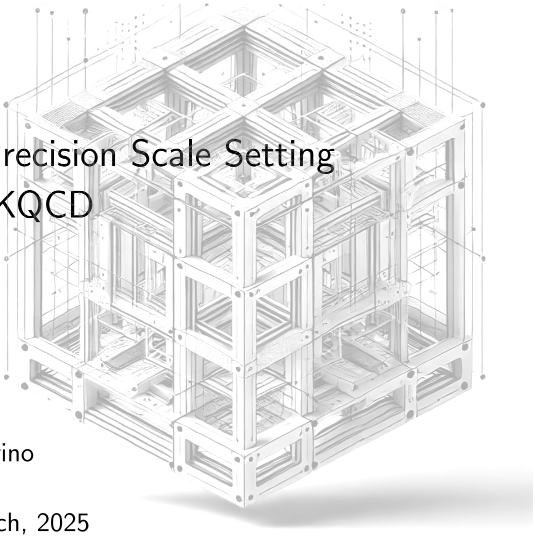
Recent Progress on High Precision Scale Setting for RBC/UKQCD



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Why high precision scale setting?

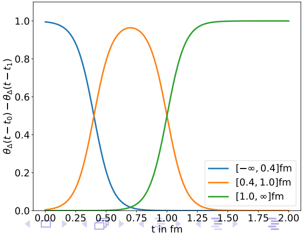
- To obtain physical quantities from a lattice simulation, we need to fix the lattice scale
- Impacts results for high precision observables, such as HVP contribution to $(g-2)_\mu$
- Since muon mass m_μ in HVP kernel $f(t, m_\mu)$ is dimensionful quantity

  [Bernecker, Meyer arxiv:1107.4388]

$$a_\mu^{\mathrm{hvp}} = \left(\frac{\alpha}{\pi}\right)^2 \int_0^\infty dt\, f(t, m_\mu)\, \frac{1}{3} \sum_{\boldsymbol{x}} \sum_{i=1}^{3} \langle j_i(\boldsymbol{x}, t) j_i(0) \rangle$$

- Vector current $j_\mu^{em} = i\left(\frac{2}{3}\bar{u}\gamma_\mu u - \frac{1}{3}\bar{d}\gamma_\mu d + \dots\right)$
- For window quantities $a_\mu^{\mathrm{hvp}} = (a_\mu^{\mathrm{hvp}})^{\mathrm{SD}} + (a_\mu^{\mathrm{hvp}})^{\mathrm{ID}} + (a_\mu^{\mathrm{hvp}})^{\mathrm{LD}}$,

  window function also depends on lattice scale



Why high precision scale setting?

- Recent results for the intermediate- and long-distance window quantities in isoQCD

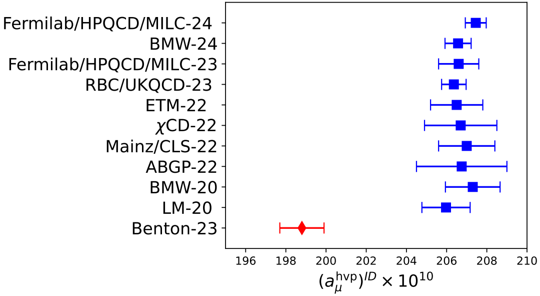


Fig. 1: Intermediate-distance window contribution

Why high precision scale setting?

- Recent results for the intermediate- and long-distance window quantities in isoQCD
- Definition of isoQCD scheme is important!

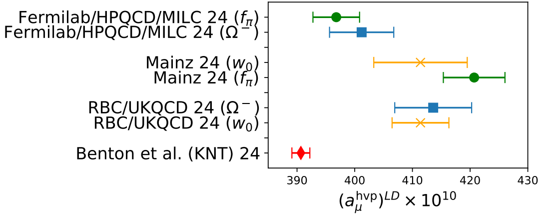


Fig. 2: Long-distance window contribution to a_μ^{hvp}

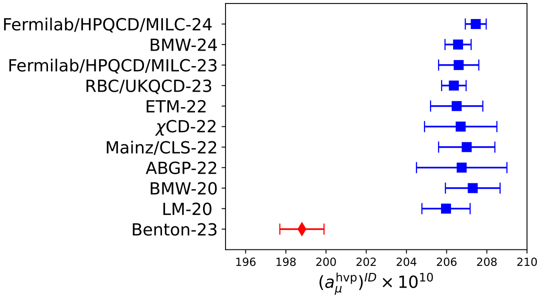


Fig. 3: Intermediate-distance window contribution

Why high precision scale setting?

What is the effect of scale setting on window contributions?

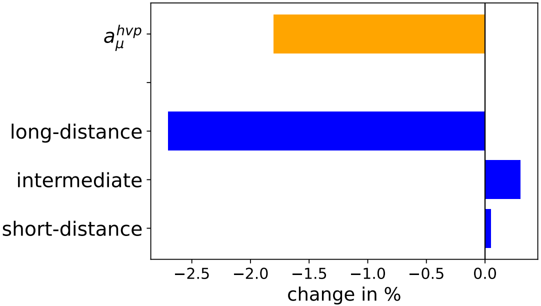
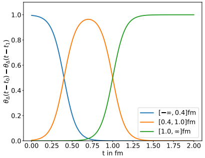


Fig. 4: Change of the different HVP window contributions for a 1% change of the lattice scale



- A +1% shift in lattice scale leads to −1.8% shift in a_μ^{hvp}
- Large cancellation in intermediate and short-distance window
- But, long-distance contributions shifts about −2.7%

Why high precision scale setting?

Entering the high precision era of lattice QCD:

- Aiming for sub-percent precision, we need to include isospin breaking corrections!
- Lattice simulations are typically performed in isospin symmetric QCD ($m_u = m_d$, $\alpha_{QED} = 0$)
- Sub-percent precision, isospin breaking effects are a significant source of error
- Effects computation of observable a_μ^{hvp} directly $\rightarrow$ many additional Wick contractions
- But, also scale setting is affected by isospin breaking corrections $\rightarrow$ Compute corrections to scale setting quantities
- Ongoing project of calculations in QCD+QED for RBC/UKQCD scale setting

Outline

1. RBC/UKQCD ensembles
2. Isospin symmetric QCD
3. Isospin breaking corrections
4. Computational strategy

Ensemble overview

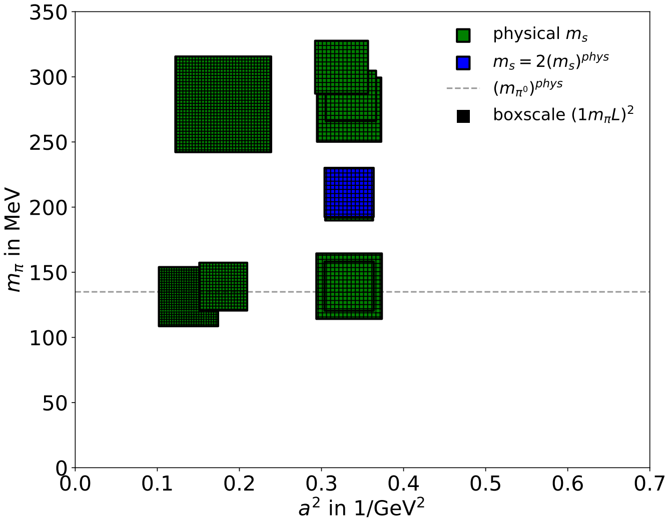
- Several new ensembles, used for recent calculations of HVP contribution to $(g-2)_\mu$ [Blum et al.arxiv:2301.08696], [arxiv:2410.20590]
- $O(a)$ improved Iwasaki gauge action
- Generated with $N_f = 2+1$ Möbius domain wall fermions, with Möbius parameters $b - c = 1$ and $b + c = 2$ [Blum et al. arxiv:1411.7017]
- Chiral symmetry on the lattice, with mild cost of non-locality
- $am_{\mathrm{res}} = O(10^{-4})$, effects are negligible (generally m_{res} effects are of similar size as bare light quark mass)
- Lattice spacing between $0.07 - 0.12$ fm

Ensemble overview

ID	a^{-1}/GeV	$L^3 \times T \times L_s/a^5$	m_π/MeV	m_K/MeV	$m_\pi L$
96I	2.6920(67)	$96^3 \times 192 \times 12$	131.29(66)	484.5(2.3)	4.7
64I	2.3549(49)	$64^3 \times 128 \times 12$	138.98(43)	507.5(1.5)	3.8
48I	1.7312(28)	$48^3 \times 96 \times 24$	139.32(30)	499.44(88)	3.9
C	1.7312(28)	$64^3 \times 96 \times 24$	139.32(30)	499.44(88)	5.2
4	1.7312(28)	$24^3 \times 48 \times 24$	274.8(2.5)	530.1(3.1)	3.8
D	1.7312(28)	$32^3 \times 48 \times 24$	274.8(2.5)	530.1(3.1)	5.1
1	1.7312(28)	$32^3 \times 64 \times 24$	208.1(1.1)	514.0(1.8)	3.8
2	1.7312(28)	$24^3 \times 48 \times 32$	285.4(2.9)	537.8(4.6)	4.0
3	1.7312(28)	$32^3 \times 64 \times 24$	211.3(2.3)	603.8(6.1)	3.9
9	2.3549(49)	$32^3 \times 64 \times 12$	278.9(0.6)	531.2(0.7)	3.8
A	1.7312(28)	$24^3 \times 48 \times 8$	307.4(3.5)	557.3(5.7)	4.2
L	2.3549(49)	$64^3 \times 128 \times 12$	278.9(0.6)	531.2(0.7)	7.6

Ensemble overview

- $N_f = 2 + 1$ Möbius domain wall ensembles
- 4 ensembles at physical pion mass
- Physical strange mass, except for one ensemble
- Ongoing thermalization of new physical point ensemble: 128I



Ensemble overview

Additional ensembles

- With $N_f = 2+1+1$ flavors to estimate sea charm effects
- Small physical pion mass ensembles with different Möbius parameters $b+c=4$
- ID ensembles have dislocation suppressing determinant ratio in action (DSDR), only used for method testing and not high-precision results (physical pion mass with low cost) [Blum et al. arxiv:1411.7017]

ID	a^{-1}/GeV	N_f	$L^3 \times T \times L_s/a^4$	$b+c$	$am_{\mathrm{res}} \times 10^4$	m_π/MeV	m_K/MeV	m_{D_s}/GeV	$m_\pi L$
5	1.7498(73)	2+1+1	$24^3 \times 48 \times 24$	2	6.7	279.8(3.5)	539.1(5.3)	1.9902(69)	3.8
7	1.7566(81)	2+1+1	$24^3 \times 48 \times 24$	2	7.9	272.5(5.9)	523(10)	1.3882(57)	3.7
24ID	1.0230(20)	2+1	$24^3 \times 64 \times 24$	4	23	142.96(30)	515.7(1.0)	–	3.4
32ID	1.0230(20)	2+1	$32^3 \times 64 \times 24$	4	23	142.96(30)	515.7(1.0)	–	4.5

Isospin symmetric QCD

Renormalization dictates to fix free parameters of the action

- In $N_f = 2 + 1$ flavor pure QCD, we need three parameters $\boldsymbol{g}^0 = (g_s^0, m_l, m_l, m_s, \alpha_{\text{EM}} = 0)$

- IsoQCD definition is ambigous, since nature is not only pure QCD

- Use scale setting quantities near physical hadron masses
- After isospin breaking corrections applied, all schemes agree
- But, size of isospin breaking corrections depend on the isoQCD scheme

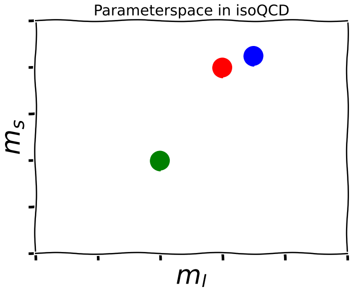


Fig. 5: Colored points: Different schemes for isoQCD

Isospin symmetric QCD

- Define renormalization scheme in isoQCD
- Use hadronic scales without experimental uncertainty
- Parameters for isoQCD in RBC/UKQCD18 scheme [Blum et al. arxiv:1801.07224]:

$$m_\pi = 135 \text{ MeV}, \qquad m_K = 495.7 \text{ MeV}, \qquad m_\Omega = 1.67225 \text{ GeV}$$

$$(m_{D_s} = 1.96847 \text{ GeV for } N_f = 2+1+1 \text{ ensembles})$$

- Another possibility (Definition of BMW20 scheme from [Blum et al.arxiv:2301.08696]):

$$m_\pi = 134.97 \text{ MeV}, \qquad m_{ss*} = 689.8 \text{ MeV}, \qquad \omega_0 = 0.17236 \text{ fm}$$

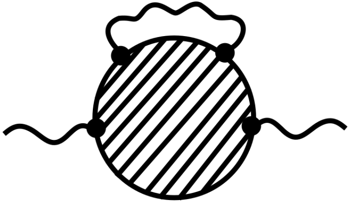
$$(m_{D_s} = 1.96847 \text{ GeV for } N_f = 2+1+1 \text{ ensembles})$$

RBC/UKQCD world

1. For RBC/UKQCD18 scheme: First compute $\frac{\partial m_\Omega}{\partial m_\pi}$, $\frac{\partial^2 m_\Omega}{\partial m_\pi^2}$ $\frac{\partial m_\Omega}{\partial m_K}$ from global analysis including systematic uncertainties [Blum et al.arxiv:2301.08696], [arxiv:2410.20590]
2. Then write m_Ω as function of m_π/m_Ω and m_K/m_Ω on each ensemble and extrapolate with information from first bullet point to the target values
3. The lattice spacing can be obtained from the global fit on each ensemble

- Repeat above procedure for w_0 using $m_\pi w_0$ $m_{ss*} w_0$ to obtain the lattice spacing in the BMW20 scheme

Isospin breaking effects



- Isospin is not a symmetry of nature
- At low energies nature is effectively QCD+QED
- Electromagnetic corrections $\to$ need to include photons
- Strong isospin breaking corrections: $m_u \neq m_d$
- Parameters for $N_f = 1+1+1$: $\boldsymbol{g} = (g_s, m_u, m_d, m_s, \alpha_{\mathrm{EM}})$
- RM123 [Divitiis et al. arxiv:1303.4896]: Expand around isospin symmetric theory $\boldsymbol{g}^0$ in

$$\frac{m_d - m_u}{\Lambda_{QCD}} \sim \alpha_{\mathrm{EM}} \sim O(\epsilon)$$

Hadronic renormalization scheme in QCD+QED

- With isospin breaking corrections, hadronic scheme is unambigous
- Use physical hadron mass shifts masses to set scale PDG 2024 [PhysRevD.110.030001]

$$\begin{aligned} m_{\pi^0} &= 134.9768(5)\ \text{MeV}, \\ m_{K^0} &= 497.611(13)\ \text{MeV}, \\ m_{K^0} - m_{K^+} &= 3.9340(2)\ \text{MeV}, \\ m_{\Omega} &= 1672.45(29)\ \text{MeV} \end{aligned}$$

- Electromagnetic coupling does not renormalize at leading order

$$(\alpha_{QED})^{-1} = 137.035999177(21)$$

- As crosscheck calculate pion mass splitting

$$m_{\pi^+} - m_{\pi^0} = 4.59359(5)\text{MeV}$$

QCD+QED: Electromagnetic corrections

- Electromagnetic corrections to expectation value of operator $O(z)$ as expansion in EM coupling $e = \sqrt{4\pi\alpha}$

$$
\begin{aligned}
\langle T\{O(z)\}\rangle_{QCD+QED} &= \{O(z)\}\rangle_{QCD} + e^2 \frac{\partial}{\partial e^2} \langle T\{O(z)\}\rangle_{QCD+QED}\Big|_{e^2=0} + O(e^4) \\
&= \langle T\{O(z)\}\rangle_{QCD} \\
&\quad - \frac{e^2}{2} \int_{x,y} G_{\nu\rho}(x,y) \langle T\{O(z) j^{em}_\nu(y) j^{em}_\rho(x)\}\rangle_{QCD} + O(e^4)
\end{aligned}
$$

- Photon propagator in Feynman gauge: $G_{\nu\rho}(x,y) = \delta_{\nu\rho} G(x,y)$

- Electromagnetic vector current $j^{em}_\mu = i\left(\frac{2}{3}\bar{u}\gamma_\mu u - \frac{1}{3}\bar{d}\gamma_\mu d - \frac{1}{3}\bar{s}\gamma_\mu s + \ldots\right)$

QCD+QED: Electromagnetic corrections

- Introduction of QED leads to new divergences→ lattice can be used as a regulator
- But, QCD+QED on the lattice has infrared problem due to massless photon
- Different proposed regularizations of QED: QED_m, QED_L, QED_r, QED_∞
- Affects choice of photon propagator $G(x, y)$
- For control over systematic uncertainty, we choose to use multiple QED versions

- QED_L: Spatial zero modes are removed [Hayakawa et al.arxiv:0804.2044]]

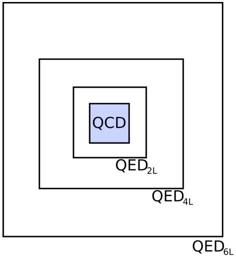
$$G(x, y) = \sum_{k \in (\frac{2\pi}{L}\mathbb{Z})^4} \frac{e^{ik(x-y)}}{(2\pi)^4} \frac{1}{k^2} (1 - \delta_{\boldsymbol{k},0})$$

QCD+QED: Electromagnetic corrections

- QED_r: Spatial zero modes are redistributed [Di Carlo et al.arxiv:2501.07936]

$$G(x,y) = \sum_{k=\frac{2\pi n}{L}, n\in\mathbb{Z}} \frac{e^{ik(x-y)}}{(2\pi)^4} \frac{(1+\delta_{|\boldsymbol{n}|,1}/6)}{k^2}(1-\delta_{\boldsymbol{k},0})$$

- QED_∞:
  - Use subsequent version of QED_L
  - E.g. QED_{2L},QED_{4L}, QED_{6L}, QED_{NL}
  - Ensures same UV-behaviour
  - Take the limit $N \to \infty$



QCD+QED: Strong isospin breaking corrections

- Strong isospin breaking corrections ($m_u \neq m_d$) are expressed via

$$\begin{aligned}\langle T\{O(z)\}\rangle_{m_f\neq\hat{m}} &= \langle T\{O(z)\}\rangle_{m_f=\hat{m}} \\ &+(m_f-\hat{m})\frac{\partial}{\partial m_f}\langle T\{O(z)\}\rangle\Big|_{m_f=\hat{m}} + O((m_f-\hat{m})^2)\end{aligned}$$

- The mass derivative is obtained by

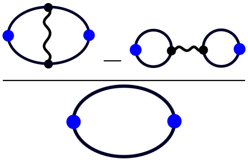
$$\frac{\partial}{\partial m_f}\langle T\{O(z)\}\rangle\Big|_{m_f=\hat{m}} = \langle T\{SO(z)\}\rangle_{m_f=\hat{m}}$$

using the insertion of a scalar current $S=\sum_x \overline{\psi}_f(x)\psi_f(x)$

QCD+QED: Pion mass splitting

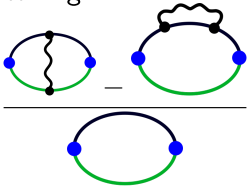
- Pion mass splitting is due to EM effects only
- Result is a direct prediction
  (older lattice QCD results: [Divitiis et al. arxiv:1303.4896] [Feng at el. arxiv:2108.05311])
- Check of QED implementation
- Only two diagrams with internal photon need to be calculated

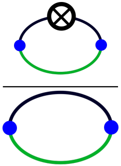
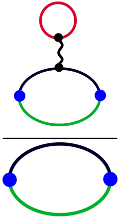
$$m_{\pi^+} - m_{\pi^0} = \frac{e^2}{2}(q_u - q_d)^2 \partial_t$$



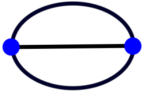
QCD+QED: Kaon mass splitting

- Kaon mass splitting (green line represents strange propagator)
- EM corrections and strong isospin breaking

$m_{K^+} - m_{K^0} = e^2(q_u^2 - q_d^2)\partial_t$ 

$-(m_d - m_u)\partial_t$  $+ e^2(q_u - q_d)\sum_f q_f \partial_t$ 

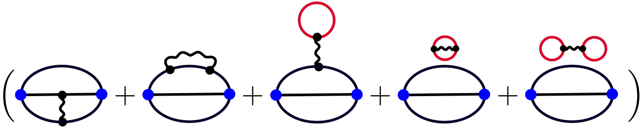
QCD+QED: Omega baryon

- Omega mass can be obtained from correlation function $\langle \Omega^{\alpha}_{\mu}(z)\Omega^{\alpha}_{\mu}(0)\rangle$ of the operator $\Omega^{\alpha}_{\mu} = \epsilon_{ijk}(s_i^T C\gamma_\mu s_j)s_k^{\alpha}$ [Blum et al. arxiv:1411.7017]
- At leading order: $C^{(0)}(t) =$ 
- Radiative corrections are small (previous electroquenched calculation by RBC/UKQCD in 2018 [Blum et al.arxiv:1801.07224])
- Only composed of strange quarks $\rightarrow$ no strong isospin breaking corrections at leading order
- Challenge: Multiple operators are needed for control of excited states, but in practice doable

QCD+QED: Omega baryon

- Omega mass can be obtained from correlation function $\langle \Omega^{\alpha}_{\mu}(z)\Omega^{\alpha}_{\mu}(0)\rangle$ of the operator $\Omega^{\alpha}_{\mu} = \epsilon_{ijk}(s_i^T C\gamma_\mu s_j)s_k^{\alpha}$ [Blum et al. arxiv:1411.7017]
- Ongoing project: compute isospin breaking corrections including seaquark effects

$C^{(1)} = e^2$



- Extract first order effective mass from $\partial_t \frac{C^{(1)}(t)}{C^{(0)}(t)}$

Computational strategy

Ok, but how do we actually implement the calculation?

Computational strategy: Wick contractions

For Wick contractions: Lattice operator toolkit (http://github.com/jparrino/lotk)

- Only python and Numpy necessary
- Lightweight easy to use symbolic manipulation of operators and contractions
- Operators are written in ASCII format
- Algebraic operations and simplifications
- Used for crosscheck
- Automatic generation of Wick contractions in LaTeX and graphically

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```
import lotk
[...]

o1=kaonMinusOperator("x")
o2=kaonPlusOperator("y")
o3=2*o1*o2-o2*o1

print(o3.simplify())


```

Listing: $O^{K^-}(x)O^{K^+}(y)$ operator

Computational strategy: Wick contractions

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```
FACTOR 1.0 0.0
UBAR x
GAMMA 5
S x
SBAR y
GAMMA 5
U y
```

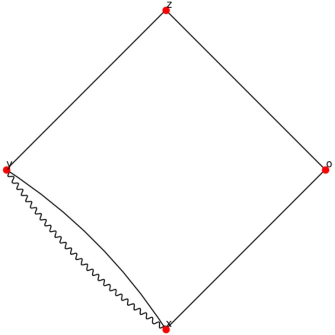
Listing: $O^{K^-}(x)O^{K^+}(y)$ operator

Computational strategy: Wick contractions

```python
import lotk
[...]
import lotk.diagrams.toLatex as tl
import lotk.diagrams.drawDiagrams as dd

fourptf = kaonNeutralOperator("z")
     *vectorCurrent(["U","D","S"],"y","NU")
     *vectorCurrent(["U","D","S"],"x","MU")
     *kaonBarNeutralOperator("o")
     *photonPropagator("x","y")

contraction = TraceContraction.contract(
    fourptf).simplify()
latex = tl.diagrams_to_latex(str(
    contraction[0]))
dd.generate_feynman_diagram(str(
    contraction[0]))

```

$\longrightarrow$

$$-\frac{8}{9}\mathrm{Tr}[S_S(z,o)\gamma^5 S_L(o,x)\gamma^\nu S_L(x,y)\gamma^\mu S_L(y,z)\gamma^5]G_0(x,y)$$



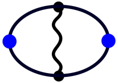
Computational strategy: Lattice QCD implementation

Lattice QCD implementation in gpt (http://github.com/lehner/gpt)

- We need to calculate correlators of type

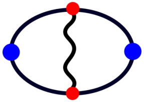
$$\int_{x,y} G_{\nu\rho}(x,y)\langle\pi^+(\boldsymbol{p},t)|T\{j_\nu^{em}(y)j_\rho^{em}(x)\}|\pi^-(\boldsymbol{p},0)\rangle_{QCD}$$

$$\supset \int_{x,y} G_{\nu\rho}(x,y)\left\langle \mathrm{Tr}\left[\gamma_5 S(0,x)\gamma_\rho S(x,(\mathbf{0},t))\gamma_5 S((\mathbf{0},t),y)\gamma_\nu S(y,0)\right]\right\rangle_U =$$



- Challenge: Double integral over x, y is effectively $V \times V$ sum
- Calculating all-to-all propagators is not feasible
- RBC/UKQCD approach: Evaluate x and y integrals stochastically

Computational strategy: Stochastic sampling



- Propagators are calculated on stochastic subset of point (Introduced in calculation of hadronic light-by-light contribution [Blum et al. arxiv:1510.07100])
- Propagator from N source points to M sink points are saved on disc
- No extra inversion needed to calculate diagram
- Can be contracted with different versions of the photon propagator

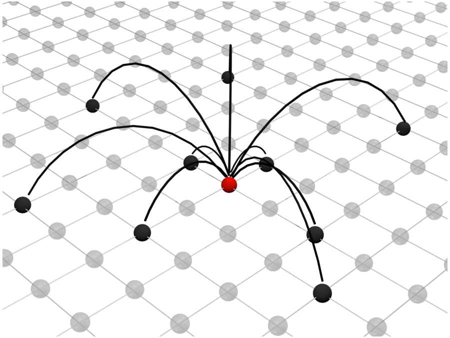
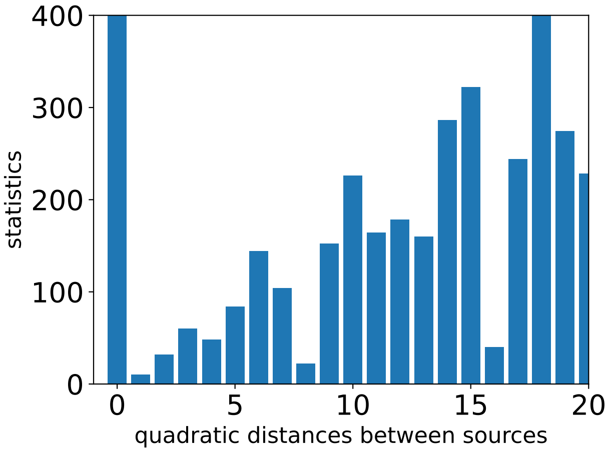


Fig. 6: Propagator for (red) source point to several (black) sink points

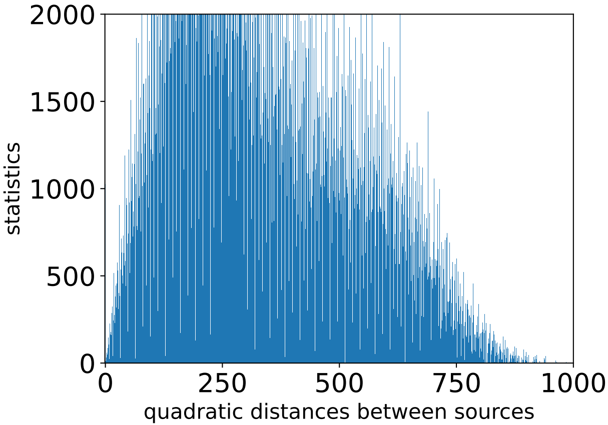
Computational strategy: Stochastic sampling

- Histogram of point source separations on $24^3 \times 48$ ensemble
- Zero-distance is sampled with high statistics
- $O(10^3)$ source positions
- $O(10^6)$ sink positions
- Number of points to sample from can be chosen on the fly



Computational strategy: Stochastic sampling

- Histogram of point source separations on $24^3 \times 48$ ensemble
- Short-distance regime with more statistics
- $O(10^3)$ source positions
- $O(10^6)$ sink positions
- Number of points to sample from can be chosen on the fly



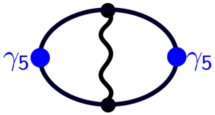
Computational strategy: Reference implementation

Crosscheck for implementation

- Do calculation on $4^3 \times 8$ box
- Compute exact all-to-all propagators
- One gauge configuration
- Full statistics < 4GB $\rightarrow$ can be run on laptop
- Simple implementation of all diagrams using Numpy code
- Check for all operator insertions and photon implementations
- Crosscheck implementation of stochastic sampling for all diagrams

Computational strategy: Reference implementation

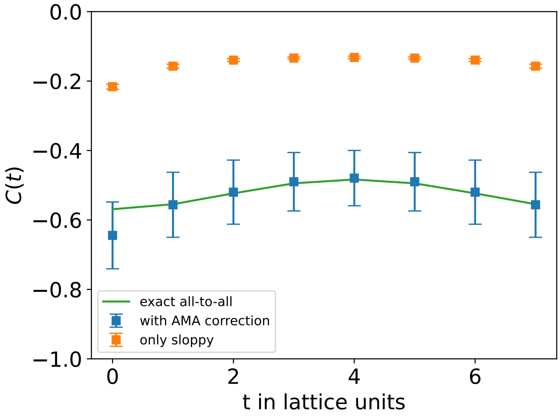
- Crosscheck diagram V for QED_L



- Between reference implementation and lattice QCD code using gpt

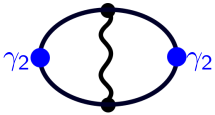
[http://github.com/lehner/gpt]

- Intentionally large AMA correction to check for correctness
- Statistical error from point-sources sampling



Computational strategy: Reference implementation

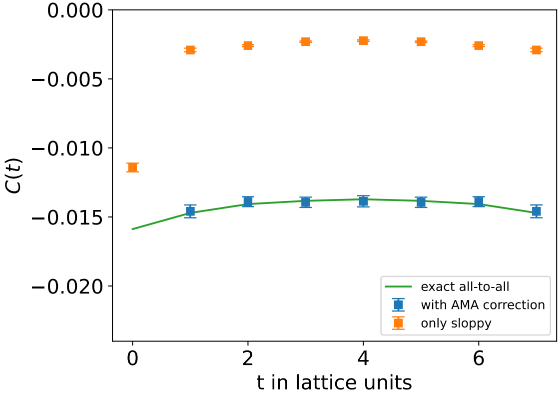
- Crosscheck diagram V for QED_{2L}



- Between reference implementation and lattice QCD code using gpt

  [http://github.com/lehner/gpt]

- Intentionally large AMA correction to check for correctness
- Statistical error from point-sources sampling



Computational strategy: Reference implementation

- Reference implementation of all diagrams for meson masses and EM corrections to HVP already carried out
- For different photons : QED_L, QED_∞ and QED_r and all necessary combinations of external operators

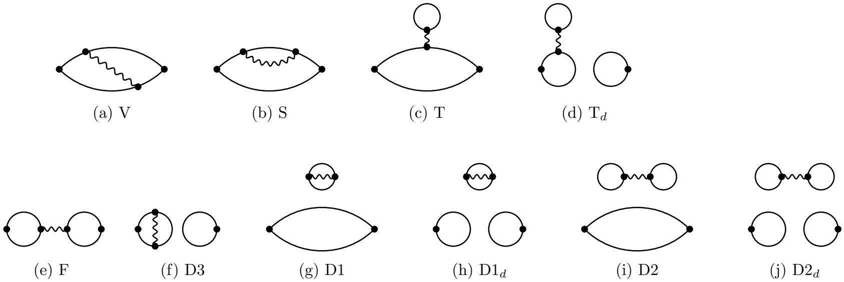


Fig. 7: EM corrections to the HVP contribution [Blum et al.arxiv:2301.08696]

First results: Pion mass splitting

- Pion mass splitting on $24^3 \times 48$ ensemble at $m_\pi = 275$ MeV
- With finite-size correction for $m_\pi L = 3.8$ for QED_L [Borsanyi et al.arxiv:1406.4088] and QED_r [Di Carlo et al.arxiv:2501.07936]
- Diagram F is neglected at the moment, contribution is very small [Feng et al.arxiv:2108.05311]
- So far, still low statistics

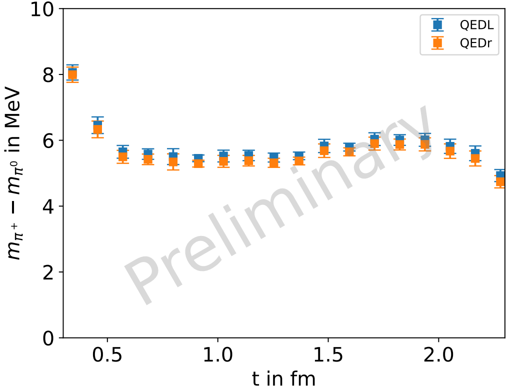
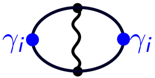


Fig. 8: Pion mass splitting at $m_\pi = 275$ MeV

First results: HVP integrand

- HVP integrand for diagram V on $24^3 \times 48$ ensemble at $m_\pi = 275$ MeV

$$\tilde{f}(t, m_\mu)\ \frac{1}{3}\sum_{i=1}^{3}$$



- With blinded HVP kernel $\tilde{f}(t, m_\mu)$
- Good signal to noise ratio
- Proof of concept for stochastic sampling method

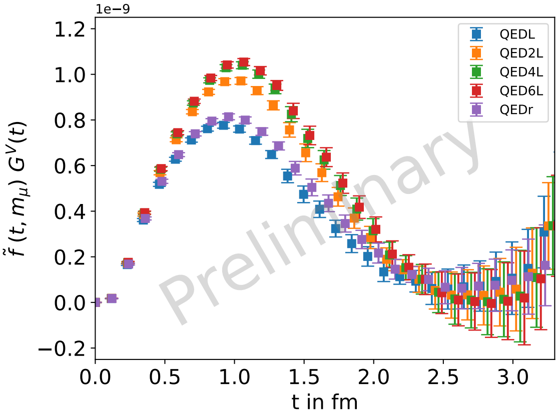


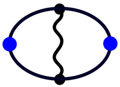
Fig. 9: Integrand for the EM contribution to the HVP (diagram V)

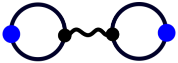
Outlook

- Optimize and test lattice QCD code for all Wick contractions
- Calculate Δm_K and m_Ω
- Increase statistics
- Extrapolation to physical point defined by the $m_\pi, m_K, \Delta m_K, m_\Omega$
- Determination of lattice spacing for RBC/UKQCD ensembles
- Use correlators for HVP project (apply blinding procedure)

Backup

Computational strategy





- EM corrections to meson masses similar to EM corrections to HVP

$$\int_{x,y} \delta_{\nu\rho} G_0(y,x) \langle T\{O^{(1)}(z) j_\nu^{em}(y) j_\rho^{em}(x) O^{(2)}(0)\}\rangle_{QCD}$$

- Versatile code implementation to allow for different operator insertions

$$O(z) = \{j_\mu^{em}(z), O^\pi(z), O^K(z)\}$$

- Different operator insertions generated with the same code
- Optimized implementation for different Wick contractions

Finite volume correction

- Leading finite volume correction for charged pion mass in QED_L and QED_r ([Borsanyi et al.arxiv:1406.4088], [Di Carlo et al.arxiv:2501.07936])

$$\Delta m_\pi^2(L) = e^2 m_\pi^2 \Big[\frac{c_2}{4\pi^2 m_\pi L} + \frac{c_1}{2\pi (m_\pi L)^2} - \frac{c_0}{(m_\pi L)^3} \Big(\frac{\langle r_\pi^2 \rangle m_\pi^2}{3} + C \Big) + O\big(\frac{1}{(m_\pi L)^4}\big) \Big]$$

- With real coefficients c_0, c_1, c_2 from [Di Carlo et al.arxiv:2501.07936]

- For QED_r: $c_0 = 0$