



RTG 2575:

Rethinking Quantum Field Theory



Error Scaling of Sea Quark Isospin-Breaking Effects

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SPECIAL ARTICLE - Tools for Experiment and Theory

THE EUROPEAN PHYSICAL JOURNAL C



openQCD code: a versatile tool for QCD+QED simulations

PDT01 collaboration

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Abstract We present the open-source package openQCD (v1.0) (openQCD.GitLab, <https://gitlab.cern.ch/cpt/openQCD>; DOI: <https://doi.org/10.5281/generic/310891>, <https://doi.org/10.1140/epjc/s10052-019-07334-w>, 2019), which has been primarily developed for lattice calculations of the combined theory of QCD and QED. It includes calculations of QCD+QED and QCD with and without Coulomb boundary conditions, and QCD+QED Wilson fermions. The size of the code is ~100,000 lines of C++ code. The code is based on a local and gauge-invariant formulation of QCD+QED in finite volume, and provides a theoretically clean way to calculate observables such as the ratio of the self-energy to the bare mass, observable from free particles. The openQCD code is based on openQCD-1.6 (Simulation program for lattice QCD (openQCD code), <https://arxiv.org/abs/hep-lat/0609025>, 2006), and on the Numerical Partial Differential Equations and Scientific Theory (NPDE) code (<https://arxiv.org/abs/math/0507077>, 2005). In particular it inherits from openQCD-1.6 several code features, such as the implementation of the time-slice operator, the locality defined solver, the frequency splitting for the HLLC or the 4th order OMP integrator.

1.2. User guide for the dynamical QCD+QED simulation program <https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/manual.pdf>

1.3. Coupling and running the main program https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/run_main.pdf

1.4. Constructing the input for latt2c <https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/latt2c.pdf>

4 Performance analysis

4.1. Code performance on parallel machines https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/perf_parallel.pdf

4.2. Low-level tests https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/perf_lowlevel.pdf

4.3. Construction of the Runhook with Fourier transforms <https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/runhook.pdf>

4.4. Performance of locally defined solver in QCD+QED https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/local_solver.pdf

4.5. Key observables for HMC simulations of QCD+QED <https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/observables.pdf>

5 Summary and outlook <https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/summary.pdf>

A Implementation of the RHM <https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/rhm.pdf>

A.1 Runhook approach <https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/runhook.pdf>

A.2 Frequency splitting and partitioned action <https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/freqsplit.pdf>

A.3 Reweighting factors <https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/reweight.pdf>

A.3.1 Reweighting factor μ_{ω} https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/reweight_mu.pdf

B Laplacian for the Fourier-accelerated molecular dynamics <https://gitlab.cern.ch/cpt/openQCD/blob/v1.0/doc/laplacian.pdf>

Motivations

Isospin symmetry is an approximation as long as the target precision is above 1%:

$$\underbrace{\left(\frac{m_d - m_u}{\Lambda_{\text{QCD}}} \right)}_{\text{Strong-IBE}} \sim 0.01$$

$$\underbrace{\frac{e^2}{4\pi}}_{\text{Electromagnetic-IBE}} \sim 0.01 \quad .$$

- Many lattice computations of hadronic observables have reached 1% precision;
- Sea-quark effects are small, but a bound needs to be included in the error;

RM123 Method [PhysRevD.87.114505]

Monte Carlo simulation of $\text{QCD}_{\text{Iso}} + \text{perturbative expansion in Isospin breaking term } S_{\text{QCD+QED}} = S_{\text{Iso}+\gamma} + S_{\text{IB}}(\delta m_{ud}, e^2)$:

$$\begin{aligned}\langle \mathcal{O} \rangle &= \frac{\int dU d\chi dA e^{-S_{\text{Iso}}[U, \chi]} e^{-S_{\text{IB}}[U, A, \chi]} e^{-S_\gamma[A]} \mathcal{O}[U, A, \chi]}{\int dU d\chi dA e^{-S_{\text{Iso}}[U, \chi]} e^{-S_{\text{IB}}[A, \chi, U]} e^{-S_\gamma[A]}} \\ &= \langle \mathcal{O} \rangle_{\text{Iso}} - \underbrace{\langle S_{\text{IB}} \mathcal{O} \rangle_{\text{Iso}\gamma, c}}_{\text{valence-valence}} + \underbrace{\frac{1}{2} \langle S_{\text{IB}} S_{\text{IB}} \mathcal{O} \rangle_{\text{Iso}\gamma, c}}_{\text{sea-valence}} + \underbrace{\langle S_{\text{IB}} S_{\text{IB}} \mathcal{O} \rangle_{\text{Iso}\gamma, c}}_{\text{sea-sea}} \\ &\quad - \underbrace{\langle S_{\text{IB}} \mathcal{O} \rangle_{\text{Iso}\gamma, c} + \frac{1}{2} \langle S_{\text{IB}} S_{\text{IB}} \mathcal{O} \rangle_{\text{Iso}\gamma, c} + \frac{1}{2} \langle S_{\text{IB}} S_{\text{IB}} \mathcal{O} \rangle_{\text{Iso}\gamma, c}}_{\text{sea-sea}} \\ &\quad + O(\delta m_{ud}^2, e^4, e^2 \delta m_{ud}) .\end{aligned}$$

Sea-sea Diagrams

From the expansion:

$$\langle \mathcal{O} \rangle = \langle \mathcal{O} \rangle_{\text{Iso}} - \langle S_{\text{IB}} \mathcal{O} \rangle_{\text{Iso}+\gamma,c} + \frac{1}{2} \langle S_{\text{IB}} S_{\text{IB}} \mathcal{O} \rangle_{\text{Iso}+\gamma,c}$$

The sea-sea diagrams are:

$$\begin{aligned}\langle \mathcal{O} \rangle_{\text{sea}} &= \sum_f \delta m_f \langle \text{mass} \circlearrowleft \mathcal{O} \rangle_{\text{Iso},c} + e^2 \sum_f q_f^2 \langle \text{tadpole} \circlearrowleft \mathcal{O} \rangle_{\text{Iso},c} \\ &\quad + e^2 \left[\sum_f q_f^2 \langle \text{lightbulb} \circlearrowleft \mathcal{O} \rangle_{\text{Iso},c} + \sum_{fg} q_f q_g \langle \text{lanterns} \circlearrowleft \mathcal{O} \rangle_{\text{Iso},c} \right].\end{aligned}$$

Scaling of the Error

Looking at the error of the insertion

$$\sigma [\langle \mathcal{D}\mathcal{O} \rangle_{\text{Iso},c}]$$

In the asymptotic limit, the gauge error factorizes [Harris et al., LATTICE2022 013]:

$$\sigma [\langle \mathcal{D}\mathcal{O} \rangle_{\text{Iso},c}] \underset{a \rightarrow 0}{\sim} \sqrt{\langle \mathcal{D}^2 \rangle_{\text{Iso},c} \langle \mathcal{O}^2 \rangle_{\text{Iso},c}}$$

The leading result is:

$$\sigma \left[\langle \textcirclearrowright \mathcal{O} \rangle_{\text{Iso},c} \right] \underset{a \rightarrow 0}{\sim} \sigma_{\mathcal{O}} a^{-1} \sqrt{V}$$

$$\sigma [\langle \mathcal{D}\mathcal{O} \rangle_{\text{Iso},c}] \underset{a \rightarrow 0}{\sim} \sigma_{\mathcal{O}} a^{-2} \sqrt{V} \text{ for } \mathcal{D} = \text{Diagram A}, \text{Diagram B}, \text{Diagram C}$$

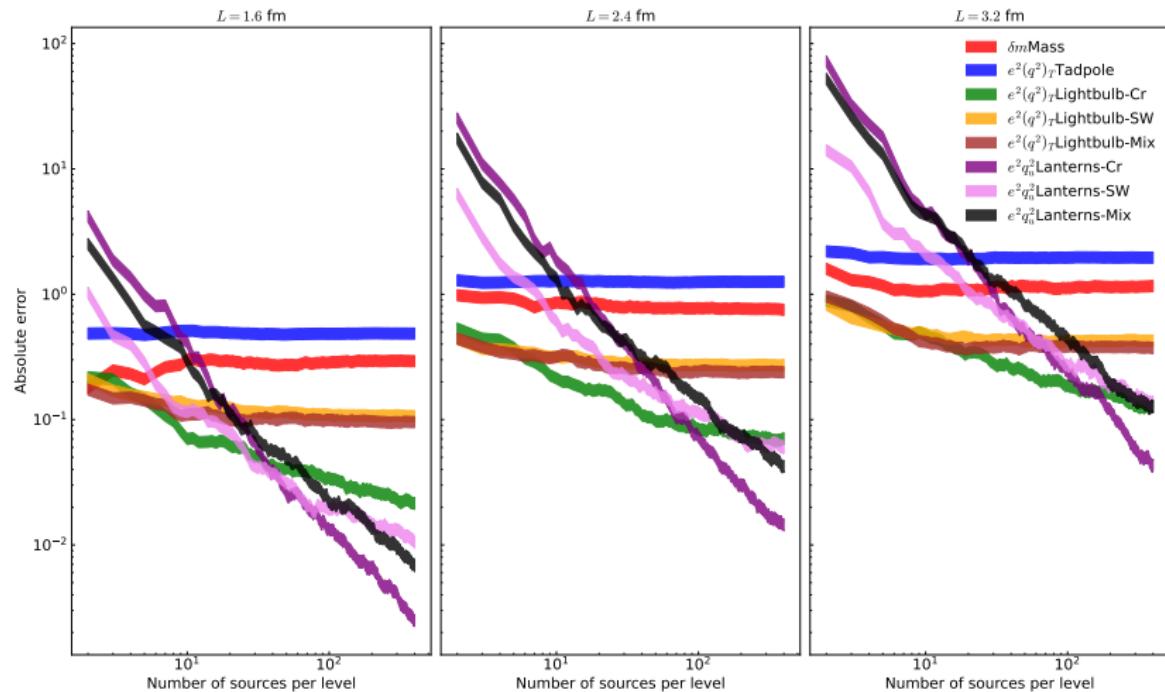
Volume Scaling

Scaling of the diagrams' error with the number of sources

ensemble	a [fm]	M_π [MeV]	$M_\pi L$	n.cnfg
A420a00b334	0.0990(7)	413(8)	3.31	50
B420a00b334	0.0991(3)	415(3)	4.98	50
C420a00b334	0.0990(1)	415(1)	6.63	50

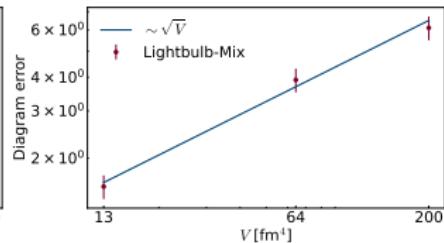
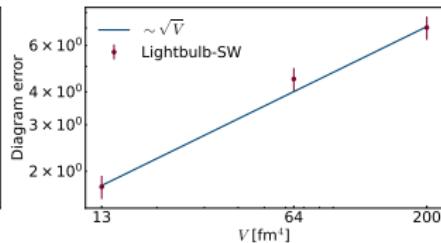
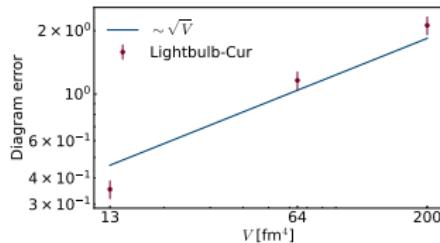
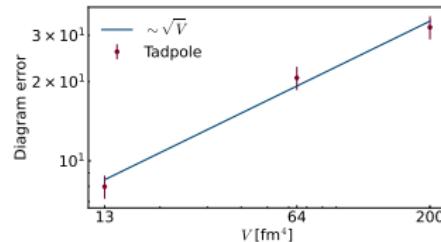
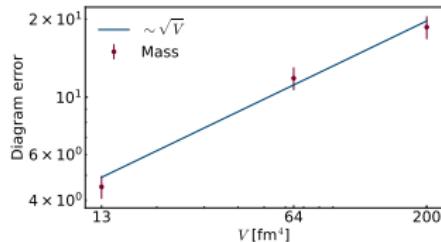


Parameters from [Bali et al., JHEP05(2023)035]



Volume Scaling

Scaling of the diagrams' error



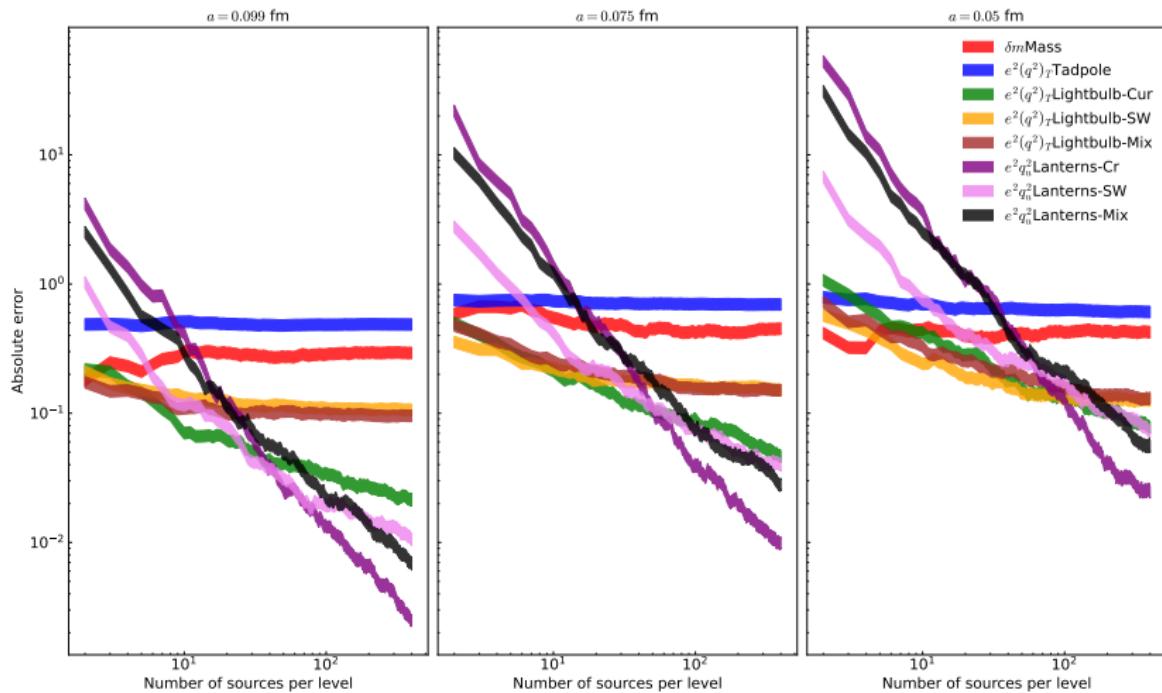
Continuum Scaling

Scaling of the diagrams' error with the number of sources

ensemble	a [fm]	M_π [MeV]	L [fm]	n.cnfg
C420a00b370	0.0499(2)	416(3)	1.596(6)	50
B420a00b346	0.0769(3)	414(2)	1.857(6)	50
A420a00b334	0.0990(7)	413(8)	1.58(1)	50

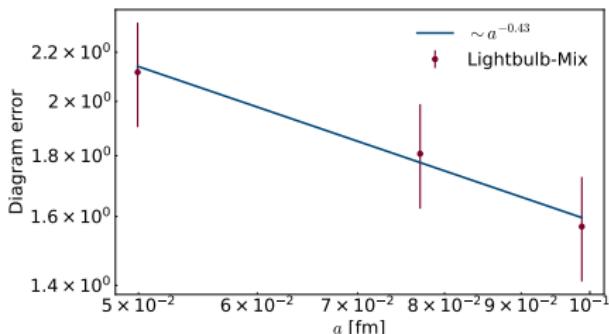
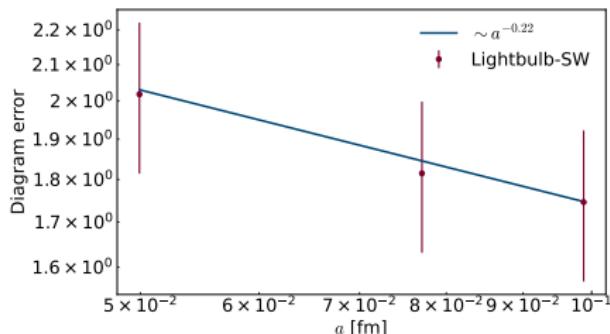
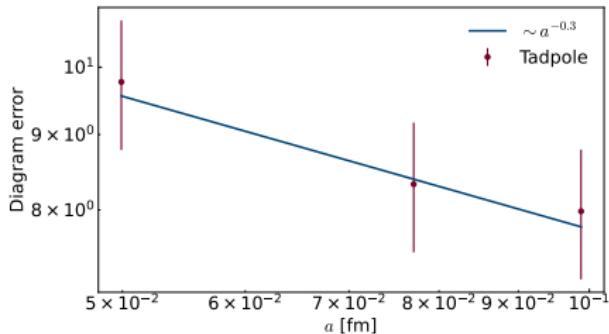
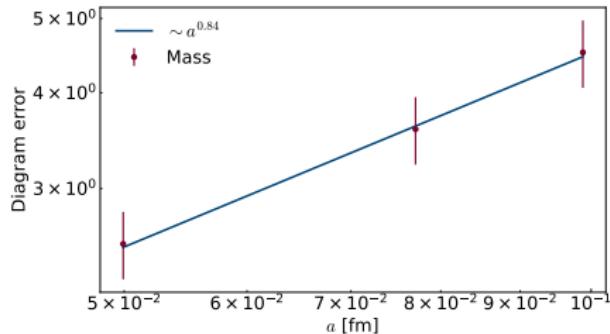


Parameters from [Bali et al., JHEP05(2023)035]



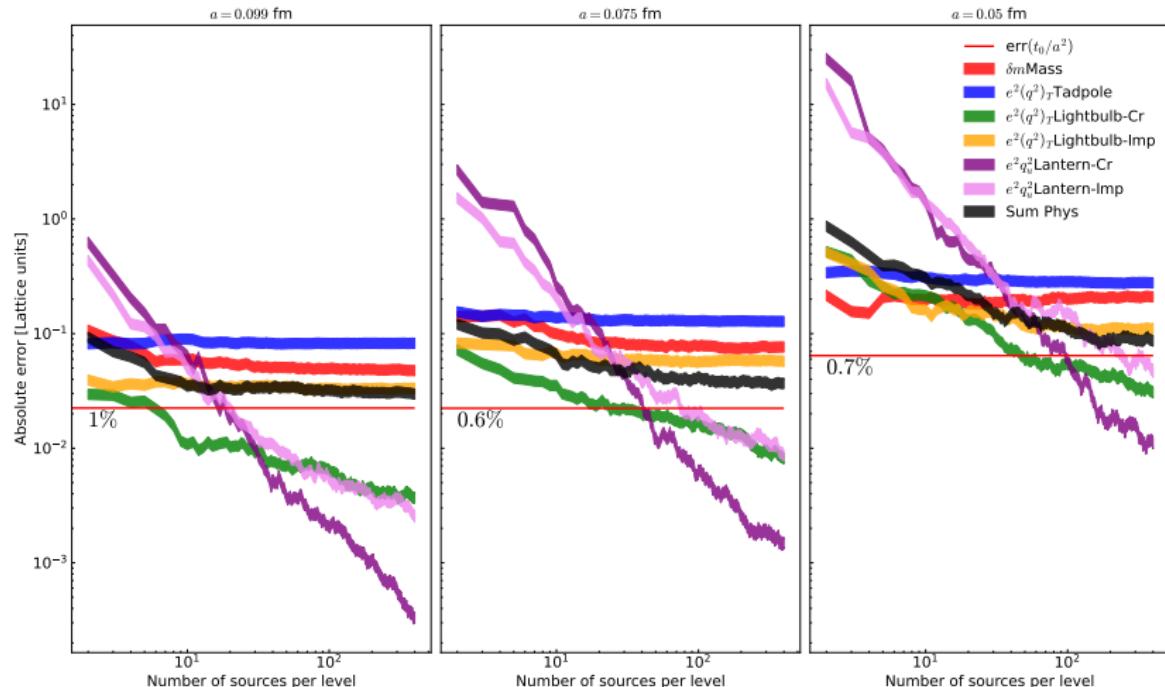
Continuum Scaling

Scaling of the diagrams' error



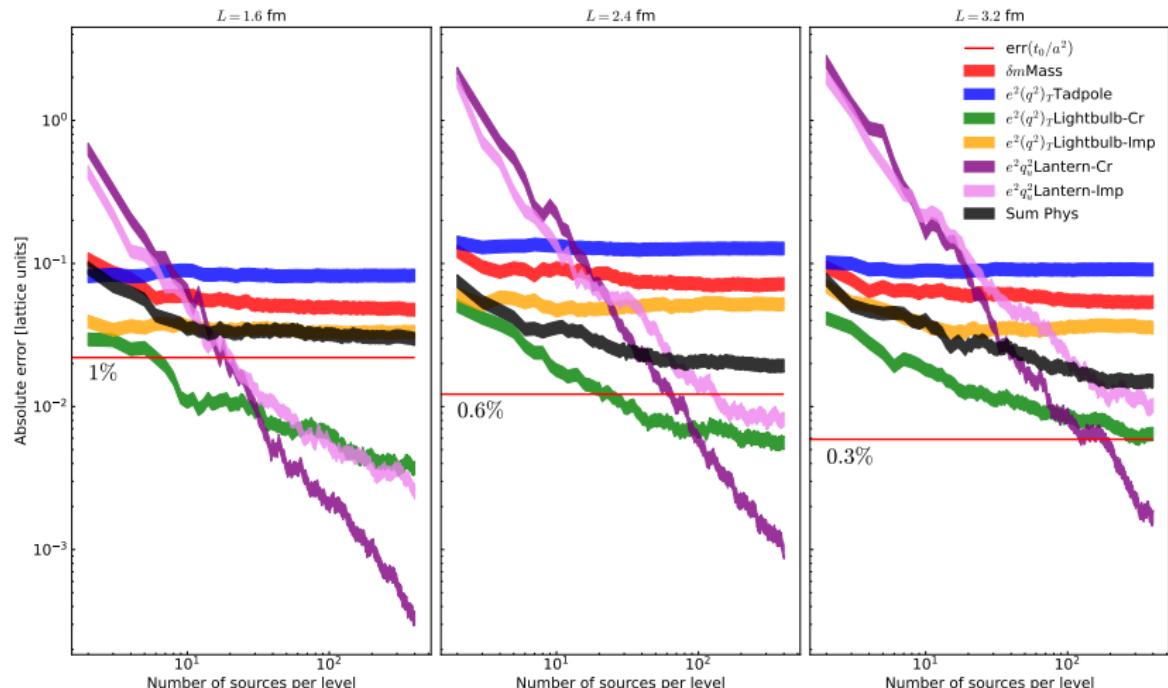
Continuum Scaling of the error of t_0/a^2

Scaling with the number of sources

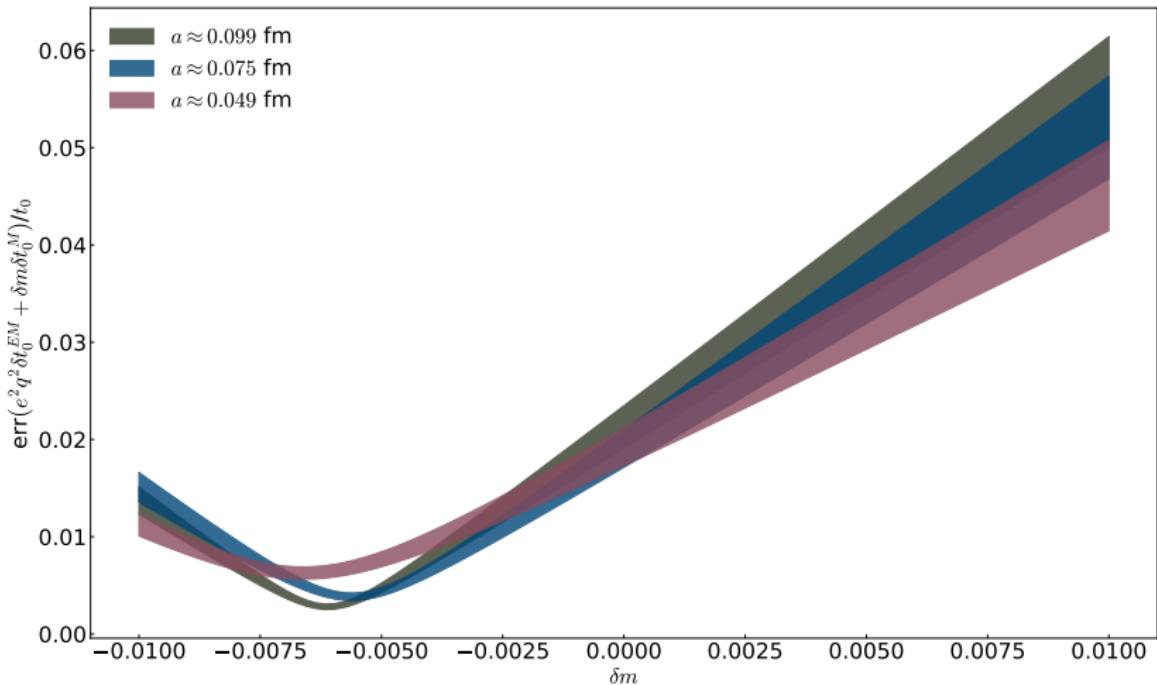


Infinite Volume Scaling of the error of t_0/a^2

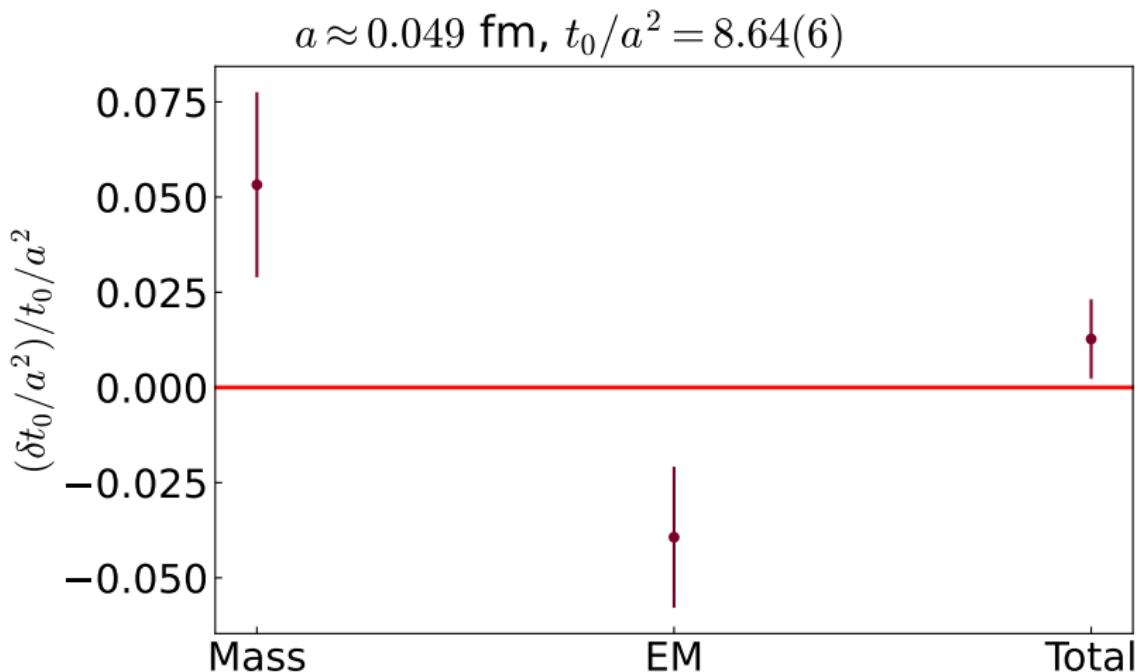
Scaling with the number of sources



Error Correlation for t_0/a^2



Correction to t_0/a^2



Conclusions and Outlook

- ✓ Sea quark isospin-breaking effects can be computed for $O(a)$ -improved Wilson fermions, reaching the gauge noise for almost all the contributions;
- ✓ The gauge error of the diagrams does not diverge in the continuum limit;
- ✓ The gauge error of the diagrams diverges in the infinite volume limit;
- ✓ The correlation between the mass term and the tadpole term can be exploited with new discretization of the mass operator;
- Extend the statistics and $m_\pi \rightarrow m_{\pi^{\text{phys.}}}$;
- Study the effects on the HVP [for the latest update, see L. Parato's talk today @ 12:10];

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Thank you for your attention!

Backup: The Diagrams

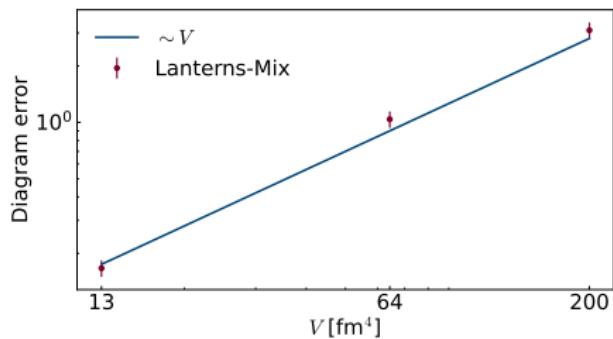
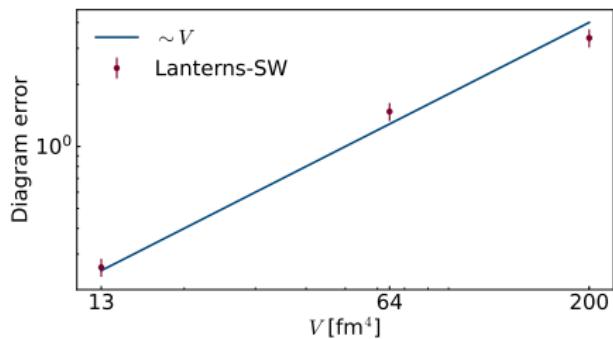
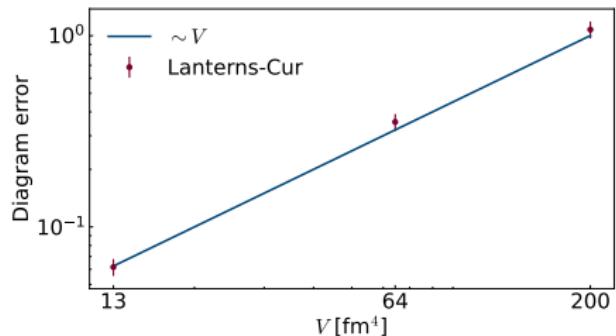
$$\frac{1}{2} \sum_x \operatorname{Re} \operatorname{tr} [D_f^{-1}(x, x)] = \circlearrowleft^f$$

$$\frac{1}{4} \sum_{xy} \langle \operatorname{Re} \operatorname{tr} [D_f^{-1}(x, y) T(y, x)] \rangle_\gamma = \circlearrowleft^f \star$$

$$\left. \begin{aligned} & \frac{1}{8} \sum_{xyzw, \mu} \langle \operatorname{Im} \operatorname{tr} [J(x, y) D_f^{-1}(y, x)] \operatorname{Im} \operatorname{tr} [J(z, w) D_g^{-1}(w, z)] \rangle_\gamma \\ & \frac{c_f c_s}{128} \sum_{xy, \mu\nu\rho\sigma} \langle \operatorname{Re} \operatorname{tr} [\sigma_{\mu\nu} \hat{A}_{\mu\nu}(x) D_f^{-1}(x, x)] \operatorname{Re} \operatorname{tr} [\sigma_{\rho\sigma} \hat{A}_{\rho\sigma}(y) D_g^{-1}(y, y)] \rangle_\gamma \\ & \frac{c_f}{16} \sum_{xyz, \mu\nu} \langle \operatorname{Re} \operatorname{tr} [\sigma_{\mu\nu} \hat{A}_{\mu\nu}(x) D_f^{-1}(x, x)] \operatorname{Im} \operatorname{tr} [J(y, z) D_g^{-1}(z, y)] \rangle_\gamma \end{aligned} \right\} = \circlearrowleft^f \text{---} \text{---} \circlearrowright^g$$

$$\left. \begin{aligned} & \frac{1}{4} \sum_{xyzw, \mu} \langle \operatorname{Re} \operatorname{tr} [J(x, y) D_f^{-1}(y, z) J(z, w) D_f^{-1}(w, x)] \rangle_\gamma \\ & - \frac{c_f^2}{64} \sum_{xy, \mu\nu\rho\sigma} \langle \operatorname{Re} \operatorname{tr} [\sigma_{\mu\nu} \hat{A}_{\mu\nu}(x) D_f^{-1}(x, y) \sigma_{\rho\sigma} \hat{A}_{\rho\sigma}(y) D_f^{-1}(y, x)] \rangle_\gamma \\ & - \frac{c_f}{8} \sum_{xyz, \mu\nu} \langle \operatorname{Im} \operatorname{tr} [\sigma_{\mu\nu} \hat{A}_{\mu\nu}(x) D_f^{-1}(x, y) J(y, z) D_f^{-1}(z, x)] \rangle_\gamma \end{aligned} \right\} = \circlearrowleft^f \text{---} \text{---} \circlearrowright^g$$

Backup: Volume Scaling for the Lanterns



Backup: Continuum Scaling for the other Diagrams

