EDMs from Lattice QCD

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Neutron Electric Dipole Moment: from Theory to Experiment
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Collaboration Members

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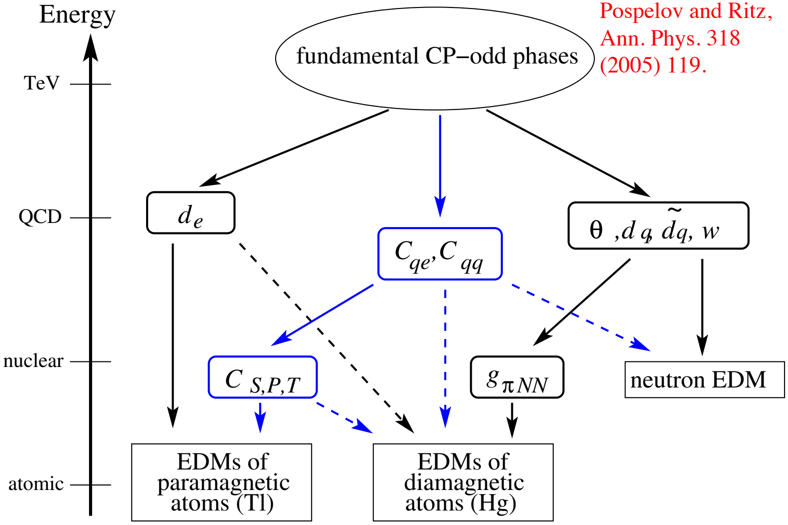
Outline

1. Introduction
2. Neutron EDM from QCD θ-term
3. Neutron EDM from Quark EDM
4. Neutron EDM from quark Chromo-EDM
5. Neutron EDM from Weinberg's three-gluon Operator
6. Conclusion

Hierarchy of EDM Scales



Pospelov and Ritz, Ann. Phys. 318 (2005) 119.

$$\mathcal{L}_{\rm CPV} = \mathcal{L}_{\rm CKM} + \mathcal{L}_{\bar{\theta}} + \mathcal{L}_{\rm BSM} \quad \longrightarrow \quad \mathcal{L}_{\rm CPV}^{\rm eff}$$

Effective CPV Lagrangian at Hadronic Scale

$$\begin{aligned}
\mathcal{L}_{\mathrm{CPV}}^{d\leq 6} &= -\frac{g_s^2}{32\pi^2}\overline{\theta}G\tilde{G} && \text{dim=4 QCD } \theta\text{-term} \\
&- \frac{i}{2}\sum_{q=u,d,s} d_q\overline{q}(\sigma\cdot F)\gamma_5 q && \text{dim=5 Quark EDM (qEDM)} \\
&- \frac{i}{2}\sum_{q=u,d,s} \tilde{d}_q g_s\overline{q}(\sigma\cdot G)\gamma_5 q && \text{dim=5 Quark Chromo EDM (CEDM)} \\
&+ d_w\frac{g_s}{6}G\tilde{G}G && \text{dim=6 Weinberg's 3g operator} \\
&+ \sum_i C_i^{(4q)}O_i^{(4q)} && \text{dim=6 Four-quark operators}
\end{aligned}$$

- $\overline{\theta} \leq \mathcal{O}(10^{-8} - 10^{-11})$: Strong CP problem
- Dim=5 terms suppressed by $d_q \approx \nu/\Lambda_{BSM}^2$; effectively dim=6
- All terms up to $d = 6$ are leading order

Calculation of Neutron EDM d_n

$$d_n = \overline{\theta} \cdot C_\theta + d_q \cdot C_{\mathrm{qEDM}} + \tilde{d}_q \cdot C_{\mathrm{CEDM}} + \cdots$$

- SM and BSM theories
  $\longrightarrow$ Coefficients of the effective CPV Lagrangian ($\overline{\theta}, d_q, \tilde{d}_q, \ldots$)
- Lattice QCD
  $\longrightarrow$ Nucleon matrix elements in presence of CPV interactions
  ($C_\theta, C_{\mathrm{qEDM}}, C_{\mathrm{CEDM}}, \ldots$)

Physical Results from Unphysical Simulations

- **Finite Lattice Spacing**

  – Simulations at finite lattice spacings $a \approx 0.045 - 0.15$ fm

  $\Rightarrow$ Extrapolate to continuum limit, $a \to 0$

- **Heavy Pion Mass**

  – Lattice simulation: Smaller quark mass $\longrightarrow$ Larger computational cost

  – Simulations at or heavier than physical pion mass

- **Finite Volume**

  – Simulations at finite lattice volume; small effect in most of the EDM calculations

- **Renormalization**

  – Lattice results $\longrightarrow$ continuum $\overline{\mathrm{MS}}$; involves complicated/divergent mixing

- **Excited state contamination**

  – Lattice interpolating operators of meson and nucleon couples to excited states

Neutron EDM from QCD θ-term

$$
\begin{aligned}
\mathcal{L}_{\rm CPV}^{d\leq 6} &= -\frac{g_s^2}{32\pi^2}\overline{\theta} G\tilde{G} && \text{dim=4 QCD } \theta\text{-term} \\
&- \frac{i}{2}\sum_{q=u,d,s} d_q \overline{q}(\sigma\cdot F)\gamma_5 q && \text{dim=5 Quark EDM (qEDM)} \\
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&+ d_w \frac{g_s}{6} G\tilde{G}G && \text{dim=6 Weinberg's 3g operator} \\
&+ \sum_i C_i^{(4q)} O_i^{(4q)} && \text{dim=6 Four-quark operators}
\end{aligned}
$$

QCD θ-term

$$S = S_{QCD} + i\bar{\theta}Q, \qquad Q = \int d^4x \frac{G\tilde{G}}{32\pi^2}$$

- Three different approaches
  - External electric field method: $\langle N\overline{N}\rangle_{\bar{\theta}}(\vec{\mathcal{E}}, t) = \langle N(t)\overline{N}(0)e^{i\bar{\theta}Q}\rangle_{\vec{\mathcal{E}}}$

    Aoki and Gocksch (1989), Aoki, Gocksch, Manohar, and Sharpe (1990), CP-PACS Collaboration (2006), Abramczyk, *et al.* (2017)
  - Simulation with imaginary $\bar{\theta}$: $\bar{\theta} = i\tilde{\theta}, \quad S^q_{\bar{\theta}} = \tilde{\theta}\frac{m_l m_s}{2m_s+m_l}\sum_x \bar{q}\gamma_5 q$

    Horsley, *et al.*, (2008), Guo, *et al.* (2015)
  - Expansion in $\bar{\theta}$:

$$\begin{aligned}\langle O(x)\rangle_{\bar{\theta}} &= \frac{1}{Z_{\bar{\theta}}}\int d[U,q,\bar{q}]O(x)e^{-S_{QCD}-i\bar{\theta}Q} \\ &= \langle O(x)\rangle_{\bar{\theta}=0} - i\bar{\theta}\langle O(x)Q\rangle_{\bar{\theta}=0} + \mathcal{O}(\bar{\theta}^2)\end{aligned}$$

Shintani, *et al.*, (2005), Berruto, Blum, Orginos, and Soni (2006)
Shindler, T. Luu, J. de Vries (2015), Shintani, Blum, Izubuchi, and Soni (2016), Alexandrou, *et al.*, (2016), Abramczyk, *et al.* (2017), Dragos, *et al.* (2019)
Bhattacharya, *et al.* (2021)

Simulation with QCD θ-term

- Expansion in $\bar{\theta}$, which is expected to be tiny

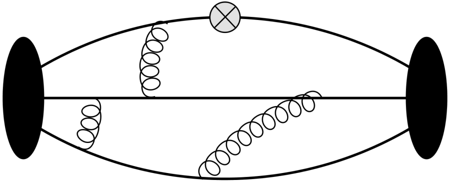
$$\langle O(x)\rangle_{\bar{\theta}} = \langle O(x)\rangle_{\bar{\theta}=0} - i\bar{\theta}\langle O(x)Q\rangle_{\bar{\theta}=0} + \mathcal{O}(\bar{\theta}^2)$$

- Do not need to generate new gauge fields (lattices) at $\bar{\theta} \neq 0$ or $d_w \neq 0$
- Neutron EDM requires calculations of
(1) vector current $O = V_\mu$, and (2) topological charge $Q_{\rm top}$
- Vector current V_μ and its renormalization
  - Reusing data generated for vector form-factor
- Topological charge $Q_{\rm top}$
  - $\mathcal{O}(a^4)$-improved gluon field strength tensor
  - Gradient flow for cooling/renormalization

$\Rightarrow$ Obtain CP violating form factor using

$$\langle N|V_\mu(q)|N\rangle_{\rm CPV} = \langle N|V_\mu(q)|N\rangle - i\bar{\theta}\langle N|V_\mu(q)Q_{\rm top}|N\rangle + \mathcal{O}(\bar{\theta}^2)$$

CPV Form Factor F_3



- F_3 is extracted from vector current in presence of CPV interactions

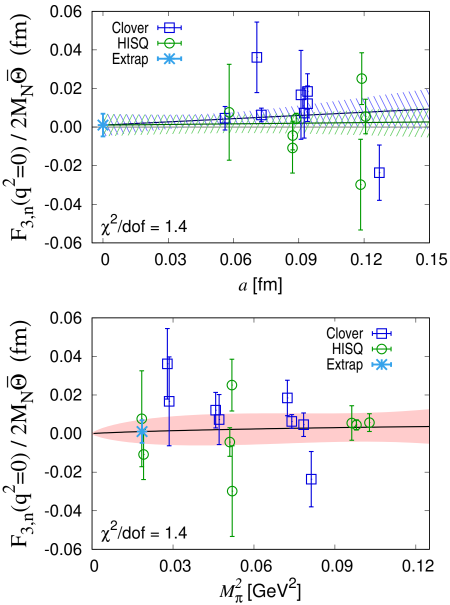
$$\langle N|V_\mu(q)|N\rangle_{\rm CPV} = \overline{u}_N \left[F_1(q^2)\gamma_\mu + i\frac{F_2(q^2)}{2M_N}\sigma_{\mu\nu}q^\nu - \frac{F_3(q^2)}{2M_N}\sigma_{\mu\nu}q^\nu\gamma_5 \right] u_N(p)$$

  Caveat: CPV interactions introduce phase in neutron mass
  $\rightarrow \gamma_4$ is not a parity operator of neutron state [Abramczyk, et al., 2017]
- Neutron EDM $d_n = |e|F_3(Q^2=0)\ /\ 2M_N$

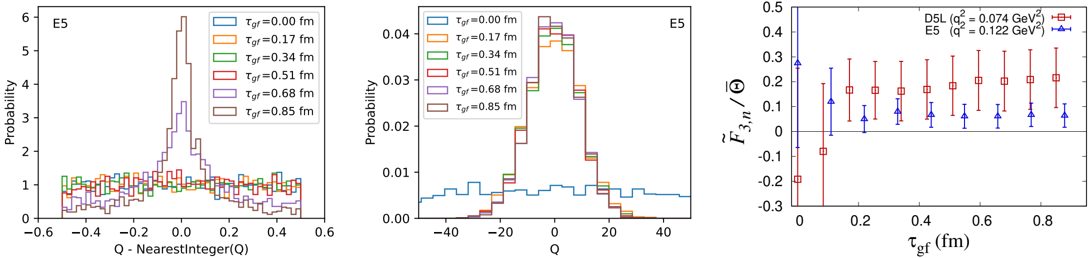
Two Lattice Discretizations in Comparison

- Previous calculation
  [Bhattacharya, *et al.* (2021)]
  - Fermion: Clover (valence) on HISQ (sea)
  - Lattice spacings: 0.057 fm – 0.151 fm
  - Pion mass: 128 MeV – 320 MeV
  - Number of configurations: 550 – 2200

- New calculation
  - Fermion: Clover (valence) on Clover (sea)
  - Lattice spacings: 0.056 fm – 0.127 fm
  - Pion mass: 167 MeV – 285 MeV
  - Number of configurations: 810 – 2100



Calculation of Topological Charges



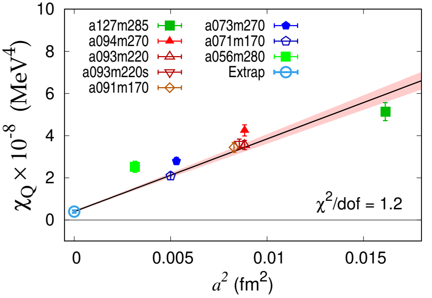
- Converging to an integer $Q_{\rm top}$ takes long flow time τ_{gf} (longer on coarser lattice)
- But $Q_{\rm top}$ and F_3 converge to a distribution with short τ_{gf}

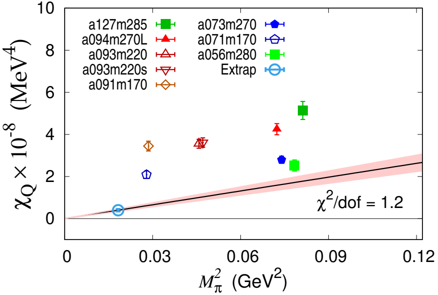
Topological Susceptibility

- Topological Susceptibility χ_Q provides a good check for the lattice calculation of Q_{top}
$$\chi_Q = \int d^4 \langle Q(x) Q(0) \rangle$$
- Fit to leading M_π- and a-dependence
$$\chi_Q = c_1 M_\pi^2 + c_2 a^2 M_\pi^2 + c_3 a^2$$
$$= [79.5(3.0)\ \text{MeV}]^4$$

c.f., $\chi_Q = [66(9)(4)\ \text{MeV}]^4$ from HISQ

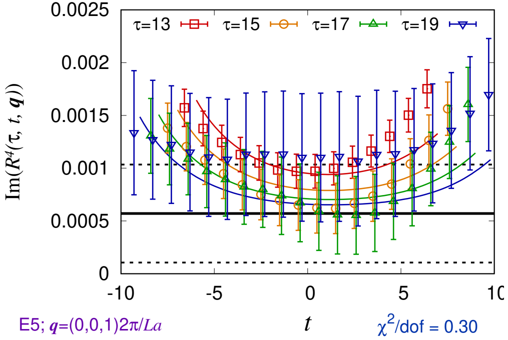
- The chiral behavior precisely agree with χPT
$$\frac{1}{\chi_Q} = \frac{1}{\chi_Q^{\text{quench.}}} + \frac{4}{M_\pi^2 F_\pi^2}\left(1 - \frac{M_\pi^2}{3M_\eta^2}\right)^{-1}$$
$$\chi_Q = [79\ \text{MeV}]^4$$

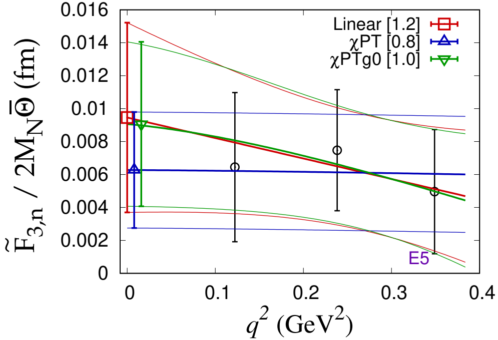




Bhattacharya, *et al.* (2021)

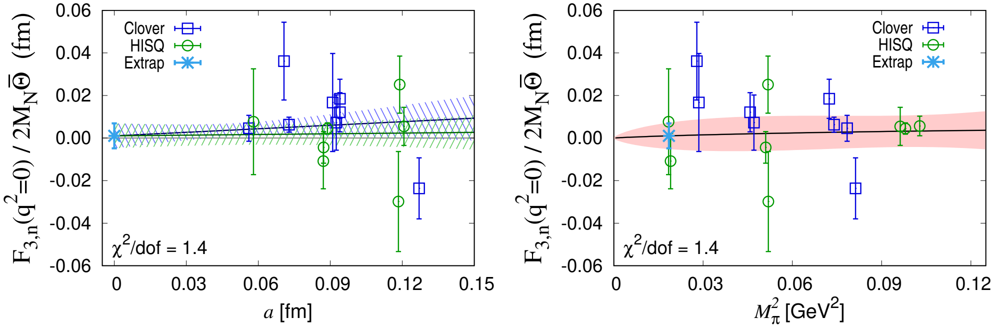
Neutron EDM from QCD θ-term on each Ensemble





- Calculate $\langle N|V_\mu(q)Q_{\rm top}|N\rangle$ and remove excited-state contamination
- Extract CPV form-factor F_3 and extrapolate to $Q^2=0$ limit
- Neutron EDM $d_n = |e|F_3(Q^2=0)\ /\ 2M_N$

Neutron EDM from QCD θ-term Extrapolated to Continuum



- Extrapolation to continuum $a \to 0$ and physical pion mass $M_\pi \to 135\mathrm{MeV}$
- Simultaneous fit to Clover-on-HISQ and Clover-on-Clover results

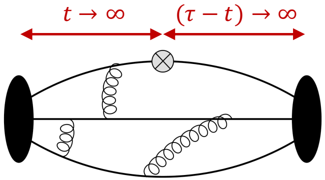
$$d_N = c_1 M_\pi^2 + c_2 M_\pi^2 \log\left(\frac{M_\pi^2}{M_N^2}\right) + c_3^{\mathrm{HISQ}} a + c_3^{\mathrm{Clover}} a = 0.0010(59)$$

PRELIMINARY; statistical error only.

- See **Tanmoy Bhattacharya**'s talk at **LATTICE2022** for details

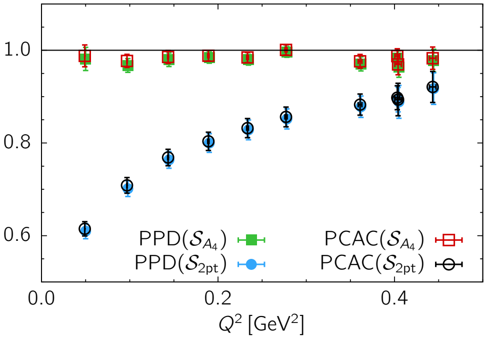
Potential Challenges: Difficult Physical Pion Mass Simulation

- On lattice, nucleon states are generated using an interpolating operator that couples to the ground-state of the nucleon but also to the excited states
- Excited-states (ES) effect exponentially diminishes for large Euclidean time
  - Separating proton sources far from each other leaves only the ground-state
  - But signal-to-noise ratio drops exponentially for baryons $(R \sim e^{(M_N - \frac{3}{2}m_\pi)\tau})$
- For reasonably small source-sink separation, fit correlators to a function including ES
  - $C_{2pt}(\tau) = \sum_i |A_i|^2 e^{-M_i \tau}$
  - $C_{3pt}^{\Gamma}(\tau, t) = \sum_{i,j} A_i A_j^* \langle i|O_\Gamma|j\rangle e^{-M_i t - M_j(\tau - t)}$
  - $C_{3pt}^{\Gamma}/C_{2pt}(\tau) \to g_\Gamma^{u-d}$ as $t \to \infty, (\tau - t) \to \infty$
- Tower of possible excited states
  - Radial excitations: $N(1440), N(1710), \ldots$
  - Multi-hadron states: $N(\mathbf{p})\pi(-\mathbf{p}), N(\mathbf{0})\pi(\mathbf{0})\pi(\mathbf{0}), \ldots$
  - But, which states contribute significantly?

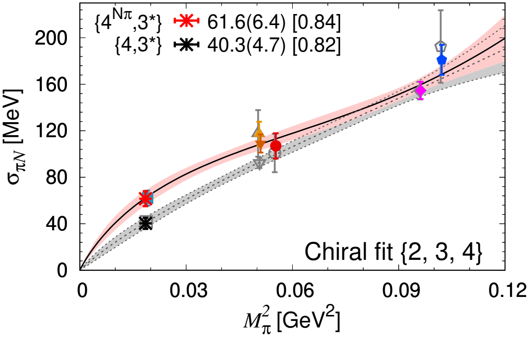


Potential Challenges: Difficult Physical Pion Mass Simulation

- Excited state fits to C_{2pt} gives large first ES mass $M_1 \gtrsim M_{N(1440)}$
- But various evidences advocate $M_1 \ll M_{N(1440)}$
  - PCAC relation between $G_A, \tilde{G}_P$, and G_P is much better satisfied with smaller M_1
  - Nucleon σ-term results are consistent with χPT when $M_1 \sim M_{N\pi, N\pi\pi}$

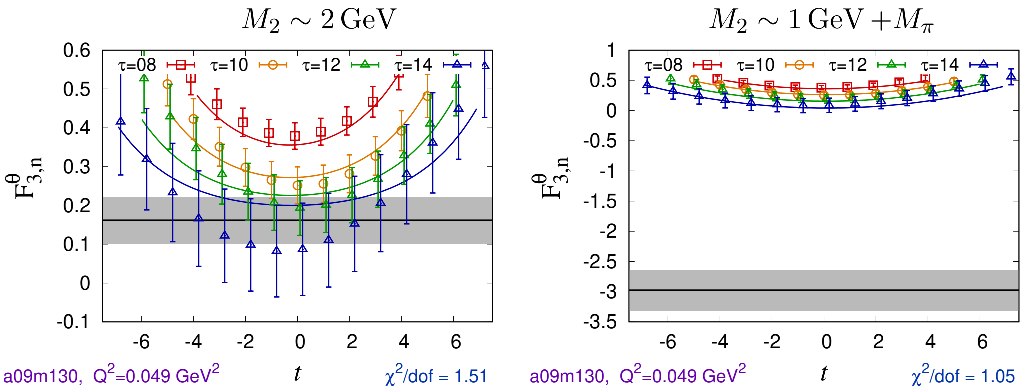


[Jang, *et al.*, (2020)]



[Gupta, *et al.*, (2021)]

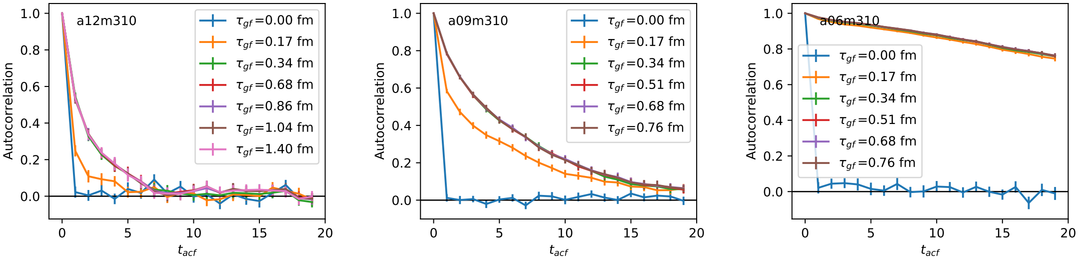
Potential Challenges: Difficult Physical Pion Mass Simulation



- Calculations at $m_\pi < 200\mathrm{MeV}$ have poor signal
- Possibly significant contamination from the $N\pi$-first-excited-state at near $m_\pi^{\mathrm{phys.}}$
  Calculation with high statistics is needed to resolve [Bhattacharya, *et al.*, (2020)]

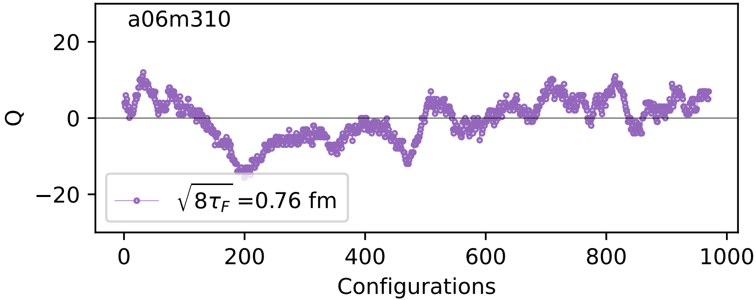
Potential Challenges: Long Autocorrelation at Fine Lattice

$a \approx 0.12$ fm | $a \approx 0.09$ fm | $a \approx 0.06$ fm



- Simulations on small a is required to reduce discretization artifact
- Topological charge Q shows longer autocorrelation on smaller a
- Clover lattices have much weaker autocorrelation, but starts to show autocorrelation at $a \approx 0.06$ fm

Potential Challenges: Long Autocorrelation at Fine Lattice



- Simulations on small a is required to reduce discretization artifact
- Topological charge Q shows longer autocorrelation on smaller a
- Clover lattices have much weaker autocorrelation, but starts to show autocorrelation at $a \approx 0.06$ fm

Neutron EDM from Quark EDM term

$$\mathcal{L}_{\text{CPV}}^{d\leq 6} = -\frac{g_s^2}{32\pi^2}\overline{\theta}G\tilde{G} \qquad \text{dim=4 QCD } \theta\text{-term}$$

$$-\frac{i}{2}\sum_{q=u,d,s} d_q \overline{q}(\sigma\cdot F)\gamma_5 q \qquad \text{dim=5 Quark EDM (qEDM)}$$

$$-\frac{i}{2}\sum_{q=u,d,s} \tilde{d}_q g_s \overline{q}(\sigma\cdot G)\gamma_5 q \qquad \text{dim=5 Quark Chromo EDM (CEDM)}$$

$$+ d_w \frac{g_s}{6} G\tilde{G}G \qquad \text{dim=6 Weinberg's 3g operator}$$

$$+ \sum_i C_i^{(4q)} O_i^{(4q)} \qquad \text{dim=6 Four-quark operators}$$

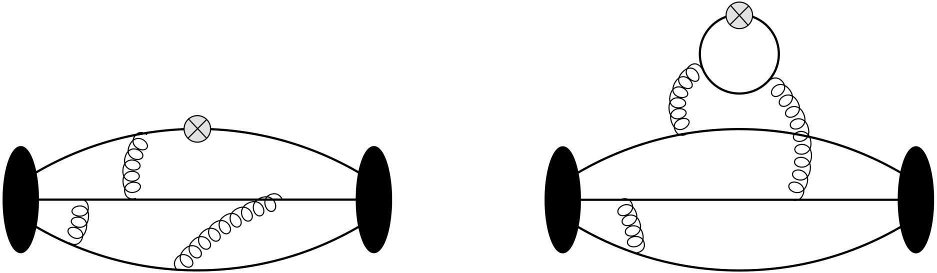
Quark EDM and Tensor Charge

- Neutron EDM (d_N) from Quark EDMs can be written in tensor charges g_T

$$-\frac{i}{2}\sum_{q=u,d,s} d_q \bar{q}(\sigma\cdot F)\gamma_5 q \quad \longrightarrow \quad d_N = d_u g_T^u + d_d g_T^d + d_s g_T^s$$

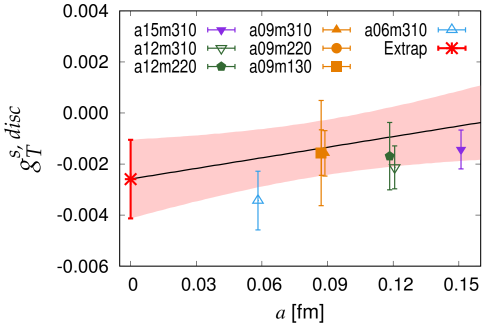
$$\langle N|\bar{q}\sigma_{\mu\nu}q|N\rangle = g_T^q \bar{u}_N \sigma_{\mu\nu} u_N$$

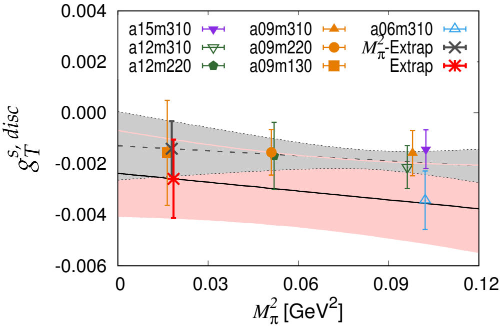
- $d_q \propto m_q$ in many models $\Rightarrow$ Precision determination of $g_T^{s,N}$ is important
- Requires computationally very expensive quark-line disconnected diagrams



Calculation of Tensor Charge

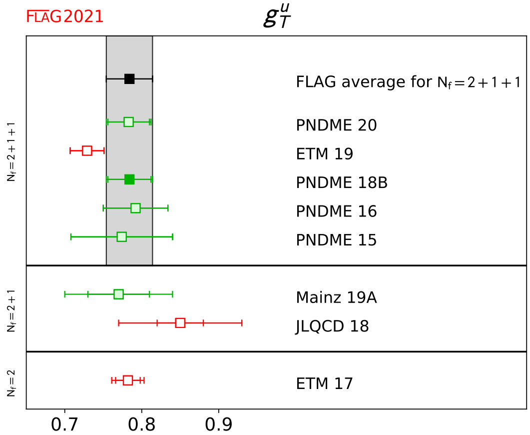
[Gupta, *et al.* (2018)]

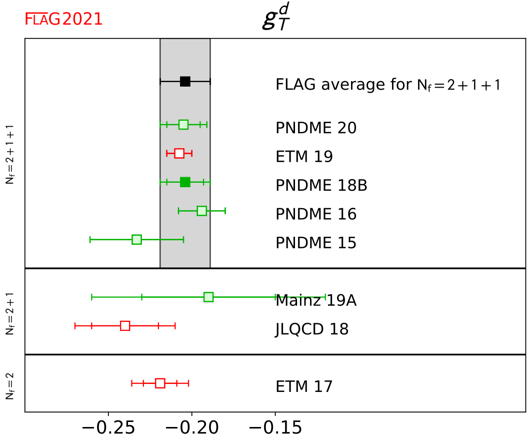




- Calculate matrix element $\langle N|\bar{q}\sigma_{\mu\nu}q|N\rangle$ and remove ESC on each ensemble
- Renormalize $g_T^{u,d,s}$ to $\overline{\mathrm{MS}}$ at 2 GeV and extrapolate the results to continuum limit
- Three-point functions that are easier to calculate than other EDM correlators
- Contributions from the disconnected diagrams, especially for g_T^s, are expensive

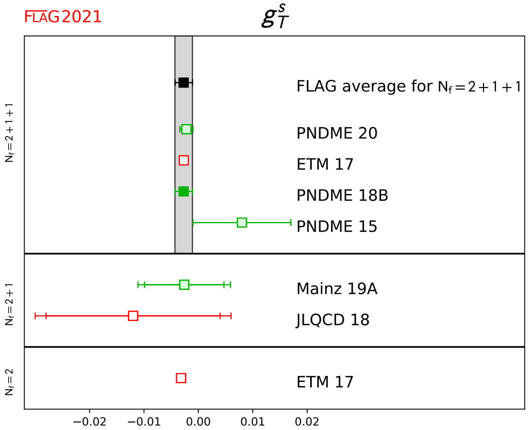
qEDM: Current Status





- $g_T^u = 0.784(28)(10)$, $g_T^d = -0.204(11)(10)$, $g_T^s = -0.0027(16)$ [PNDME 18B]
- See **Sungwoo Park**'s talk at **LATTICE2022** for updated PNDME results

qEDM: Current Status



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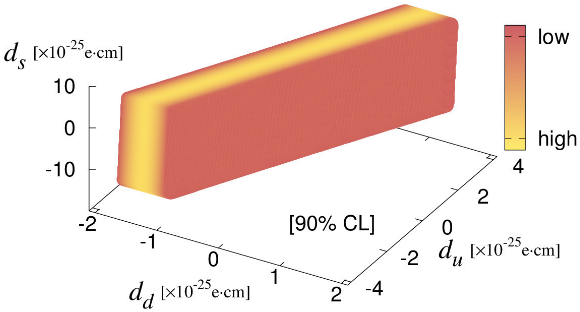
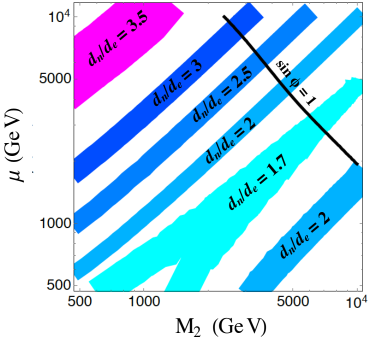
BSM Constraints from qEDM

$$d_N = d_u g_T^u + d_d g_T^d + d_s g_T^s$$





[Bhattacharya, *et al.* (2015), Gupta, *et al.* (2018)]

(L) Constraints on the BSM couplings $d_{u,d,s}$,
assuming that these couplings give dominant contribution to nEDM

(R) Regions in gaugino (M_2) and Higgsino (μ) mass plane
corresponding to various values of d_n/d_e in split SUSY

Neutron EDM from quark Chromo-EDM (CEDM)

$\mathcal{L}_{\text{CPV}}^{d\leq 6} = -\frac{g_s^2}{32\pi^2}\overline{\theta}G\tilde{G}$	dim=4 QCD θ-term
$-\frac{i}{2}\sum_{q=u,d,s} d_q\overline{q}(\sigma \cdot F)\gamma_5 q$	dim=5 Quark EDM (qEDM)
$-\frac{i}{2}\sum_{q=u,d,s} \tilde{d}_q g_s\overline{q}(\sigma \cdot G)\gamma_5 q$	dim=5 Quark Chromo EDM (CEDM)
$+d_w\frac{g_s}{6}G\tilde{G}G$	dim=6 Weinberg's 3g operator
$+\sum_i C_i^{(4q)}O_i^{(4q)}$	dim=6 Four-quark operators

Lattice QCD approaches for CEDM

$$S = S_{QCD} + S_{CEDM}; \qquad S_{CEDM} = \frac{g_s}{2} \sum_{q=u,d,s} \tilde{d}_q \int d^4x \overline{q} (\sigma \cdot G) \gamma_5 q$$

- Three different approaches developed
  - Schwinger source method [Bhattacharya, *et al.* (2016)]:

$$D_{clov} \to D_{clov} + \frac{i}{2} \varepsilon \sigma^{\mu\nu} \gamma_5 G_{\mu\nu}$$

  - Expansion in $\tilde{d}_q$ [Abramczyk, *et al.* (2017)]:

$$\langle N V_\mu \overline{N} \rangle_{CEDM} = \langle N V_\mu \overline{N} \rangle + \tilde{d}_q \langle N V_\mu \overline{N} \sum_x O_{CEDM} \rangle + \mathcal{O}(\tilde{d}_q^2)$$

  - External electric field method [Abramczyk, *et al.* (2017)]:

$$\langle N \overline{N} \rangle_{CEDM} (\vec{\mathcal{E}}, t) = \langle N(t) \overline{N}(0) O_{CEDM} \rangle_{\vec{\mathcal{E}}}$$

Power-divergent Mixing

- CEDM operator has power-divergent mixing with the pseudoscalar operator
  [Bhattacharya, *et al.* (2015), Constantinou, *et al.* (2015)]
  - Gradient-flow technique can remove the power-divergent mixing
  - Alternative approach: define a new operator to subtract power-divergence

$$\tilde{C} \equiv i\bar{\psi}\sigma^{\mu\nu}\gamma_5 G_{\mu\nu}T^a\psi - \frac{iA}{a^2}\bar{\psi}\gamma_5 T^a\psi$$

[Bhattacharya, *et al.* (2022)]

  - The coefficient A should be set to cancel the ultraviolet divergence
  - Determine A so that $\tilde{C}$ does not create pion $\langle\Omega|\tilde{C}|\pi(\vec{p}=0)\rangle = 0$

- At $p=0$, isovector P can be rotated away using non-anomalous Ward identity

$$Z_A(1+b_A ma)\partial\cdot A + iaZ_A c_A \partial^2 P + 2miP - iaK\tilde{C} \approx 0$$

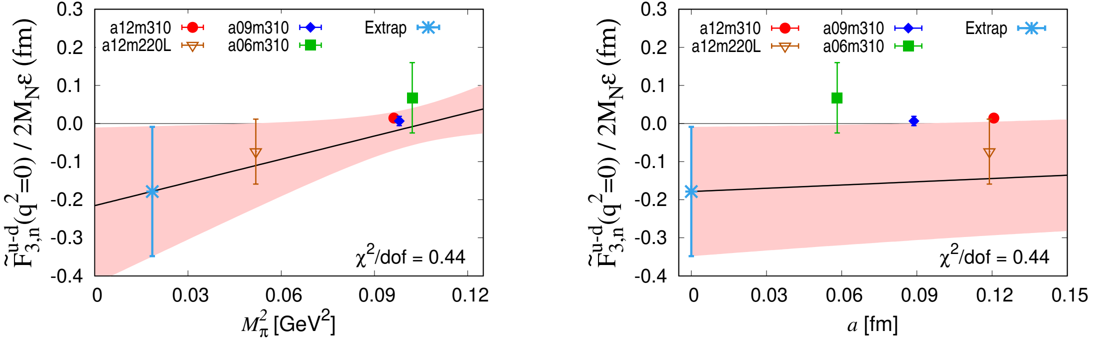
  - All below three combinations describe the same physics

$$\left(aC - A\frac{P}{a}\right), \qquad \left(\frac{\bar{y}}{\bar{x}} - A\right)\frac{P}{a}, \qquad \left(1 - \frac{A\bar{x}}{\bar{y}}\right)aC$$

where A, $\bar{x}$, and $\bar{y}$ are the coefficients that can be determined from pion correlators

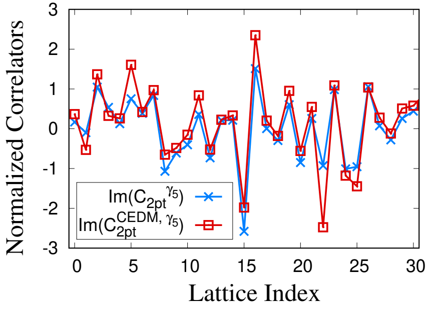
Results

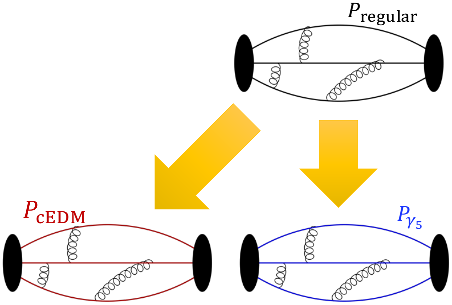
[Bhattacharya, *et al.* (2022)]



- Preliminary data of bare (power-divergent-subtracted) operator $\tilde{C}$
- Results seem to have better signal than QCD θ-term for $M_\pi \approx 300$ MeV

Machine Learning Predictions for CEDM Observables

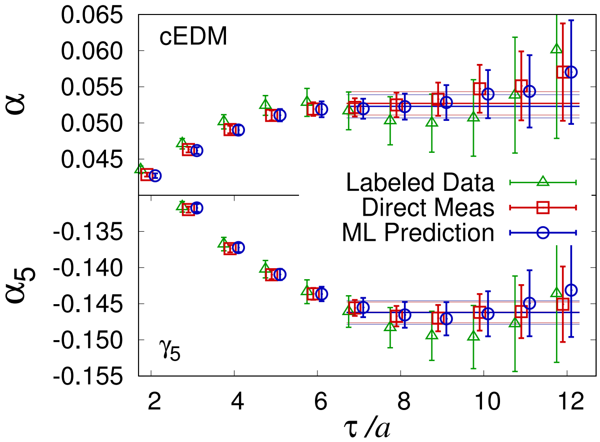




- Calculation of quark propagators including CEDM interactions are expensive
- Plain C_{2pt} is highly correlated with the C_{2pt}^{CEDM}
- Machine learning can learn the correlation pattern and predict C_{2pt}^{CEDM} from C_{2pt}
- ML prediction error can be estimated statistically – unbiased estimators

[Yoon, *et al.* (2019)]

Prediction of C_{2pt}^{CEDM} from C_{2pt}



- CP violating phase
  $(ip_\mu\gamma_\mu + me^{-2i\alpha\gamma_5})\tilde{u} = 0$
- Training on 70 confs,
  bias correction on 50 confs,
  prediction for 400 confs
- ML algorithm is able to learn the computation of CPV observables
- Prediction errors are statistically included in the errorbars (unbiased eatimates)

Neutron EDM from Weinberg's ggg

$$\mathcal{L}_{\rm CPV}^{d\leq 6} = -\frac{g_s^2}{32\pi^2}\overline{\theta}G\tilde{G}$$ dim=4 QCD θ-term

$$-\frac{i}{2}\sum_{q=u,d,s} d_q\overline{q}(\sigma\cdot F)\gamma_5 q$$ dim=5 Quark EDM (qEDM)

$$-\frac{i}{2}\sum_{q=u,d,s} \tilde{d}_q g_s\overline{q}(\sigma\cdot G)\gamma_5 q$$ dim=5 Quark Chromo EDM (CEDM)

$$+\, d_w\frac{g_s}{6}G\tilde{G}G$$ dim=6 Weinberg's 3g operator

$$+\sum_i C_i^{(4q)}O_i^{(4q)}$$ dim=6 Four-quark operators

Weinberg's 3g Op: Current Status and Future Prospects

$$\mathcal{L}_{W_{ggg}} = \frac{1}{6} d_w g_s G\tilde{G}G$$

- No publications yet, except a few preliminary studies
  [Yoon, *et al.* (2019), Bhattacharya, *et al.* (2022)]
- Calculation is almost the same as the QCD θ-term, but signal seems to be noisier
- Requires renormalization
  - RI-MOM scheme and its perturbative conversion to $\overline{\mathrm{MS}}$ is available
    [Cirigliano, Mereghetti, and Stoffer (2020)]
  - Gradient flow scheme is a favorable option due to the complex mixing structure
    [Rizik, Monahan, and Shindler (2020)]

Renormalization with Gradient Flow

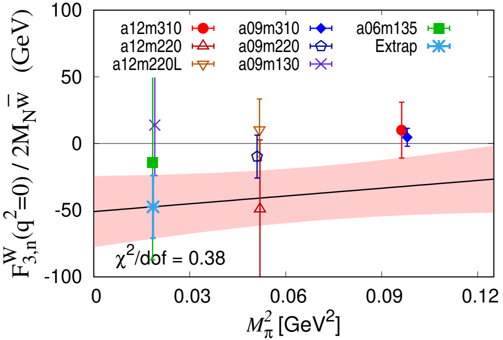
Gradient flow [Lüscher and Weisz (2011)]:

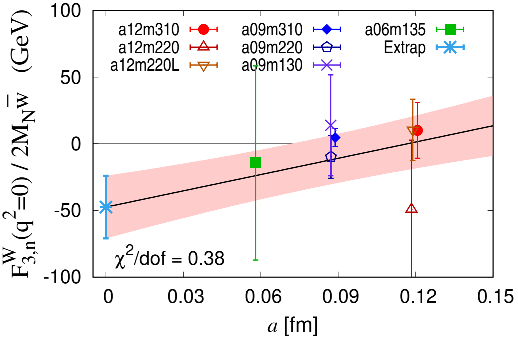
$$\partial_t B_\mu(t) = D_\nu G_{\nu\mu}, \qquad B_\mu(x, t=0) = A_\mu(x),$$
$$\partial_t \chi(t) = \Delta^2 \chi, \qquad \chi(x, t=0) = \psi(x)$$

- Smear (flow) gluon and quark fields along the gradient of an action to a fixed physical size τ_{gf} (sets ultraviolet cutoff of the theory)
- The flowed operators have finite matrix elements except for an universal Z_ψ $\longrightarrow$ Allow us to take continuum limit without power-divergent subtractions
- Mixing and connection to the $\overline{\mathrm{MS}}$: simpler continuum perturbation calculation
- Related studies for CPV ops are recently started [Rizik, Monahan, and Shindler (2020)]

Results

[Bhattacharya, *et al.* (2022)]





- Preliminary data of bare operator in Gradient Flow scheme ($\tau_{gf} \approx 0.34$ fm)
- W_{ggg} in Gradient flow scheme has $\mathcal{O}(1/\tau_{gf})$ mixing with topological charge

  [Rizik, Monahan, and Shindler (2020)]
- Resutls sensitive to τ_{gf}

Conclusion

- We are calculating matrix elements for neutron EDM from SM and BSM
- The matrix elements will play a crucial role in connecting experiments and BSM
- Significant progress has been made in
  formulating problems and carrying out preliminary studies
- Large computational resources will be needed
- Inputs from phenomenologists will help us formulating the problems
  and guiding the continuum/chiral/excited-state extrapolations