Update on the lattice calculation of direct CP-violation in K decays

(aka “Update on K=>pi pi & All That”)

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Motivation and previous result
Motivation

- Likely explanation for matter/antimatter asymmetry in Universe, baryogenesis, requires violation of CP.
- Amount of CPV in Standard Model appears too low to describe measured M/AM asymmetry: tantalizing hint of new physics.
- Direct CPV first observed in late 90s at CERN (NA31/NA48) and Fermilab (KTeV) in $K^0 \rightarrow \pi\pi$:

  \[\eta_{00} = \frac{A(K_L \rightarrow \pi^0\pi^0)}{A(K_S \rightarrow \pi^0\pi^0)}, \quad \eta_{+-} = \frac{A(K_L \rightarrow \pi^+\pi^-)}{A(K_S \rightarrow \pi^+\pi^-)}.\]

  \[\text{Re}(\epsilon'/\epsilon) \approx \frac{1}{6} \left( 1 - \left| \frac{\eta_{00}}{\eta_{\pm}} \right|^2 \right) = 16.6(2.3) \times 10^{-4} \quad \text{(experiment)}\]

- Small size of $\epsilon'$ makes it particularly sensitive to new direct-CPV introduced by many BSM models.
- In terms of isospin states: $\Delta I=3/2$ decay to $I=2$ final state, amplitude $A_2$
  $\Delta I=1/2$ decay to $I=0$ final state, amplitude $A_0$

  \[A(K^0 \rightarrow \pi^+\pi^-) = \sqrt{\frac{2}{3}} A_0 e^{i\delta_0} + \sqrt{\frac{1}{3}} A_2 e^{i\delta_2},\]

  \[A(K^0 \rightarrow \pi^0\pi^0) = \sqrt{\frac{2}{3}} A_0 e^{i\delta_0} - 2\sqrt{\frac{1}{3}} A_2 e^{i\delta_2}.\]

  \[\omega = \frac{\text{Re}A_2}{\text{Re}A_0}, \quad \epsilon' = \frac{i\omega e^{i(\delta_2-\delta_0)}}{\sqrt{2}} \left( \frac{\text{Im}A_2}{\text{Re}A_2} - \frac{\text{Im}A_0}{\text{Re}A_0} \right)\]

  ($\delta_i$ are strong scattering phase shifts.)
Overview of calculation

- Hadronic energy scale $\ll M_W$ – use weak effective theory.

- $K \to \pi\pi$ decays require single insertion of $\Delta S=1$ Hamiltonian:

$$H_{W}^{\Delta S=1} = \frac{G_F}{\sqrt{2}} V_{ud}^* V_{us} \sum_{j=1}^{10} [z_j(\mu) + \tau y_j(\mu)] Q_j$$

10 effective four-quark operators

Perturbative Wilson coeffs.

Renormalization matrix (mixing)

Use RI-SMOM and convert to MSbar perturbatively

LL finite-volume correction

$$\tau = - \frac{V_{ts}^* V_{td}}{V_{us}^* V_{ud}} = 0.0014606 + 0.00060408i$$

Imaginary part solely responsible for CPV (everything else is pure-real)

$$A^I = F \frac{G_F}{\sqrt{2}} V_{ud} V_{us} \sum_{i=1}^{10} \sum_{j=1}^{7} \left[ (z_i(\mu) + \tau y_i(\mu)) Z_{i,j}^{\text{lat}} \to \overline{\text{MS}} M_j^{I,\text{lat}} \right]$$

$$M_j^{I,\text{lat}} = \langle (\pi\pi)_I | Q_j | K \rangle \text{ (lattice)}$$
Summary of published results


- \( A_2 \) computed on RBC/UKQCD 64\( ^3 \times 128 \) and 48\( ^3 \times 96 \) 2+1f Mobius DWF ensembles with the Iwasaki gauge action and physical pion mass.
- \( a^{-1} = 2.36 \text{ GeV} \) and 1.73 GeV resp - continuum limit taken.
- Statistical errors sub-percent, dominant systematic errors due to truncation of PT series in computation of RI-SMOM to MSbar matching and Wilson coefficients.
- 10\% and 12\% total errors on Re(\( A_2 \)) and Im(\( A_2 \)) resp.


- \( A_0 \) computed on 216cfgs of 32\( ^3 \times 64 \) Mobius DWF with Iwasaki+DSDR gauge action and physical pion mass.
- G-parity BCs in 3 directions to give physical kinematics.
- Single, coarse lattice with \( a^{-1} = 1.38 \text{ GeV} \) but large physical volume to control FV errors.
- 21\% and 65\% stat errors on Re(\( A_0 \)) and Im(\( A_0 \)) due to disconn. diagrams and, for Im(\( A_0 \)) a strong cancellation between \( Q_4 \) and \( Q_6 \).
- Dominant, 15\% systematic error is due again to PT truncation errors exacerbated by low renormalization scale 1.53 GeV.
Result for $\varepsilon'$

- $\text{Re}(A_0)$ and $\text{Re}(A_2)$ from expt.
- Lattice values for $\text{Im}(A_0)$, $\text{Im}(A_2)$ and the phase shifts

$$\text{Re} \left( \frac{\varepsilon'}{\varepsilon} \right) = \text{Re} \left\{ \frac{i\omega e^{i(\delta_2-\delta_0)}}{\sqrt{2\varepsilon}} \left[ \frac{\text{Im} A_2}{\text{Re} A_2} - \frac{\text{Im} A_0}{\text{Re} A_0} \right] \right\}$$

$$= 1.38(5.15)(4.43) \times 10^{-4}, \quad \text{(calculated)}$$

$$16.6(2.3) \times 10^{-4}, \quad \text{(experiment)}$$

- Error is dominated by that on $A_0$.
- Total error on $\text{Re}(\varepsilon'/\varepsilon)$ is $\sim 3x$ the experimental error.
- Result is in tension with Standard Model at $2.1\sigma$ level.
The “ππ puzzle” and multi-operator fits
On the importance of the $\pi\pi$ state

- Understanding $I=0 \pi\pi$ system is crucial:
  - Energy is needed for time dependence of correlation function from which we extract finite-volume $K \to \pi\pi$ matrix element.
  - Phase shift enters Lellouch-Luscher finite-volume correction to matrix element.
  - Phase shifts also enter in formula relating $A_{\perp}$ to $\epsilon'$ itself

- 2015 calculation of $\delta_0$ in 2σ tension with dispersion theory calculation:
  $$\delta_0 = 23.8(4.9)(2.2)^\circ \text{ (latt)}$$
  $$= 34^\circ \text{ (G.Colangelo et al)}$$

- This observation prompted increased focus on $\pi\pi$ system.
Increased statistics

- To resolve the “pi-pi puzzle” we increased statistics from 216 to 1438 (a 6.6x increase!). However this did not resolve the situation:

\[
\delta_0 = 23.8(4.9)(2.2)^\circ \rightarrow 19.1(2.5)(1.2)^\circ
\]
Resolving the pi-pi puzzle

- Most likely explanation is excited state contamination masked by rapid growth of statistical errors.
- To resolve this we turned to multi-operator fits which provide much greater resolution on excited states time dependence alone.
- Obtain parameters by simultaneous fitting to matrix of correlation functions

\[ C_{ij}(t) = \langle 0|O_i^\dagger(t)O_j(0)|0\rangle = C + \sum_{\alpha} A_{i,\alpha} A_{j,\alpha} e^{-E_\alpha t} \]

- Increased from 1 → 3 operators: \( \pi\pi(111) \quad \pi\pi(311) \quad \sigma \) [cf T.Wang Monday]
- 741 configurations measured with 3 operators.

round-the-world single pion propagation small compared to errors - drop
Effect of multiple operators on $\pi\pi$

Result compatible with dispersive value $t_{\text{min}}$ of fit

Preliminary results only

Stat Errs Only

Fitted energy (lattice units)

From dispersion theory + expt. data

Result compatible with dispersive value
Effect of multiple operators on $K \rightarrow \pi\pi$ (case I)

[741 configs PRELIMINARY]

Ground-state projected data

$\pi\pi(111)+\sigma$

$\pi\pi(111)+\pi\pi(311)+\sigma$

$\pi\pi(111)$
Effect of multiple operators on $K \to \pi\pi$ (case II)

Dramatic improvement in both precision and plateau quality!

[741 configs PRELIMINARY]
Other systematic error improvements
Systematic error improvements

<table>
<thead>
<tr>
<th>Description</th>
<th>Error</th>
<th>Description</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Finite lattice spacing</td>
<td>12%</td>
<td>Finite volume</td>
<td>7%</td>
</tr>
<tr>
<td>Wilson coefficients</td>
<td>12%</td>
<td>Excited states</td>
<td>≤ 5%</td>
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<tr>
<td>Parametric errors</td>
<td>5%</td>
<td>Operator renormalization</td>
<td>15%</td>
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<td>Unphysical kinematics</td>
<td>≤ 3%</td>
<td>Lellouch-Lüscher factor</td>
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<tr>
<td>Total (added in quadrature)</td>
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<td>27%</td>
</tr>
</tbody>
</table>

NPR+Wilson Coefficients

- NPR error large due to use of 1-loop PT to match to MSbar at low, 1.53 GeV renormalization scale.
- Since 2015 have improved NPR error 15% → 8% (preliminary) by increasing scale to 2.29 GeV using step-scaling procedure.
- Inclusion of dim.6 gauge-invariant operator $G_1$ which mixes with $Q_i$ under renormalization, effects demonstrated to be %-scale as expected.
- Do not expect significant improvement in Wilson coeffs error from scale increase as it is overshadowed by use of PT to cross the charm threshold (1.29 GeV).
- Working on circumventing this by computing 3 → 4 flavor matching non-perturbatively.
- Requires $\mu \ll m_c$. At these low energies, MOM-scheme NPR severely hampered by increased mixing with tower of gauge-noninvariant operators.
- Circumvent using position-space NPR which does not require gauge fixing.

[RBC&UKQCD PRL 115 (2015) 21, 212001]  
[cf Masaaki Tomii Tuesday]
Related projects on the horizon:

- Performing calculation taking advantage of modern multi-operator techniques to fit excited-state $\pi\pi\pi$ contributions directly, without G-parity BCs. [Cerdà-Sevilla, Gorbahn, Jäger, Kokulu]
- Laying the groundwork for non-perturbatively computing the effects of isospin breaking and electromagnetism. [EPJ Web Conf. 175 (2018) 13016]
Advances in statistical techniques
Dealing with autocorrelations

- With increased statistics we now have evidence for (limited) autocorrelation effects: $\tau_{\text{int}} \sim 4$ MDTU (1 cfg).
- Naively expect $\sim 1.4x$ larger errors.
- Standard approach is to bin (average) data over blocks sufficiently large to make the blocks independent.

- Pion and kaon energies behave as expected with binning
\(I=0 \, \pi \pi \, 2\text{pt function}\)

- \(\pi \pi\) errors continue growing with bin size and do not stabilize. Why?
- Covariance matrix is 66x66 here!
- As bin size increased, fewer data points enter determination of covariance matrix, matrix becomes less and less well resolved.
- Fluctuations of low eigenvalues increase, causing error growth unrelated to autocorrelation.
Scrambled data

- Isolate effect of loss of resolution of covariance matrix by randomly scrambling data to destroy autocorrelations

- Error growth essentially the same!
To prevent loss of resolution of covariance matrix while still taking into account autocorrelations, we perform **block jackknife**.

Regular, binned jackknife: generate $n/B$ "reduced ensembles" of $n/B-1$ numbers by successively dropping values.

With binning, covariance matrix obtained from just $n/B-1$ numbers.
Block jackknife II

block jackknife: From \textit{unbinned} data generate $n/B$ reduced ensembles but of size $n-B$ values by throwing away successive \textbf{blocks} of size $B$

\begin{itemize}
  \item Covariance matrix obtained from $n-B$ values!
  \item Jackknife procedure ensures correct statistical error
\end{itemize}
$I=0$ ππ 2pt function with block jackknife

Now obtain expected behavior
Goodness of fit

- Large number (741) of configurations encourages more sophisticated statistical techniques.
- In particular, well-controlled correlated fits allow for reliable goodness-of-fit metrics which aid fitting and systematic error estimation.
- Goodness-of-fit described by a p-value - the probability of getting a worse fit allowing for only statistical fluctuations.

With covariance matrix obtained from sample covariance:

\[
C_{tt'} = \frac{1}{n(n-1)} \sum_{i=1}^{n} [v_{i,t} - \bar{v}_t] [v_{i,t'} - \bar{v}_{t'}]
\]
P-value issues

- Despite high degree of stability under changing fit ranges, goodness of fit for $\pi\pi$ typically quite poor.

- Importance of reliable $\pi\pi$ fits strongly motivates resolving this issue.

- Key is to recognize that the $\chi^2$ distribution does not account for fluctuations in the covariance matrix over the population.

- When cov. mat. is determined from data, finite statistics effects broaden the distribution of $q^2$ as the matrix fluctuates along with the data.

- For ensembles of uncorrelated Gaussian data (not QCD path integral-distributed!) the corrected distribution can be determined analytically: It is the Hotelling $T^2$ distribution, $T^2(k, n-1)$ for $n$ samples.

- However in general there is no analytic result.

- Even if we assume Gaussian data, numerical tests indicate strong autocorrelation effects that can only be removed by binning to large bin sizes (a no-go for us!).
Non-overlapping block bootstrap (NBB)

- The **bootstrap** technique allows us to estimate properties of the population from just one ensemble, by randomly resampling (with replacement).

- The (non-overlapping) block variant resamples blocks rather than single configurations, much like block jackknife, in order to account for autocorrelations:
Computing p-values via bootstrap

- Use NBB to directly compute the distribution of $q^2$!
  - No normality assumption
  - Blocking accounts for autocorrelations without binning
- Minor subtlety: bootstrap ensemble means $\overline{b}^\alpha$ distributed about ensemble mean $\overline{\mathcal{V}}$ *not population mean*
- Results in broader distribution of $q^2$ with larger mean
- Correct by “recentering”: $\overline{b}^\alpha(t) \rightarrow \overline{b}^\alpha(t) + [f(t, \bar{p}) - \bar{e}(t)]$

Gaussian data, no autocorrelations, 400 samples
I=0 ππ fit bootstrap p-value

The graph shows the relationship between block size and p-value. As the block size increases, the p-value also increases, indicating a stronger fit in the bootstrap analysis.
p-values for uncorrelated fits!

- Conventional wisdom is that one cannot obtain the goodness-of-fit for uncorrelated fits. Using the bootstrap technique we can!

\[
q^2 / \text{dof} = 0.4 \pm 0.2
\]
Conclusions
Conclusions

- Multi-operator techniques appear to resolve discrepancy with dispersive prediction for $I=0$ $\pi\pi$ phase shift.
- Marked improvement in quality of plateaus in $K\rightarrow\pi\pi$, better control over excited state systematics.
- Programmes for reducing other systematic errors in progress.
- Already achieved 2x improvement in NPR error via step scaling.
- Potential near-term reduction in Wilson coeff. systematic through NNLO PT calculation. In longer term we aim for a non-perturbative matching through the charm threshold.
- Advanced statistical techniques allow for more reliable p-values and enable us to account for mild autocorrelation effects without exploding our statistical error through binning.
- Expect no further hurdles to completion of project and we aim to publish within the next few months.

Thank you!
Is the Hotelling distribution sufficient?

- Numerical experiments with fake data show Hotelling $T^2$ relatively tolerant of non-normality.

- **However** $T^2$ relies on independent configurations: *extremely* sensitive to autocorrelations.

- Even with binning, slow convergence to true distribution:

  ![Graph showing convergence](image)

  - Fake gaussian data
  - 400 configs, sep ~ $\tau_{int}=5$
  - (Metropolis algorithm)

  - $B=1$, $B=2$, $B=4$, $B=8$, $B=12$

- Wish to avoid binning due to explosion in statistical error from reduced resolution of covariance matrix
Demonstration II - log-normal

400 cfgs, log-normal

μ=0  σ=0.7

Stat error and bias fall as $n, B \to \infty$ ($B \ll n$)

No autocorrelations

Autocorrelations, cfg sep $\sim \tau_{int}$