Bringing near-physical QCD+QED calculations beyond the electro-quenched approximation

Ryan Hill

RBC-UKQCD

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Lattice 2024

THE UNIVERSITY of EDINBURGH

The RBC & UKQCD collaborations

Boston University
Nobuyuki Matsumoto

BNL and BNL/RBRC
Peter Boyle
Taku Izubuchi
Christopher Kelly
Shigemi Ohta (KEK)
Amarji Soni
Masaaki Tomii
Xin-Yu Tuo
Shuhei Yamamoto

University of Cambridge
Nelson Lachini

CERN
Matteo Di Carlo
Felix Erben
Andreas Jüttner (Southampton)
Tobias Tsang

Columbia University
Norman Christ
Sarah Fields
Ceran Hu
Yikai Huo
Joseph Karpie (JLab)
Erik Lundstrum
Bob Mawhinney
Bigeng Wang (Kentucky)

University of Connecticut
Tom Blum
Jonas Hildebrand
Luchang Jin
Vaishakhi Moningi
Anton Shcherbakov
Douglas Stewart
Joshua Swaim

DESY Zeuthen
Raoul Hodgson

Edinburgh University
Luigi Del Debbio
Vera Gülpers
Maxwell T. Hansen
Nils Hermansson-Truedsson
Ryan Hill
Antonin Portelli
Azusa Yamaguchi

Johannes Gutenberg University of Mainz
Alessandro Barone

Liverpool Hope/Uni. of Liverpool
Nicolas Garron

LLNL
Aaron Meyer

Autonomous University of Madrid
Nikolai Husung

University of Milano Bicocca
Mattia Bruno

Nara Women's University
Hiroshi Ohki

Peking University
Xu Feng
Tian Lin

University of Regensburg
Andreas Hackl
Daniel Knüttel
Christoph Lehner
Sebastian Spiegel

RIKEN CCS
Yasumichi Aoki

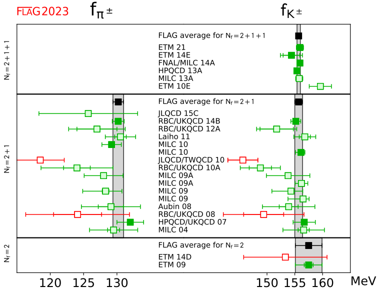
University of Siegen
Matthew Black
Anastasia Boushmelev
Oliver Witzel

University of Southampton
Bipasha Chakraborty
Ahmed Elgaziari
Jonathan Flynn
Joe McKeon
Rajnandini Mukherjee
Callum Radley-Scott
Chris Sachrajda

Stony Brook University
Fangcheng He
Sergey Syritsyn (RBRC)

Motivation

- FLAG[1] reports averages for observables calculable from $K \to \ell\overline{\nu}$, $\pi \to \ell\overline{\nu}$ at a sub-percent level.
  - $N_f = 2+1$ $\quad f_{\pi^\pm} = 130.2(0.8)$ MeV (0.61%)
  - $N_f = 2+1+1$ $\quad f_{K^\pm} = 155.7(0.3)$ MeV (0.19%)
  - $N_f = 2+1$ $\quad f_{K^\pm} = 155.7(0.7)$ MeV (0.45%)
- These inform $|V_{us}|/|V_{ud}|$.



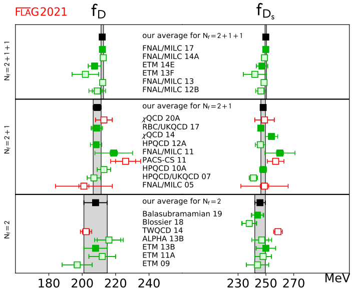
- Lattice results based on partial evaluation of first-order isospin-breaking corrections (or χPT).
- $< 1\%$ errors without a full *ab-initio* correction?

Plot from FLAG Review 2021 (February 2024 Revision). Full citation list at end of talk.

[1] FLAG Review 2021 (February 2024 Revision), http://flag.unibe.ch/2021/

Motivation

- Similar situation for $D \to \ell\overline{\nu}$, $D_s \to \ell\overline{\nu}$.
  - $N_f = 2+1+1$ $f_D = 212.0(0.7)$ MeV (0.33%)
  - $N_f = 2+1$ $f_D = 209.0(2.4)$ MeV (1.15%)
  - $N_f = 2+1+1$ $f_{D_s} = 249.9(0.5)$ MeV (0.2%)
  - $N_f = 2+1$ $f_{D_s} = 248.0(1.6)$ MeV (0.65%)



- Important to include a complete *ab-initio* calculation of first-order isospin-breaking corrections.

Plot from FLAG Review 2021 (February 2024 Revision). Full citation list at end of talk.

Previous Work

Several published results addressing disconnected QED IB:

- *Electromagnetic Splittings and Light Quark Masses in Lattice QCD*
  Duncan *et al.* 1996 Phys. Rev. Lett. 76, 3894
- *Computing electromagnetic effects in fully unquenched QCD*
  Duncan *et al.* 2005 Phys. Rev. D 71, 094509
- *Full QED+QCD Low-Energy Constants through Reweighting*
  Ishikawa *et al.* 2012 Phys. Rev. Lett. 109, 072002
- *1+1+1 flavor QCD+QED simulation at the physical point*
  Aoki *et al.* 2012 Phys. Rev. D 86, 034507
- *Isospin splittings of meson and baryon masses from three-flavor lattice QCD + QED*
  Horsley *et al.* 2016 J. Phys. G: Nucl. Part. Phys. 43 10LT02

Previous Work

Quark-disconnected $O(\alpha)$ diagrams have also been calculated for $g_\mu - 2$ HVP:

- *Leading hadronic contribution to the muon magnetic moment from lattice QCD*
  Borsanyi *et al.* 2021 Nature 593, 51–55
- *High precision calculation of the hadronic vacuum polarisation contribution to the muon anomaly*
  Boccaletti *et al.* 2024 [arXiv:2407.10913]

Lattice Strategy: RM123 method

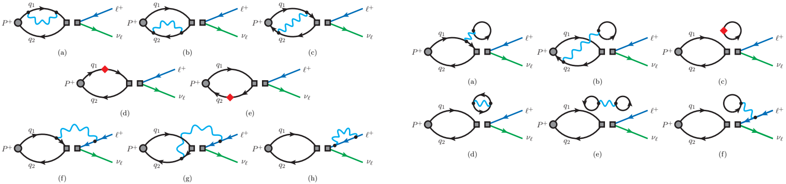
- Working at $\mathcal{O}(\alpha)$: $m_u = m_d$.
- Introduce IB effects using the RM123 method[1] [2]:
  - IB corrections *via* perturbative expansion in $\alpha = \frac{e^2}{4\pi}$, m.

$$\langle O \rangle = \langle O \rangle \Big|_{e=0} + \underbrace{\frac{1}{2}\left(e^{\phi}\right)^2 \left[\frac{\partial}{\partial e}\frac{\partial}{\partial e}\langle O \rangle\right]_{e=0}}_{\text{QED IB}} + \underbrace{\left(m^{\phi} - m^{(0)}\right)\left[\frac{\partial}{\partial m}\langle O \rangle\right]_{e=0}}_{\text{Strong IB}} + \ldots \quad (1)$$

  - IB corrections take the form of additional diagrams evaluated in the isospin-symmetric limit.
  - m^{ϕ} = physical mass, $m^{(0)}$ = simulation-point mass.

[1] de Divitiis *et al.* JHEP 04 (2012) 124 [arXiv:1110.6294]
[2] de Divitiis *et al.* PRD 87 (2013) 114505 [arXiv:1303.4896]

Lattice Strategy: Isospin-Breaking Corrections to $P \to \ell\overline{\nu}$



Diagrams from Boyle *et al.* JHEP 02 (2023) 242. Red diamonds: scalar insertions.

- Quark-connected contributions (left) to the isospin-breaking correction have been calculated for $P \to \ell\overline{\nu}$ in lattice QCD[1] [2].
- Quark-disconnected contributions (right) omitted.
- Referred to as the "electro-quenched" approximation.
- Uncontrolled systematic.

[1] Di Carlo *et al.* PRD 100 (2019) 034514 [arXiv:1904.08731]

[2] Boyle *et al.* JHEP 02 (2023) 242 [arXiv:2211.12865]

Lattice Strategy: Propagator Loops in Lattice QCD

- Quark-disconnected diagrams are difficult to estimate—loops given by factors like $D^{-1}(x,x)$.
- This requires one propagator solve per lattice site.
  $\rightarrow$ Computationally infeasible.
- Instead stochastically estimate Dirac operator inverse using noise vectors η obeying

$$\left\langle \eta(y)\eta^\dagger(x) \right\rangle_\eta = \delta_{xy}, |\eta(x)|^2 = 1, \langle \eta(x) \rangle_\eta = 0, \qquad (2)$$

where $\langle \cdot \rangle_\eta$ is an average over η. This gives

$$D^{-1}(x,x) = \sum_y D^{-1}(x,y)\delta_{xy} \qquad (3)$$

$$\approx \frac{1}{N_\eta} \sum_\eta \left(\sum_y D^{-1}(x,y)\eta(y) \right) \eta^\dagger(x). \qquad (4)$$

Lattice Strategy: EM Currents in the Isospin Limit

- $\mathcal{O}(\alpha)$ correlation function for operator O:

$$\sum_x \sum_y \langle J_\mu(x) A_\mu(x) J_\nu(y) A_\nu(y) O \rangle \qquad (5)$$

- EM current insertions: $J_\mu(x) = \sum_f Q_f \overline{\psi}_f(x) \gamma_\mu \psi_f(x)$.
  - $2+1f$: Consider sum over quark flavours $f \in \{u, d, s\}$.
  - Q_f: EM charge (*i.e.* $Q_u = 2/3$, $Q_d = -1/3$, $Q_s = -1/3$).
- u and d terms sum in single-propagator loops.
  - Light and strange quarks equally-weighted; relative minus sign.
  - $\Rightarrow J_\mu(x) = 1/3 \left(\overline{\psi}_l(x) \gamma_\mu \psi_l(x) - \overline{\psi}_s(x) \gamma_\mu \psi_s(x) \right) A_\mu$.
  - This leads to differences of single-propagator traces in several disconnected diagrams.

Lattice Strategy: Split-Even Estimator

Giusti *et al.*[1] have demonstrated a successful variance-reduction strategy for differences of single-propagator loops:
"split-even" estimators.

For *e.g.* Wilson, DWF Dirac Operators differing only by mass,

$$D_1^{-1} - D_2^{-1} = D_1^{-1}\left(D_2 - D_1\right) D_2^{-1}, \quad (6)$$
$$= (m_2 - m_1) D_1^{-1} D_2^{-1}. \quad (7)$$

Choice in how to stochastically estimate propagator traces:

"Standard" $$(m_2 - m_1)\mathrm{Tr}\left\{\gamma^\mu \left\{D_1^{-1} D_2^{-1} \eta\right\}(x)\eta^\dagger(x)\right\}, \quad (8)$$

"Split-Even" $$(m_2 - m_1)\mathrm{Tr}\left\{\gamma^\mu \left\{D_1^{-1} \eta\right\}(x)\{\eta^\dagger D_2^{-1}\}(x)\right\}, \quad (9)$$

→ *c.f.* Raoul Hodgson 11:35 2nd August – Use in rare K decays

[1] Giusti *et al.* EPJC 79, 586 (2019) [arXiv:1903.10447]

Lattice Strategy: Ensemble Parameters

Current run performed on the RBC-UKQCD 'C0' ensemble.

- $2+1$ flavour, $L^3 \times T = 48^3 \times 96$, $a^{-1} = 1.73$ GeV.
- Physical-scale light-, strange-quark masses.
- zMöbius Domain-Wall action.
  $\rightarrow$ Cheaper than Möbius DWF; requires bias correction step.
  $\rightarrow$ Accumulate statistics on cheaper zMöbius estimator.
- Light quarks deflated with 2000 low modes.
- Following techniques developed on non-physical mass 'C1' ensemble for quark-disconnected diagrams (Harris *et al.*[1])

Runs also planned on the 'M0' ensemble.

- 2+1 flavour, $L^3 \times T = 64^3 \times 128$, $a^{-1} = 2.36$ GeV.
- Same physical volume as C0.
- Also at physical-scale light-, strange-quark masses.

[1] Harris *et al.* PoS LATTICE2022 (2023) 013 [arXiv:2301.03995]

Lattice Strategy: Photon Action

- Finite volume + periodic boundary conditions:
  $\rightarrow$ Charged states forbidden by Gauss' Law.
- Need to choose a QED prescription.
  - QED_L: Remove spatial zero-mode[1].
    $\rightarrow$ Can express as a special case of $\mathrm{QED}_L^{\mathrm{IR}}$ [2]
    $\rightarrow$ Large finite-volume effects at $\mathcal{O}(1/L^3)$ for $K \rightarrow \ell\overline{\nu}$?[3]
  - QED_r: Redistribute zero-mode to neighbouring modes[4] [5].
    $\rightarrow$ Investigated to remove $\mathcal{O}(1/L^3)$ finite-volume effects
    $\rightarrow$ Also a particular case of $\mathrm{QED}_L^{\mathrm{IR}}$
    $\rightarrow$ Used for this project.

[1] Hayakawa and Uno, PTP 120 (2008) 413 [arXiv:0804.2044]

[2] Davoudi *et al.* PRD 99 (2019) 034510 [arXiv:1810.05923]

[3] Boyle *et al.* JHEP02(2023)242 arXiv: [2211.12865]

[4] Di Carlo, PoS LATTICE2023 (2024) 120 [arXiv:2401.07666]

[5] Hermansson-Truedsson *et al.*, PoS LATTICE2023 (2024) 265 [arXiv:2310.13358]

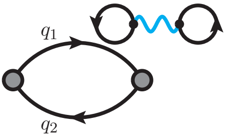
Lattice Strategy: Software

- Calculation performed with **Grid**[1], and the Grid-based workflow management software **Hadrons**[2].
- Split-even and quark-disconnected diagram contractions implemented as Hadrons modules (code review TBC).
- Thanks to Antonin Portelli, Raoul Hodgson, and Tim Harris for assisting with code development.

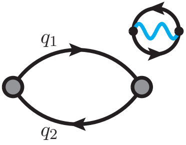
[1] https://github.com/paboyle/Grid

[2] https://github.com/aportelli/Hadrons

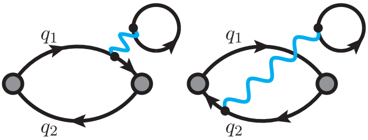
$\mathcal{O}(\alpha)$ Quark-Disconnected Diagrams for $P \to P$



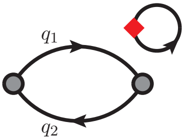
‘Specs’ diagram



‘Burger’ diagram



Tadpole diagram

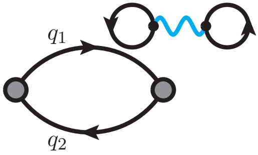


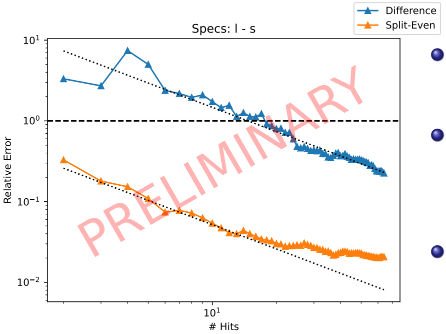
Sea-loop diagram

[Schematics courtesy of Matteo Di Carlo.]

Specs error analysis

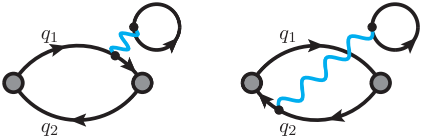
- Specs subdiagram contains two $l - s$ loops.
- Can be computed as a difference of propagators or with the split-even estimator.

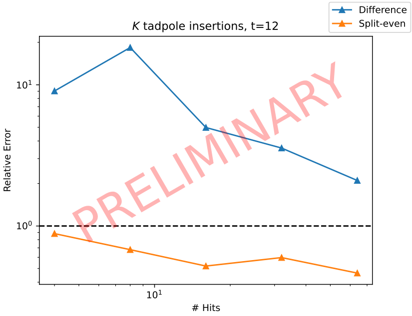




- Left: error scaling of specs **subdiagram**.
- Significant reduction in error with the split-even estimator.
- Reaching the gauge noise with ∼32 Z2 noise hits.

Tadpole error analysis

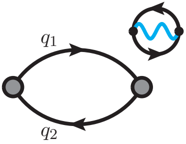




- Tadpole diagrams also feature an $l - s$ loop.
- **Left:** Relative error of the kaon tadpole diagrams.
- Once again, the split-even estimator significantly reduces the error.

Burger error analysis

- 'Burger' diagram $\rightarrow$ same flavour in both propagators.
- $e_q^2 \rightarrow$ no relative cancellation between diagrams.

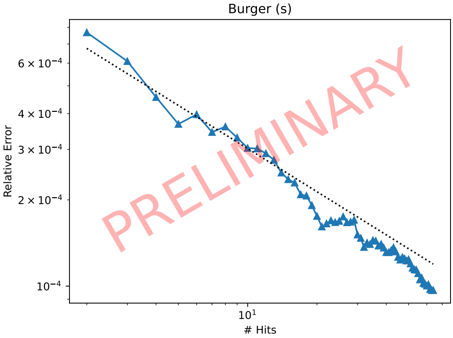


- 'Burger' diagram falls off exponentially with propagator separation $\Rightarrow$ short-distance dominated.
- Prior study on non-physical mass 'C1' ensemble (Harris *et al.*[1]): concentrate computational effort on short-distance behaviour.
  - Volume-averaged stochastic estimation of all-to-all propagators within a radius $|x - y| < R$.
  - Random point sources for $|x - y| >= R$.

[1] Harris *et al.* PoS LATTICE2022 (2023) 013 [arXiv:2301.03995]

Burger error analysis

- **Right:** Error scaling of the strange burger **subdiagram** (R=4).
- Volume-averaging strategy provides an efficient method for obtaining a small error.
- Not yet at gauge noise with 64 hits.



Summary

- Quark-disconnected QED IB corrections are challenging, but important to quantify.
- Diagrams at $\mathcal{O}(\alpha)$ have exploitable characteristics:
  - Precision of 'Specs' and Tadpole diagrams can be greatly improved with the split-even estimator.
  - 'Burger' diagram is short-distance dominated.
- Findings at non-physical masses reproduced on a physical-point ensemble.
- Building towards a physical-point electro-unquenched calculation of $P \to \ell\nu$.

Backup

FLAG $f_{\pi^\pm}$, $f_{K^\pm}$ Citation List

Dowdall *et al.* PRD 88 (2013) 074504
Carrasco *et al.* PRD 91 (2015) 054507
Bazavov *et al.* PRD 98 (2018) 074512
Miller *et al.* PRD 102 (2020) 034507
Alexandrou *et al.* PRD 104 (2021) 074520
Follana *et al.* PRL 100 (2008) 062002
Bazavov *et al.* PoS LATTICE2010 (2010) 074
Durr *et al.* PRD 81 (2010) 054507
Blum *et al.* PRD 93 (2016) 074505
Durr *et al.* PRD 95 (2017) 054513
Bornyakov *et al.* PLB 767 (2017) 366–373
Blossier *et al.* JHEP 07 (2009) 043

FLAG f_D, f_{D_s} Citation List

Balasubramamian, Blossier EPJC 80 (2020) 5, 412

Carrasco *et al.* JHEP 03 (2014) 016

Davies *et al.* PRD 82 (2010) 114504

Bazavov *et al.* PRD 85 (2012) 114506

Boyle *et al.* JHEP 12 (2017) 008

Yang *et al.* PRD 92 (2015) 034517

Na *et al.* PRD 86 (2012) 054510

Bazavov *et al.* PRD 98 (2018) 074512

Carrasco *et al.* PRD (2015) 054507