Exploiting hidden symmetries to accelerate the lattice calculation of $K \to \pi\pi$ decays with G-parity boundary condititons

Christopher Kelly

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The RBC & UKQCD collaborations

University of Bern & Lund
Dan Hoying

BNL and BNL/RBRC
Peter Boyle (Edinburgh)
Taku Izubuchi
Yong-Chull Jang
Chulwoo Jung
Christopher Kelly
Meifeng Lin
Nobuyuki Matsumoto
Shigemi Ohta (KEK)
Amarjit Soni
Raza Sufian
Tianle Wang

CERN
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
Luchang Jin (RBRC)
Douglas Stewart
Joshua Swaim
Masaaki Tomii

Edinburgh University
Matteo Di Carlo
Luigi Del Debbio
Felix Erben
Vera Gülpers
Maxwell T. Hansen
Tim Harris
Ryan Hill
Raoul Hodgson
Nelson Lachini
Zi Yan Li
Michael Marshall
Fionn Ó hÓgáin
Antonin Portelli
James Richings
Azusa Yamaguchi
Andrew Z.N. Yong

Liverpool Hope/Uni. of Liverpool
Nicolas Garron

LLNL
Aaron Meyer

University of Milano Bicocca
Mattia Bruno

Nara Women's University
Hiroshi Ohki

Peking University
Xu Feng

University of Regensburg
Davide Giusti
Andreas Hackl
Daniel Knüttel
Christoph Lehner
Sebastian Spiegel

RIKEN CCS
Yasumichi Aoki

University of Siegen
Matthew Black
Anastasia Boushmelev
Oliver Witzel

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

Stony Brook University
Fangcheng He
Sergey Syritsyn (RBRC)

Motivation and approach

- Direct CPV in $K \to \pi\pi$ decay a sensitive probe for such physics.
  - May help explain matter dominance in Universe.
- Experimental result with ~10% error available (CERN/FNAL, 1990s)
- Standard Model calculation only recently possible due to large non-perturbative contributions: Lattice QCD!
- Lattice calculation via 3-flavor weak effective theory:

Measure of direct CPV (*not including EM, isospin breaking)

$$\epsilon' \propto \frac{\mathrm{Re}(A_2)}{\mathrm{Re}(A_0)} \left(\frac{\mathrm{Im}(A_2)}{\mathrm{Re}(A_2)} - \frac{\mathrm{Im}(A_0)}{\mathrm{Re}(A_0)} \right)$$

Effective 4-quark operators

$$A_I = \underbrace{\langle (\pi\pi)_I | H_W | K^0 \rangle}_{}$$

lattice

isospin

$$H_W \propto \sum_{i=1}^{10} c_i(\mu) Q_i(\mu)$$

Perturbative 3f Wilson coeffs (high energy physics)

NB: Renormalization in consistent scheme ($\overline{\mathrm{MS}}$) required

NB2: Lellouch-Lüscher finite-volume correction required!

Calculation status

[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:

[Phys.Rev.D 102 (2020) 5, 054509]

$$\mathrm{Re}(\epsilon'/\epsilon) = 21.7\underbrace{(2.6)}_{\text{stat}}\underbrace{(8.0)}_{\text{sys}} \times 10^{-4} \quad \text{[Lattice]}$$

$$16.6(2.3) \times 10^{-4} \quad \text{[Experiment]}$$

- Agrees with experiment but with ~4x the total error

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Error budget and ways forward

- Dominated by systematic errors:
  - (~12%) Perturbation theory in Wilson coeffs to match 3f – 4f weak EFT at m_c
    - Improve with 4f calculation (active charm) : computationally infeasible?
    - Non-perturbative calculation of matching matrix : investigation underway

      [*M.Tomii, PoS* LATTICE2018 (2019) 216]
  - (~23%) Lack of EM+isospin-breaking contributions in lattice calculation
    - Lattice measurement of these effects extremely challenging but approach is being formulated.

      [*Phys.Rev.D* 106 (2022) 1, 014508]
      [*Christ, PoS* LATTICE2021 (2022) 312]
  - (~12%) Use of single lattice spacing to compute I=0 amplitude
    - Repeat calculation with multiple, finer lattice spacings: **my current focus**

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Physical kinematics and GPBC

- Issue:

  $\pi\pi$ ground-state is 2 pions at rest, energy ~ 270 MeV $\ll m_K \sim$ 500 MeV

  Signal dominated by unphysical decay!

- Options:
  - Attempt to extract physical decay as excited state contribution [cf M.Tomii, Thurs @2.30pm]
  - Manipulate boundary conditions (BCs) to change ground-state pion momenta.

- For I=0 channel, G-parity BCs make pions antiperiodic while conserving isospin: $$\hat{G}\pi^{\pm,0} = -\pi^{\pm,0}$$

GPBC	vs	Periodic
$p_{x,y,z} = (2n+1)\pi/L$		$p_{x,y,z} = 2n\pi/L$

$$E_{\pi\,\mathrm{gnd}} = \sqrt{m_\pi^2 + 3\frac{\pi^2}{L^2}} \Rightarrow E_{\pi\pi\,\mathrm{gnd}} = 2E_{\pi\,\mathrm{gnd}}(L) + \Delta_{\mathrm{int}}(L)$$

Interactions (Lüscher)

Tune L to match $E_{\pi\pi\,\mathrm{gnd}} = m_K$ Measured 0.348(1) vs 0.3559(1)

(2% different)

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GPBC on quarks

- G-parity mixes quark flavors: $$\hat{G}\begin{pmatrix} u \\ d \end{pmatrix}\hat{G}^{-1} = \begin{pmatrix} -C\bar{d}^T \\ C\bar{u}^T \end{pmatrix}$$

charge-conjugation (spin) matrix

- Rewrite as new "flavor doublet"

$$\hat{G}\underbrace{\begin{pmatrix} d \\ C\bar{u}^T \end{pmatrix}}_{\psi}\hat{G}^{-1} = \begin{pmatrix} C\bar{u}^T \\ -d \end{pmatrix} \qquad \hat{G}\psi\hat{G}^{-1} = i\sigma_2\psi$$

- G-parity BC becomes a "flavor rotation" occurring at the boundary
- Gauge invariance demands complex-conjugate (charge conjugate) BCs for gauge links.

GPBC Dirac operator

$\pm\sigma_2$ at spatial boundaries, 1 otherwise
<u>induces GPBC</u>

$$\mathcal{M}(x,y) = \frac{1}{2}\sum_\mu \left[\tilde{U}_\mu(x)\gamma_\mu B^+_\mu(x_\mu)\delta_{x+\hat{\mu},y} - B^-_\mu(x_\mu)\tilde{U}^\dagger_\mu(x)\gamma_\mu\delta_{x-\hat{\mu},y}\right] + m\delta_{x,y}$$

$$\begin{pmatrix} U_\mu(x) & 0 \\ 0 & U^*_\mu(x) \end{pmatrix}$$

- Use of two-flavor operator **doubles the cost** of applying Dirac op.
- HMC even more expensive: $\det(\mathcal{M}^\dagger\mathcal{M})$ is a 4-flavor determinant!
  - 2f light quarks requires *square-root* of determinant (RHMC or “EOFA” [for DWF])
  - 1f heavy quark requires *fourth root* (RHMC)
  - Overheads of these algorithms also limit tuning opportunities (e.g. Hasenbusch)

Gauge field generation **very** expensive
Strong motivation for improved algorithms

Complex conjugate relation

$$X = C\gamma^5 \Rightarrow X^{-1}\gamma_\mu^* X = \gamma_\mu$$

- X relates gamma-matrices to their complex conjugates

$$\sigma_2 \tilde{U}_\mu^* \sigma_2 = \tilde{U}_\mu$$

$$\begin{pmatrix} U_\mu(x) & 0 \\ 0 & U_\mu^*(x) \end{pmatrix}$$

- σ_2 relates (G-parity) gauge links to their complex conjugates

$$\Xi = -i\sigma_2 X \Rightarrow \Xi^{-1}\mathcal{M}^*(x,y)\Xi = \mathcal{M}(x,y)$$

Makes Ξ Hermitian

- **Ξ relates Dirac matrix to its complex conjugate!**

a curious property – useful?

Flavor structure

$$\mathcal{M} = \Xi^{-1}\mathcal{M}^*\Xi$$

$$\begin{pmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ \mathcal{M}_{21} & \mathcal{M}_{22} \end{pmatrix} = \begin{pmatrix} X^{-1}\mathcal{M}_{22}^*X & -X^{-1}\mathcal{M}_{21}^*X \\ -X^{-1}\mathcal{M}_{12}^*X & X^{-1}\mathcal{M}_{11}^*X \end{pmatrix}$$

Equate lower rows

$$\mathcal{M} = \begin{pmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ -X^{-1}\mathcal{M}_{12}^*X & X^{-1}\mathcal{M}_{11}^*X \end{pmatrix}$$

Dirac matrix rows are related by complex conjugation!
Does this imply some kind of “degeneracy”?

A real-ly interesting relation

$$\mathcal{M} = \begin{pmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ -X^{-1}\mathcal{M}_{12}^{*}X & X^{-1}\mathcal{M}_{11}^{*}X \end{pmatrix}$$

$$\boxed{X^2 = -1}$$

Introduce unitary matrix

$$R = \frac{\overset{\text{phase}}{\alpha}}{\sqrt{2}} \begin{pmatrix} -X & i \\ -1 & iX \end{pmatrix}$$

$$\boxed{\Xi = -RR^T}$$

$$R^\dagger \mathcal{M} R = \begin{pmatrix} -\mathrm{Re}(X\mathcal{M}_{11}X + X\mathcal{M}_{12}) & -\mathrm{Im}(X\mathcal{M}_{11} + X\mathcal{M}_{12}X) \\ -\mathrm{Im}(\mathcal{M}_{11}X + \mathcal{M}_{12}) & \mathrm{Re}(\mathcal{M}_{11} + \mathcal{M}_{12}X) \end{pmatrix} = \mathcal{M}_{\mathrm{re}}$$

The G-parity Dirac operator can be rotated with a unitary matrix into a real matrix!

Can we exploit this?

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Real-ly big savings?

Standard pseudofermion integral

$\phi' = R\phi$

$\phi' = \phi'_r + i\phi'_i$

$$\det(\mathcal{M}^\dagger\mathcal{M}) = \int [d\phi_r][d\phi_i] \exp\left(-\phi^\dagger(\mathcal{M}^\dagger\mathcal{M})^{-1}\phi\right)$$

$$= \int [d\phi'_r][d\phi'_i] \exp\left(-\phi'^\dagger(\mathcal{M}^\dagger_{\rm re}\mathcal{M}_{\rm re})^{-1}\phi'\right)$$

$$= \int [d\phi'_r][d\phi'_i] \exp\left(-\phi'^T_r(\mathcal{M}^\dagger_{\rm re}\mathcal{M}_{\rm re})^{-1}\phi'_r - \phi'^T_i(\mathcal{M}^\dagger_{\rm re}\mathcal{M}_{\rm re})^{-1}\phi'_i\right)$$

$$= \left[\int [d\phi'_r] \exp\left(-\phi'^T_r(\mathcal{M}^\dagger_{\rm re}\mathcal{M}_{\rm re})^{-1}\phi'_r\right)\right]^2$$

Four-flavor determinant

real pseudofermions

G-parity squared-operator determinant is an exact square!

$$\boxed{\det(\mathcal{M}^\dagger\mathcal{M})^{1/2} = \int [d\phi'_r] \exp\left(-\phi'^T_r(\mathcal{M}^\dagger_{\rm re}\mathcal{M}_{\rm re})^{-1}\phi'_r\right)}$$

Two-flavor determinant

No need for EOFA / RHMC for light quarks!

X-conjugate vectors

$\mathcal{M}_{\mathrm{re}}$ is a complicated operator that is hard to implement

$$\begin{pmatrix} \phi'_{r,1} \\ \phi'_{r,2} \end{pmatrix}$$

Transform to a more convenient form!

$$-\phi_r'^{\,T}(\mathcal{M}_{\mathrm{re}}^\dagger \mathcal{M}_{\mathrm{re}})^{-1}\phi'_r = -\phi_r'^{\,T} R^\dagger (\mathcal{M}^\dagger \mathcal{M})^{-1} R\phi'_r$$
$$= -\chi^\dagger (\mathcal{M}^\dagger \mathcal{M})^{-1}\chi$$

Choose $\alpha = 1$

$$\chi \equiv R\phi'_r = \frac{1}{\sqrt{2}}\begin{pmatrix} -X\phi'_{r,1} + i\phi'_{r,2} \\ -\phi'_{r,1} + iX\phi'_{r,2} \end{pmatrix} = \begin{pmatrix} \chi_1 \\ -X\chi_1^* \end{pmatrix}$$

"X-conjugate vector"

Write in terms of new, complex fields but with half as many complex degrees of freedom as a standard pseudofermion due to "X-conjugacy"

X-conjugate Dirac operator

$$\psi = \mathcal{M}\chi = \begin{pmatrix} \mathcal{M}_{11} & \mathcal{M}_{12} \\ -X^{-1}\mathcal{M}_{12}^* X & X^{-1}\mathcal{M}_{11}^* X \end{pmatrix} \begin{pmatrix} \chi_1 \\ -X\chi_1^* \end{pmatrix}$$

$$= \begin{pmatrix} \mathcal{M}_{11}\chi_1 - \mathcal{M}_{12}X\chi_1^* \\ -X\left[\mathcal{M}_{11}\chi_1 - \mathcal{M}_{12}X\chi_1^*\right]^* \end{pmatrix} = \begin{pmatrix} \psi_1 \\ -X\psi_1^* \end{pmatrix}$$

- Dirac operator preserves X-conjugacy
- Need only solve for ψ_1, reconstruct $-X\psi_1^*$ afterwards

Acts only between "bulk" sites

Acts only across boundary

$$\psi_1 = \mathcal{M}_{11}\chi_1 - \mathcal{M}_{12}X\chi_1^*$$
$$\equiv \mathcal{M}_X\chi_1$$

<u>Looks like a new (unflavored) Dirac operator with "X-conjugate" BCs!</u>

$$\hat{T}^{-1}\psi(L-1)\hat{T} = -X\psi^*(0)$$

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X-ceptional gains!

$$\det(\mathcal{M}^\dagger\mathcal{M})^{1/2} = \int [d\phi_r'] \exp\left(-\phi_r'^T (\mathcal{M}_{\rm re}^\dagger \mathcal{M}_{\rm re})^{-1} \phi_r'\right)$$
$$= \int [d\chi_{1,r}][d\chi_{1,i}] \exp\left(-\chi_1^\dagger (\mathcal{M}_X^\dagger \mathcal{M}_X)^{-1} \chi_1\right)$$

- X-conjugate Dirac op easy to implement, just a new BC
- As an unflavored operator, application cost ½ of regular GPBC operator
- Evaluation of 2f determinant same as regular 2f determinant
  - No need for square-root!

Dramatic reduction in evolution cost!

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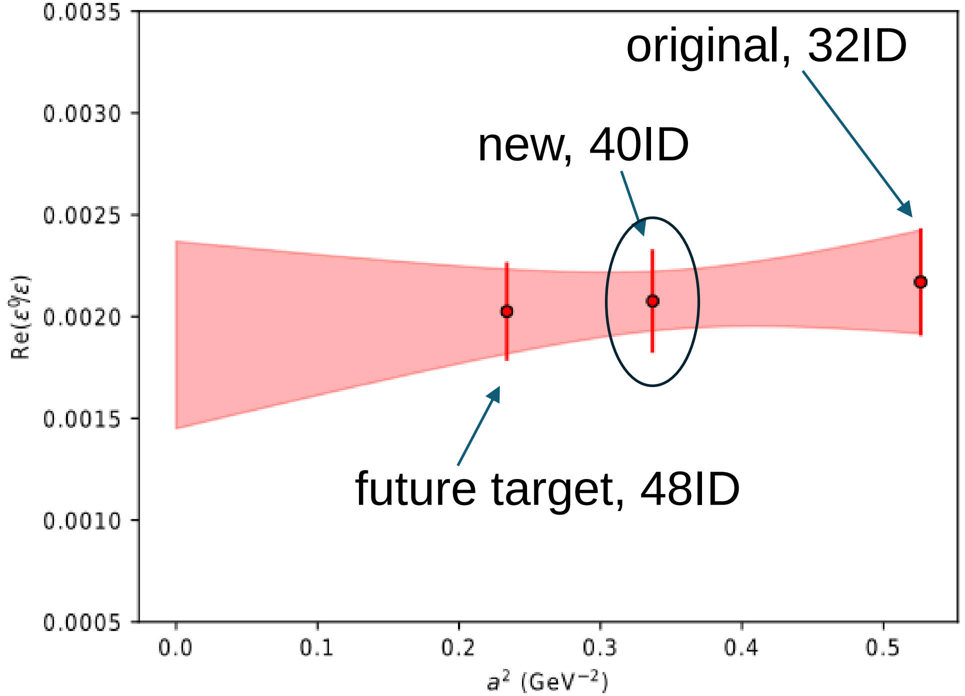
40ID ensemble

- $40^3 \times 64$ 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

>1300 trajectories generated in ~1 month (avg ~45/day)
~ 1/5(?) of target statistics!

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Eigenvectors of Hermitian Dirac Op

$$\mathcal{M}^\dagger \mathcal{M}\psi = \lambda\psi \quad \Longrightarrow \quad R^\dagger \mathcal{M}^\dagger \mathcal{M} R(R^\dagger\psi) = \lambda(R^\dagger\psi)$$

$$\Longrightarrow \quad \mathcal{M}_{\mathrm{re}}^T \mathcal{M}_{\mathrm{re}}(R^\dagger\psi) = \lambda\underbrace{(R^\dagger\psi)}_{v_r}$$

- $\mathcal{M}_{\mathrm{re}}^T \mathcal{M}_{\mathrm{re}}$ is real, symmetric:
  - evecs v_r can be chosen to be real vectors

$$\psi \equiv R v_r = \frac{1}{\sqrt{2}} \begin{pmatrix} -X v_{r,1} + i v_{r,2} \\ -v_{r,1} + i v_{r,2} \end{pmatrix} = \begin{pmatrix} \psi_1 \\ -X\psi_1^* \end{pmatrix}$$

- Evecs ψ can be expressed as X-conjugate vectors!
- Possible to solve for using X-conjugate Dirac op

2x cost reduction in generating evecs!
2x reduction in memory and disk footprint for storing!

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Conclusions and Outlook

- Improving lattice calculation of ϵ' requires addressing sys. errors.
- Continuum limit will reduce/eliminate a dominant, 12% error. Expensive due to G-parity BCs.
- Exploiting properties of the G-parity Dirac op, re-expressed fermion determinant in terms of a cheaper, “X-conjugate” op.
- Achieve 4x speed-up on same hardware for finer, “40ID” ensemble (2.7x for more efficient job layout)
- Sufficient trajectories for repeat analysis expected to be completed this year as a result!
- 2x speed-up also achieved in eigenvector generation for measurements.