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

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Motivation for studying $K \to \pi\pi$ Decays

- 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 $K^0 \to \pi\pi$:

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

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

- 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 $A_0$

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

$$A(K^0 \to \pi^0\pi^0) = \sqrt{\frac{2}{3}} A_0 e^{i\delta_0} - 2 \sqrt{\frac{1}{3}} A_2 e^{i\delta_2}. \quad \omega = \text{Re}A_2/\text{Re}A_0$$

$$\epsilon' = \frac{i\omega e^{i(\delta_2 - \delta_0)}}{\sqrt{2}} \left(\frac{\text{Im}A_2}{\text{Re}A_2} - \frac{\text{Im}A_0}{\text{Re}A_0}\right) \quad (\delta_i \text{ are strong scattering phase shifts.})$$

- Small size of $\epsilon'$ makes it particularly sensitive to new direct-CPV introduced by many BSM models.
Summary of 2015 published result


- $A_2$ previously computed on lattice precisely (12% total error)

- Computed $A_0$ on $32^3 \times 64$ Mobius DWF ensemble with Iwasaki+DSDR gauge action. G-parity BCs in 3 directions to give physical kinematics.

- Single, coarse lattice with $a^{-1} = 1.38$ GeV but large physical volume to control FV errors.

- Re($A_0$) and Re($A_2$) from expt.

- Lattice values for Im($A_0$), Im($A_2$) and the phase shifts.

\[
\text{Re} \left( \frac{\epsilon'}{\epsilon} \right) = \frac{1.38(5.15)(4.43)}{16.6(2.3)} \times 10^{-4}
\]  

(our result)

(our result)  

(experiment)

- Find reasonable consistency with experimental value (at 2.1σ level).
- Total error on is ~3x the experimental error.
- “This is now a quantity accessible to lattice QCD”!

- Focus since has been to improve statistics and reduce / improve understanding of systematic errors.
The $\pi\pi$ puzzle

1438 cfgs
(PRELIMINARY)

(From dispersion theory + expt. data)
Resolving the $\pi\pi$ puzzle

- Since 2015 publication have been working to resolve discrepancy between our lattice I=0 $\pi\pi$ phase shift ($\delta_0=23.8(4.9)(1.2)$) and that predicted by dispersion theory ($\sim 34^\circ$). [RBC&UKQCD PRL 115 (2015) 21, 212001] [Colangelo et al, Nucl.Phys. B603 (2001) 125-179]

- Increased statistics from 216 to almost 1400 configurations, a 6.5x increase. Observed discrepancy becomes more significant.

- Alongside existing 1s hydrogen wavefunction pion source smearing we added a 2s form and a scalar ($\sigma=\bar{u}d$) $\pi\pi$ operator to the 2-pt function calculation.

- Also added 2s pion sources to $K\to\pi\pi$ calculation.

- While 2s data appears too noisy, combined fits (or GEVP) to $\pi\pi\to\pi\pi$, $\sigma\to\pi\pi$ and $\sigma\to\sigma$ correlators result in considerably lower ground-state energy: [cf. T.Wang, prev. talk]

  $508(5)$ MeV [1386 cfgs] from $\pi\pi\to\pi\pi$ alone
  vs
  $483(1)$ MeV [501 cfgs] from sim. fit of all 3 correlators.

- Strong new evidence for nearby excited finite-volume $\pi\pi$ state. Indeed such a state with $E \sim 770$ MeV is predicted by dispersion theory.
**Implications for K → ππ and resolution**

- Despite vast increase in statistics, *this state cannot be resolved based on the time dependence using only a single ππ operator.*
- Possibly a significant underestimate of excited state systematic in K → ππ calculation that can only be resolved by adding additional operators.
- In response we have **expanded the scope of the calculation:**
  - **Added K → σ matrix elements.** This involved significant work in both deriving the Wick contractions and in implementing/optimizing the parallel code.
  - **Added more pion momenta.** Previously we computed only zero-momentum ππ-states with pion momenta in the set (±1,±1,±1)π/L (8-total). We have now added 24 new momenta: (±3,±1,±1)π/L + perms.
- Result is **3x increase in the number of S-wave ππ operators in K → ππ**
- Using sim. fits / GEVP to 2-pt function data can then determine appropriate linear comb. of these 3 sets of matrix elements that best projects onto the ground-state.
- Also added ππ 2pt functions with non-zero total ππ momenta. Will allow calculation of phase shift at several (smaller) additional center-of-mass energies.
  - Additional points that can be compared to dispersive result / experiment
  - Improve ~11% systematic on Lellouch-Luscher factor associated with slope of phase shift.
Effect of projecting 2pt data onto ground-state using existing data (c/o T.Wang)

Expect even better ground-state projection with new higher-momentum operators in upcoming analysis.
Scaling of $\pi \pi$ contraction timing

- On 512-nodes of BG/Q, computing the $8 \times 8 = 64$ $\pi \pi$ contractions with 0 total $\pi \pi$ momentum takes 13.6 mins.

- However: 32 pion momenta, computing all contractions with $p_{\pi \pi} = (0, 0, 0), (\pm 2\pi/L, 0, 0), (\pm 2\pi/L, \pm 2\pi/L, 0), (\pm 2\pi/L, \pm 2\pi/L, \pm 2\pi/L) + \text{perms}$
  Number rises to 7848 contractions: $\sim 27.8$ hours on the $\pi \pi$ contractions alone!

- To make tractable take advantage of symmetries.
  Take care to use only those that do not significantly affect statistical error.

- To determine symmetries to use, we studied our $\pi \pi$ data including 121 cfgs of new data at non-zero $\pi \pi$ momentum computed using saved meson fields.

- Examined:
  
  Parity: exchange $\vec{p} \rightarrow -\vec{p}$

  Axis permutation: global interchange of momentum components
  (GPBC in 3 dirs so all spatial dirs equivalent)
"Auxiliary diagram" symmetry:

Source/sink timeslice interchange coupled with $\gamma^5$ hermiticity relates $\pi\pi$ correlators (after temporal folding/config avg):

$$\langle C(\vec{p}_{\text{src}}^{\pi_1}, \vec{p}_{\text{snk}}^{\pi_1}, \vec{p}_{\text{tot}}) \rangle \equiv$$

$$\langle C(-\vec{p}_{\text{tot}} + \vec{p}_{\text{snk}}^{\pi_1}, \vec{p}_{\text{tot}} - \vec{p}_{\text{src}}^{\pi_1}, -\vec{p}_{\text{tot}}) \rangle$$

[Parity + aux.diag together preserve $p_{\text{tot}}$]
\( p_{\text{tot}} = 0 \)

- Observe all symmetries individually well realized and do not significantly affect statistical error.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Orig (64 diags)</th>
<th>Pty+perm (10 diags)</th>
<th>Aux+pty+perm (8 diags)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(</td>
<td>A_{\pi\pi}</td>
<td>^2)</td>
<td>0.1609(22)</td>
</tr>
<tr>
<td>(E_{\pi\pi})</td>
<td>0.3686(33)</td>
<td>0.3690(36)</td>
<td>0.3672(36)</td>
</tr>
<tr>
<td>(C_{\pi\pi})</td>
<td>3(10) \times 10^{-5}</td>
<td>3(10) \times 10^{-5}</td>
<td>-1(11) \times 10^{-5}</td>
</tr>
<tr>
<td>(\chi^2/\text{dof})</td>
<td>1.30(57)</td>
<td>1.25(54)</td>
<td>1.10(52)</td>
</tr>
</tbody>
</table>

- 8x reduction in #correlators for base pion momentum set!

\( p_{\text{tot}} = (\pm 2,0,0)\pi/L + \text{perms} \)

- Applied globally, utilizing parity for 2x reduction in diags does not affect error, but axis permutation does: suggests (2,0,0), (0,2,0) and (0,0,2) largely uncorrelated.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Orig (96 diags)</th>
<th>Pty (48 diags)</th>
<th>Pty+perm (16 diags)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(</td>
<td>A_{\pi\pi}</td>
<td>^2)</td>
<td>0.3466(41)</td>
</tr>
<tr>
<td>(E_{\pi\pi})</td>
<td>0.3869(23)</td>
<td>0.3869(23)</td>
<td>0.3879(40)</td>
</tr>
<tr>
<td>(C_{\pi\pi})</td>
<td>2(1) \times 10^{-4}</td>
<td>2(1) \times 10^{-4}</td>
<td>4(2) \times 10^{-4}</td>
</tr>
</tbody>
</table>

- Take second column and allow parity, axis perm and aux. diag. to relate the 48 diags:

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Pty (48 diags)</th>
<th>Pty+perm+aux (21 diags)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(</td>
<td>A_{\pi\pi}</td>
<td>^2)</td>
</tr>
<tr>
<td>(E_{\pi\pi})</td>
<td>0.3869(23)</td>
<td>0.3868(23)</td>
</tr>
<tr>
<td>(C_{\pi\pi})</td>
<td>2(1) \times 10^{-4}</td>
<td>2(1) \times 10^{-4}</td>
</tr>
</tbody>
</table>
• 4.5x reduction in #diagrams with no observed increase in errors.

• Similar picture observed for \((\pm 2, \pm 2, 0)\pi/L\) and \((\pm 2, \pm 2, \pm 2)\pi/L\):
  Different orientations (up to parity) largely uncorrelated but applying symmetries for fixed \(p_{\text{tot}}\) leaves errors unchanged.

• For our extended calculation
  Using parity to exclude 1/2 of diags with \(p_{\text{tot}} \neq 0\): 7848 diags \(\rightarrow\) 4436
  Then applying symmetries with fixed \(p_{\text{tot}}\):

<table>
<thead>
<tr>
<th>(p_{\text{tot}})</th>
<th>Total</th>
<th>pty</th>
<th>pty+perm</th>
<th>pty+perm+aux</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0, 0, 0)</td>
<td>1024</td>
<td>512</td>
<td>102</td>
<td>62</td>
</tr>
<tr>
<td>(2, 0, 0)</td>
<td>1200</td>
<td>1200</td>
<td>654</td>
<td>357</td>
</tr>
<tr>
<td>(2, 2, 0)</td>
<td>768</td>
<td>768</td>
<td>408</td>
<td>228</td>
</tr>
<tr>
<td>(−2, 2, 0)</td>
<td>768</td>
<td>768</td>
<td>384</td>
<td>216</td>
</tr>
<tr>
<td>(2, 2, 2)</td>
<td>169</td>
<td>169</td>
<td>33</td>
<td>21</td>
</tr>
<tr>
<td>(−2, 2, 2)</td>
<td>507</td>
<td>507</td>
<td>267</td>
<td>153</td>
</tr>
<tr>
<td>Total</td>
<td>4436</td>
<td></td>
<td>1037</td>
<td></td>
</tr>
</tbody>
</table>

• Overall 7.6x reduction in diagram count, reducing time (pre-optimization) to 3.7 hours.
## BG/Q Timings and Status

<table>
<thead>
<tr>
<th>Description</th>
<th>Time (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Light quark Lanczos</td>
<td>5.78</td>
</tr>
<tr>
<td>Light quark A2A vectors</td>
<td>4.48</td>
</tr>
<tr>
<td>Heavy quark A2A vectors</td>
<td>2.68</td>
</tr>
<tr>
<td>Gauge fix</td>
<td>0.31</td>
</tr>
<tr>
<td>Kaon 2pt function</td>
<td>0.44</td>
</tr>
<tr>
<td>Kaon WW meson fields</td>
<td>0.08</td>
</tr>
<tr>
<td>$K \to \sigma$ contractions</td>
<td>0.67</td>
</tr>
<tr>
<td>Sigma 2pt function</td>
<td>0.02</td>
</tr>
<tr>
<td>Light-light 1s pion meson fields</td>
<td>5.23</td>
</tr>
<tr>
<td>$\pi\pi \to \sigma$ 2pt function</td>
<td>0.06</td>
</tr>
<tr>
<td>$K \to \pi\pi$ contractions</td>
<td>7.02</td>
</tr>
<tr>
<td>Pion 2pt function</td>
<td>0.01</td>
</tr>
<tr>
<td>$\pi\pi$ 2pt contractions</td>
<td>1.51</td>
</tr>
<tr>
<td>Configuration total</td>
<td><strong>29.10</strong></td>
</tr>
</tbody>
</table>

- Currently running on 3x 512-node partitions of BG/Q at BNL
- Timing per configuration ~29 hours
- $\pi\pi$ contraction time only 1.5 hours after utilizing symmetries and code optimizations.
- Currently have measured 44 configurations (as of last night)
- New data can be combined with existing 1400 configs using super-jackknife procedure
- **Expect to be able to start serious analysis when ~100 configs, i.e. within the month.**
Conclusions

- Inclusion of additional scalar $\pi\pi$ operator in order to attempt to understand discrepancy with dispersion theory reveals nearby excited state.
- State unresolvable with just single operator, even with 6.5x more statistics.
- Suggests excited state systematic on published $K \rightarrow \pi\pi$ calculation significantly underestimated.
- In response added scalar operator and 24 additional pion momenta to $K \rightarrow \pi\pi$ calc, **increasing # of S-wave $\pi\pi$ operators in $K \rightarrow \pi\pi$ by 3x**
- Using 2pt data will ascertain appropriate linear combination that best projects onto ground state.
- New pion momenta and inclusion of non-zero CoM $\pi\pi$ momenta in 2pt calculation required utilization of symmetries to make computationally tractable.
- Generating 5 new measurements every 2 days on 3x 512-node BG/Q machines.

We hope to have enough new data to begin serious analysis within the next few weeks

Thank you!
Statistics increase

- Original goal was a 4x increase in statistics over 216 configurations used in 2015 analysis.
- 4x reduction in configuration generation time obtained via algorithmic developments (exact one-flavor implementation)
- Large-scale programme performed involving many machines:

<table>
<thead>
<tr>
<th>Source</th>
<th>Determinant computation</th>
<th>Independent configs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blue Waters</td>
<td>RHMC</td>
<td>34+18+4+3</td>
</tr>
<tr>
<td>KEKSC</td>
<td>RHMC</td>
<td>106</td>
</tr>
<tr>
<td>BNL</td>
<td>RHMC</td>
<td>208</td>
</tr>
<tr>
<td>DiRAC</td>
<td>RHMC</td>
<td>151</td>
</tr>
<tr>
<td>KEKSC</td>
<td>EOFA</td>
<td>275+215</td>
</tr>
<tr>
<td>BNL</td>
<td>EOFA</td>
<td>245</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1259 total</td>
</tr>
</tbody>
</table>

- Measurements performed using IBM BG/Q machines at BNL and the Cori computer (Intel KNL) at NERSC largely complete.
- Including original data, now have 6.7x increase in statistics!
1438 cfgs vs 216 cfgs (PRELIMINARY)
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>
</tr>
<tr>
<td>Parametric errors</td>
<td>5%</td>
<td>Operator renormalization</td>
<td>15%</td>
</tr>
<tr>
<td>Unphysical kinematics</td>
<td>≤ 3%</td>
<td>Lellouch-Lüscher factor</td>
<td>11%</td>
</tr>
<tr>
<td>Total (added in quadrature)</td>
<td></td>
<td></td>
<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. [PoS LATTICE2016 (2016) 308]
- Inclusion of dim.6 gauge-invariant operator $G_1$ which mixes with $Q_i$ under renormalization, effects demonstrated to be %-scale as expected. [G. McGlynn arxiv:1605.08807]

Do not expect significant improvement in Wilson coeffs. error as dominated 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.
Discretization error

- Currently have results only on single lattice with coarse lattice spacing $a^{-1}=1.38(1)$ GeV.
- Require second lattice spacing. Going to finer lattice requires more lattice sites; prohibitively expensive for current gen. computers.
- Promising alternative is to go to a coarser lattice spacing, $a^{-1} \sim 1.0$ GeV. Preliminary studies suggest discretization errors remain under control. [EPJ Web Conf. 175 (2018) 02006]

Related projects on the horizon:

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