From Hadron Structure to Fundamental Symmetry

Bridging Theory and Experiment with the Gradient Flow

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IRN Terascale Montpellier 24.11.2025

Bridge Between QCD and Experiment

Experiments measure things like

- Cross sections and differential distributions
- Decay rates and lifetimes
- Asymmetries, EDM signals, form factors, etc.

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short-distance physics
(perturbative / BSM)

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hadronic matrix elements
non-perturbative QCD

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- High-energy experiments (LHC, future colliders, EIC)

  PDFs, GPDs → Higgs & BSM searches
- Flavor physics (Belle II, LHCb)

  ΔF=1,2 operators (four-fermion, chromomagnetic, etc.) matrix elements → Belle II / LHCb
- Fundamental symmetry tests (EDM searches, nuclear/atomic experiments)

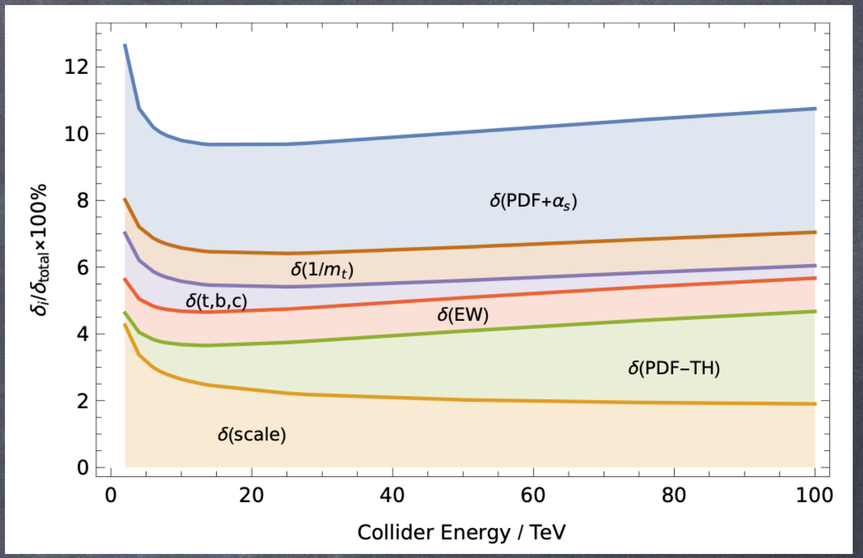
  CP-odd matrix elements → EDM experiments

Motivations

- ## Higgs boson production

PDF uncertainty is still one of the largest sources of theoretical uncertainty affecting the predictions for Higgs boson production

LHC Higgs Cross section Working Group (2016)
Snowmass 2021 White paper



- ## SM parameters

PDFs contribute to precise extraction of the SM parameters from the LHC data ->

- strong coupling constant
- W boson mass

for which different PDF sets yield results that are significantly different as compared to the size of statistical and systematic uncertainties

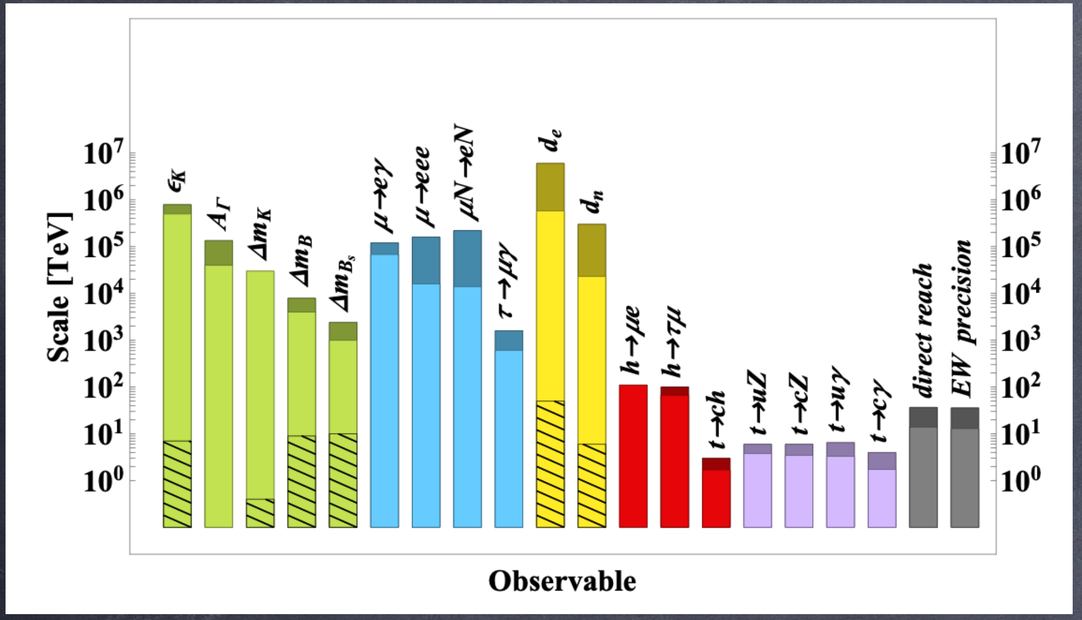
- ## New physics searches

PDF uncertainties become sizeable at large-x due to the lack of precise experimental constraints in that region
Large uncertainty in the predictions for the high-energy tails of the measured distributions,
where programs of indirect new physics searches focus

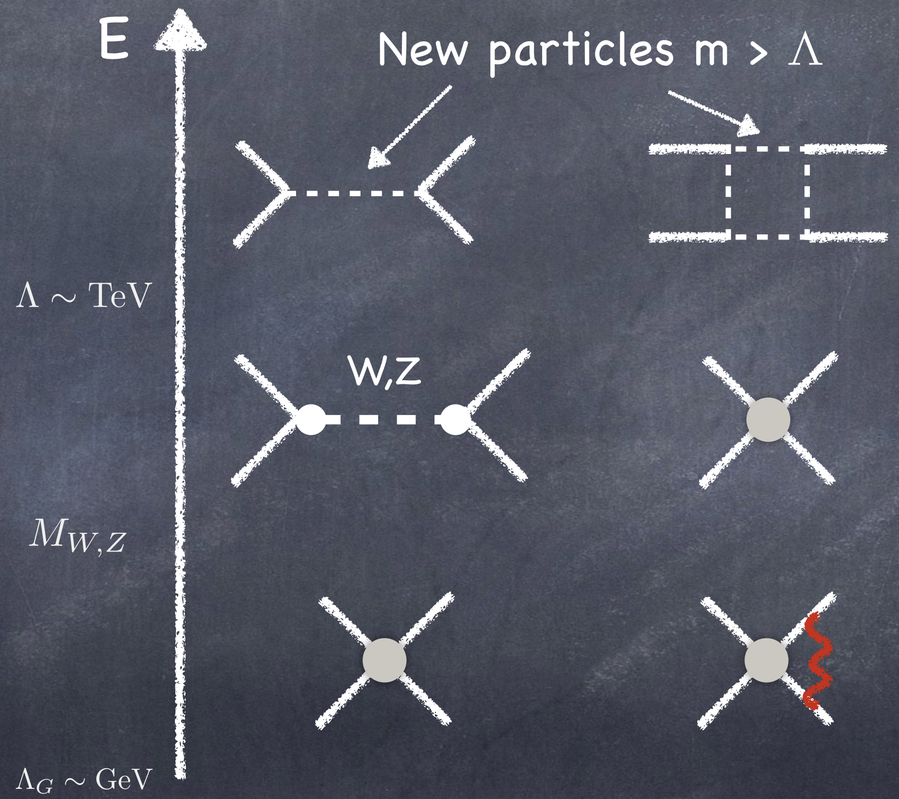
Ball, Candido, Forte, Hekhorn, Nocera, Rojo, Schwan (2022)

Effective operators

Cirigliano, Ramsey-Musolf (2013)
Engel, Ramsey-Musolf, Van Kolck (2013)



European Strategy for Particle Physics Preparatory Group, Physics Briefing Book: Input for the European Strategy for Particle Physics Update (2020) [arXiv:1910.11775 [hep-ex]]



$$\mathcal{L}_{BSM}$$

$$\mathcal{L}_{SM} + \sum_{d\geq 5} \frac{\alpha_n^{(d)}}{\Lambda^{d-4}} \mathcal{O}_n^{(d)}$$

$$\mathcal{L}_{Fermi} + \sum_i \frac{c_i}{\Lambda^2} \mathcal{O}_i$$

$$+\mathcal{L}_{QCD} + \mathcal{L}_{QED}$$

What Are the Non-Perturbative Tools?

Can we determine hadronic matrix elements non-perturbatively?

In principle yes — several frameworks exist

- **Lattice QCD** (fully non-perturbative, systematically improvable)
- **QCD sum rules** (analytic constraints + non-perturbative inputs)
- **Large N_c expansions** (useful organizing principles)

But if lattice QCD is the ideal tool…
…do we actually know how to compute these matrix elements with the required precision?

Gradient flow

Narayanan, Neuberger (2006)

Lüscher (2010)
Lüscher, Weisz (2011)

$$A_\mu(x) \overset{\text{gradient flow}}{\longrightarrow} B_\mu(x,t)$$

$$\partial_t B_\mu(x,t) = D_\nu G_{\nu\mu}(x,t)$$

$$B_\mu(x,t)|_{t=0} = A_\mu(x)$$

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

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

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

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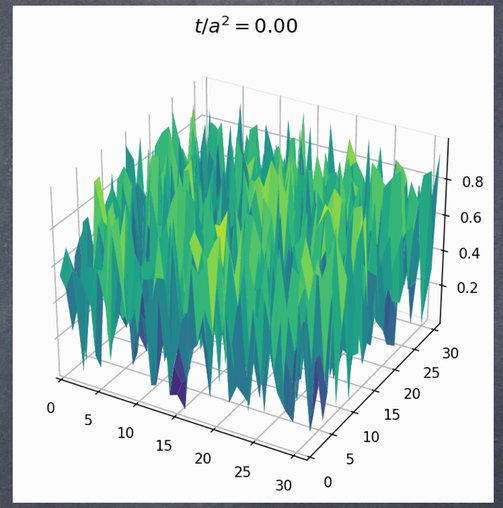

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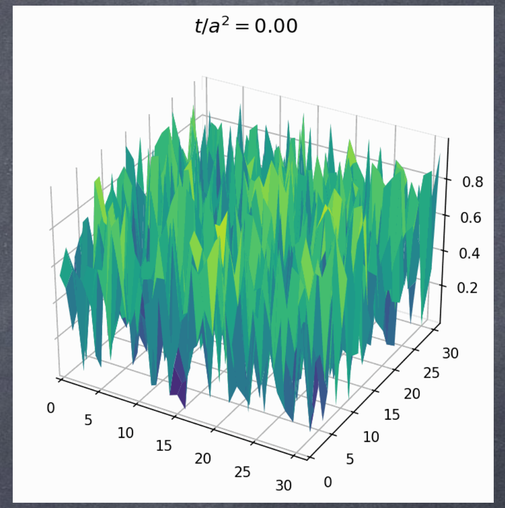

- Gaussian damping at large momenta
- Smoothing at short distance over a range $\sqrt{8t}$

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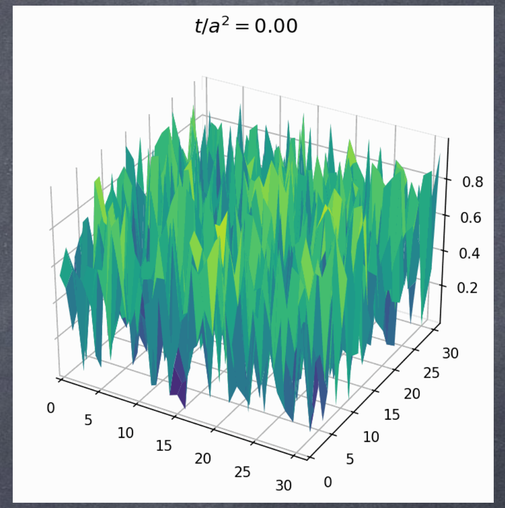

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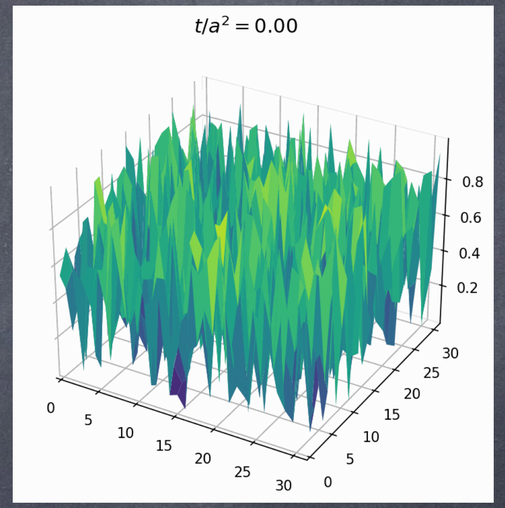

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$$\langle \cdots B_\mu(x,t) \cdots \rangle \qquad t > 0 \qquad \text{finite}$$

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Gradient flow

Lüscher (2013)

$$\psi(x) \overset{\text{gradient flow}}{\longrightarrow} \chi(x,t)$$

$$\partial_t \chi(x,t) = \Delta \chi(x,t)$$

$$\partial_t \bar{\chi}(x,t) = \bar{\chi}(x,t) \overleftarrow{\Delta}$$

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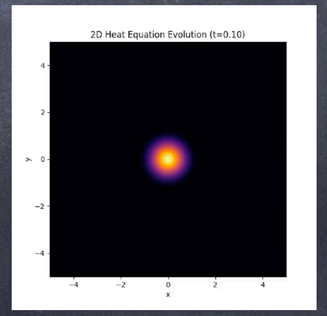

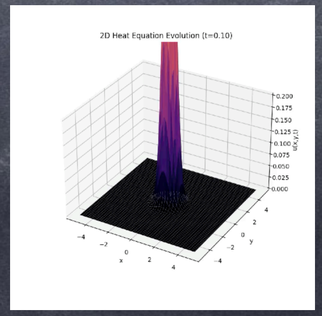

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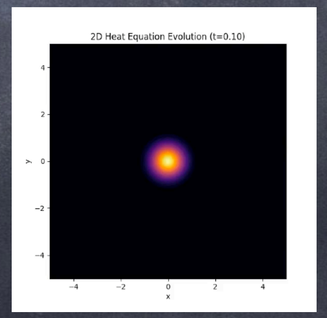

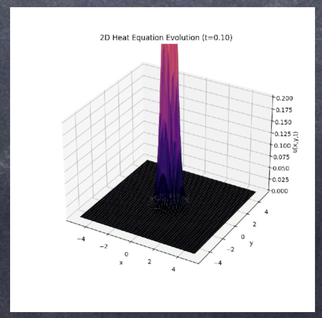

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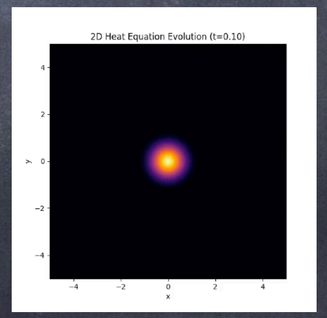

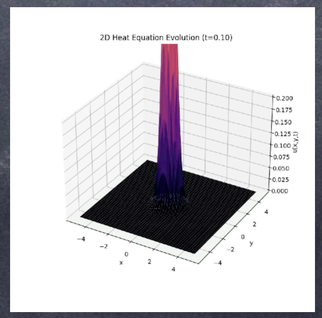

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$$\chi_R(x,t) = Z_\chi^{1/2}\chi(x,t)$$

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$$\mathcal{O}_R = Z_\chi \mathcal{O}$$

$$\Sigma_t = \langle \overline{\chi}(x,t)\chi(x,t)\rangle$$

$$\Sigma_{t,R} = Z_\chi \Sigma_t$$

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No additive divergences

Continuum limit finite after normalizing fermion fields

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"Ringed" fields

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

Makino, Suzuki (2014)

$$\chi^{r,\mathrm{MS}}(x,t) = (8\pi t)^{\epsilon/2}\,\zeta_\chi^{1/2}\mathring{\chi}^r(x,t) \qquad \zeta_\chi = 1 - \frac{\overline{g}^2}{(4\pi)^2}C_F\left(3\log(8\pi\mu^2 t) - \log(432)\right)$$

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

Harlander, Kluth, Lange (2018)

Artz et al. (2019)

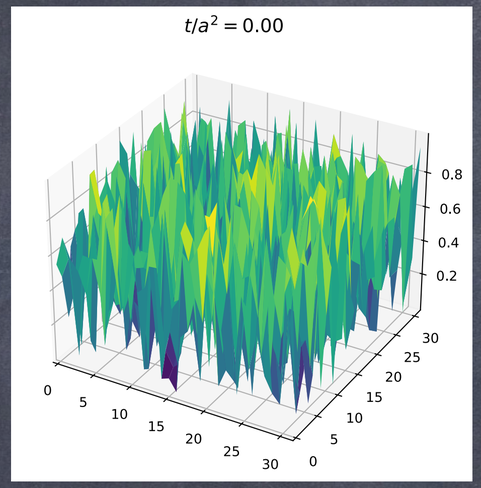
NNLO

$$D = 4 - 2\epsilon$$

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

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

Gradient flow



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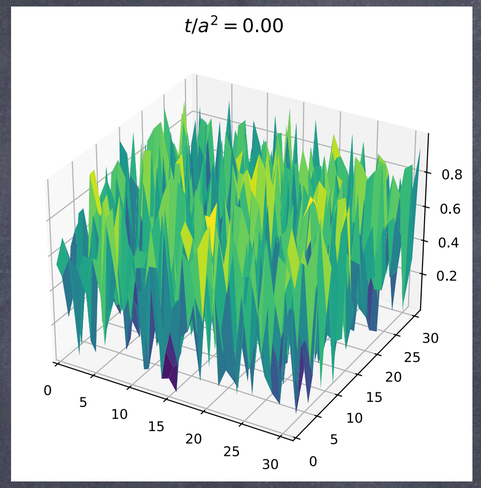

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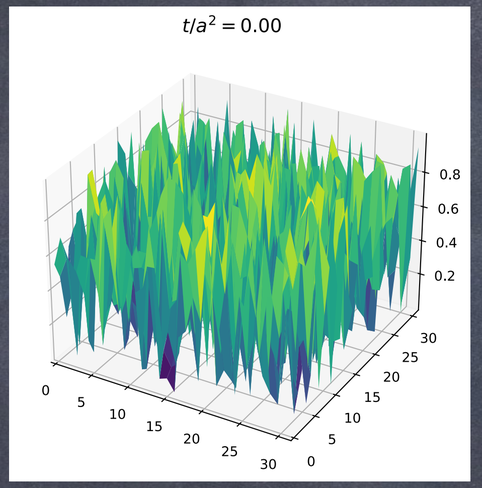

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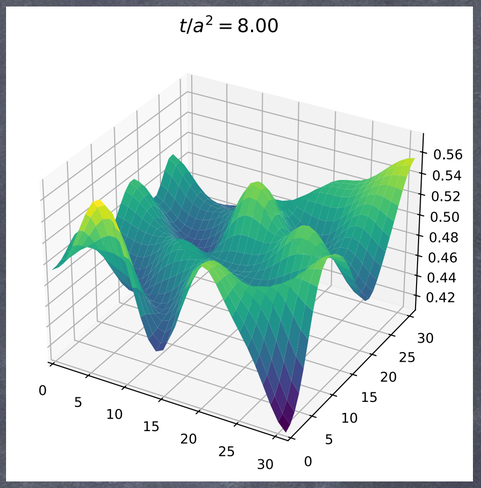

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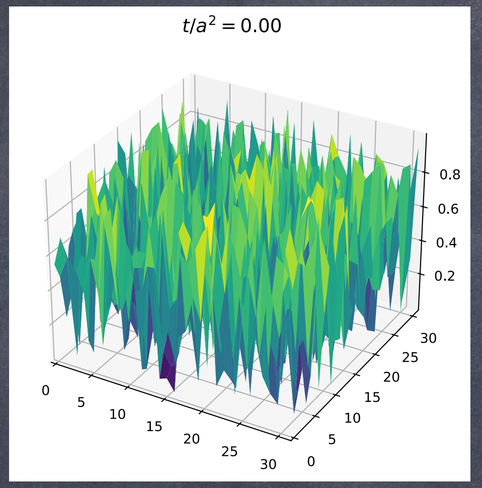

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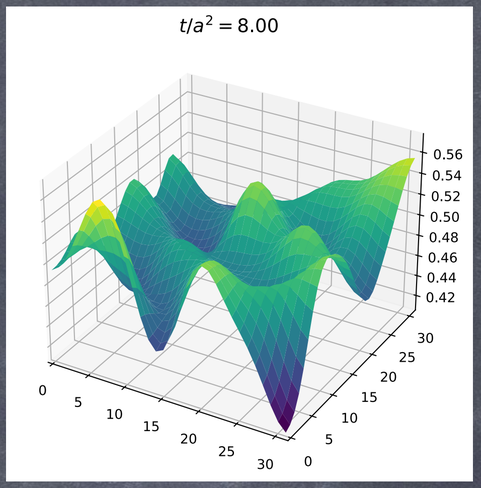

?

Short-flow-time expansion

Lüscher (2013)

$$\mathring{\mathcal{O}}_i(t) = \sum_j \zeta_{ij}(t,\mu)\,[O_j(t=0,\mu)]_{\mathrm{R}} + O(t)$$

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LQCD

PT - LQCD

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A.S., Luu, de Vries (2014-2015)
Dragos, Luu, A.S. de Vries (2018-2019)
Rizik, Monahan, A.Sh. (2018-2020)
A.Sh.: (2020)
Kim, Luu, Rizik, A.Sh. (2020)
Mereghetti, Monahan, Rizik, A.Sh., Stoffer (2021)
Monahan, Rizik, A.Sh., Stoffer (2023)
A.Sh. (2023)
Harlander, Kohnen, A.Sh. (2025)

- **New UV regulator** that preserves continuum symmetries
- **Simplifies renormalization** and improves removal of the hard lattice cutoff
- **Enables new strategies** for hadronic matrix elements.

Hadron Structure

PDF and Lattice QCD

$$\langle x^{n-1} \rangle_q^h(\mu) = \int_0^1 dx\, x^{n-1} \left[q^h(x,\mu) + (-1)^n\, \overline{q}^h(x,\mu) \right]$$

Curci, Furmanski, Petronzio (1980)
Collins, Soper (1982)

$$\langle h(p) \,|\, \widehat{O}^{qq}_{\{\mu_1 \cdots \mu_n\}} \,|\, h(p) \rangle = 2\, \langle x^{n-1} \rangle_q^h(\mu)\ (p_{\mu_1} \cdots p_{\mu_n} - \text{traces})$$

$$\widehat{O}^{qq}_{\{\mu_1 \cdots \mu_n\}}(x) = \overline{\psi}^q(x)\, \gamma_{\{\mu_1} \overleftrightarrow{D}_{\mu_2} \cdots \overleftrightarrow{D}_{\mu_n\}}\, \psi^q(x) - \text{traces}$$

Kronfeld, Photiadis (1985)
Martinelli, Sachrajda (1987 - 1988)

- Continuum limit too difficult for $\langle x^n \rangle$ for n>3
- For n=2,3 the need of non-vanishing external spatial momenta degrades the signal-to-noise ratio
- Realistically only the lowest moments of PDFs and GPDs could be computed directly
- Power divergences and large gauge noise restrict the calculation to $\langle x \rangle$ and (very poorly) to $\langle x^2 \rangle$ and $\langle x^3 \rangle$

PDF and Lattice QCD

Approaches have been developed to determine the x-dependence of the PDFs

- Hadronic tensor — Liu, Dong (1994) Liang et al. (2019)
- Auxiliary scalar field — Aglietti et al. (1998)
- quasi-PDF (LaMET) — Ji (2013)
- pseudo-PDF — Radyushkin (2017) Karpie, Radyushkin, Orginos, Zafeiropoulos: (2017-2018)
- Fictitious heavy quark — Detmold, Lin (2005)
- Auxiliary scalar quark — Braun, Müller (2008)
- Compton amplitude + OPE — Chambers et al. (2017)
- Good Lattice Cross Sections — Ma, Qiu (2018)
- PDF without Wilson line — Zhao (2024)

- 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)

Intrinsic tension: Need small separations (twist control) and large hadron momenta (Ioffe time),
Lattices reach only $P_z \lesssim 3\ \mathrm{GeV}$ $\Rightarrow$ limited ν window.

High-momentum systematics: Large P_z worsens excited states and noise ==>
precision saturates unless lattices get much finer or new strategies are used

Flowed moments

A.Sh. (2023)

Calculate matrix elements of flowed twist-2 fields -> renormalize multiplicatively

$$\left\langle h(p)|\hat{\mathring{O}}_n(t)|h(p)\right\rangle = 2\left(p_{\mu_1}\cdots p_{\mu_n} - \text{trace terms}\right)\left\langle x^{n-1}\right\rangle_h(t)$$

Renormalize flowed fermion fields or build appropriate ratios. Continuum limit is finite and O(a) improved for any n, m

$$\frac{\left\langle x^{n-1}\right\rangle_h(t)}{\left\langle x^{m-1}\right\rangle_h(t)} \quad n \neq m \quad n \geq 3,\ m \geq 2$$

Construct fields based on irreps of O(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

Compute matching factors in perturbation theory. Matching is multiplicatively in the continuum

$$\left\langle x^{n-1}\right\rangle_h^{\overline{\text{MS}}}(\mu) = \langle x\rangle_h^{\overline{\text{MS}}}(\mu)\frac{c_2(t,\mu)}{c_n(t,\mu)}\frac{\left\langle x^{n-1}\right\rangle_h(t)}{\langle x\rangle_h(t)}$$

Test case: Heavy pion at SU(3) flavor-symmetric point

- Stabilized Wilson Fermions (SWF)
- Lüscher-Weisz gauge action

$m_u = m_d = m_s$

label	a [fm]	t_0/a^2	β	$\kappa_{ud} = \kappa_s$	$T/a \times (L/a)^3$	N_{cfg}
a12m412_mL6.0 (a12)	0.12	1.4868(04)	3.685	0.1394305	96×24^3	838
a094m412_mL6.2 (a094)	0.094	2.4400(01)	3.8	0.138963	96×32^3	700
a077m412_mL7.7 (a077)	0.077	3.6239(12)	3.9	0.138603	96×48^3	400
a064m412_mL6.4 (a064)	0.064	5.2471(26)	4.0	0.138272	96×48^3	500

OPEN LATtice initiative

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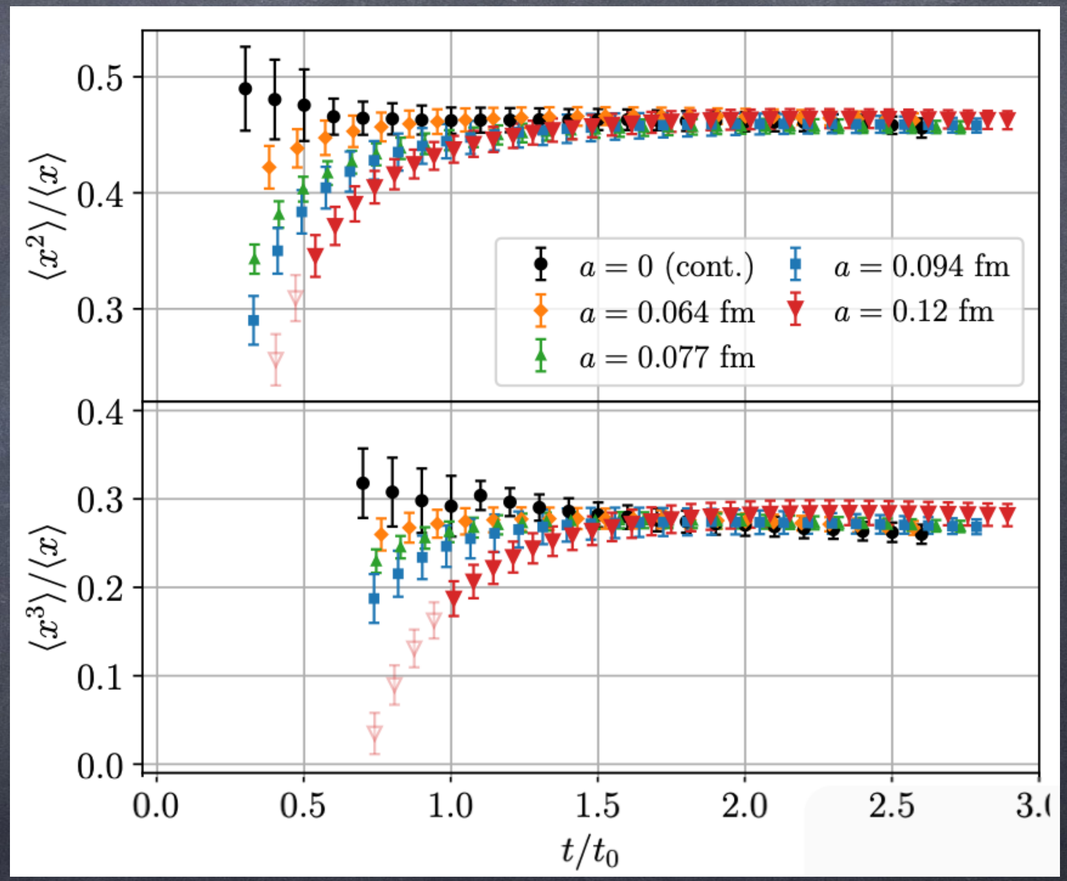
https://openlat1.gitlab.io

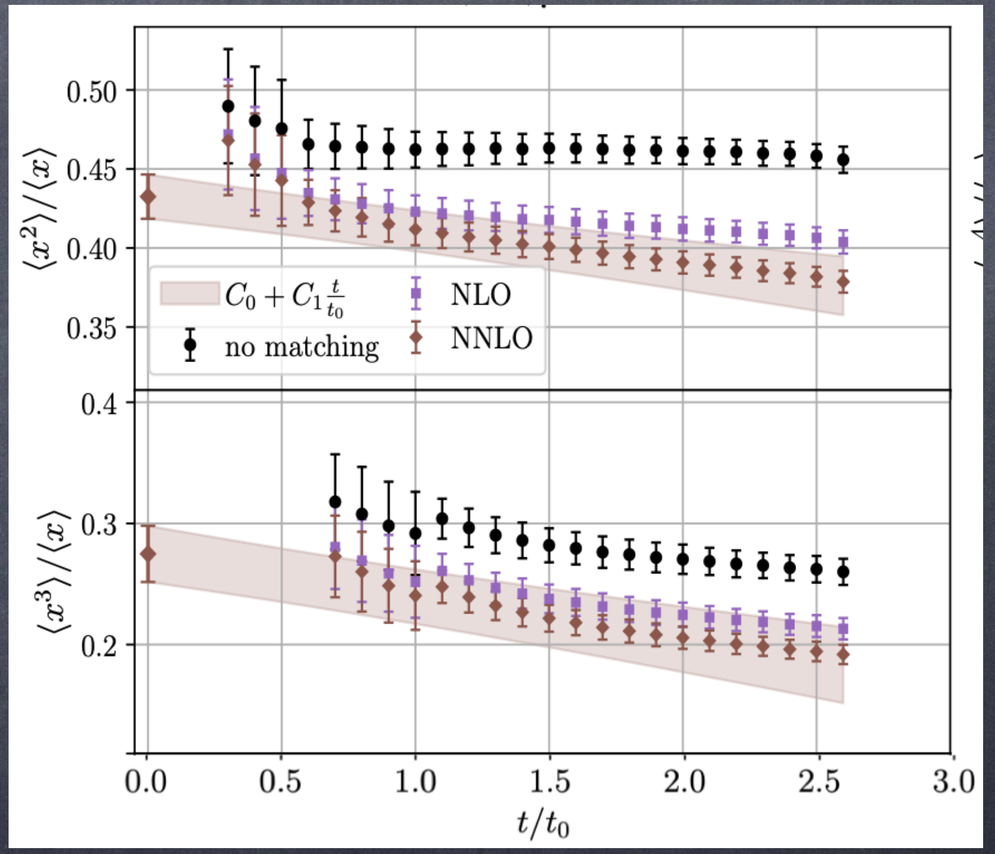


Matching and $t \to 0$

- NLO calculation — A.Sh. (2023)
- NNLO calculation — Harlander, Kohnen, A.Sh. 2511.17145

$$\mathring{\widehat{O}}^{rs}_{\{\mu_1 \cdots \mu_n\}}(t) = \zeta_n(t,\mu)\, \widehat{O}^{rs}_{\{\mu_1 \cdots \mu_n\}}(\mu) + O(t)$$

$$\frac{\langle x^{n-1} \rangle^{\overline{\rm MS}}(\mu)}{\langle x^{m-1} \rangle^{\overline{\rm MS}}(\mu)} = \frac{\zeta_m(t,\mu)}{\zeta_n(t,\mu)} \frac{\langle x^{n-1} \rangle(t)}{\langle x^{m-1} \rangle(t)} + O(t)$$



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Comparison with experiment

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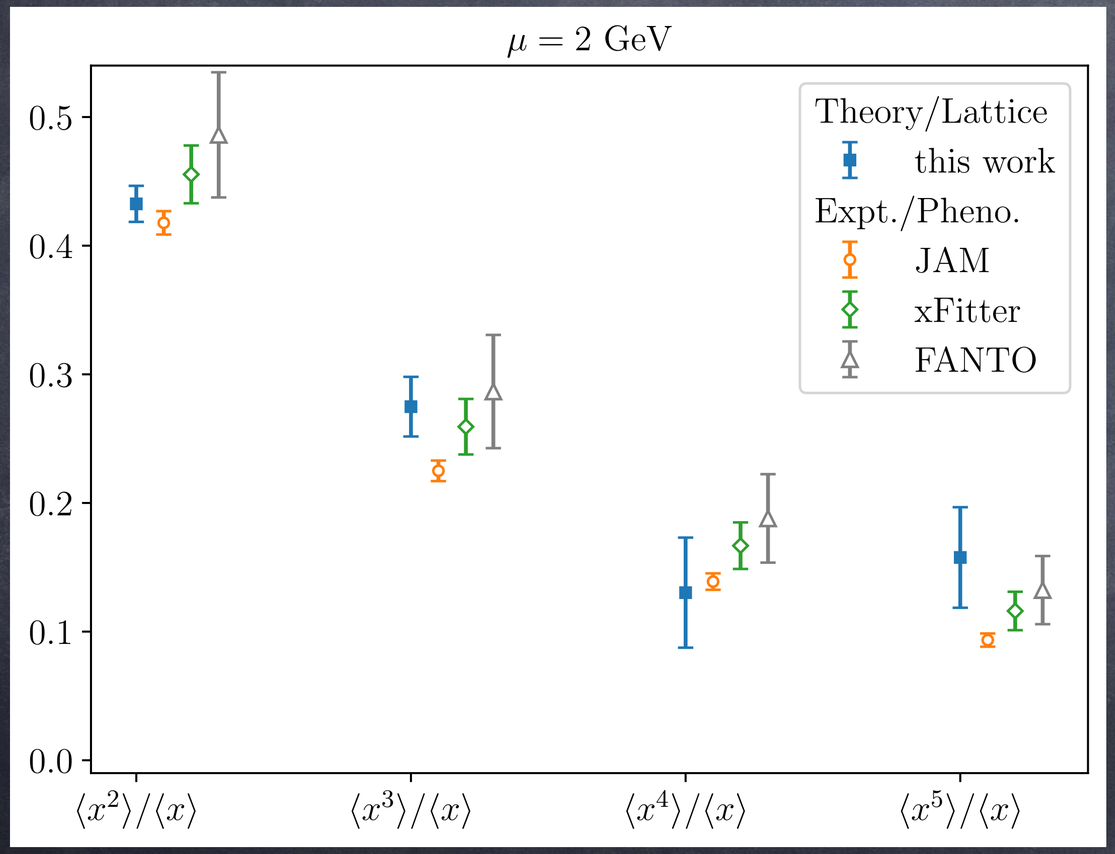
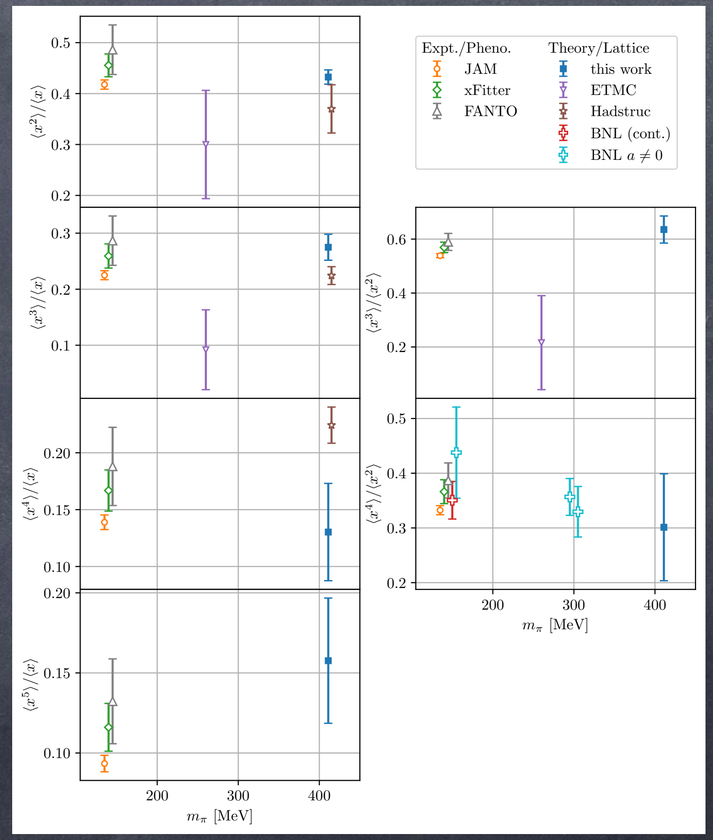
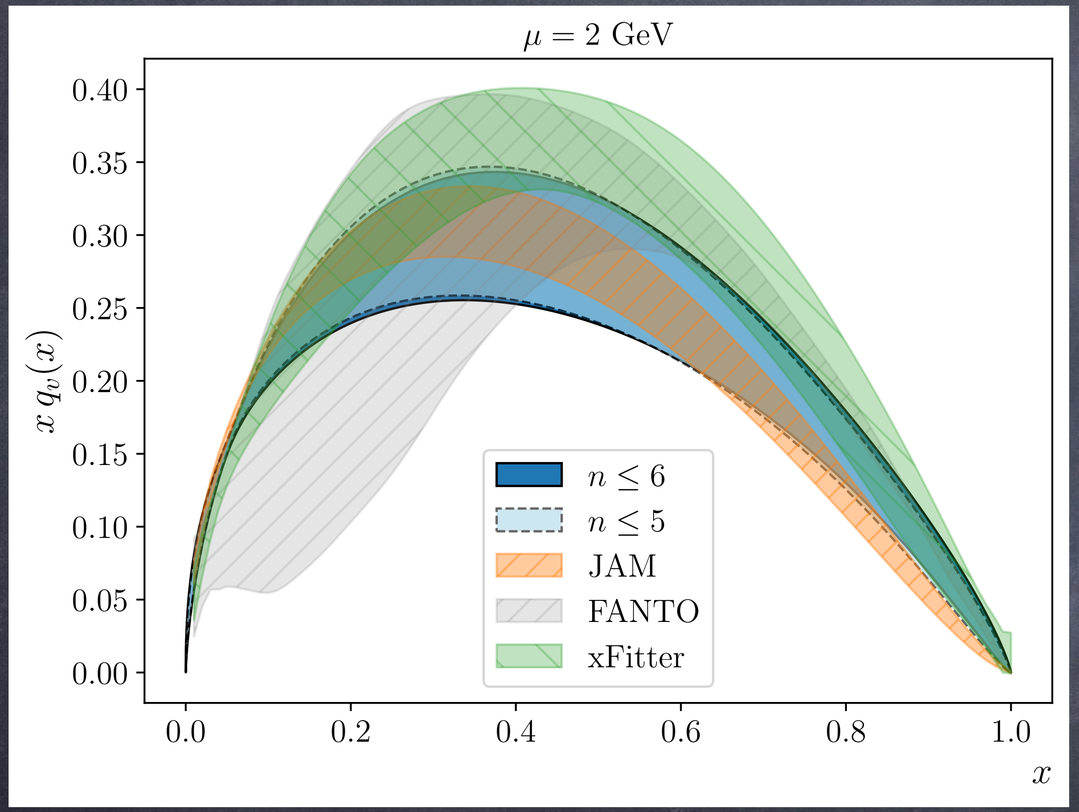


JAM: 2108.05822
xFitter: 2002.02902
FANTO: 2505.13594e



ETMC: Alexandrou et al. (2020-2021)
Joó et al. (2019)
Gao et al. (2022)

PDF reconstruction



$$q_v(x) = \mathcal{N}\, x^{\alpha}(1-x)^{\beta}\, p(x)$$

- Non-trivial use of priors to stabilize fit
- Difficulties in constraining α but large x parameter $\beta \sim 1$ across all fit variations
- Plans to use Gaussian Processes (underway by UC Berkeley PhD student Rohith Karur)

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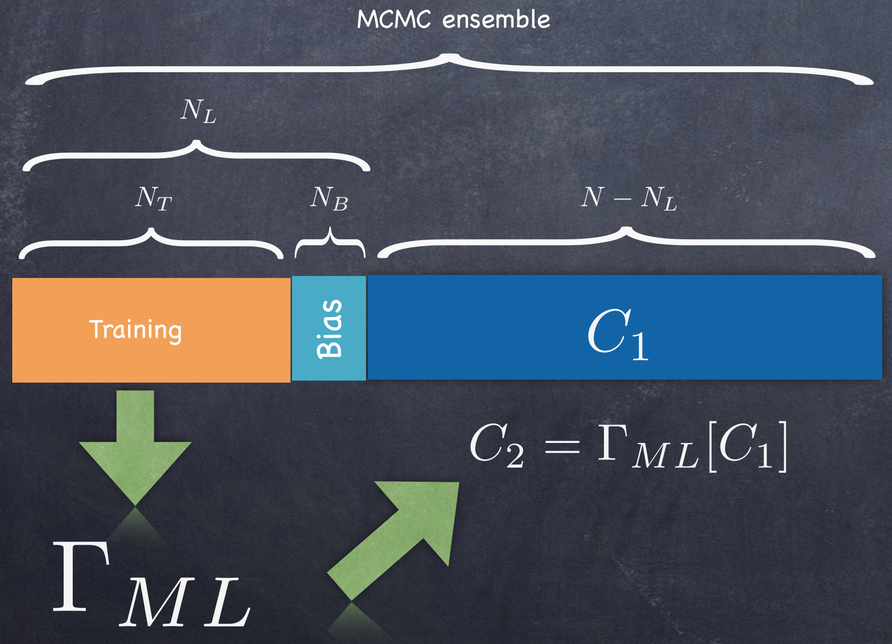
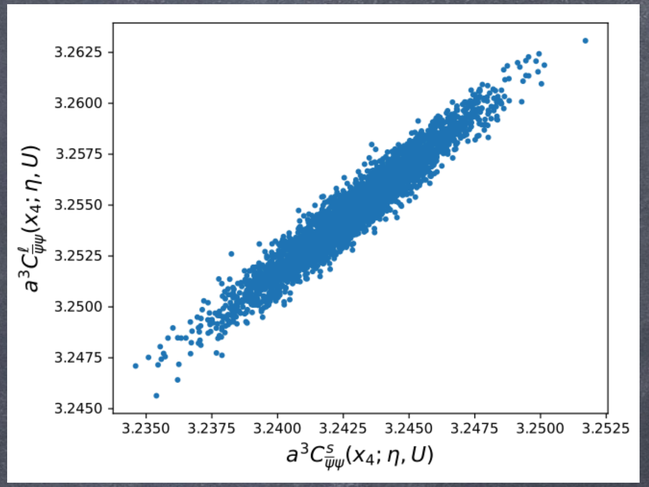
Machine Learning

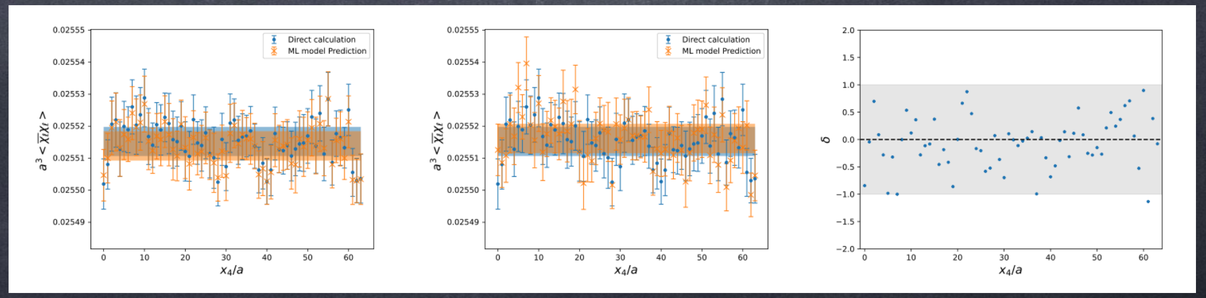
J. Kim, G. Pederiva, A.Sh. (2024)

Method based on supervised ML to accelerate the computation of hadron correlators

- DTs can map correlations between lattice QCD data Yoon et al. (2019)
- Trained a DT to reconstruct fermion disconnected diagrams with different parameters (quark mass, flow time,...)





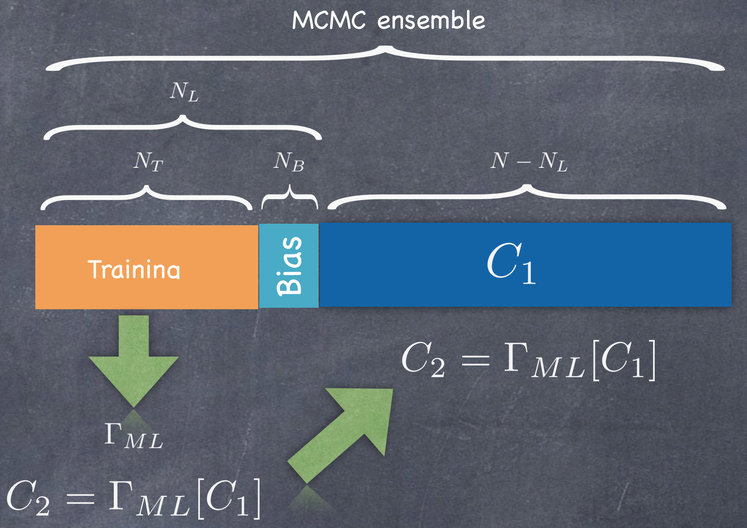


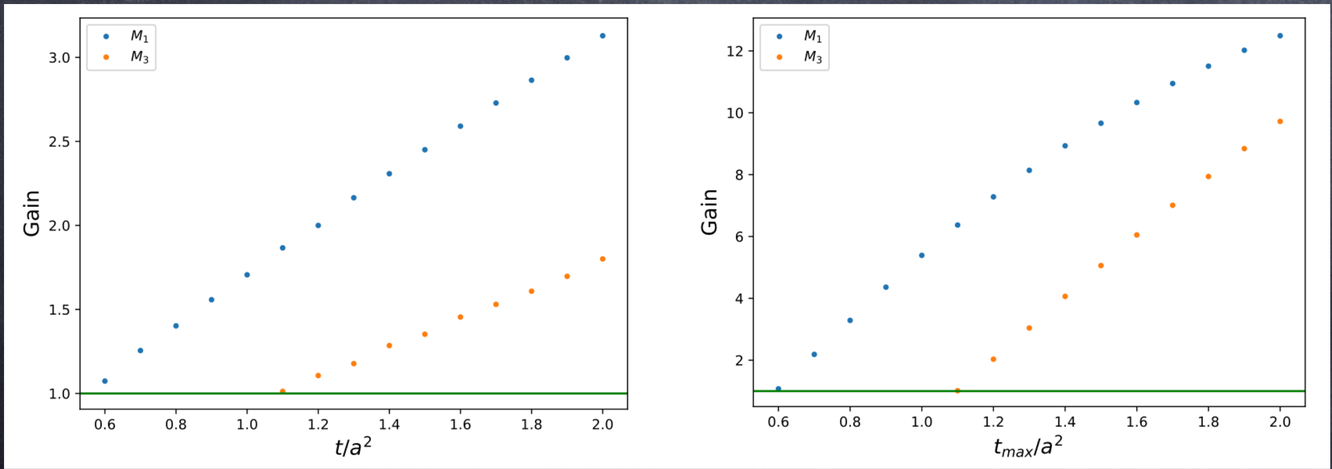
Machine Learning

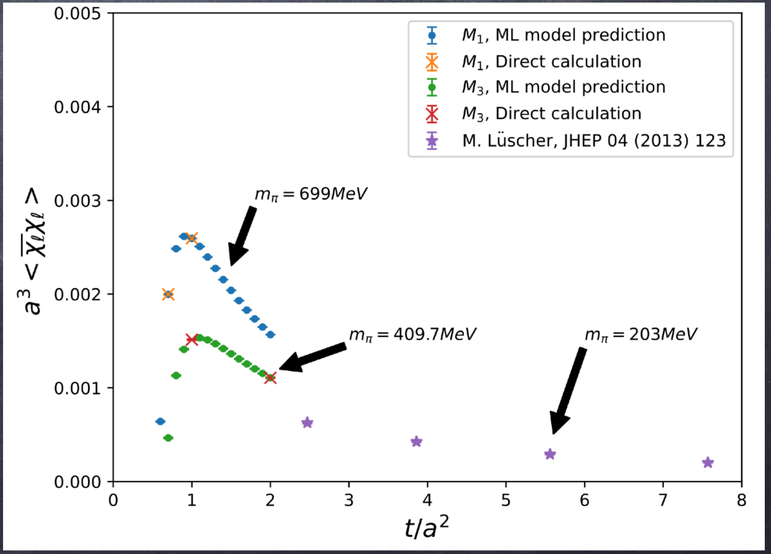
J. Kim, G. Pederiva, A.Sh. (2024)

Gain factors

Ens.	Input	Obs.	Direct	ML	N_T	N_B	N_U	Gain
M_1	$a^3 \langle\overline{\psi}\psi\rangle\|_{m_s}$	$a^3 \langle\overline{\psi}\psi\rangle\|_{m_\ell}$	3.252553(25)	3.252554(24)	50	349	399×19	1.31
M_3	$a^3 \langle\overline{\psi}\psi\rangle\|_{m_s}$	$a^3 \langle\overline{\psi}\psi\rangle\|_{m_\ell}$	3.254626(31)	3.254622(26)	50	400	450×19	1.39
M_1	$a^3 \langle\overline{\chi}\chi\rangle\|_{t=0.5}$	$a^3 \langle\overline{\chi}\chi\rangle\|_{t=0.7}$	0.0019974(48)	0.0019970(47)	50	349	399×19	1.26
M_1	$a^3 \langle\overline{\chi}\chi\rangle\|_{t=0.5}$	$a^3 \langle\overline{\chi}\chi\rangle\|_{t=1.0}$	0.0025947(35)	0.0025946(34)	50	349	399×19	1.71
M_3	$a^3 \langle\overline{\chi}\chi\rangle\|_{t=1.0}$	$a^3 \langle\overline{\chi}\chi\rangle\|_{t=2.0}$	0.0011067(37)	0.0011070(33)	50	400	450×29	1.80





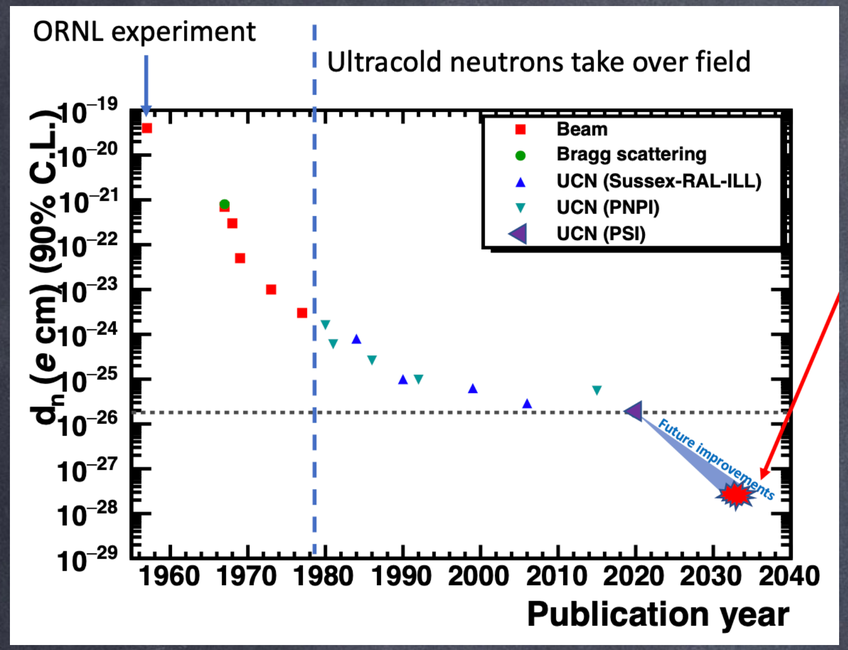


Summary - PDF

- **First direct QCD extraction** of flavor non-singlet pion PDF moment ratios using the gradient flow, resolving the **power-divergence problem** for higher moments
- General method to compute PDF moments of any order, valid for any lattice action
- Uses a **gradient-flow regulator**, simplifying the **continuum limit** and restoring O(4) before **continuum PT matching**
- Matrix elements computed at **zero external momentum ratios** further improve S/N and continuum control
- Moments up to $\langle x^5 \rangle$ show **very good agreement** with phenomenology even with modest statistics
- Provides **high-precision inputs** useful for global PDF analyses
- **Future extensions:** physical-pion limit, proton, singlet+gluon, helicity/transversity, GPD form factors, higher twist

Electric dipole moment θ-term

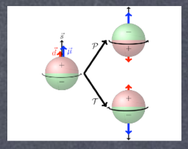
Neutron EDM

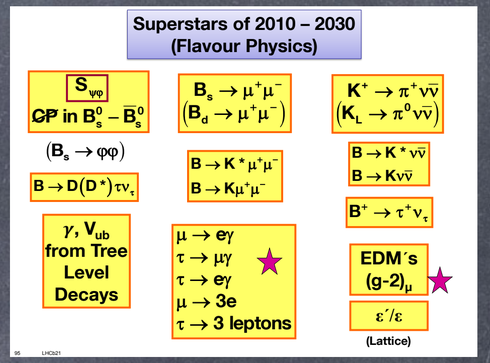


$$|d_n| < 1.8 \times 10^{-26}\ e\ \text{cm}\ (90\%\ \text{C.L.})$$

PSI: Abel et al. (2020)

$$H = -\mu\, \underline{B} \cdot \frac{\underline{S}}{|S|} - d\, \underline{E} \cdot \frac{\underline{S}}{|S|}$$





Buras: LHCb21

Alarcon et al. (2022)
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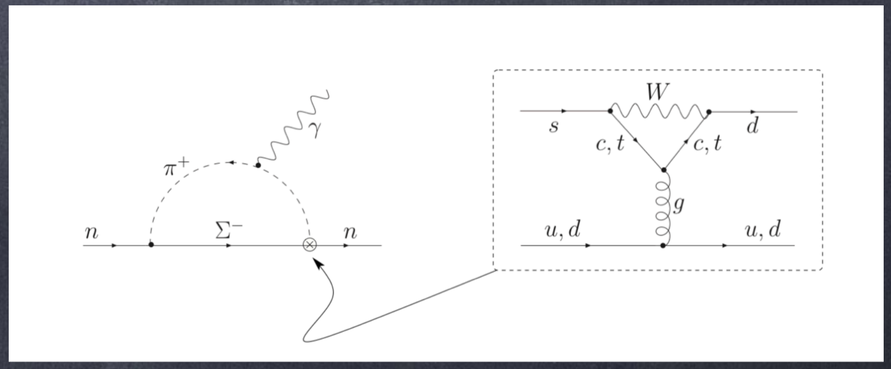
Experiment: Facility	Neutron Source	Measurement Cell	Measurement Techniques	90% C.L. (10^{-28} e-cm) With 300 Live Days	Year 90% C.L. Data Acquired
Crystal: JPARC	Cold Neutron Beam	Solid	Crystal Diffraction (High Internal $\vec{E}$)	< 100	Development
Beam: ESS	Cold Neutron Beam	Vacuum	Pulsed Beam	< 50	~ 2030
PNPI: ILL	ILL Turbine (UCN) PNPI/LHe (UCN)	Vacuum	Ramsey Technique, $\vec{E} = 0$ Cell for Magnetometry	Phase 1 < 100 < 10	Development Development
n2EDM: PSI	Solid D_2 (UCN)	Vacuum	Ramsey Technique, External Cs Magnetometers, Hg Co-Magnetometer	< 15	~ 2026
PanEDM ILL/Munich	Superfluid ^{4}He (UCN), Solid D_2 (UCN)	Vacuum	Ramsey Technique, Hg Co-External ^{3}He and Cs Magnetometers	< 30	~ 2026
TUCAN: TRIUMF	Superfluid ^{4}He (UCN)	Vacuum	Ramsey Technique, Hg Co-Magnetometer, External Cs Magnetometers	< 20	~ 2027
nEDM: LANL	Solid D_2 (UCN)	Vacuum	Ramsey Technique, Hg Co-Magnetometer, Hg External Magnetometer, OPM	< 30	~ 2026
nEDM@SNS: ORNL	Superfluid ^{4}He (UCN)	^{4}He	Cryogenic High Voltage, ^{3}He Capture for ω, ^{3}He Co-Magnetometer with SQUIDs, Dressed Spins, Superconducting Magnetic Shield	< 20 < 3	~ 2029 ~ 2031

$$(d_n)_{\text{SM}} = (1-6) \times 10^{-32} e\ \text{cm}$$

Shabalin (1978-1980) Khriplovich, Zhitnitsky (1982)
Gavela et al. (1982) Seng (2015)



CP-violating sources

$$\mathcal{L}_{\mathrm{QCD}+\theta} = \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu} + \sum_{f=u,d,s,\ldots} \overline{\psi}_f(x) \left\{ \gamma_\mu \left[\partial_\mu + g A^a_\mu T^a \right] + m_f \right\} \psi_f(x) - i\bar{\theta} q(x)$$

$$q(x) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \mathrm{tr} \left\{ G_{\mu\nu}(x) G_{\rho\sigma}(x) \right\}$$

Topological charge density

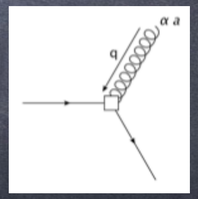
- Full list of dimension 5 and 6 operators is known

Buchmuller, Wyler (1986)
de Rujula et al. (1991)
Grzadkowski et al (2010)

$$O^f_{\mathrm{q}}(x) = \overline{\psi}_f(x) \gamma_5 \sigma_{\mu\nu} \psi_f(x) F_{\mu\nu}$$

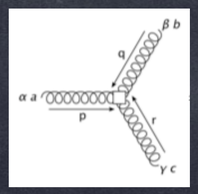
Quark EDM

$$O^f_{\mathrm{CE}}(x) = \overline{\psi}_f(x) \gamma_5 \sigma_{\mu\nu} G^a_{\mu\nu} T^a \psi_f(x)$$



Quark-chromo EDM

$$O_{3\mathrm{g}}(x) = \frac{1}{6} i f^{abc} G^a_{\mu\rho}(x) G^b_{\nu\rho}(x) G^c_{\lambda\sigma}(x) \epsilon_{\mu\nu\lambda\sigma}$$



3-gluon CP-odd

Weinberg (1989)

CP-violating sources

$$\mathcal{L}_{\rm QCD+\theta} = \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu} + \sum_{f=u,d,s,\ldots} \overline{\psi}_f(x) \left\{ \gamma_\mu \left[\partial_\mu + g A^a_\mu T^a \right] + m_f \right\} \psi_f(x) - i\bar{\theta} q(x)$$

$$q(x) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} {\rm tr} \left\{ G_{\mu\nu}(x) G_{\rho\sigma}(x) \right\}$$

Topological charge density

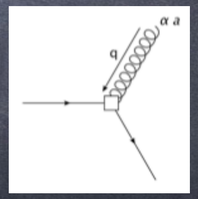
- Full list of dimension 5 and 6 operators is known

Buchmuller, Wyler (1986)
de Rujula et al. (1991)
Grzadkowski et al (2010)

$$O^f_{\rm q}(x) = \overline{\psi}_f(x) \gamma_5 \sigma_{\mu\nu} \psi_f(x) F_{\mu\nu}$$

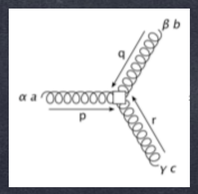
Quark EDM

$$O^f_{\rm CE}(x) = \overline{\psi}_f(x) \gamma_5 \sigma_{\mu\nu} G^a_{\mu\nu} T^a \psi_f(x)$$



Quark-chromo EDM

$$O_{\rm 3g}(x) = \frac{1}{6} i f^{abc} G^a_{\mu\rho}(x) G^b_{\nu\rho}(x) G^c_{\lambda\sigma}(x) \epsilon_{\mu\nu\lambda\sigma}$$



3-gluon CP-odd

Weinberg (1989)

Hadronic matrix elements

$$d_{\rm N} = M^{\theta}_{\rm N}\bar{\theta} + \left(\frac{v}{\Lambda}\right)^2 \sum_i M^{(i)}_{\rm N}\tilde{d}_i \qquad \langle N|J_\mu \mathcal{O}_{\not{C}\not{P}}|N\rangle \to d\ \underline{E}\cdot\underline{S}$$

$$d_f \sim e\, q_f \sin(\delta_{\rm CPV}) \left(\frac{g^2}{16\pi^2}\right)^{\ell} \xi_{\rm FV} \frac{m_f}{M^2_{\rm NP}}.$$

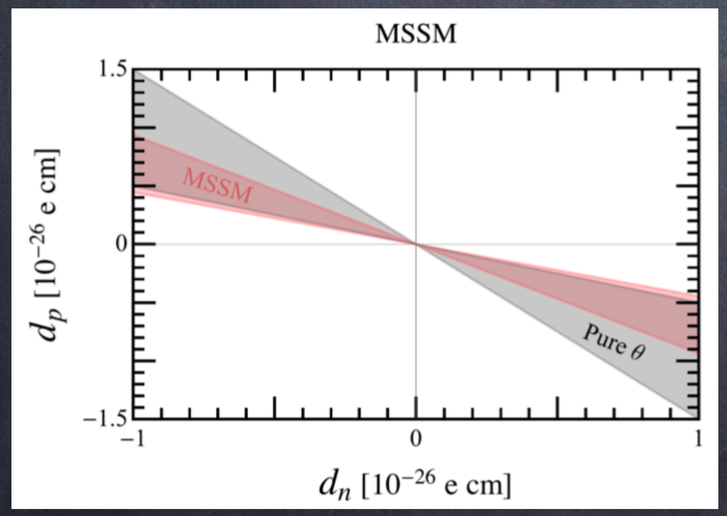
$M^{\theta}_{\rm N}$ → Hadronic matrix element topological charge

$M^{(i)}_{\rm N}$ → Hadronic matrix element CP odd operators

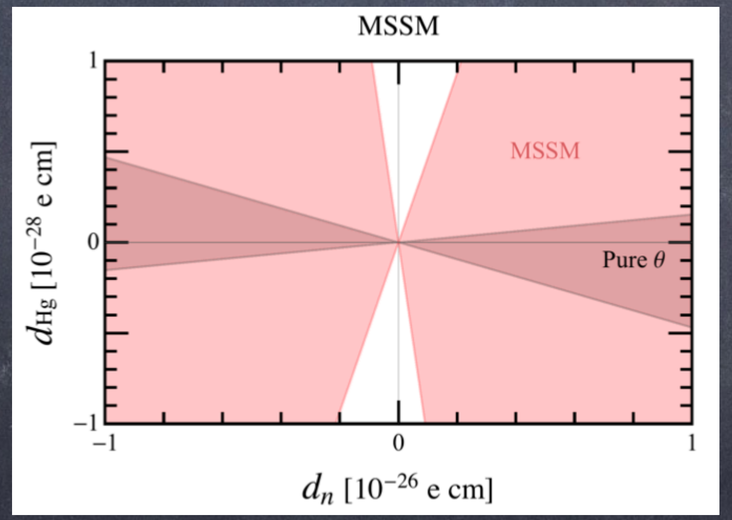
$$M_{\rm NP} \gtrsim \sqrt{\frac{10^{-29}\, e\,{\rm cm}}{d_e^{\rm max}}} \times \begin{cases} 50\ {\rm TeV} & \ell = 1 \\ 2\ {\rm TeV} & \ell = 2 \end{cases}$$

$$\begin{aligned} d_n = &- (1.5 \pm 0.7)\cdot 10^{-3}\bar{\theta} e\ {\rm fm} \\ &- (0.2 \pm 0.01) d_u + (0.78 \pm 0.03) d_d + (0.0027 \pm 0.016) d_s \\ &- (0.55 \pm 0.28) e\tilde{d}_u - (1.1 \pm 0.55) e\tilde{d}_d + (50 \pm 40)\,{\rm MeV} e\tilde{d}_G \end{aligned}$$

Dragos, Luu, A.Sh., de Vries, Yousif (2019)



de Vries et al.: (2021)



Alarcon et al.: (2022)
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Shintani et al. (2005)
Berruto, Blum, Orginos, Soni (2006)
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$$d_f \sim e\,q_f \sin(\delta_{\rm CPV})\left(\frac{g^2}{16\pi^2}\right)^{\ell} \xi_{\rm FV}\frac{m_f}{M^2_{\rm NP}}.$$

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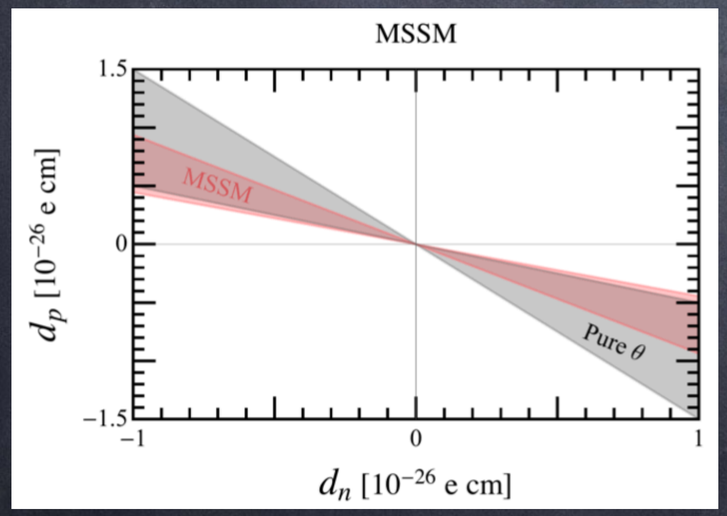
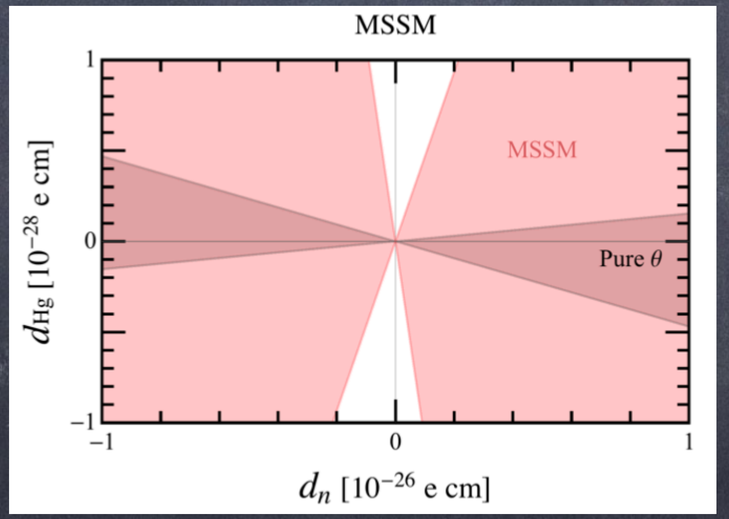
$$d_n = \begin{aligned} &- \quad (1.5 \pm 0.7)\cdot 10^{-3}\bar{\theta} e\ {\rm fm} \\ &- \quad (0.2 \pm 0.01)d_u + (0.78 \pm 0.03)d_d + (0.0027 \pm 0.016)d_s \\ &- \quad (0.55 \pm 0.28)e\tilde{d}_u - (1.1 \pm 0.55)e\tilde{d}_d + (50 \pm 40){\rm MeV} e\tilde{d}_G \end{aligned}$$

Dragos, Luu, A.Sh., de Vries, Yousif (2019)



de Vries et al.: (2021)



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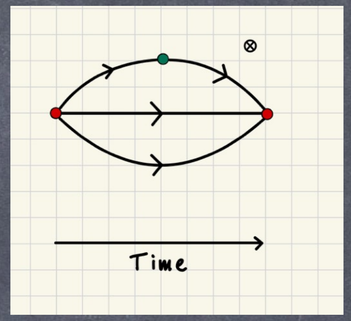
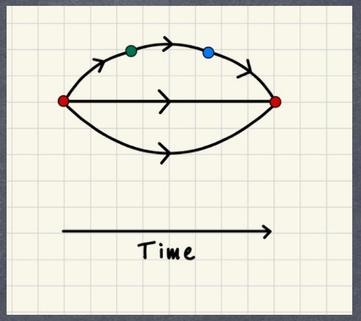
Yoon, Bhattacharya, Cirigliano, Gupta, Mereghetti: (2015-2021)

How to calculate nEDM

$$\left\langle N J_\mu^{\rm em} \overline{N} \right\rangle_{\not{CP}} \simeq \left\langle N J_\mu^{\rm em} O_{\not{CP}} \overline{N} \right\rangle_{\rm QCD} \quad \Rightarrow \quad \left\langle N(p_1) | J_\mu^{\rm em} | N(p_2) \right\rangle_{\not{CP}}$$





$$\left\langle N(p_1) | J_\mu^{\rm em} | N(p_2) \right\rangle_{\not{CP}} = \overline{u}_N(p_1) \Gamma_\mu^{\not{CP}}(Q^2) u_N(p_2)$$

$$\Gamma_\mu^{\not{CP}}(Q^2) \simeq F_1(q^2)\gamma_\mu + \frac{i}{2M_N} F_2(q^2)\sigma_{\mu\nu}q_\nu + i\bar{d}_{\not{CP}} \frac{1}{2M_N} F_3(q^2)\sigma_{\mu\nu}\gamma_5 q_\nu \qquad |d_N| = F_3(0)/2M_N \qquad q = p_1 - p_2$$

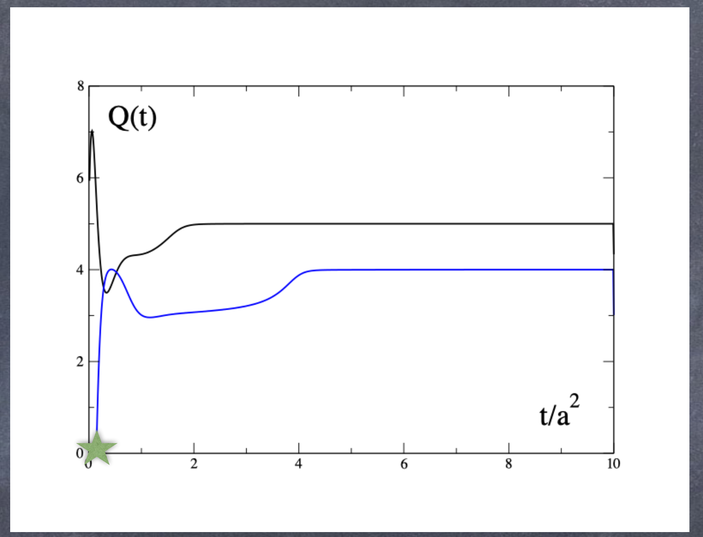
Challenges on the lattice

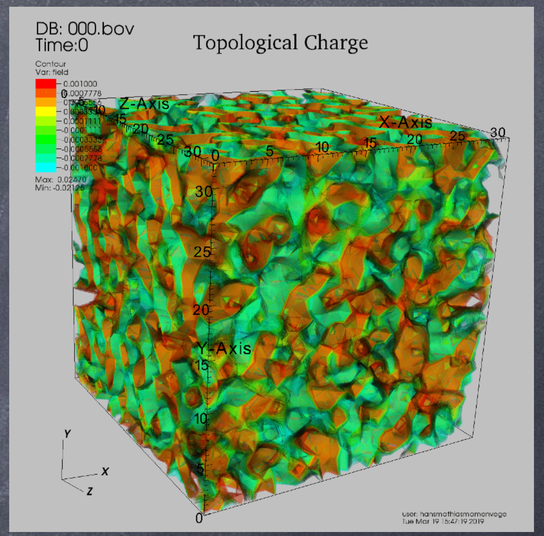
- Renormalization of $O_{\not{CP}}$ and continuum limit a -> 0
- Excited states contaminations $\sum_i a_i \, e^{-m_i x_4} \qquad E_0 < E_1 < \cdots$
- Signal-to-noise ratio

Gradient flow and topological charge

Lüscher (2010)

$$Q(t) = \int d^4x \; q(x,t) \qquad q(x,t) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \mathrm{Tr}\left\{ G_{\mu\nu}(x,t) G_{\rho\sigma}(x,t) \right\}$$





Pederiva, Vege, A.Sh. (2018)
LatViz

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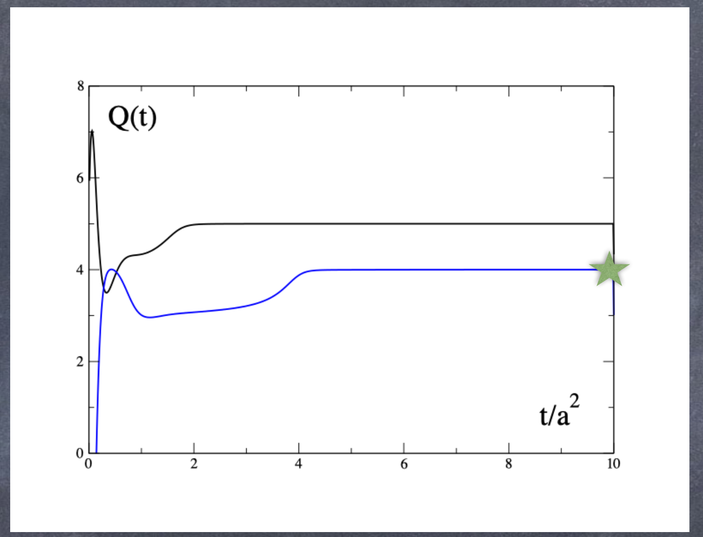

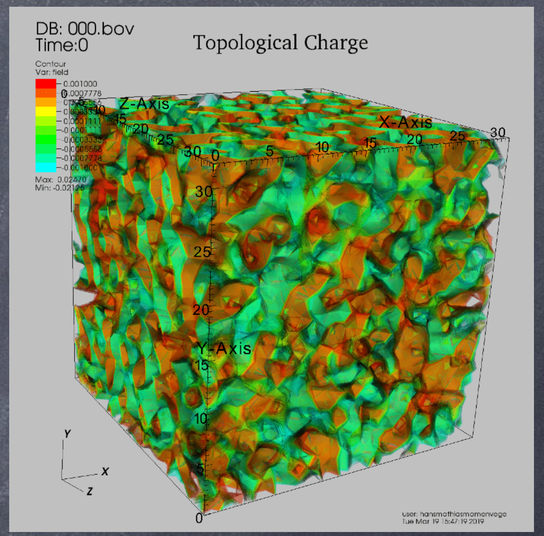

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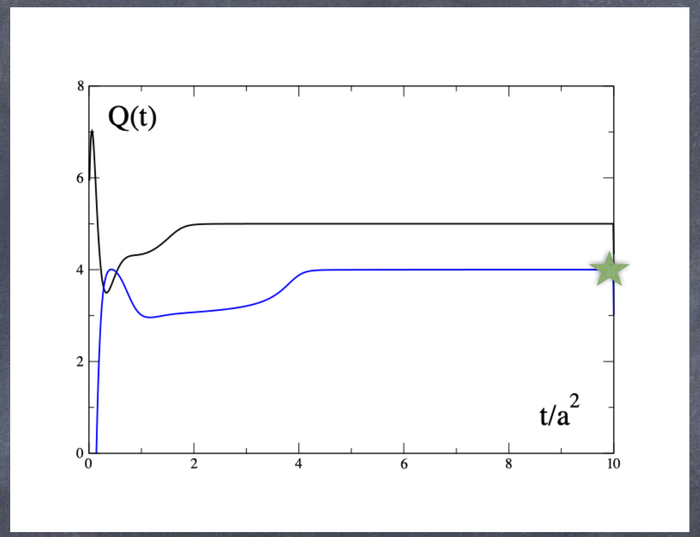
$\delta B_\mu(x,t) = \partial_t B_\mu \delta t$ + Bianchi identities

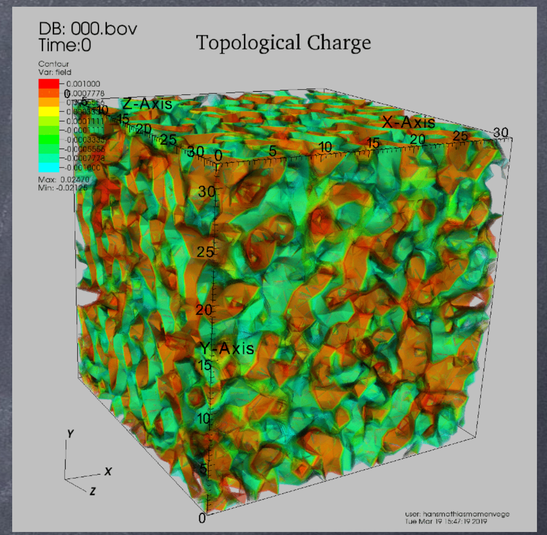
$$\partial_t q(x,t) = \partial_\mu \mathcal{K}_\mu(x,t)$$

$$Q = \int d^4x\ q(x,t)$$

$$\langle \cdots [Q(t)]_R \cdots \rangle = \langle \cdots Q(t) \cdots \rangle$$

$$\boxed{\partial_t Q(t) = 0}$$





Pederiva, Vege, A.Sh. (2018)
LatViz

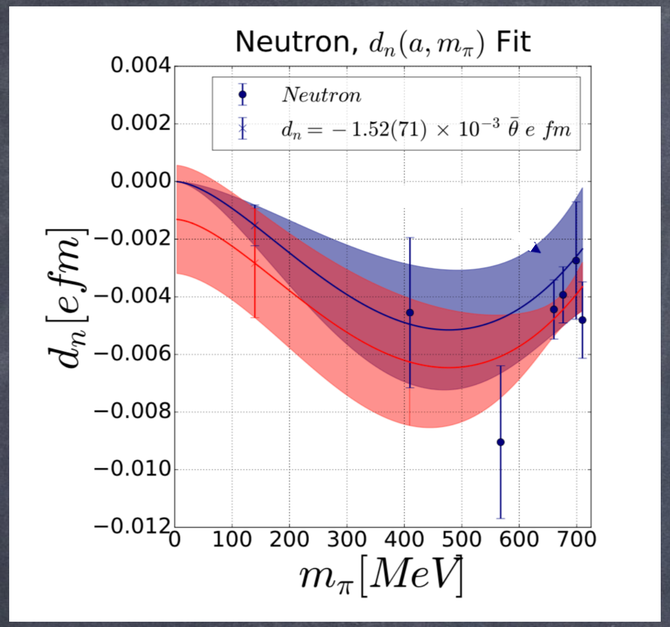
Equivalent to fermionic definition

$$\mathcal{K}_\mu(x,t) = \frac{1}{8\pi^2}\epsilon_{\mu\nu\rho\sigma}\,\mathrm{Tr}\left[G_{\nu\rho}(x,t)D_\alpha G_{\alpha\sigma}(x,t)\right]$$

Polyakov (1987), Lüscher (2010) Ce', Consonni, Engel, Giusti (2015) Lüscher (2021) Lüscher, Weisz (2021)

Neutron EDM from theta term

Dragos, Luu, A.Sh., de Vries, Yousif (2019)



$$d_n(\bar{\theta}) = \bar{d}_n - \frac{e g_A \bar{g}_0^{\bar{\theta}}}{8\pi^2 F_\pi} \ln \frac{m_\pi^2}{M_N^2}$$

Ottnad et al. (2010)
Mereghetti et al. (2011)

$$d_{n/p}(a, m_\pi) = C_1^{n/p} m_\pi^2 + C_2^{n/p} m_\pi^2 \ln \frac{m_\pi^2}{M_N^2} + C_3^{n/p} a^2$$

$$d_n^{\rm phys} = -0.00152(71)\ \bar{\theta}\ e\ \text{fm}$$

$$|\bar{\theta}| < 1.98 \times 10^{-10} (90\%\text{CL})$$

$$\bar{g}_0^{\bar{\theta}} = -1.28(64) \cdot 10^{-2} \bar{\theta}$$

Ab-initio determination of $\bar{g}_0^{\bar{\theta}}$

$$\bar{g}_0^{\bar{\theta}} = -1.47(23) \cdot 10^{-2} \bar{\theta}$$

Crewther et al. (1980)
de Vries et al. (2015)

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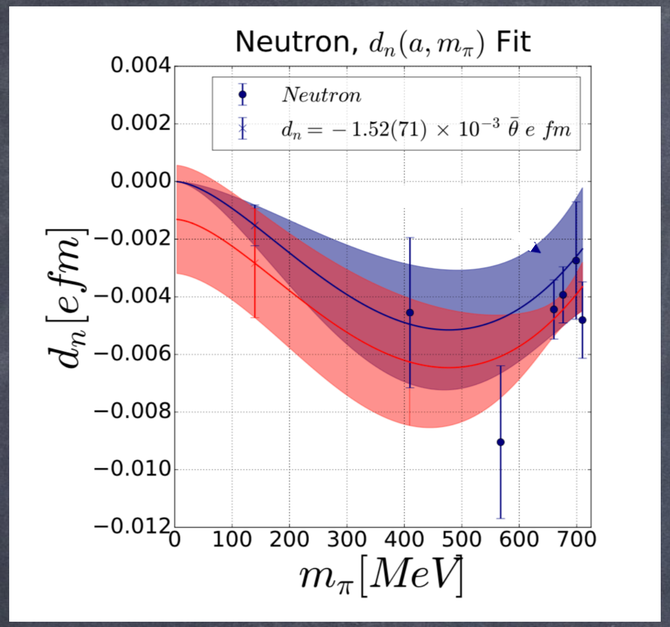

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$$d_n(m_\pi = 412\ \text{MeV}) = -0.00095(50)\ \bar{\theta}\ e\ \text{fm}$$

PRELIMINARY

OpenLat: Kim, A.Sh. (2025)

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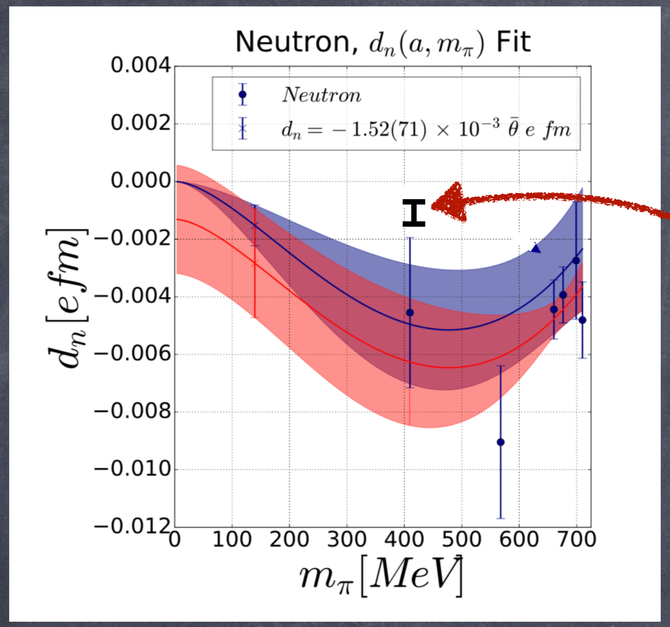

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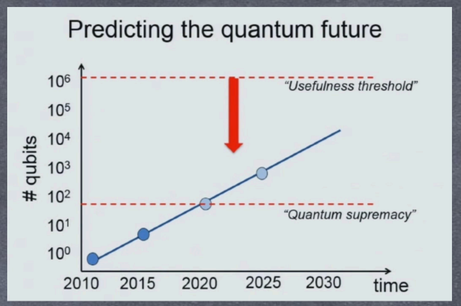
Crewther et al. (1980)
de Vries et al. (2015)

A. Bazavov, B. Henke, L. Hostetler, D. Lee,
H.-W. Lin, G. Pederiva, A. Sh. (2023)

Algorithms for quantum states preparation

θ term in Euclidean space -> complex action
Real time calculation (Minkowski) -> sign problem
3+1 LQCD ==> 10^5 - 10^6 qubits vs. IBM Eagle 127 qubits

Byrnes, Yamamoto (2005)



L. Vandersypen (2017)

1+1 Schwinger model + θ term

E. Chakraborty, Honda, Izubuchi, Kikuchi, Tomiya (2022)
Hamer, Weihong, Oitmaa (1997)

$$H = -i \sum_{n=1}^{N-1} \left(\frac{1}{2a} - (-1)^n \frac{m}{2} \sin\theta \right) \left[\chi_n^\dagger e^{i\phi_n} \chi_{n+1} - \text{h.c.} \right] + m \cos\theta \sum_{n=1}^{N} (-1)^n \chi_n^\dagger \chi_n + \frac{g^2 a}{2} \sum_{n=1}^{N-1} L_n^2$$

Adiabatic State Preparation (ASP)

- Simple, limited by discretization + adiabatic time
- Needs many steps; small gains from step-size tuning

Quantum Approximate Optimization Algorithm (QAOA)

- High precision but requires heavy classical optimization
- Accuracy drops as system grows, even with blocked ansatz

Rodeo Algorithm (RA)

- Can prepare any eigenstate, not just ground state
- Performance depends on overlap; can be combined with others

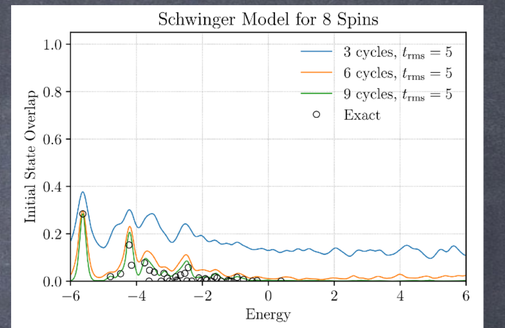


FIG. 6. Spectral overlap factors for the $|10101010\rangle$ initial state from the rodeo algorithm.

Method	# of Steps	# of CNOT/Qubit	E_0	GS Overlap
ASP $L1$	10	45	-1.7140	0.9827
ASP $S1$	10	45	-1.6751	0.9599
ASP $C1$	10	45	-1.7144	0.9827
ASP $L2$	10	75	-1.7089	0.9729
ASP $S2$	10	75	-1.7204	0.9847
ASP $C2$	10	75	-1.7260	0.9880
QAOA	2	18	-1.7353	0.9975
QAOA	3	27	-1.7357	0.9977
RA	9	37	-1.7387	0.9991

Quark-Chromo EDM
&
3-gluon CP-odd

Challenges with BSM operators

- Operators mix with lower dimensional operators
- Power divergences need to be subtracted non-pertubatively

Maiani, Martinelli, Sachrajda (1992)

- Additional complicated mixing pattern

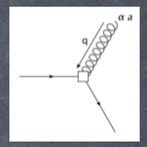
Bhattacharya, Cirigliano, Gupta, Mereghetti, Yoon (2015)

Cirigliano, Mereghetti, Stoffer (2020)

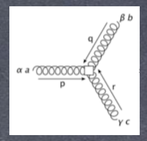
$$[O_{\rm CE}]_R = Z_{\rm CE}\left[O_{\rm CE} - \frac{C}{a^2}P\right] + \cdots$$

$$[O_{3g}]_R = Z_{3g}\left[O_{3g} - \frac{C'}{a^2}q\right] + \cdots$$

$$O^f_{\rm CE}(x) = \overline{\psi}_f(x)\gamma_5\sigma_{\mu\nu}G^a_{\mu\nu}T^a\psi_f(x)$$



$$O_{3g}(x) = \frac{1}{6}if^{abc}G^a_{\mu\rho}(x)G^b_{\nu\rho}(x)G^c_{\lambda\sigma}(x)\epsilon_{\mu\nu\lambda\sigma}$$



$$P^f(x) = \overline{\psi}_f(x)\gamma_5\psi_f(x)$$

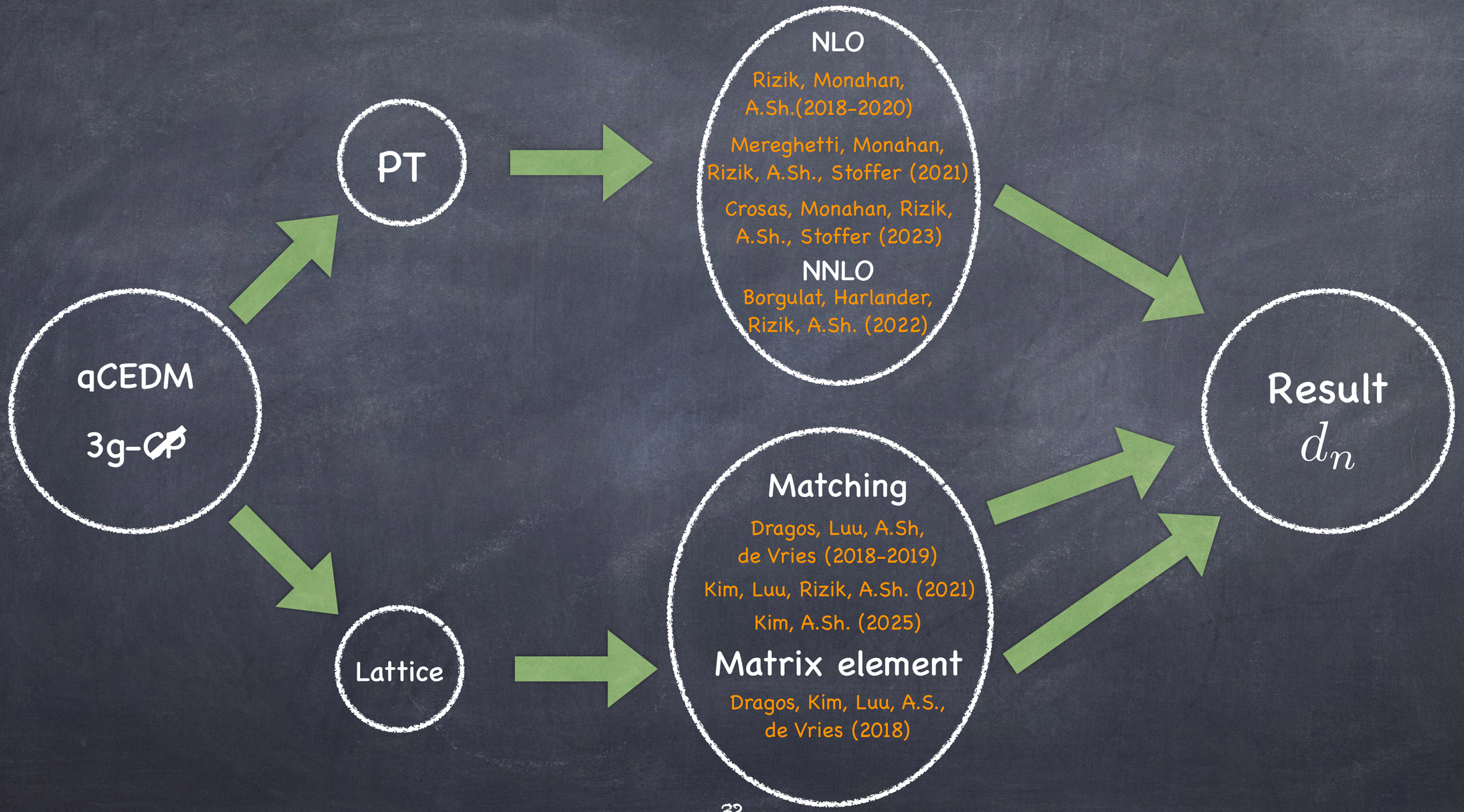
$$q(x) = \frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\,\mathrm{tr}\,\{G_{\mu\nu}(x)G_{\rho\sigma}(x)\}$$

qCEDM with RI-MOM Off-shell

$\frac{1}{a}$ d=4 —> 2 operators + 3 O(m)

$\log a$ d=5 —> 3 operators + (7 + 5) O(m,m²) + 4 “nuisance”

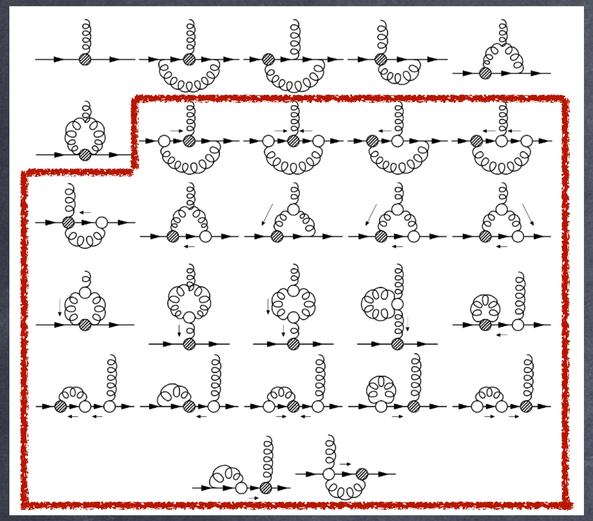
BSM contributions



Quark-Chromo EDM

Rizik, Monahan, A.Sh. (2020)
Mereghetti, Monahan, Rizik, A.Sh., Stoffer (2021)

$\zeta_{\mathrm{CE,CE}}(t,\mu)$



$$\zeta_{\mathrm{CE,CE}}(t,\mu) = \zeta_\chi^{-1} + \frac{\alpha_s}{4\pi}\left[2(C_F - C_A)\log(8\pi\mu^2 t) - \frac{1}{2}\Big((4+5\delta_{\mathrm{HV}})C_A + (3-4\delta_{\mathrm{HV}})C_F\Big)\right]$$

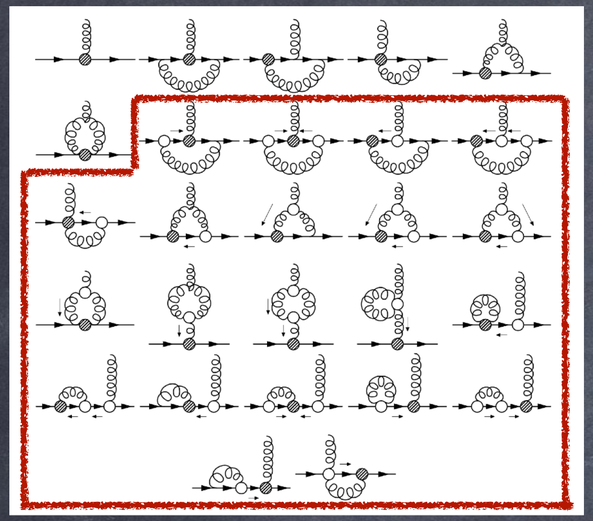
$$= 1 + \frac{\alpha_s}{4\pi}\Bigg[(5C_F - 2C_A)\log(8\pi\mu^2 t) - \frac{1}{2}\Big((4+5\delta_{\mathrm{HV}})C_A + (3-4\delta_{\mathrm{HV}})C_F\Big) - \log(432)C_F\Bigg]$$

- Expand integrands of loop integrals in all scales excluding t
  - Analytic structure altered —> distortion of IR structure
  - in matching equation the IR modification drops out in the difference
  - Expanding loop integrals in the RHS vanish in DR —> UV and IR are identical
  - The LHS is UV-finite, beside the renormalization of the bare parameters and flowed fermion fields
  - The IR singularities on the LHS exactly match the UV MS counterterms

Quark-Chromo EDM

Rizik, Monahan, A.Sh. (2020)
Mereghetti, Monahan, Rizik, A.Sh., Stoffer (2021)

$\zeta_{\mathrm{CE,CE}}(t,\mu)$



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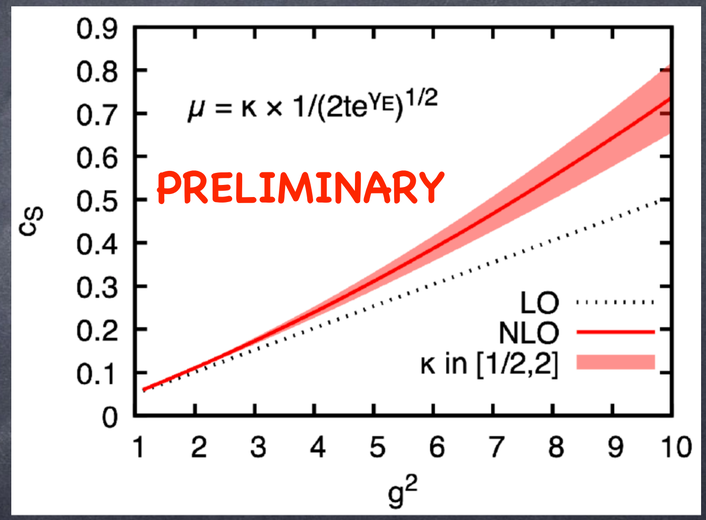
Borgulat, Harlander, Rizik, A.Sh.: in progress



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Warm-up MDM —> 2-loops (226 - 3375 FD)

Summary - Neutron EDM

Quark EDM —>
simplest calculation with Lattice QCD. Precision 3%-5%. No Disc.

Theta-term nucleon EDM —> few calculations: 2 σ effect

—> new result have stronger signal

3 gluon operator —> Preliminary lattice QCD calculation on power divergence, 1-loop matching

4-fermion operators —> No Lattice QCD calculation, 1-loop matching

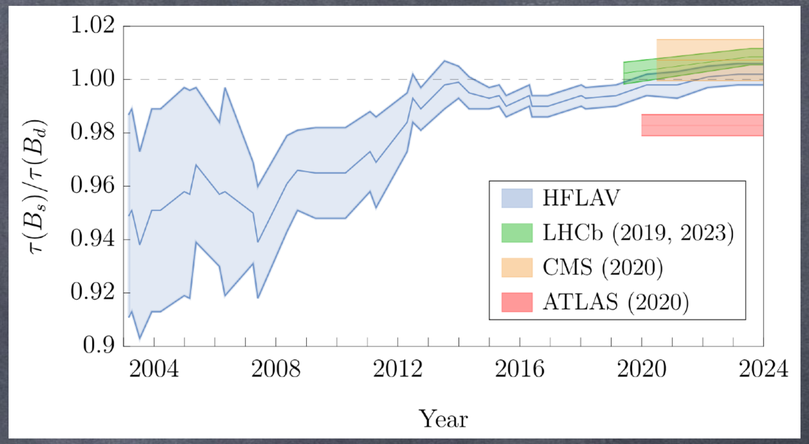
Quark-chromo EDM —>
First result with LO renormalization
New promising approach based on gradient flow —>
1-loop matching, NP power divergence,
2-loop in progress

	Renormalization	Continuum limit	Chiral extrapolation	Finite Volume	Excited States
θ - term					
quark EDM					
quark-chromo					
3-gluon					
4-fermion					

Heavy-quark physics

B-mesons lifetimes

- B-meson lifetimes are measured experimentally to high precision
- Key observables for probing New Physics → high precision in theory needed!



Albrecht et al. (2024)

- For B lifetimes, we use the Heavy Quark Expansion
- $\langle \tilde{O}_6 \rangle$ are leading uncertainties for B lifetime differences

$$\Gamma(H_Q) = \Gamma_3 \langle O_3 \rangle + \Gamma_5 \frac{\langle O_5 \rangle}{m_Q^2} + \Gamma_6 \frac{\langle O_6 \rangle}{m_Q^3} + \ldots + 16\pi^2 \left[\tilde{\Gamma}_6 \frac{\langle \tilde{O}_6 \rangle}{m_Q^3} + \tilde{\Gamma}_7 \frac{\langle \tilde{O}_7 \rangle}{m_Q^4} + \ldots \right]$$

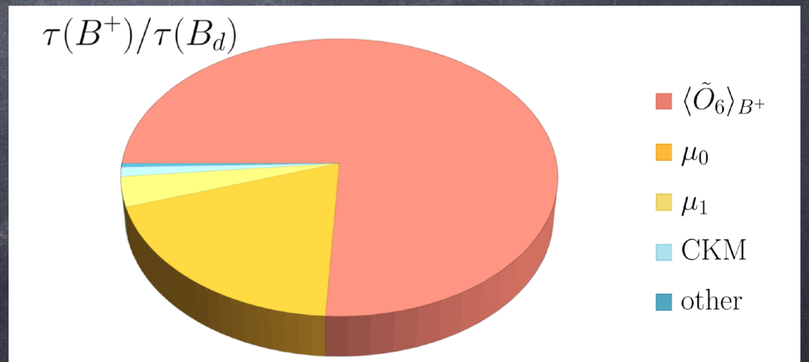


Fig. 7 Composition of the theoretical error in the HQE prediction of $\tau(B^+)/\tau(B_d)$.

Past attempts

- Four-quark $\Delta B = 0$ and $\Delta B = 2$ matrix elements can be determined from lattice QCD simulations
- $\Delta B = 2$ well-studied by several groups -> precision increasing
  - preliminary $\Delta K = 2$ for Kaon mixing study with gradient flow

ETMC (2013)
RBC (2014)
FNAL/MILC (2016)
HPQCD (2019)

Taniguchi (2019) Suzuki et al. (2020)

- $\Delta B = 0$ -> exploratory studies from ~20 years ago + new developments for lifetime ratios
  - contributions from disconnected diagrams
  - mixing with lower dimensional operators

Lin, Detmold, Meinel (2022)

DiPierro, Sachrajda (1998)
DiPierro, Sachrajda, Michael (1999)
Becirevic (2001)

1. Establish gradient flow renormalisation procedure with $\Delta B = 2$ matrix element
2. Pioneer $\Delta B = 0$ matrix elements calculations
3. Tackle disconnected contributions

Matrix elements

- In the Standard Model 4 operators contribute

$$\mathcal{O}_1 = (\bar{b}\gamma_\mu(1-\gamma_5)q)(\bar{q}\gamma_\mu(1-\gamma_5)b), \qquad \langle\mathcal{O}_1(\mu)\rangle = f_{B_q}^2\, M_{B_q}^2\, B_1^q(\mu),$$

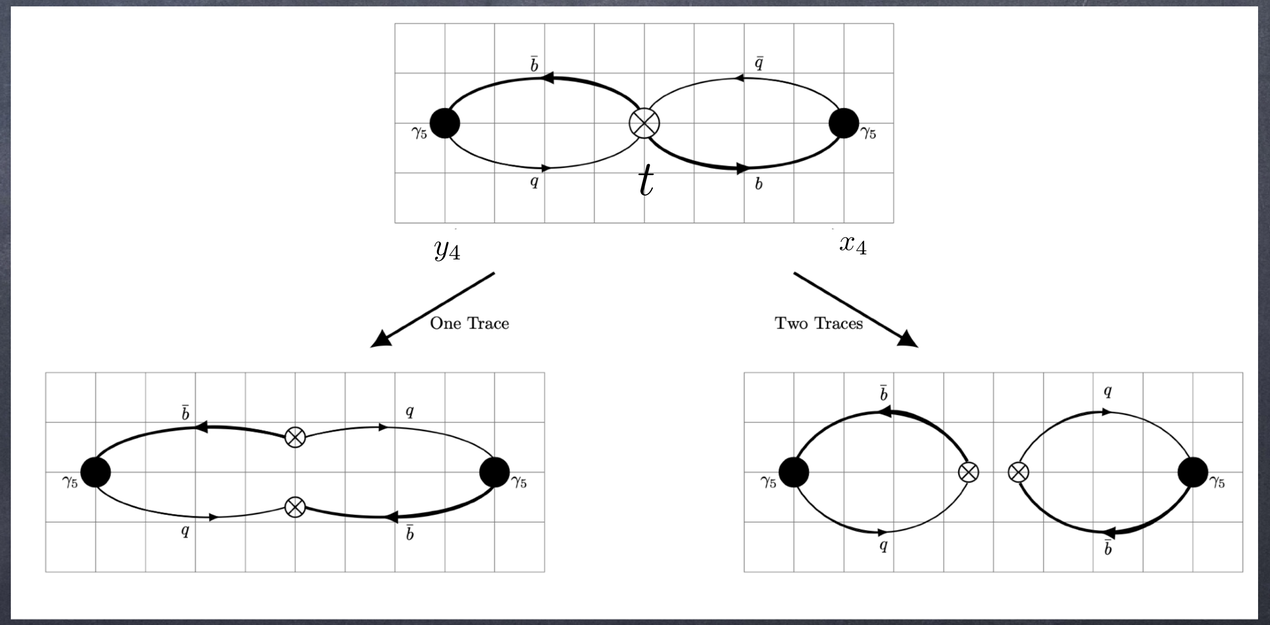
$$\mathcal{O}_2 = (\bar{b}(1-\gamma_5)q)(\bar{q}(1+\gamma_5)b), \qquad \langle\mathcal{O}_2(\mu)\rangle = \frac{M_{B_q}^2}{(m_b+m_q)^2}\, f_{B_q}^2\, M_{B_q}^2\, B_2^q(\mu),$$

$$T_1 = (\bar{b}\gamma_\mu(1-\gamma_5)T^A q)(\bar{q}\gamma_\mu(1-\gamma_5)T^A b), \qquad \langle T_1(\mu)\rangle = f_{B_q}^2\, M_{B_q}^2\, \epsilon_1(\mu),$$

$$T_2 = (\bar{b}(1-\gamma_5)T^A q)(\bar{q}(1+\gamma_5)T^A b), \qquad \langle T_2(\mu)\rangle = \frac{M_{B_q}^2}{(m_b+m_q)^2}\, f_{B_q}^2\, M_{B_q}^2\, \epsilon_2(\mu)$$

- Four-quark operators inserted in three-point correlation functions

- Flowed fermion fields renormalized



Continuum limit & matching

Black, Harlander, Lange, Rago, A.Sh., Witzel (2023-in progress)

$$t\,\partial_t \widetilde{O}(t) = \widetilde{\gamma}(a_s(\mu),\, L_{\mu t})\;\widetilde{O}(t)$$

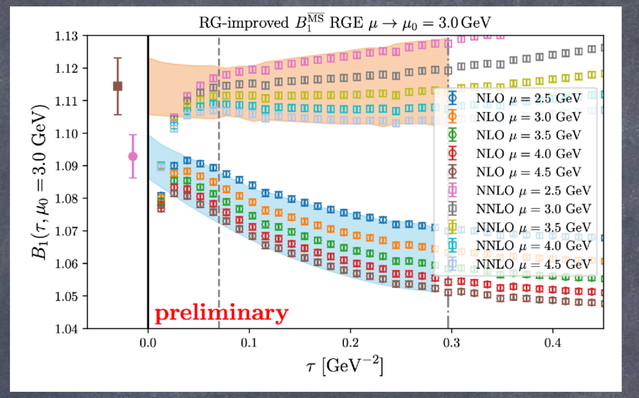
$$\widetilde{\gamma}(a_s(\mu),\, L_{\mu t}) = \big(t\,\partial_t \zeta(t,\mu)\big)\,\zeta^{-1}(t,\mu)$$

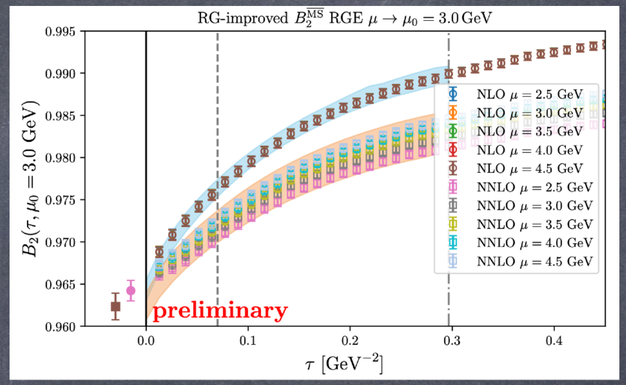
$$O(\mu) = \zeta^{-1}(t_\mu,\mu)\,\exp\left[\int_t^{t_\mu} dt'\,\widetilde{\gamma}(a_s(\mu),\, L)\right]\widetilde{O}(t)$$

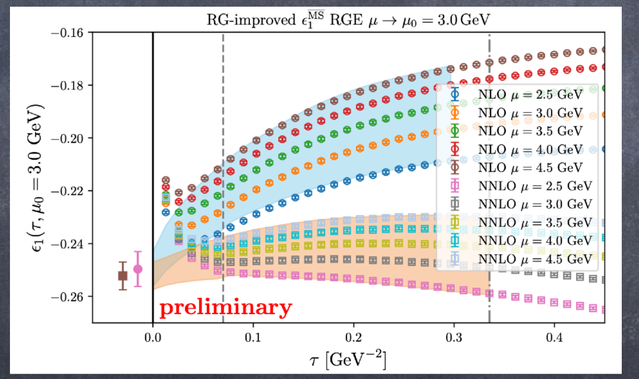
$$t_\mu = e^{-\gamma_E}/(2\mu^2)$$

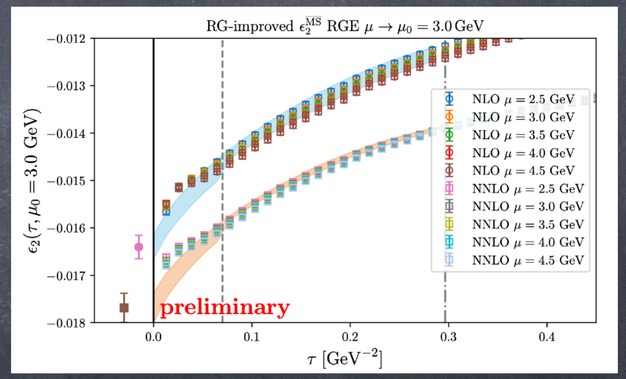
Status and outlook

- B-physics hadronic matrix elements are amenable to computation
- ΔB = 0 four-quark matrix elements are the final target
- Standard renormalization introduces mixing with lower dimensional operators









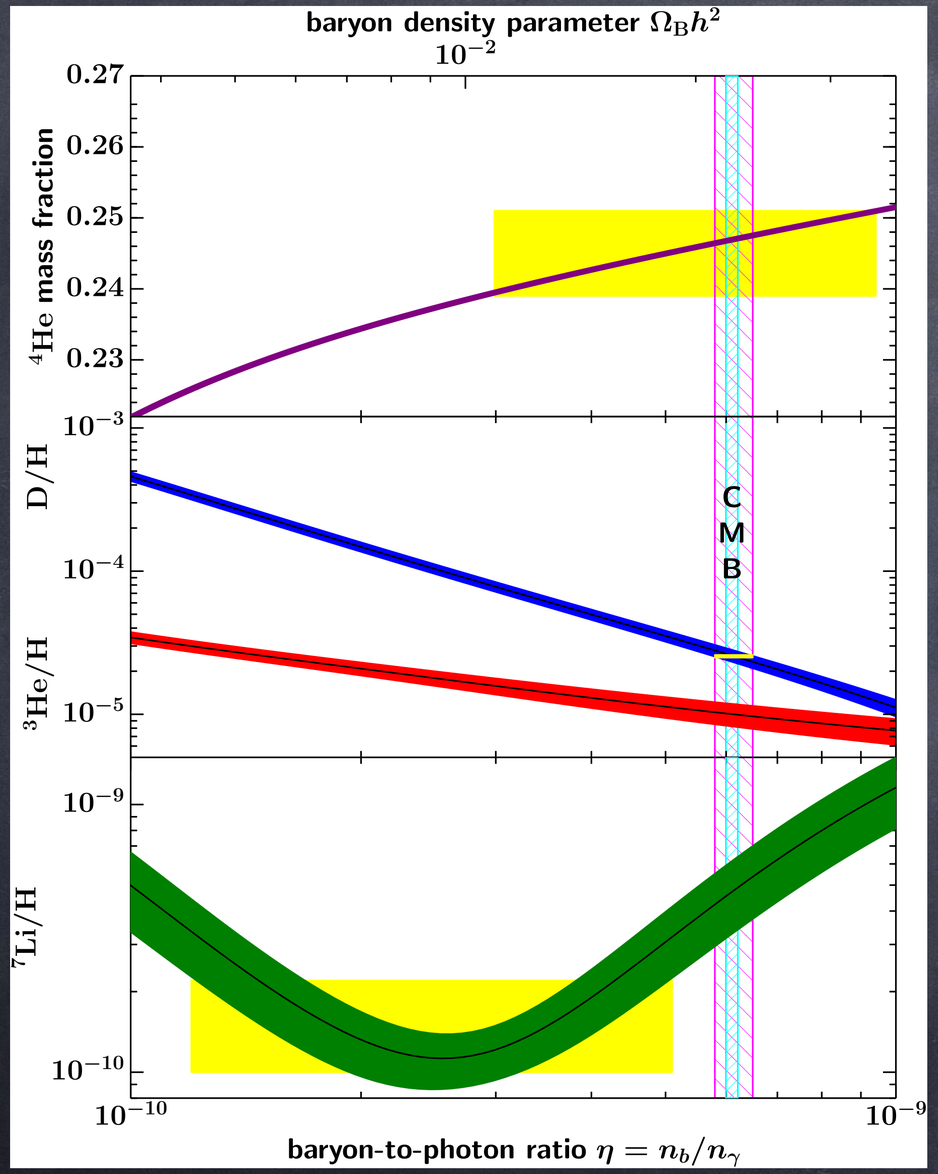
Summary

- **Gradient flow tames renormalization**, turning complicated lattice operators into clean, continuum-like objects
- **Acts as an additional UV regulator**, restoring continuum symmetries before the continuum limit
- **Direct impact on experiments:** more reliable inputs for PDFs, EDMs, B-physics lifetimes, scalar charges, ...
- Greatly reduces operator mixing and power divergences — essential for precision matrix elements
- **Improves signal quality**, though the autocorrelation window must be controlled
- Matching coefficients are perturbatively calculable, enabling controlled connection to QCD
- Nonperturbative elimination of power divergences becomes possible (observable by observable)
- Open questions: the $t \to 0$ limit and the optimal window for connecting to experiment

Thanks!

Backup slides

Matter antimatter asymmetry



PDG 2021

$$\eta = \frac{n_B}{n_\gamma} \qquad n_B = n_b - n_{\bar{b}} \qquad \eta = \frac{\text{(matter) - (antimatter)}}{\text{relic photons}}$$

$$\eta = (6.143 \pm 0.190) \times 10^{-10}$$ Concordance range

$$\Omega_b = \frac{\rho_b}{\rho_{\rm crit}} \simeq \eta h^{-2}/274 \times 10^{10} = 0.02244 \pm 0.00069\ h^{-2}$$

$$\Omega_b h^2 = 0.02230 \pm 0.00021 \Rightarrow \eta = (6.104 \pm 0.058) \times 10^{-10}$$ PLANCK

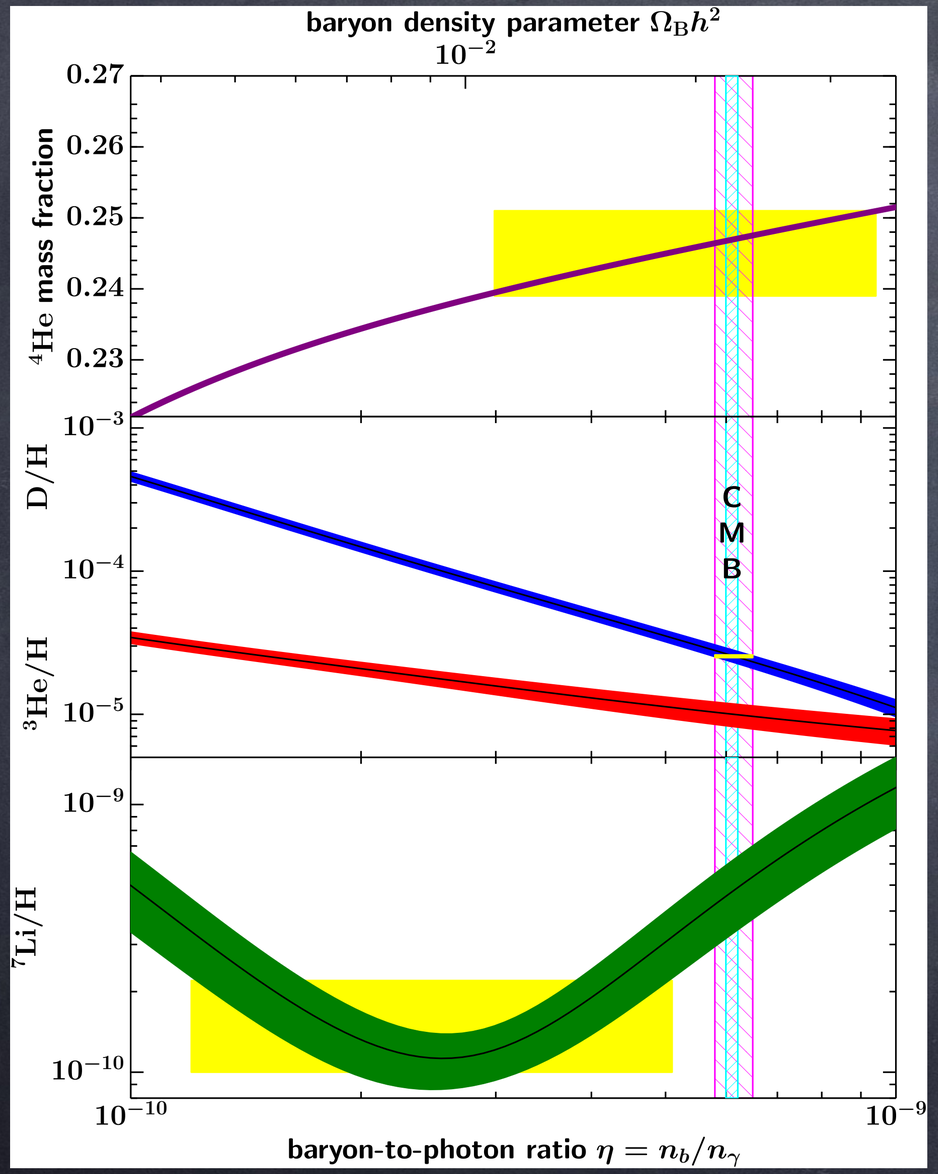
Fields, Olive, Yeh, Young: 2020

$$\eta_{SM} \sim 10^{-26}$$ Gavela, Hernandez, Orloff, Pene: 1994

Huet, Sather: 1995

Rules out any mechanism of electroweak baryogenesis that does not make use of a new source of CP violation.

Matter antimatter asymmetry



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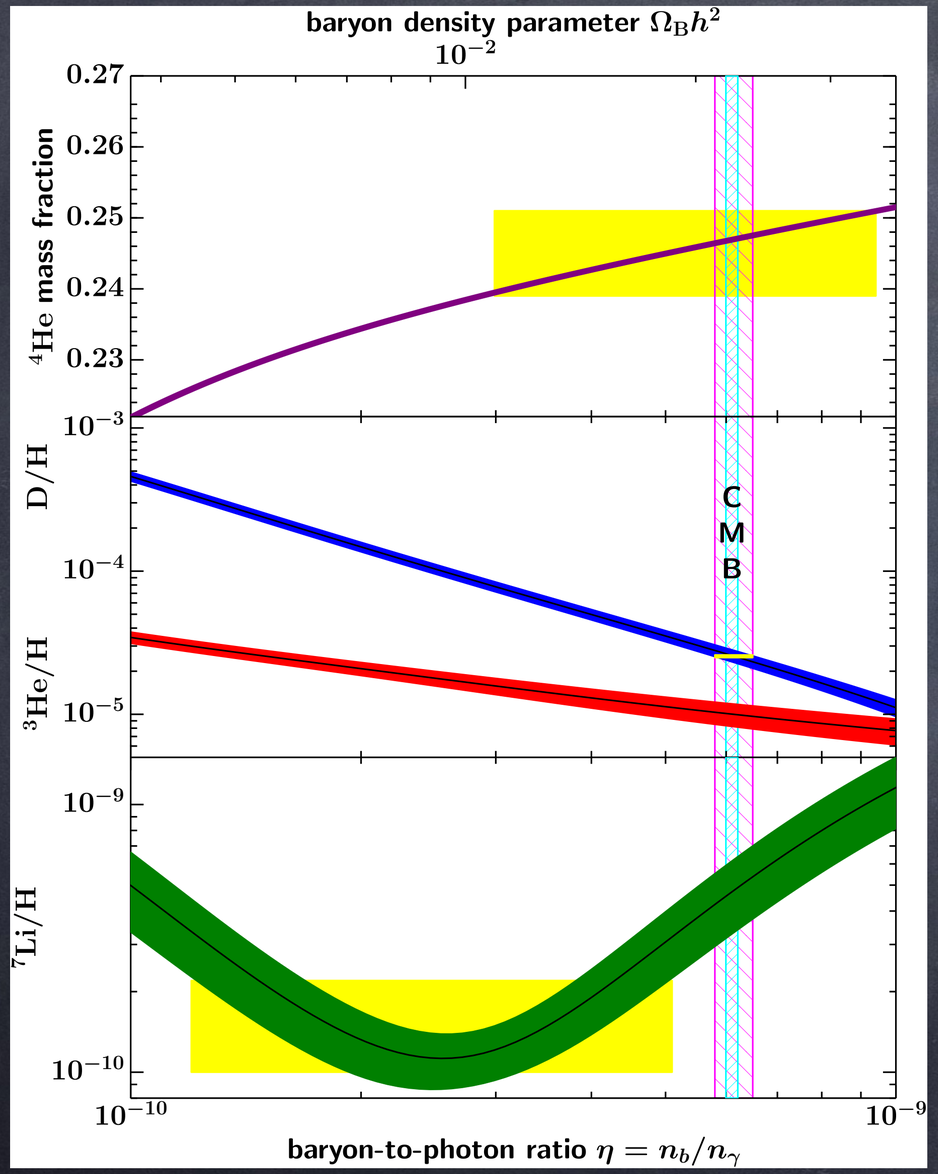

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New source of CP violation

Quark-Chromo EDM: power divergences

Kim, Luu, Rizik, A.S.:2020

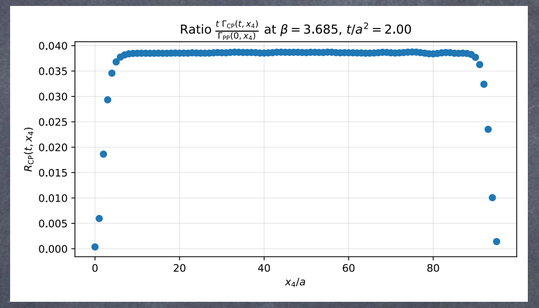
$$\mathring{\mathcal{O}}_{\mathrm{CE}}(t) = \frac{\zeta_{\mathrm{OP}}(t,\mu)}{t} P_{\mathrm{R}}(0,\mu) + \sum_i \zeta_{\mathrm{CE},i}(t,\mu)\mathcal{O}_{i,\mathrm{R}}(0,\mu)$$

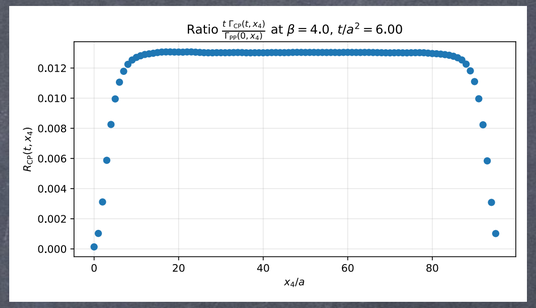
$$\Gamma_{CP}(t,x_4) = a^3 \sum_{\mathbf{x}} \left\langle \mathcal{O}^{ij}_{CE}(t,\mathbf{x},x_4) P^{ji}(0,\mathbf{0},0) \right\rangle$$

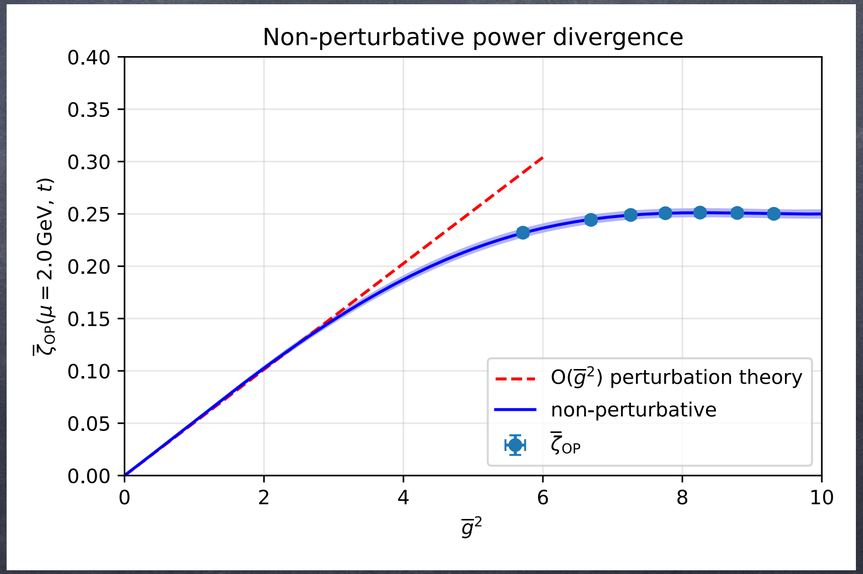
$$\Gamma_{PP}(x_4) = a^3 \sum_{\mathbf{x}} \left\langle P^{ij}(x_4,\mathbf{x}) P^{ji}(0,\mathbf{0}) \right\rangle$$

$$R_{\mathrm{CP}}(t,x_4) = t \frac{\langle 0|\mathcal{O}_{\mathrm{CE}}(t)|\pi\rangle}{\langle 0|P|\pi\rangle}$$

$$\overline{\zeta}_{\mathrm{OP}}(t,\mu) = t \frac{\left\langle 0|\mathring{\mathcal{O}}_{\mathrm{CE}}(t)|\pi\right\rangle}{\langle 0|P_{\mathrm{R}}(0,\mu)|\pi\rangle}$$







Kim, A.S. (OpenLat): 2025

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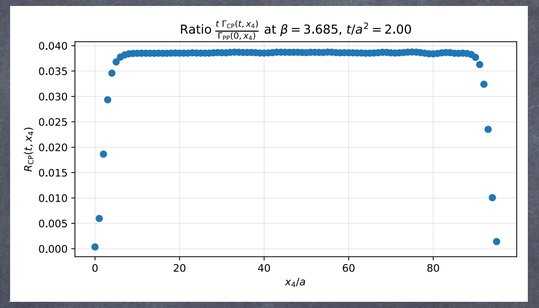
$$\Gamma_{PP}(x_4) = a^3 \sum_{\mathbf{x}} \left\langle P^{ij}(x_4,\mathbf{x}) P^{ji}(0,\mathbf{0}) \right\rangle$$

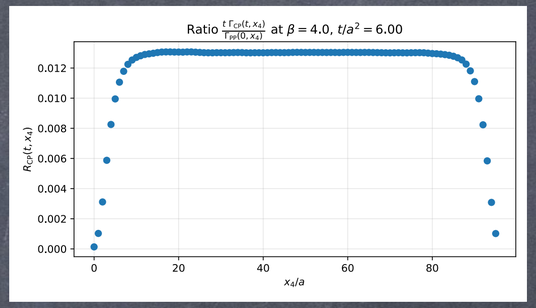
$$R_{\mathrm{CP}}(t,x_4) = t \frac{\langle 0|\mathcal{O}_{\mathrm{CE}}(t)|\pi\rangle}{\langle 0|P|\pi\rangle}$$

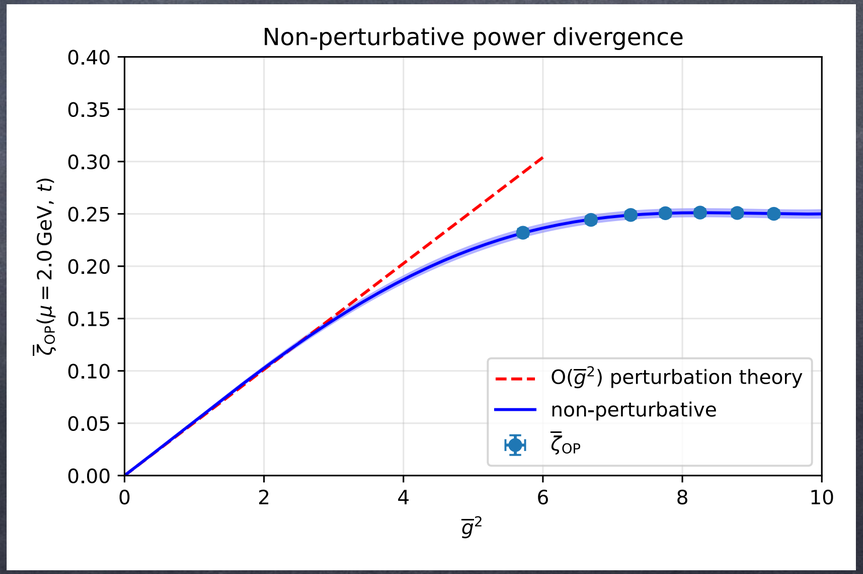
$$\overline{\zeta}_{\mathrm{OP}}(t,\mu) = t \frac{\left\langle 0|\mathring{\mathcal{O}}_{\mathrm{CE}}(t)|\pi\right\rangle}{\langle 0|P_{\mathrm{R}}(0,\mu)|\pi\rangle}$$

$$\overline{\zeta}_{\mathrm{OP}}(t,\mu) = \frac{1}{2\pi^2}\overline{g}^2 + \Delta^{(2)}\overline{g}^4 + \Delta^{(3)}\overline{g}^4 + \Delta^{(4)}\overline{g}^8$$

Rizik, Monahan, A.S.: 2018–2020







Kim, A.S. (OpenLat): 2025

3-gluon CP-odd

Crosas, Monahan, Rizik, A.S., Stoffer : 2023

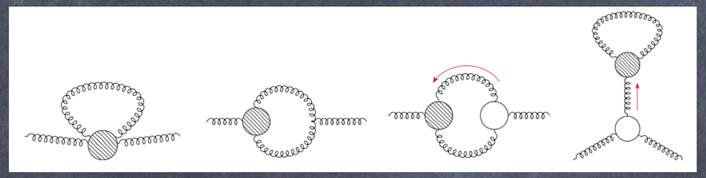
$$\mathcal{O}^R_{\widetilde{G}}(x,t) = \frac{1}{g^2}\mathrm{tr}[G_{\mu\nu}G_{\nu\lambda}\widetilde{G}_{\lambda\mu}] \qquad \zeta_{ij}(t,\mu) = \delta_{ij} + \frac{\alpha_s(\mu)}{4\pi}\zeta^{(1)}_{ij}(t,\mu) + O(\alpha_s^2)$$

$$\mathcal{O}^R_{\widetilde{G}}(x,t) = \sum_i \zeta_i(t,\mu)\mathcal{O}^{\mathrm{MS}}_i(x,\mu) + \sum_i \zeta_{\mathcal{N}_i}(t,\mu)\mathcal{N}^{\mathrm{MS}}_i(x,\mu) + \sum_i \zeta_{\mathcal{E}_i}(t,\mu)\mathcal{E}^{\mathrm{MS}}_i(x,\mu)$$

$$\mathcal{O}_\theta = \frac{1}{g_0^2}\mathrm{tr}[G_{\mu\nu}\widetilde{G}_{\mu\nu}]$$

$$\mathcal{O}_{CE} = (\bar{q}\tilde{\sigma}_{\mu\nu}\mathcal{M}t^a q)G^a_{\mu\nu}$$

$$\zeta^{(1)}_\theta = -\frac{9C_A}{4}\frac{1}{t}$$



$$\mathcal{O}_{\widetilde{G}} = \frac{1}{g_0^2}\mathrm{tr}[G_{\mu\nu}G_{\nu\lambda}\widetilde{G}_{\lambda\mu}]$$

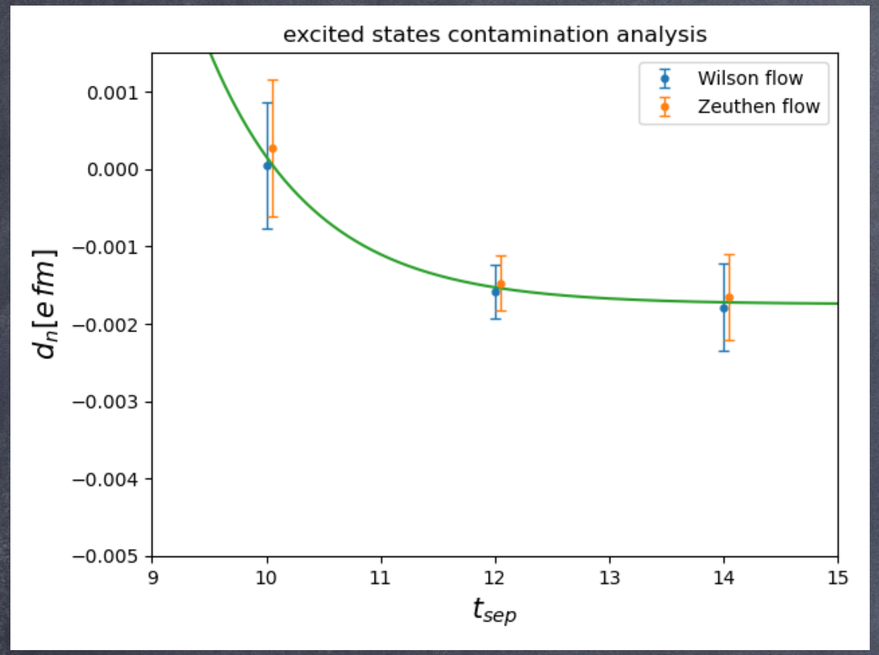
$$\zeta^{(1)}_{\widetilde{G}} = C_A\left[\frac{1}{3} + 6\log(8\pi\mu^2 t)\right] \qquad \zeta^{(1)}_{CE} = \frac{i\,C_A}{8}\left[\frac{31}{6} + 3\log(8\pi\mu^2 t)\right]$$

$$\mathcal{O}_{\partial G} = \frac{1}{g_0^2}\partial_\nu \mathrm{tr}[(D_\mu G_{\mu\lambda})\widetilde{G}_{\nu\lambda}]$$

$$\zeta^{(1)}_{\partial G} = -\frac{179C_A}{24} \qquad \zeta^{(1)}_{\Box\theta} = 0$$

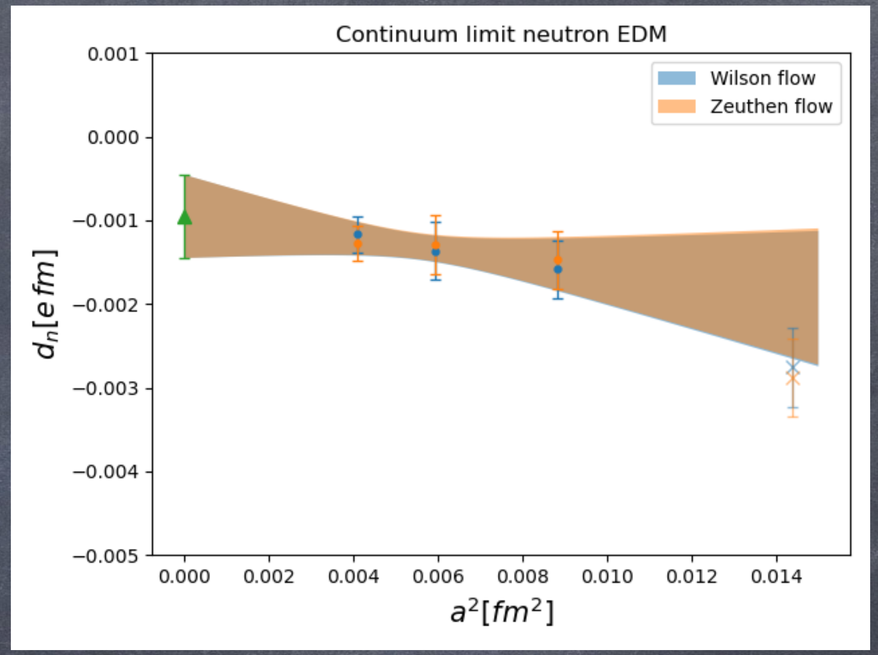
$$\mathcal{O}_{\Box\theta} = \frac{1}{g_0^2}\Box\,\mathrm{tr}[G_{\mu\nu}\widetilde{G}_{\mu\nu}]$$

Systematics



$$d_n(t_{\rm sep}) = d_n + A \cdot e^{-\delta t_{\rm sep}}$$

- ESC under control for $t_{\rm sep} \gtrsim 1.1$ fm for $m_\pi \simeq 410$ MeV
- Compare with χPT predictions



- Topological charge computed $\sqrt{8t} \simeq 0.56$ fm
- Results consistent with expected O(a) improvement
- Zeuthen flow Sint, Ramos: 2015

Topological charge on the lattice

Discretize $\longrightarrow$ $q(x) = \frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}\left\{G_{\mu\nu}(x)G_{\rho\sigma}(x)\right\}$

Continuity in space is lost
On the lattice it has no topological significance

Geometrical definition:

extend the lattice gauge field to a continuous one
Field between lattice points -> judicious interpolation
Smooth gauge fields (bound on field tensor)

Lüscher: 1982
Phillips, Stones: 1986

Fermionic definition:

Anomalous Ward Identity

Smit: 1980

$$\partial_\mu A_\mu = 2mP + \text{extra terms}$$

$$\partial_\mu A_\mu = 2mP + 2iN_f q_L$$

$$Q_L \propto m\sum_x \mathrm{Tr}\left(\gamma_5 S\right)$$

$$Q = n_+ - n_-$$

Atiyah, Singer: 1971

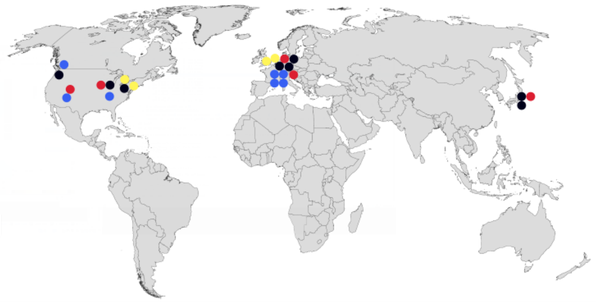
P. Hasenfratz: 1998
P. Hasenfratz, Laliena, Niedermeyer: 1998

EDM experiments in the world

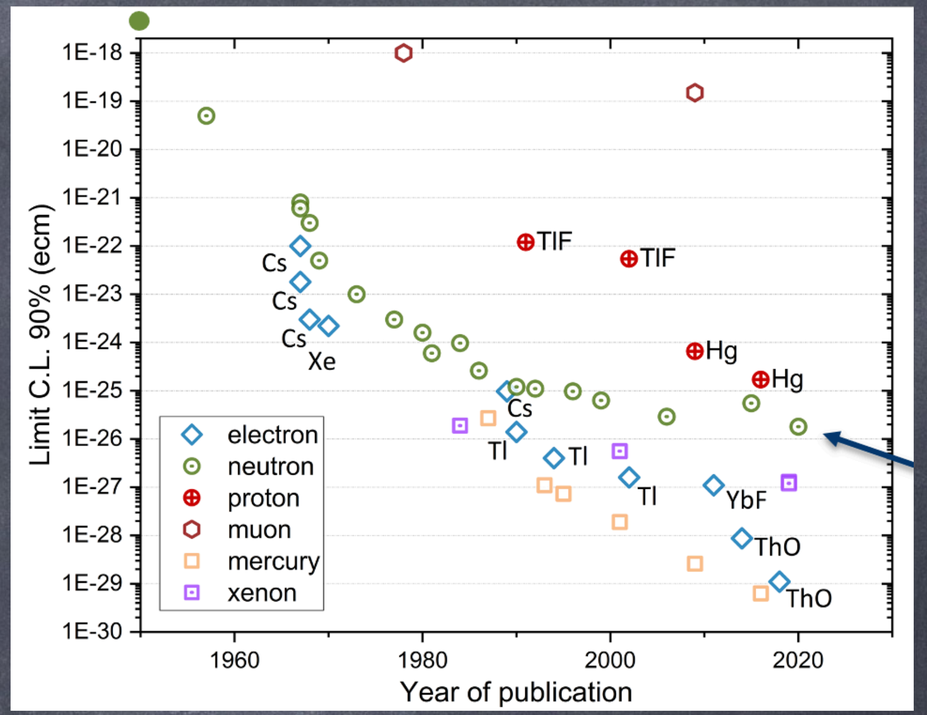
Neutrons: (~ 200 ppl.)
- Beam EDM @ Bern
- LANL nEDM @ LANL
- nEDM @ PSI
- nEDM @ SNS
- PanEDM @ ILL
- PNPI/FTI/ILL @ ILL
- TUCAN @ TRIUMF

Storage rings: (~ 400 ppl.)
- CPEDM/JEDI
- muEDM @ PSI
- g-2 @ FNAL
- g-2 @ JPARC

Atoms: (~ 60 ppl.)
- Cs @ Penn State
- Fr @ Riken
- Hg @ Bonn
- Hg @ Seattle
- Ra @ Argonne
- Xe @ Heidelberg
- Xe @ PTB
- Xe @ Riken



Molecules: (~ 55 ppl.)
- BaF (EDM^3) @ Toronto
- BaF (NLeEDM) @ Groningen/Nikhef
- HfF+ @ JILA
- ThO (ACME) @ Yale
- YBF @ Imperial



$|d_n| < 1.8 \times 10^{-26}\ e\ \text{cm}\ (90\%\ \text{C.L.})$ Abel et al.: 2020 PSI

$|d_{^{199}Hg}| < 7.4 \times 10^{-30}\ e\ \text{cm}\ (95\%\ \text{C.L.})$ Griffith et al.: 2009, Graner et al.: 2017

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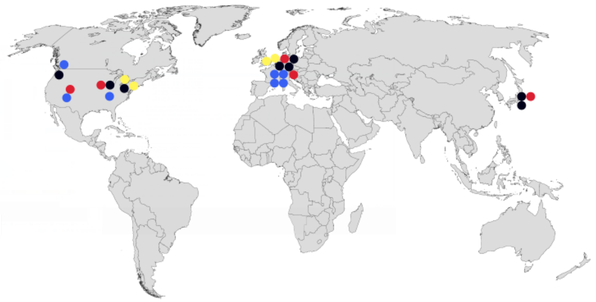

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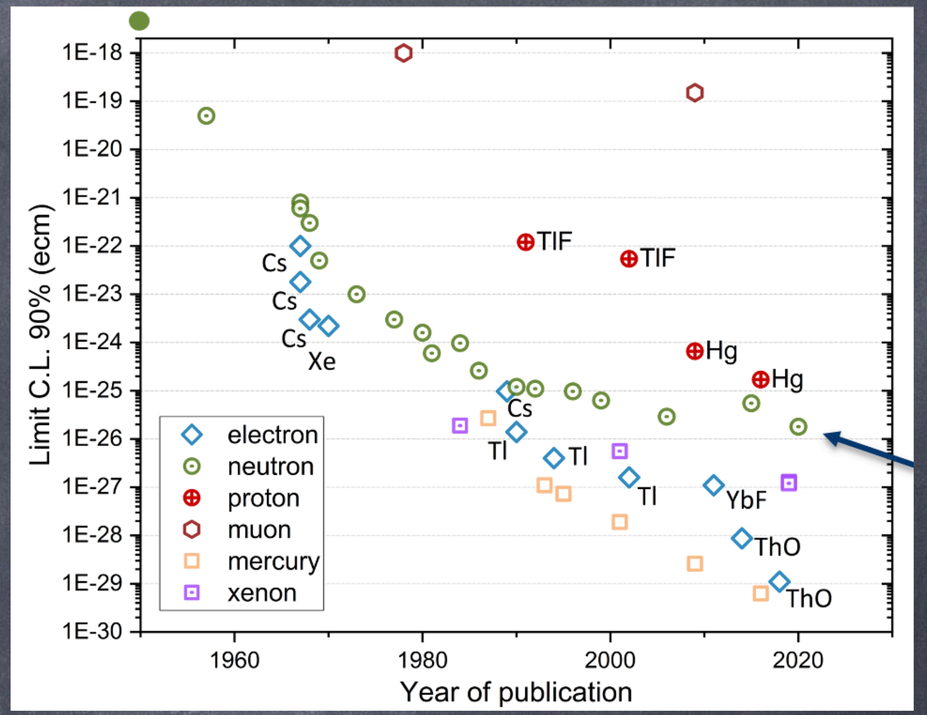

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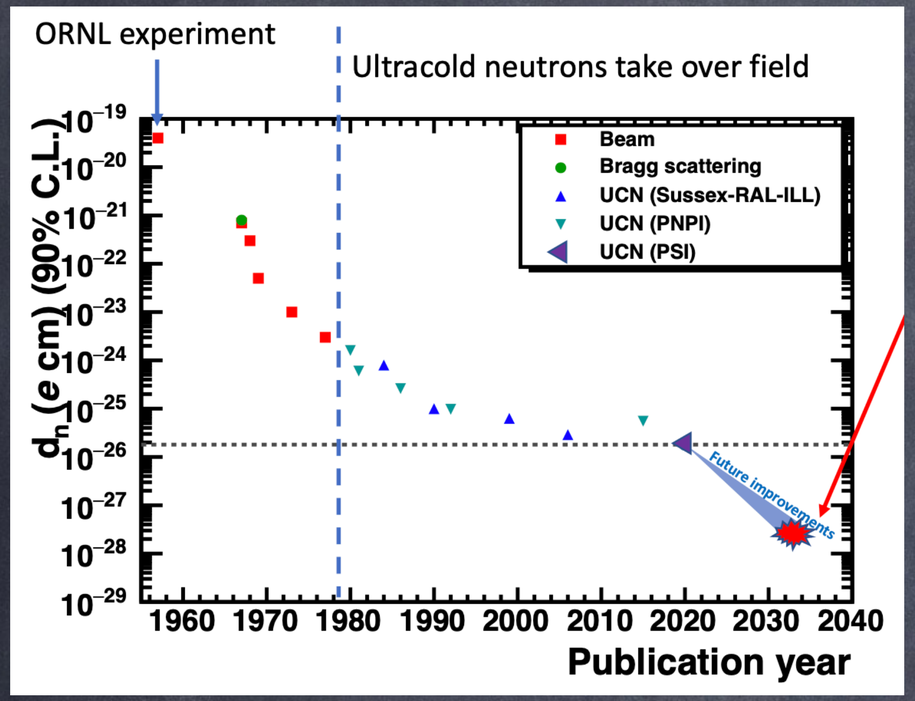
5 (10) yrs

$|d_n| \lesssim 1 - 3 \times 10^{-27}\ e\ \mathrm{cm}\ (2 \times 10^{-28}\ e\ \mathrm{cm})$ SNS

$|d_{^{199}Hg}| \lesssim 5 \times 10^{-31}\ e\ \mathrm{cm}\ (5 \times 10^{-32}\ e\ \mathrm{cm})$ Bonn

$|d_{^{225}Ra}| \lesssim 3 \times 10^{-27}\ e\ \mathrm{cm}$ ANL

Neutron EDM



Experiment	Location	UCN source	Features
n2EDM	PSI	Spallation, SD_2	Ramsey method, double cell, ^{199}Hg comagnetometer
PanEDM	ILL	Reactor, LHe	Ramsey method, double cell, ^{199}Hg comagnetometer
LANL nEDM	LANL	Spallation, SD_2	Ramsey method, double cell, ^{199}Hg comagnetometer
Tucan	TRIUMF	Spallation, LHe	Ramsey method, double cell, ^{129}Xe comagnetometer
nEDM@SNS	ORNL	In-situ production in LHe	Cryogenic, double cell, ^{3}He comagnetometer, ^{3}He as the spin analyzer

$$\nu = -2(\mu \cdot B + d \cdot E)/h$$

$$\sigma_{d_n} \sim \frac{\hbar}{2\alpha E T_{f_p} \sqrt{N}}$$

Control over systematics (factor 5)
B non-uniformity

Alarcon et al.: 2022
Snowmass Summer Study Report

$$|d_n| < 1.8 \times 10^{-26}\ e\ \text{cm}\ (90\%\ \text{C.L.})$$

Abel et al.: 2020
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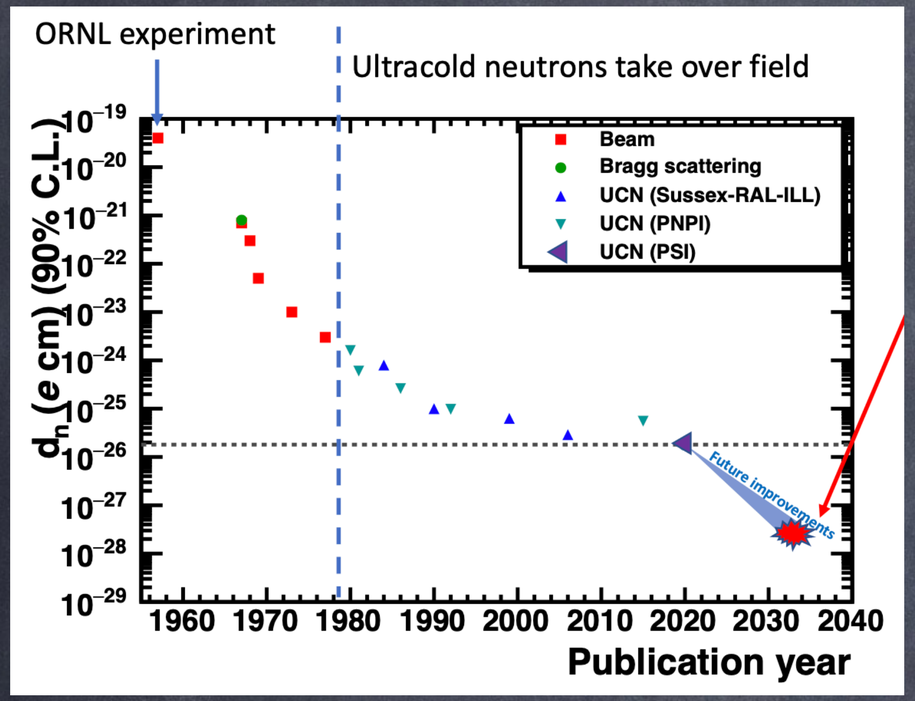
Neutron EDM



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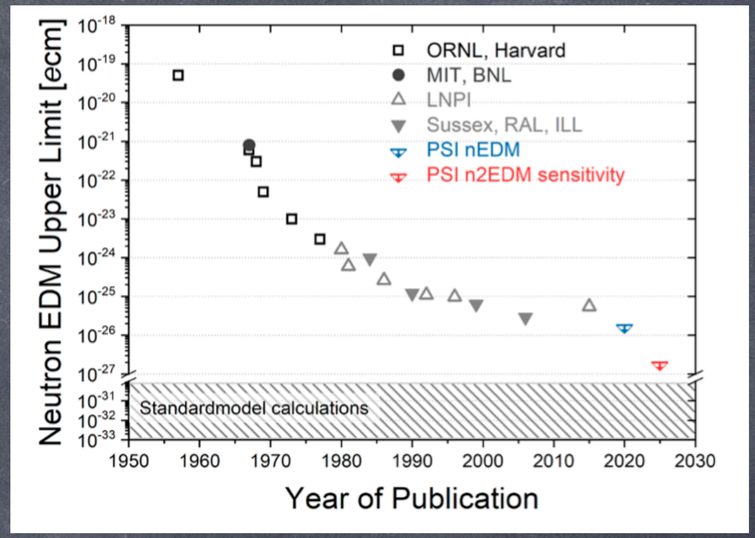

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Control over systematics (factor 5)
B non-uniformity

$$(d_n)_{\mathrm{SM}} = (1-6) \times 10^{-32} e \ \ \mathrm{cm}$$

Shabalin: 1978-1980
Khriplovich, Zhitnitsky: 1982
Gavela et al. : 1982
Seng: 2015

Alarcon et al.: 2022
Snowmass Summer Study Report

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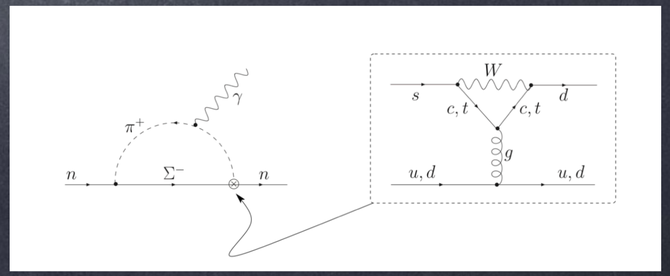
PSI



Moments of the PDF: standard method

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

- 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

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

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

$\mu_1 \neq \mu_2 \neq \mu_3$ → $\langle h(p)|O_n|h(p)\rangle = 2\ (p_{\mu_1}\cdots p_{\mu_n} - \text{ trace terms})\left\langle x^{n-1}\right\rangle_h$

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

4+1 Local field theory

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

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

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- Wick contractions

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- Wick contractions
- Renormalization. All order proof

Lüscher, Weisz: 2013
Hieda, Makino, Suzuki: 2017

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- Wick contractions
- Renormalization. All order proof
- Chiral symmetry and Ward identities

Lüscher, Weisz: 2013
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Lüscher: 2013
A.S.:2013

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- Wick contractions
- Renormalization. All order proof
- Chiral symmetry and Ward identities
- Wilson twisted mass

Lüscher, Weisz: 2013
Hieda, Makino, Suzuki: 2017

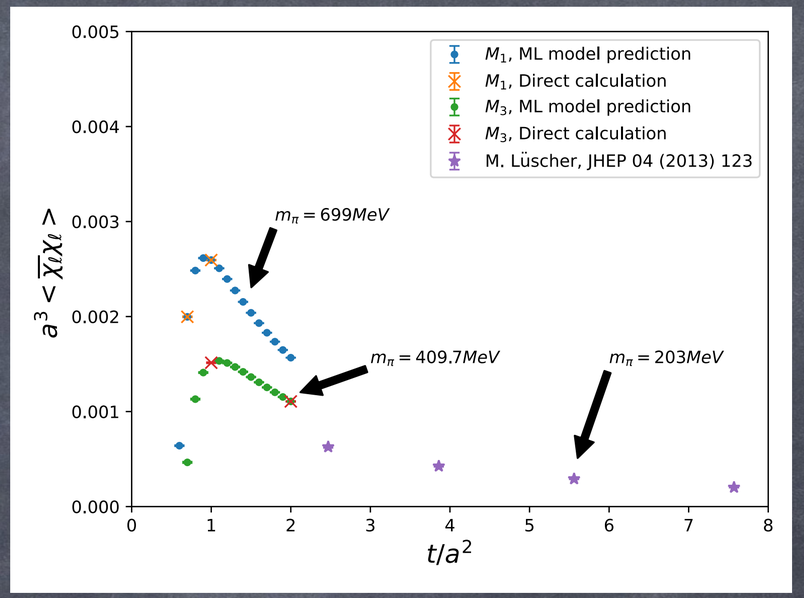
Lüscher: 2013
A.S.:2013

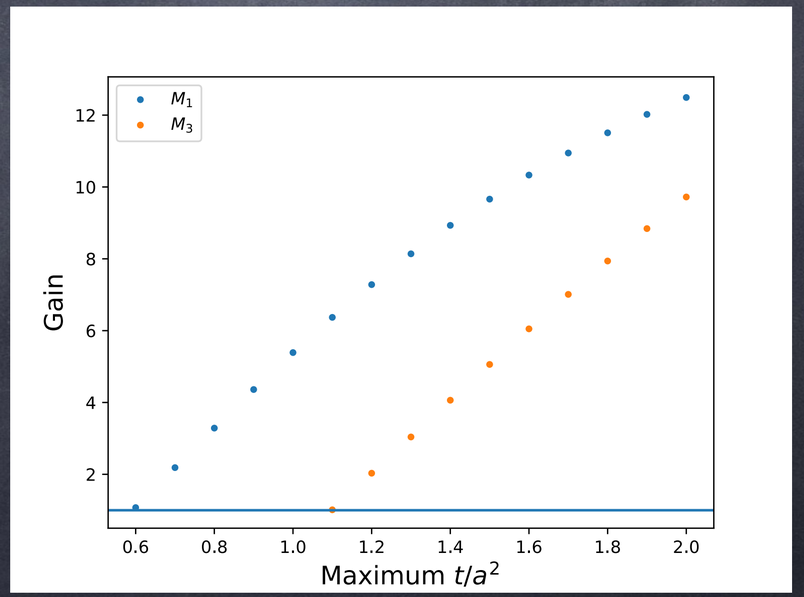
A.S.: 2013

Scalar condensate

Kim, Pederiva, A.S.: 2024

- Strong correlation between quark disconnected diagrams at different flow times
- Use of translation invariance beneficial
- Decision Tree algorithms reproduces correct distribution
- Results are compatible well below the statistical fluctuations of the lattice QCD direct calculation
- No need to large ensemble for training making use of time translation invariance





Machine Learning

Machine Learning

We propose a new method based on SML to accelerate the computation of hadron correlators

MCMC ensemble + stoch. sources + x_4

Training $C(m_1)$ $C(m_2)$

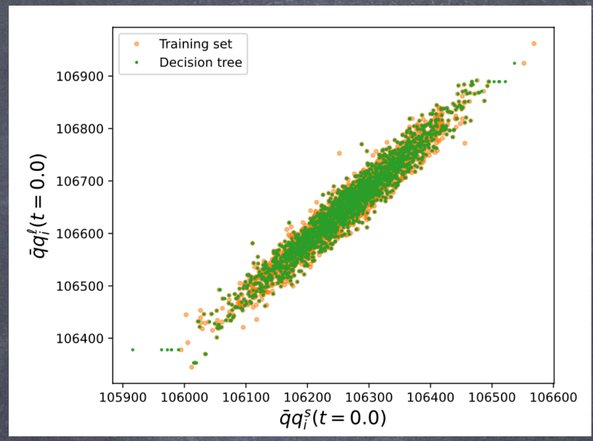
$C(m_1)$

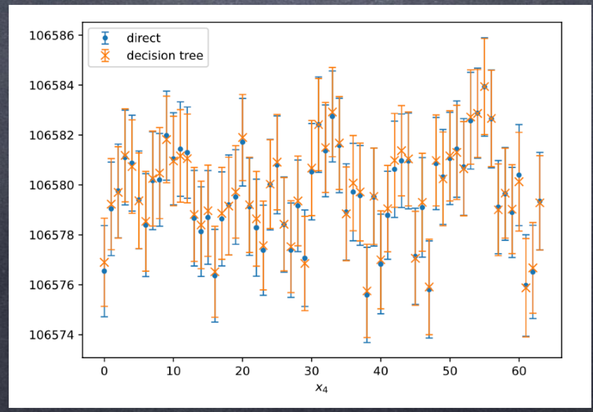
$C(m_2) = \Gamma_{ML}[C(m_1)]$

Γ_{ML}

$C(m_2) = \Gamma_{ML}[C(m_1)]$

J. Kim, G. Pederiva, A.S.





Outlook

- Further investigate our proposal
- Extension to eigenvector calculations
- Solver preconditioning

Synergies

- LQCD & S/N improvement. Krylov subspace methods, Data-driven iterative methods
- New or existing efforts in ML School of Computer Science and Statistics

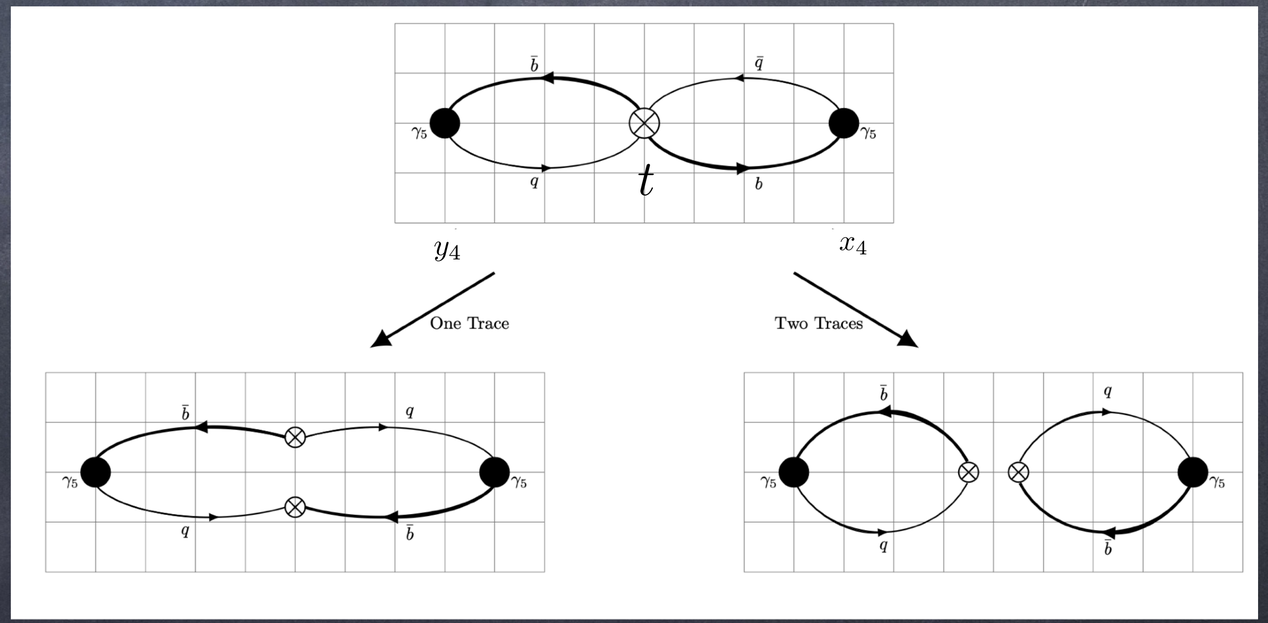
Matrix elements

$$O_1 = (\bar{b}_i \gamma_\mu (1-\gamma_5) q_i)(\bar{b}_j \gamma_\mu (1-\gamma_5) q_j) \qquad \langle O_1(\mu) \rangle = \frac{8}{3} M_{B_q}^2 \, f_{B_q}^2 \, B_1(\mu)$$

$$C^{\text{2pt}}_{\Gamma_I \Gamma_J}(x_4) = a^3 \sum_{\mathbf{x}} \left\langle \Gamma_J(\mathbf{x}, x_4) \Gamma_I^\dagger(0,0) \right\rangle \qquad C^{\text{2pt}}_{\Gamma_I \Gamma_J}(x_4) = \sum_n \frac{\langle 0|\Gamma_J|n\rangle\langle n|\Gamma_I^\dagger|0\rangle}{2M^{(n)}} \left(e^{-M^{(n)} x_4} \pm e^{-M^{(n)}(T-x_4)} \right)$$

$$C^{\text{3pt}}_{O_1}(x_4, y_4, t) = a^6 \sum_{\mathbf{x},\mathbf{y}} \left\langle P(\mathbf{x}, x_4) O_1(0,t) P^\dagger(\mathbf{y}, y_4) \right\rangle$$

$$R^{\text{Bag}}_{O_1}(x_4, y_4, t) = \frac{C^{\text{3pt}}_{O_1}(x_4, y_4, t)}{\frac{8}{3} C^{\text{2pt}}_{AP}(y_4, t) C^{\text{2pt}}_{AP}(x_4, t)}$$



Lattice details

- Gauge configurations RBC/UKQCD's 2+1 flavour Shamir DWF + Iwasaki gauge action ensembles
  Shamir: 1993
  Iwasaki, Yoshie: 1984
  Iwasaki: 1985
- To remove additional extrapolations in valence sector, we simulate at physical charm and strange
  - "neutral Ds" meson mixing
- Fully relativistic DWF for valence quarks
- Strange tuned to physical value (Shamir DWF)
- Heavy c quarks tuned for physical Ds mass (Möbius DWF)
  -> $am_c < 0.7$ with stout smearing of gauge fields Morningstar, Peardon: 2003
- Z2 wall sources for all quark propagators Boyle et al. :2018
  - Sources for strange propagators are also Gaussian smeared Allton et al.: 1993

	L	T	L_s	a^{-1}/GeV	am_l^{sea}	am_s^{sea}	am_s^{val}	M_π/MeV	# cfgs	# sources
C1	24	64	16	1.785	0.005	0.040	0.03224	340	101	32
C2	24	64	16	1.785	0.010	0.040	0.03224	433	101	32
M1	32	64	16	2.383	0.004	0.030	0.02477	302	79	32
M2	32	64	16	2.383	0.006	0.030	0.02477	362	89	32
M3	32	64	16	2.383	0.008	0.030	0.02477	411	68	32
F1S	48	96	12	2.785	0.002144	0.02144	0.02167	267	98	24

Allton et al.: 2008
Aoki et al.: 2010
Blum et al.: 2014
Boyle et al.: 2017

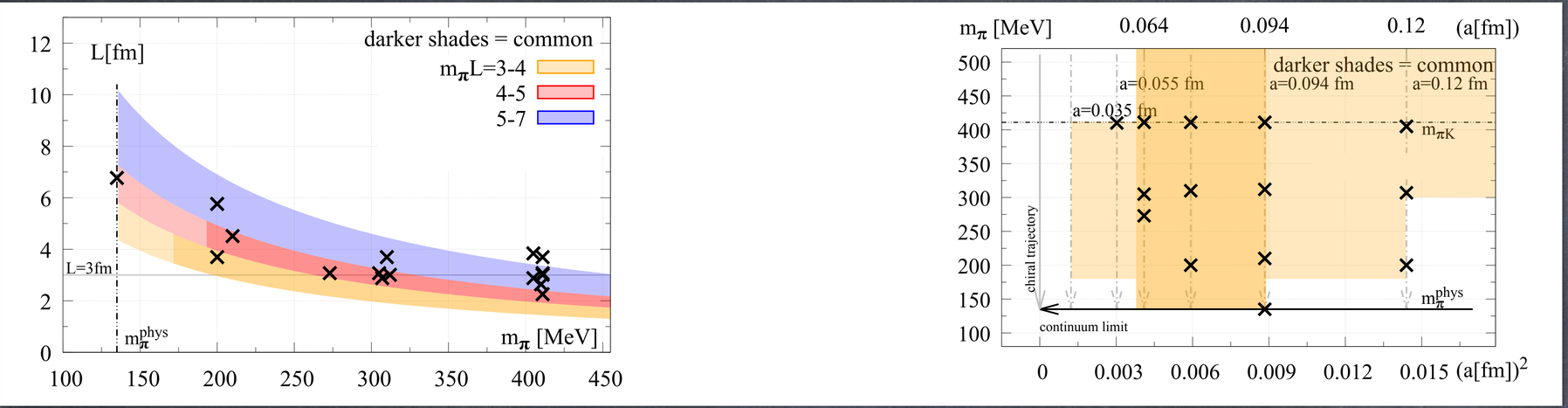
What is OpenLat

https://openlat1.gitlab.io

- OpenLat provides open access to cutting-edge (2+1)-flavor QCD gauge field ensembles, enabling the study of strong interaction phenomena with state-of-the-art simulations.
- The initiative bridges the gap for researchers without access to large-scale collaborations, fostering innovation and inclusivity in lattice QCD.
- Strategic choice of stabilized Wilson fermion framework for precision and stability in QCD simulations.

OpenLat: Current Status & Key Research Projects

OpenLat has made significant progress in producing and sharing high-quality lattice QCD ensembles.
Our two main research projects focus on precision studies of the thetaEDM parameter and advancements in lattice PDF calculations.



Project	Main Goal	Progress
EDM	Improve constraints on CP-violating effects in strong interactions (SM & BSM)	New lattice ensembles generated; analysis ongoing.
PDF	Develop new lattice techniques for parton distribution function (PDF) determination	Implementation of flowmom method; preliminary results obtained
Multi-hadron interactions		
Flavor physics		

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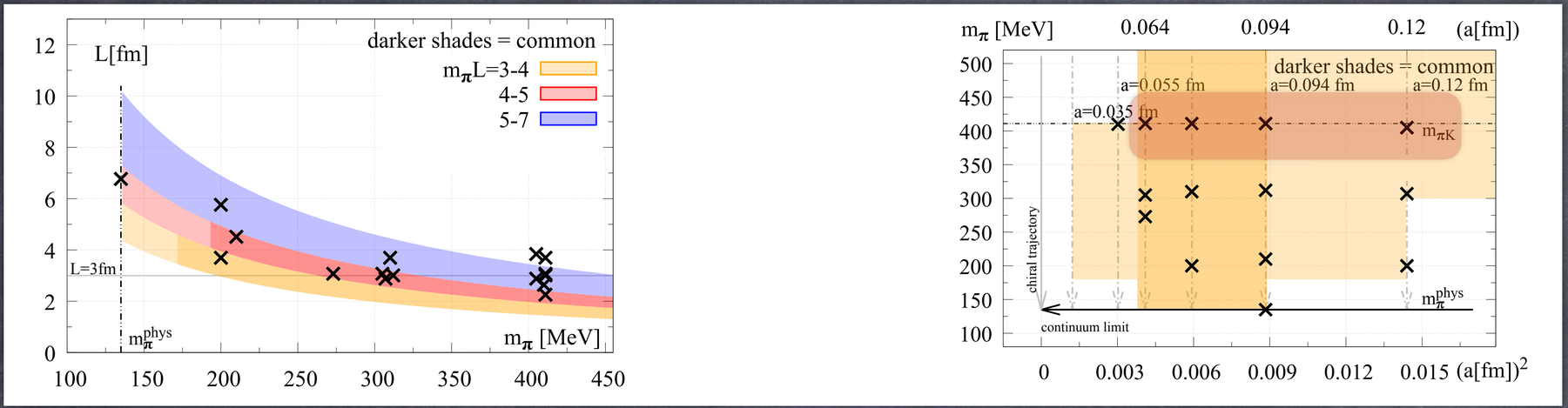

Stage 1

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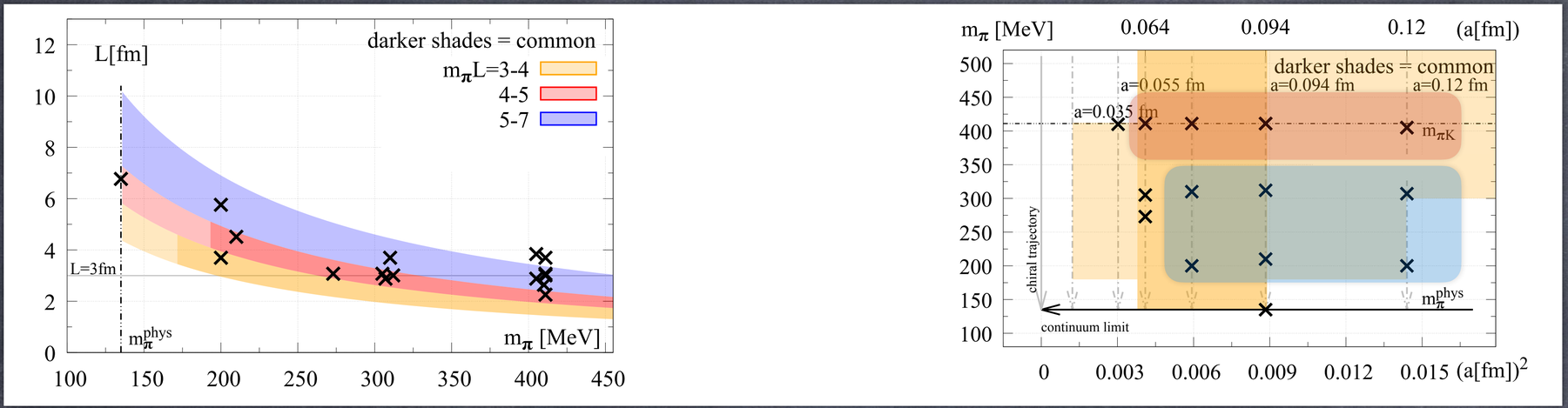

Stage 1

Stage 2

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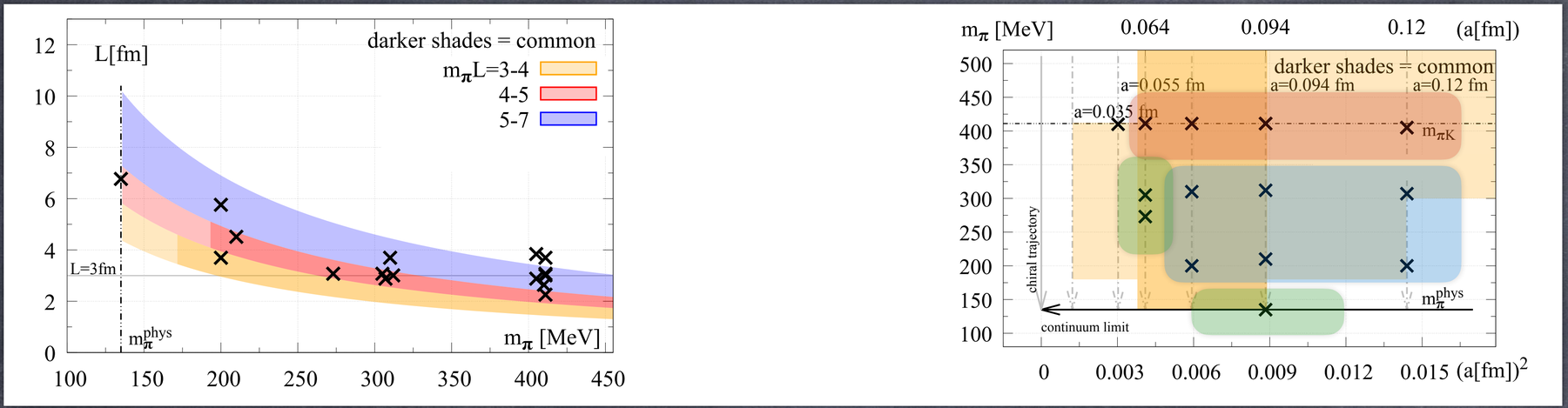

Stage 1

Stage 2

Stage 3

Project	Main Goal	Progress
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Multi-hadron interactions		
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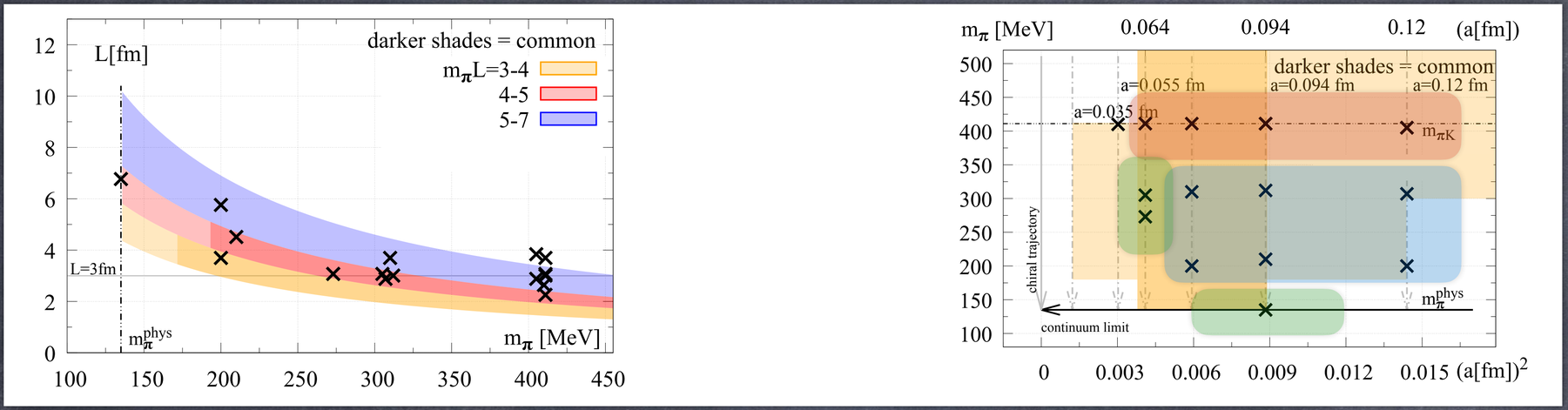

Stage 1 ✅

Stage 2 WORK IN PROGRESS

Stage 3 WORK IN PROGRESS

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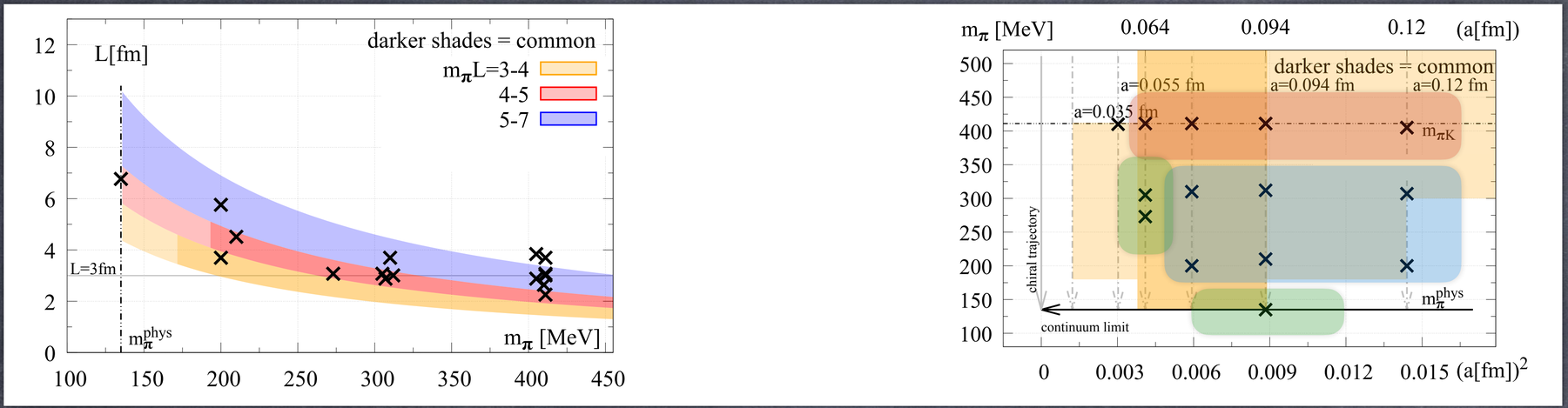


Stage 1 ✅

Stage 2 WORK IN PROGRESS

Stage 3 WORK IN PROGRESS

Perlmutter (NERSC)

JUWELS (FZJ)

Irene Joliot-Curie

PRACE
EuroHPC
Gauss

O(4) irreducible representations

GL(4) irrep $$T_{\{\mu_1\cdots\mu_n\}} = \frac{1}{n!} \sum_{\substack{\sigma\in\text{all}\\ \text{permutations}}} T_{\mu_{\sigma(1)}\cdots\mu_{\sigma(n)}}$$

In O(4) an additional operation is allowed that commutes with orthogonal trafo: contraction of 2 indices

$$T^{(12)}_{\mu_1\cdots\mu_n} = T_{\alpha\alpha\mu_3\cdots\mu_n} = \delta_{\mu_1\mu_2} T_{\mu_1\cdots\mu_n}$$ rank n-2 tensor

Subspace of traceless tensors is invariant under O(4), i.e. the traceless rank n tensors are transformed among themselves under O(4)

Always possible to decompose $$T_{\mu_1\cdots\mu_n} = \widehat{T}_{\mu_1\cdots\mu_n} + \delta_{\mu_1\mu_2} T^{(12)}_{\mu_1\cdots\mu_n} + \cdots$$ Invariant under O(4)

n(n-1)/2 terms

E.g. $$\widehat{T}_{\mu_1\mu_2} = T_{\mu_1\mu_2} - \frac{1}{4}\delta_{\mu_1\mu_2} T_{\alpha\alpha} \qquad \widehat{T}_{\mu_1\mu_2\mu_3} = T_{\mu_1\mu_2\mu_3} - \frac{1}{6}\left[\delta_{\mu_1\mu_2} T_{\alpha\alpha\mu_3} + \delta_{\mu_1\mu_3} T_{\alpha\mu_2\alpha} + \delta_{\mu_2\mu_3} T_{\mu_1\alpha\alpha}\right]$$

Traceless tensors invariant under vector index permutations —> starting point to construct all the irreducible representations of O(4) (Young symmetrizers)

Traceless and symmetrized rank-n tensors are an irreducible representation of O(4)

Matching coefficients

- Consider flowed twist-2 operators $O_n^{rs}(x,t) = \overline{\chi}^r(x,t)\gamma_{\{\mu_1}\overleftrightarrow{D}_{\mu_2}\cdots\overleftrightarrow{D}_{\mu_n\}}\chi^s(x,t)$

- Renormalize flowed twist-2 operators —> renormalization is ALWAYS multiplicative

$$O_n^{rs}(t) = Z_n O_{n,B}^{rs}(t)\,, \quad Z_n = Z_\chi \qquad \left\langle \mathring{\overline{\chi}}(x,t)\overleftrightarrow{\not{D}}\mathring{\chi}(x,t)\right\rangle = -\frac{N_c}{(4\pi)^2 t^2}$$

- Perform a short flow time expansion —> consider O(4) irreps —> traceless operators

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

Continuum limit is finite for any n

$$\left\langle h(p)|\widehat{\mathring{O}}_n(t)|h(p)\right\rangle = 2\left(p_{\mu_1}\cdots p_{\mu_n} - \text{trace terms}\right)\left\langle x^{n-1}\right\rangle_h(t)$$

- Matching is multiplicative for traceless operators

$$\widehat{\mathring{O}}_n^{rs}(t) = c_n(t,\mu)\widehat{O}_n^{rs,\overline{\text{MS}}}(\mu) + O(t)$$

- Calculate matching coefficients in PT

Matching coefficients

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

- Expand integrands of loop integrals in all scales excluding t
  - Analytic structure altered —> distortion of IR structure
  - in matching equation the IR modification drops out in the difference
  - Expanding loop integrals in the RHS vanish in DR —> UV and IR are identical
  - The LHS is UV-finite, beside the renormalization of the bare parameters and flowed fermion fields
  - The IR singularities on the LHS exactly match the UV MS counterterms

$$c_n(t,\mu) = 1 + \frac{\overline{g}^2(\mu)}{(4\pi)^2} c_n^{(1)}(t,\mu) + O(\overline{g}^4) \qquad c_n^{(1)}(t,\mu) = C_F\left[\gamma_n \log\left(8\pi\mu^2 t\right) + B_n\right] \qquad \gamma_n = 1 + 4\sum_{j=2}^{n}\frac{1}{j} - \frac{2}{n(n+1)}$$

Gross, Wilczek: 1974

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

Makino, Suzuki: 2014

$$B_n = \frac{2-4n^2(n+2)}{n(n+1)^2} + \frac{2(2n+1)}{n(n+1)}H_n - \frac{4}{n}\log(2) - 3\log(3) - 4\sum_{j=2}^{n}\frac{1}{j(j-1)}\frac{1}{2^j}\phi(1/2,1,j)$$

Ablinger, Blümlein, Schneider: 2013

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

O(a) improvement

$$O_n^{rs}(x) = O^{rs}_{\mu_1 \cdots \mu_n}(x) = \overline{\psi}^r(x)\gamma_{\{\mu_1} \overleftrightarrow{D}_{\mu_2} \cdots \overleftrightarrow{D}_{\mu_n\}}\psi^s(x) \qquad \left\langle h(p)|\widehat{O}_n|h(p)\right\rangle = 2\, p_{\mu_1} \cdots p_{\mu_n} \left\langle x^{n-1}\right\rangle_h$$

- Beside the O(a) from the lattice theory twist-2 fields are affected by specific O(a) that depend on n
- Improvement coefficients are known only for n=2 and only in PT
- Only GW fermions or Wtm at maximal twist removes these O(a)

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

$$\left\langle h(p)|\mathring{\widehat{O}}_n(t)|h(p)\right\rangle = 2\left(p_{\mu_1} \cdots p_{\mu_n} - \text{trace terms}\right)\left\langle x^{n-1}\right\rangle_h(t)$$

- Hadronic matrix elements of flowed operators beside the O(a) from the lattice theory are only affected by O(am)
- Short distance O(a) negligible at large physical distances
- The O(am) are independent on n (depend only on the fermion content)
- With ratios discretization effects are $O(a^2)$ —> clover fermions are back in the game

$$\frac{\left\langle x^{n-1}\right\rangle_h(t)}{\left\langle x^{m-1}\right\rangle_h(t)} \quad n \neq m \quad n \geq 3,\ m \geq 2$$

Finite continuum limit and O(a) improved

Potential systematics

$$\left\langle x^{n-1}\right\rangle_h^{\rm MS}(\mu) = \left\langle x^{m-1}\right\rangle_h^{\rm MS}(\mu) \frac{c_m(t,\mu)}{c_n(t,\mu)} \frac{\left\langle x^{n-1}\right\rangle_h(t)}{\left\langle x^{m-1}\right\rangle_h(t)}, \quad m \neq n \quad n \geq 3 \; m \geq 2$$

Finite volume effects — at finite a the extension of the local operators is (n-1)a $n \sim 10 - 12$

Discretization errors $\sqrt{8t} \gtrsim na$

Perturbative matching $\mu = 2$ GeV

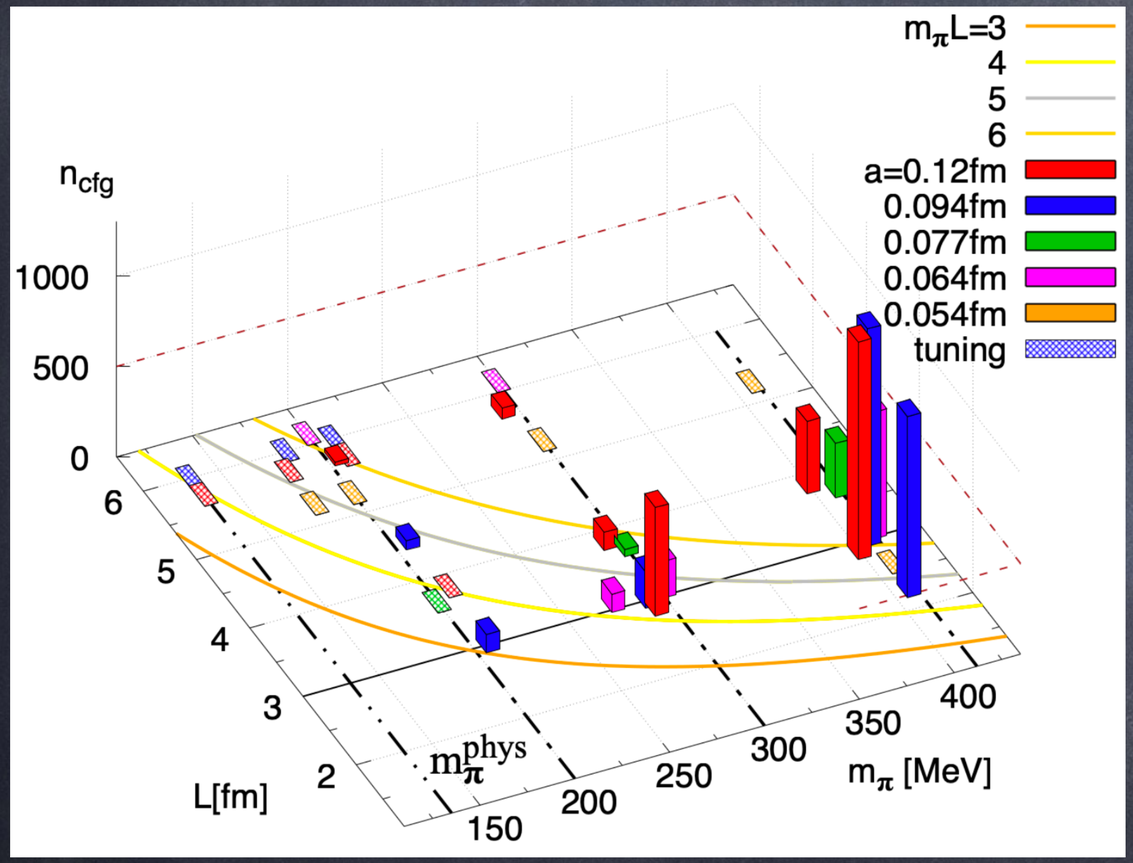
Excited state contamination

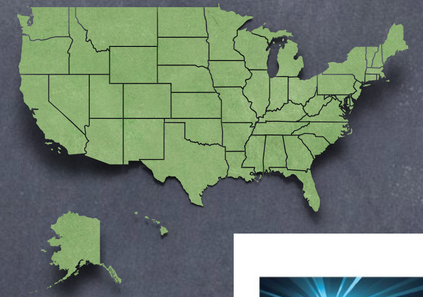
OpenLAT

Neutron EDM with Stabilized Wilson Fermions: the theta term

Hadron structure with stabilized Wilson fermions

- OpenLat: open science initiative. Gauges with SWF open to the whole community





NERSC

https://openlat1.gitlab.io