

U.S. DEPARTMENT OF

Update on the lattice calculation of $K \rightarrow \pi \pi$ decays with G-parity boundary conditions on a second lattice spacing

Christopher Kelly Lattice 2024, University of Liverpool, UK 08/01/24



<u>Boston University</u> Nobuyuki Matsumoto

BNL and BNL/RBRC

Peter Boyle Taku Izubuchi Christopher Kelly Shigemi Ohta (KEK) Amarjit Soni Masaaki Tomii Xin-Yu Tuo Shuhei Yamamoto

University of Cambridge

Nelson Lachini

<u>CERN</u>

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

The RBC & UKQCD collaborations

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

<u>LLNL</u> Aaron Meyer

<u>Autonomous University of Madrid</u> Nikolai Husung

<u>University of Milano Bicocca</u> Mattia Bruno

<u>Nara Women's University</u> 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

- The RBC & UKQCD collaborations have a long-running series of lattice QCD calculations of **Direct CPviolation in** $K \rightarrow \pi\pi$ **decays**.
- Comparing theory to experiment allows us to probe for new physics.
- Such new sources of CPV are needed to explain the dominance of matter over antimatter in the Universe.
- CERN/FNAL (1990s) experimental result available with ~15% error.
- <u>Reliable, 1st principles calculation only</u> <u>possible in lattice QCD due to NP final-</u> <u>state interactions.</u>







Strategy



- A₂ relatively straightforward with conventional methods, high precision (3% stat., 12% sys.)
- <u>A₀ much more challenging due to disconnected diagrams +</u> <u>nearby excited states.</u>



The Ground-state Conundrum

- $\pi\pi$ ground-state energy (~270 MeV) \ll kaon mass (~500 MeV)
 - Ground-state matrix element is unphysical!
- For A₂ solve using antiperiodic BCs on downquark in $n \le 3$ spatial dirs.:

$$E_{\pi^{\pm}\,gnd}^{2} \stackrel{\bullet}{=} m_{\pi}^{2} + n(\pi/L)^{2}$$

- Tune $\pi\pi$ energy via n, L
- Only works for charged pions, breaks isospin (workaround only for I=2)
- For A₀ we might use periodic BCs and extract physical matrix elem as excited state.
 - Challenging due to large statistical errors *



• Or...

G-parity Boundary Conditions

- Under the GPBC charged and neutral pions pick up a sign at the boundary.
 - Isospin is preserved.
- But we cannot directly control the BCs of composite particles, only those of their constituent quarks.
- G-parity on quarks is more complicated!
- GPBC calculation much more expensive
 - Requires explicit 2-flavor Dirac op (x2 cost)
 - Requires custom ensembles (x? cost)
 - Ensembles more expensive to generate as $det(M^{\dagger}M)$ is 4-flavor: need sqrt for light quarks (4th root for strange) (x4 cost)

$$\Rightarrow \hat{G}\pi^{\pm,0}\hat{G}^{-1} = -\pi^{\pm,0}$$

$$E_{\pi^{\pm,0}\,gnd}^2 = m_{\pi}^2 + n(\pi/L)^2$$





spin matrix



The Past and the Present

[Phys.Rev.Lett. 115 (2015) 21, 212001]

- RBC & UKQCD performed first complete calculation of ϵ' in 2015.
- Improved result in 2020:
 - +3.5x statistics
 - multiple $\pi\pi$ operators to better control excited state systematics.
- Result: $\begin{array}{c|c} \text{direct CPV} & \text{stat} & \text{sys} & [Phys.Rev.D \, 102 \, (2020) \, 5, \, 054509] \\ \hline \text{Re}(\epsilon'/\epsilon) &= 21.7(2.6)(8.0) \times 10^{-4} & [\text{Lattice}] \\ \hline \text{indirect CPV} & 16.6(2.3) \times 10^{-4} & [\text{Experiment}] \end{array}$
- Agrees with experiment but with ~4x the total error.
- Systematics dominated: Wilson coeffs. (~12%), E&M (~23%), <u>A₀</u> discretization (~12%)



unclear how reliable this estimate is!

The Edge (boundary) of Tomorrow?

- We are focusing on repeating calculation with finer lattices.
- Advent of multi-operator/variational techniques has opened the possibility of *reliably extracting the physical decay as an excited state with periodic BCs*.
 - Can reuse existing ensembles and eigenvectors where appropriate.
 - Measurements and ensemble generation much cheaper.
 - Possibility of including E&M effects in future (not so with GPBC?)
- RBC & UKQCD pilot calculation (led by M.Tomii) on coarse (1 GeV) lattice with ~1/3 of statistics of 2020 calc demonstrated method is effective: $\operatorname{Re}(\epsilon'/\epsilon) = 29.4(5.2)(12.2) \times 10^{-4}$

 $\operatorname{Re}(\epsilon'/\epsilon) = 21.7(2.6)(8.0) \times 10^{-4}$



[Phys.Rev.D 108 (2023) 9, 094517] -4 [periodic, a⁻¹=1.0 GeV] [G-parity , a⁻¹=1.4 GeV]

- Repeated calculation on finer lattice currently underway
 - For preliminary results including continuum limit, cf. M. Tomii talk 02/08 12:35pm (tomorrow)
- Should we then abandon G-parity?



X Reasons To Continue

- Under SciDAC-5 I have developed a series of "X-conjugate" algorithms exploiting a subtle symmetry of the GPBC Dirac Op.
 Av cost reduction in second.
 - 4x cost reduction in ensemble generation
 - 2x cost & memory reduction for eigenvectors
 - 2x cost reduction for inversions (for select sources)
- Ensemble gen. now as cheap as periodic BCs.
- Measurement cost substantially reduced.



- GPBC has different finite-volume systematics including reduced round-the-world pion propagation and differing $\pi\pi$ energy spectra.
- GPBC physical signal is dominant whereas periodic requires projecting out subdominant contribution.
- At this stage, a comprehensive cost-benefit analysis has not been performed of the two approaches.
- Our two analyses are somewhat independent (teams, lattices, techniques) which is beneficial given the lack of external competition for the calculation.
- Also: "general purpose" periodic lattices are trending towards larger physical volumes where the physical decay will be a higher excited state, much harder to extract.
 - Periodic will likely also need custom ensembles in the future!



(or lots of operators and large statistics!)



40ID GPBC ensemble

- $40^3 \times 64$ DWF+Iwasaki-DSDR ensemble
 - $a^{-1} = 1.73$ GeV vs 1.38 GeV previous
 - Same physical volume, physical masses
- Evolving on Perlmutter GPU





- Switched to X-conjugate action and retuned evolution:
 - Original: 4.36hrs (32 nodes) 139.5 node-hrs
 - New : 1.12hrs (32 nodes) 35.8 node-hrs
 : 1.61hrs (16 nodes) 25.76 node-hrs

5.4x (or 3.9x) reduction in cost, 2.7x (or 3.9x) speedup

Ensemble status



- Excluding thermalization, ~9700 trajectories.
- $\tau_{int} \sim 5 \text{ MDTU} => 10 \text{ traj between independent.}$
- Sampling every 20th trajectory (conservative) this is <u>enough for 485 measurements</u>.
- Very close to target ensemble size! (750 meas.)





Measurements

- K → ππ measurements performed on Polaris under ALCC allocation.
 ~6.2 hrs on 80 nodes Polaris (492 node-hours)
- Use all the latest performance tricks:
 - All-to-all propagators (disconn. diags.)
 - 2000 single-prec evecs w Block Lanczos
 - Deflated, split-Grid mixed-prec CG
 - Fourier-accelerated gauge fixing
 - 3 operators to control excited states
- Timing includes 2x reduction in Lanczos / inversion times due to X-conjugate algorithms.
- <u>To-date 81 complete measurements</u> (sep 40MDTU)





Results I



Results II

.





14

Conclusions

- Excellent progress towards repeating the GPBC calculation on a finer lattice.
 - Ensemble generation nearly complete
 - Measurements tuned and under production running. ~10% towards ultimate target.
- New algorithms have reduced cost to be comparable to periodic calc*
- Todo:
 - Lots more statistics!
 - NPR required; either custom periodic lattice or RI-SMOM with GPBC
 - Requires theory development



