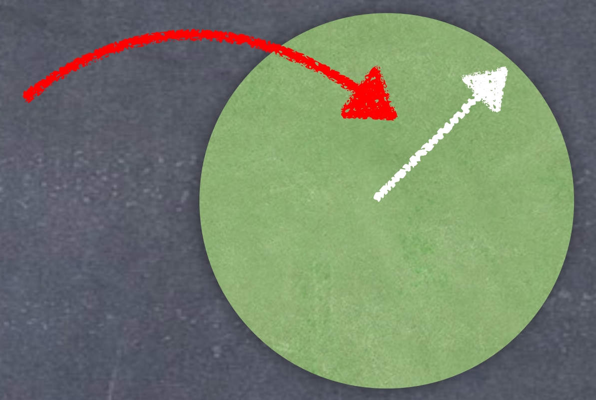

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No additive divergences

Continuum limit finite after normalizing fermion fields

Strategy - Short flow-time expansion

$$\underset{\underset{\text{LQCD}}{\uparrow}}{[\mathcal{O}_i(t)]_{\mathrm{R}}} = \sum_i \underset{\underset{\text{PT - LQCD}}{\uparrow}}{c_{ij}(t,\mu)} \boxed{[\mathcal{O}_i(t=0,\mu)]_{\mathrm{R}}} + O(t)$$

$$c_{ij}(t,\mu) = \delta_{ij} + \frac{\alpha_s(\mu)}{4\pi} c_{ij}^{(1)}(t,\mu) + O(\alpha_s^2)$$

Lüscher: 2013

A.S., Luu, de Vries: 2014-2015
Dragos, Luu, A.S. de Vries: 2018-2019
Rizik, Monahan, A.S.: 2018-2020
A.S.: 2020
Kim, Luu, Rizik, A.S.: 2020
Mereghetti, Monahan, Rizik, A.S., Stoffer: 2021

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- Calculation of matrix elements with flowed fields
  - Multiplicative renormalization (no power divergences and no mixing)
- Calculation of Wilson coefficients
  - Insert OPE in off-shell amputated 1PI Green's functions
- Power divergences subtracted non-perturbatively (LQCD)
- Determination of the physical renormalized matrix element at zero flow-time

Flowed twist-2 operators

$$O_n^{rs}(x,t) = \overline{\chi}^r(x,t)\gamma_{\{\mu_1}\overleftrightarrow{D}_{\mu_2}\cdots\overleftrightarrow{D}_{\mu_n\}}\chi^s(x,t)$$

$$O_n^{rs}(t) = Z_n O_{n,B}^{rs}(t)\,, \quad Z_n = Z_\chi$$

$$\left\langle \mathring{\overline{\chi}}_r(x,t)\overleftrightarrow{\not{D}}\mathring{\chi}_r(x,t)\right\rangle = -\frac{N_c}{(4\pi)^2t^2}$$

Makino, Suzuki: 2014

$$\chi^{r,\mathrm{MS}}(x,t) = (8\pi t)^{\epsilon/2}\,\zeta_\chi^{1/2}\mathring{\chi}^r(x,t)$$

$$\overline{\chi}^{r,\mathrm{MS}}(x,t) = (8\pi t)^{\epsilon/2}\,\zeta_\chi^{1/2}\mathring{\overline{\chi}}_r(x,t)$$

$$D = 4 - 2\epsilon$$

$$\zeta_\chi = 1 - \frac{\overline{g}^2}{(4\pi)^2}C_F\left(3\log(8\pi\mu^2 t) - \log(432)\right)$$

$$C_F = \frac{N_c^2 - 1}{2N_c}$$

$$\log\mu^2 = \log\overline{\mu}^2 + \gamma_E - \log 4\pi$$

NNLO

Harlander, Kluth, Lange: 2018

Artz et al.: 2019

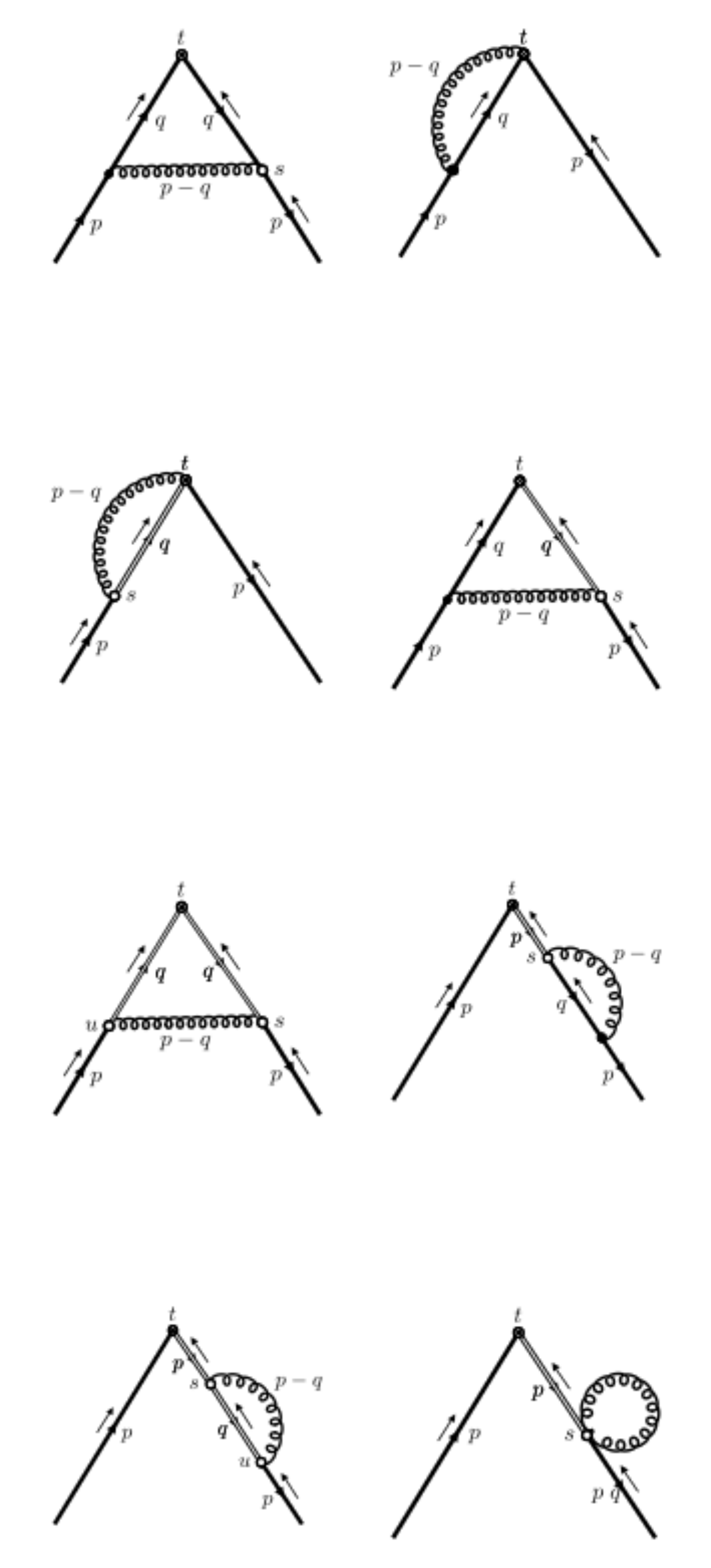
Matching coefficients

$$\hat{\mathring{O}}_n^{rs}(x,t) = \bar{\mathring{\chi}}^r(x,t)\gamma_{\{\mu_1}\overleftrightarrow{D}_{\mu_2}\cdots\overleftrightarrow{D}_{\mu_n\}}\mathring{\chi}^s(x,t) - \text{terms with } \delta_{\mu_i\mu_j}$$

Continuum limit is finite for any n

$$\left\langle h(p)|\hat{\mathring{O}}_n(t)|h(p)\right\rangle = p_{\mu_1}\cdots p_{\mu_n}\left\langle x^{n-1}\right\rangle_h(t)$$

$$\hat{\mathring{O}}_n^{rs}(t) = c_n(t,\mu)\hat{O}_n^{rs,\mathrm{MS}}(\mu) + O(t)$$



Matching equations

$$\left\langle \psi^r\hat{\mathring{O}}_n^{rs}(t)\overline{\psi}^s\right\rangle = c_n(t,\mu)\left\langle \psi^r\hat{O}_n^{rs,\mathrm{MS}}(t=0,\mu)\overline{\psi}^s\right\rangle$$

The matching coefficients are determined considering off-shell amputated one-particle irreducible (1PI) Green's functions containing the flowed operators

Mereghetti, Monahan, Rizik,
A.S., Stoffer: 2021

$$c_n(t,\mu) = 1 + \frac{\overline{g}^2(\mu)}{(4\pi)^2}c_n^{(1)}(t,\mu) + O(\overline{g}^4)$$

$$c_n^{(1)}(t,\mu) = C_F\left[\gamma_n\log\left(8\pi\mu^2 t\right) + B_n\right]$$

$$\gamma_n = 1 + 4\sum_{j=2}^{n}\frac{1}{j} - \frac{2}{n(n+1)}$$

Gross, Wilczek: 1974

$$B_n = \frac{4}{n(n+1)} + 4\frac{n-1}{n}\log 2 + \frac{2-4n^2}{n(n+1)}\gamma_E - \frac{2}{n(n+1)}\psi(n+2) + \\ + \frac{4}{n}\psi(n+1) - 4\psi(2) - 4\sum_{j=2}^{n}\frac{1}{j(j-1)}\frac{1}{2^j}\phi(1/2,1,j) - \log(432)$$

$n = 2$ Makino, Suzuki: 2014

$$\phi(z,s,a) = \sum_{k=0}^{\infty}\frac{z^k}{(k+a)^s}$$

Strategy

$$\left\langle h(p)|\widehat{\mathring{O}}_n(t)|h(p)\right\rangle = p_{\mu_1}\cdots p_{\mu_n}\left\langle x^{n-1}\right\rangle_h(t)$$

Continuum limit is finite for any n

$$\left\langle x^{n-1}\right\rangle_h^{\mathrm{MS}}(\mu) = c_n(t,\mu)^{-1}\left\langle x^{n-1}\right\rangle_h(t) + O(t)$$

Matching is multiplicative for any n

n=4 $$\widehat{O}_{4444} = O_{4444} - \frac{3}{4}O_{\{\alpha\alpha 44\}} + \frac{1}{16}O_{\{\alpha\alpha\beta\beta\}}$$

Vanishing spatial momenta for any n

$$\left\langle x^{n-1}\right\rangle_h^{\mathrm{MS}}(\mu) = \left\langle x^{n-2}\right\rangle_h^{\mathrm{MS}}(\mu)\frac{c_{n-1}(t,\mu)}{c_n(t,\mu)}\frac{\left\langle x^{n-1}\right\rangle_h(t)}{\left\langle x^{n-2}\right\rangle_h(t)}, \quad n > 2$$

Potential systematics

$$\left\langle x^{n-1}\right\rangle_h^{\mathrm{MS}}(\mu) = \left\langle x^{n-2}\right\rangle_h^{\mathrm{MS}}(\mu)\frac{c_{n-1}(t,\mu)}{c_n(t,\mu)}\frac{\left\langle x^{n-1}\right\rangle_h(t)}{\left\langle x^{n-2}\right\rangle_h(t)}\,, \quad n>2$$

Finite volume effects

at finite a the extension of the local operators is (n-1)a $\quad n \sim 10-12$

Discretization errors

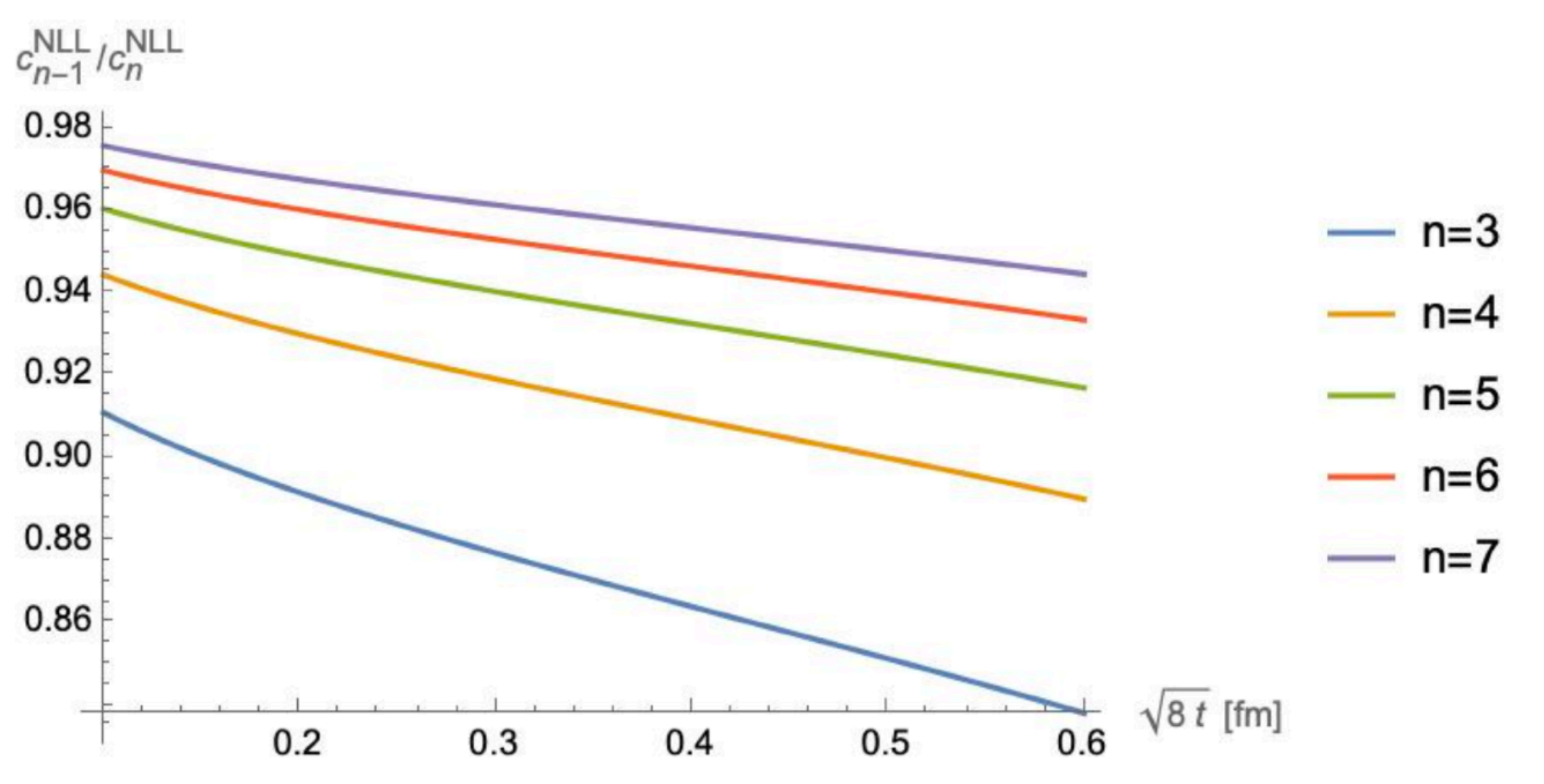
$\sqrt{8t} \gtrsim na$

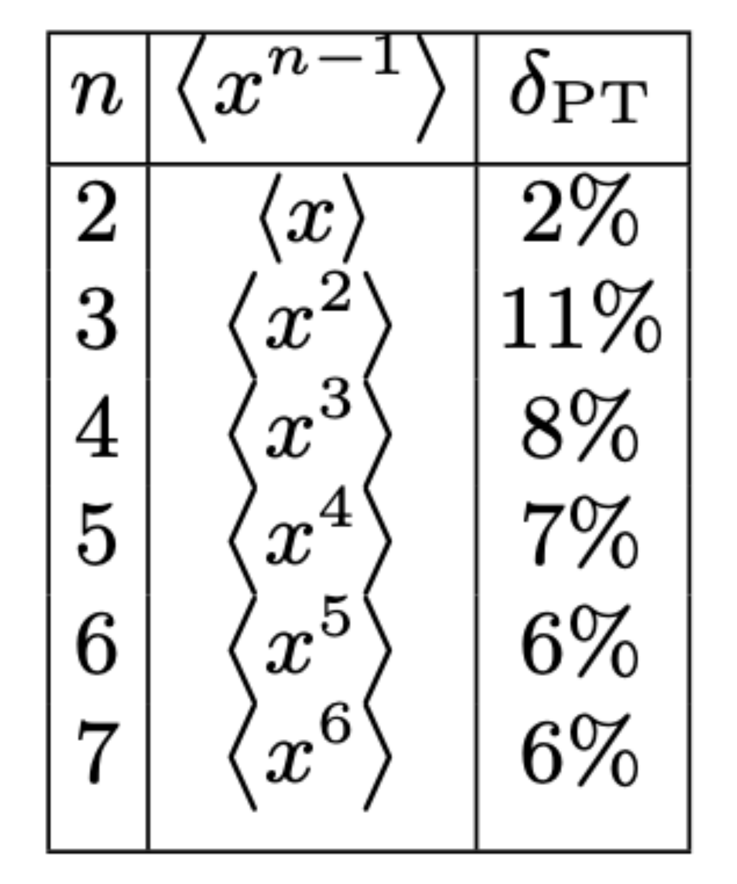
- no reason to expect larger cutoff effects than other similar calculations
- ratios are expected to reduce cutoff effects -> effect already observed
- for clover-like fermions ratios contain only O(a²) effects

Perturbative matching

$\mu = 2\ \mathrm{GeV}$

$$c_n^{\mathrm{NLL}}(t,\mu,\overline{g}(\mu)) = c_n(t,q,\overline{g}(q))\mathrm{exp}\left\{-\int_{\overline{g}(\mu)}^{\overline{g}(q)} dx\frac{\gamma_n(x)}{\beta(x)}\right\}$$





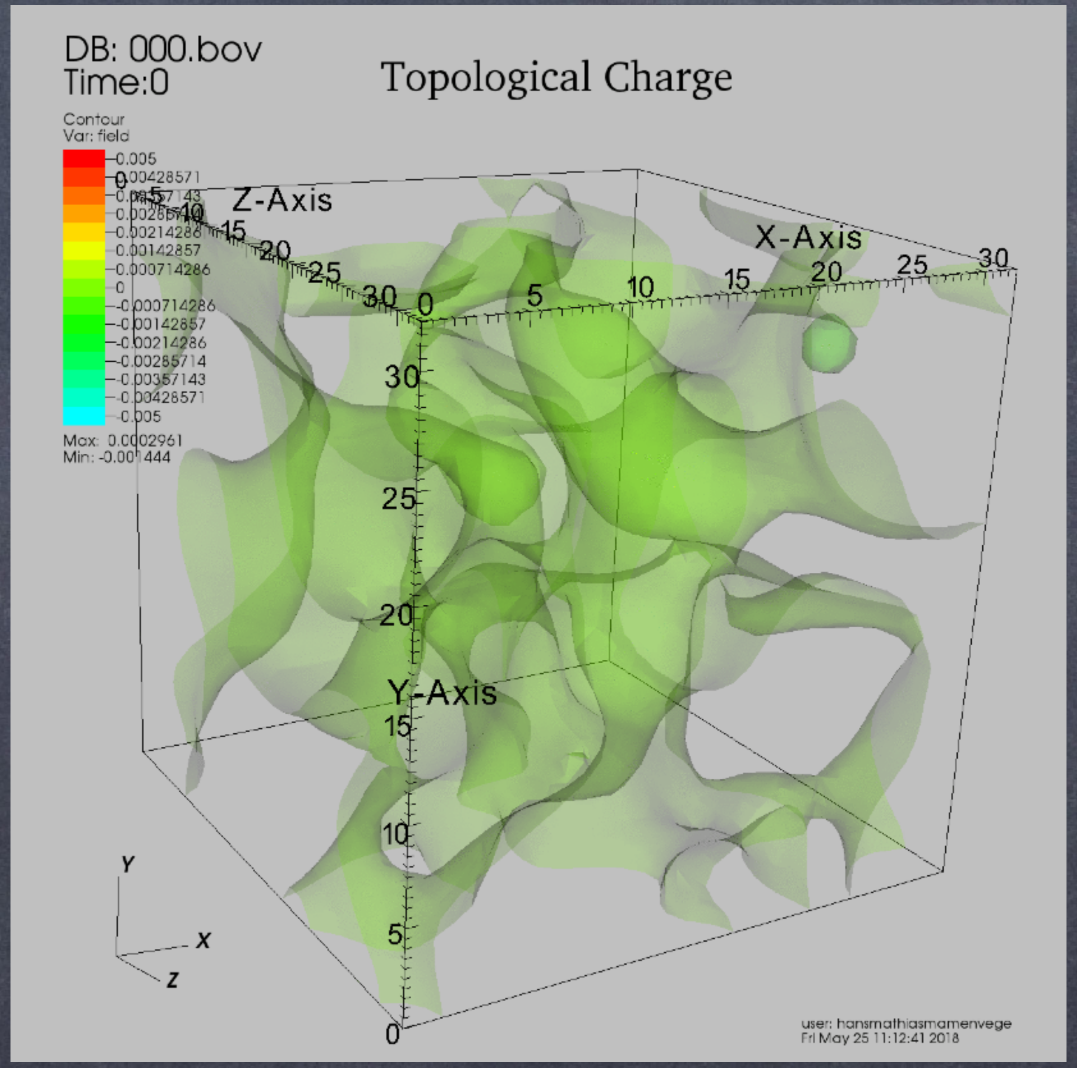
n	$\left\langle x^{n-1}\right\rangle$	δ_{PT}
2	$\left\langle x\right\rangle$	2%
3	$\left\langle x^2\right\rangle$	11%
4	$\left\langle x^3\right\rangle$	8%
5	$\left\langle x^4\right\rangle$	7%
6	$\left\langle x^5\right\rangle$	6%
7	$\left\langle x^6\right\rangle$	6%

$$\sqrt{8t} = 2(n-1)a$$
$$a = 0.05\ \mathrm{fm}$$

Summary

- New method to calculate moments of any order from lattice QCD
- We make use of an intermediate regulator (GF) that simplifies the continuum limit
- After recovering O(4) symmetry the matching is done using continuum PT
- Matrix elements can be all calculated with vanishing external momenta
- Ratios of matrix elements improve further continuum limit and S/N
- Systematic errors from perturbative matching range from 2-11% at NNL

Thank you!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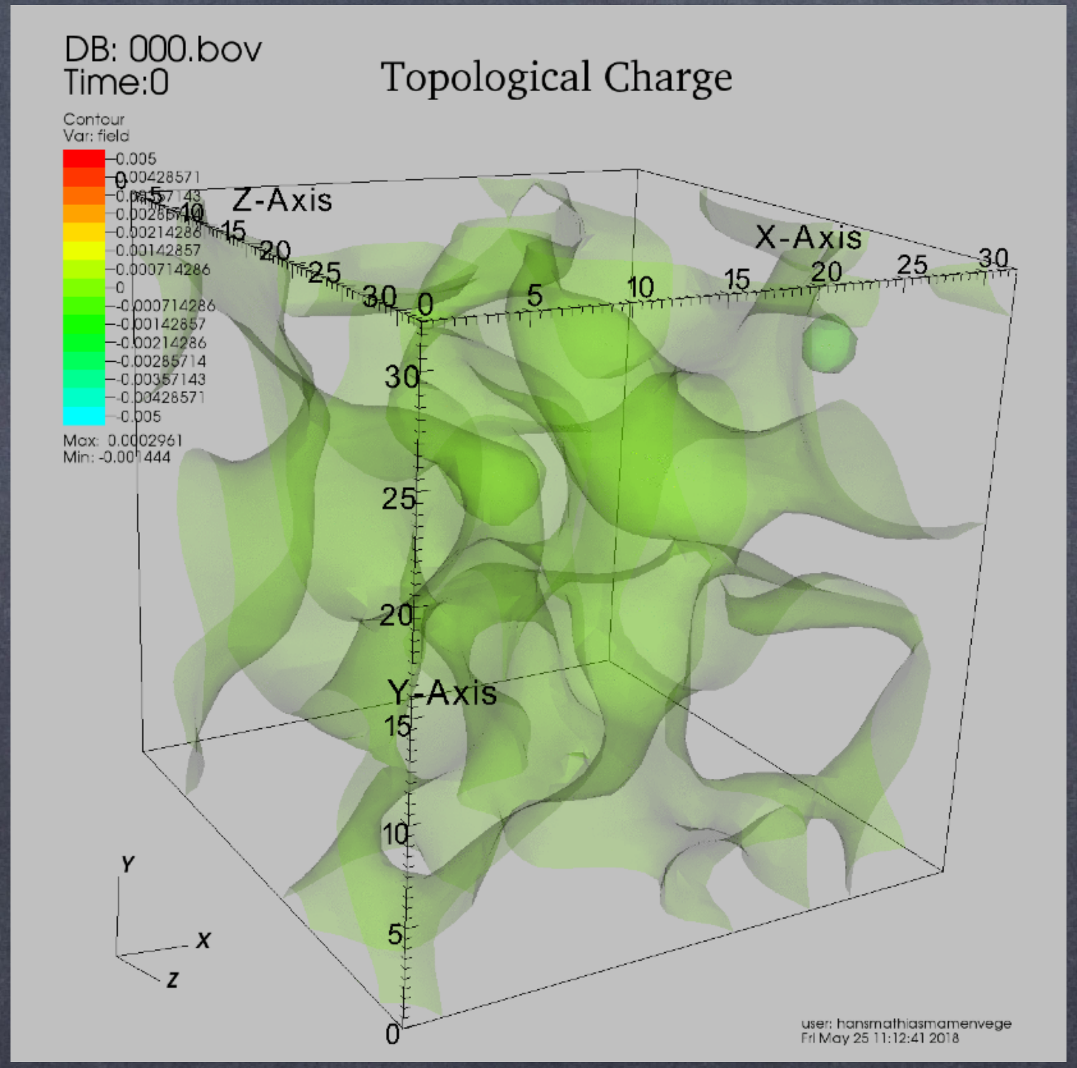
Thank you!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Backup Slides

4+1 Local field theory

Lüscher
2010-2013

$$S = S_{\mathrm{G}} + S_{\mathrm{G,fl}} + S_{\mathrm{F,QCD}} + S_{\mathrm{F,fl}}$$

$$S_{\mathrm{F,fl}} = \int_0^\infty dt \int d^4x \left[\overline{\lambda}(t,x)\left(\partial_t - \Delta\right)\chi(t,x) + \overline{\chi}(t,x)\left(\overleftarrow{\partial}_t - \overleftarrow{\Delta}\right)\lambda(t,x)\right]$$

- Wick contractions
- Renormalization. All order proof for gauge sector — Lüscher, Weisz: 2011
- Chiral symmetry and Ward identities — Lüscher: 2013 A.S.:2013
- Wilson twisted mass — A.S.: 2013

Composite operators

Scalar density $\mathcal{S}(x) = \overline{\psi}(x)\psi(x)$

$$\overline{\psi}(x)\psi(y) \overset{x\to y}{\sim} C_m(x-y)\frac{m}{|x-y|^2} + C_{m^3}(x-y)\ m^3 + C_S(x-y)\mathcal{S}(x) + \cdots$$

$$\mathcal{S}_R(x) = Z_S(a)\left[c_0(a)\frac{1}{a^3} + c_1(a)\frac{m}{a^2} + c_2(a)\frac{m^2}{a} + c_3(a)m^3 + \mathcal{S}(x)\right]$$

Absent for chirally symmetric actions