Progress Towards the First Measurement of Direct CP-Violation in $K \rightarrow \pi\pi$ Decays From First Principles

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$K \to \pi\pi$ Decays

- Direct CP-violation first observed in $K \to \pi\pi$ decays.
- Two types of decay (Bose statistics forbids $I=1$):

\[
\begin{align*}
\Delta I = 3/2 : & \quad K^+ \to (\pi^+\pi^0)_{I=2} \quad \text{with amplitude } A_2 \\
\Delta I = 1/2 : & \quad K^0 \to (\pi^+\pi^-)_{I=0} \quad \text{with amplitude } A_0 \\
& \quad K^0 \to (\pi^0\pi^0)_{I=0}
\end{align*}
\]

- Direct CP-violation:

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

where

\[\omega = \frac{\text{Re} A_2}{\text{Re} A_0}\] and $\delta_I$ are strong scattering phase shifts.

- $\epsilon'$ is highly sensitive to BSM sources of CPV.
- Strong interactions very important – origin ([arXiv:1212.1474]) of the so-called $\Delta I = 1/2$ rule: preference to decay to $I = 0$ final state.
- Lattice QCD is the only known technique for accurately studying strong dynamics in the hadronic regime.
**Brief Interlude: Lattice Methods**

- Discretize QCD Lagrangian in Euclidean space on finite volume.
- Integrate fermions out of path integral:
  \[ Z = \int dU \, \det(D[U]) \exp(-S_g[U]) \]
- U are gauge links: \( U_\mu = e^{ia A^a_\mu T^a} \in SU(3) \)
- Sample configurations of links from probability distribution Z using Monte Carlo methods.
**Lattice Measurements**

- Measure amplitudes on each link configuration and average.

\[
\int d^3 \vec{x} \langle 0 | \bar{d}(x) \gamma^5 u(x) \bar{u}(0) \gamma^5 d(0) | 0 \rangle
\]

\[
= \frac{1}{N} \sum_{i=1}^{N} \int d^3 \vec{x} \, \text{tr} \left( \gamma^5 D^{-1}_d(0, x)[U_i] \gamma^5 D^{-1}_u(x, 0)[U_i] \right)
\]

\[
= a_0 e^{-m_\pi x_4} + a_1 e^{-E_1 x_4} + \ldots
\]

- Ground state of system extracted in limit of large time separation.

- Excited state with energy \( E_i \) \( (i > 0) \) requires multi-exponential fits to time dependence – typically very noisy and should be avoided if possible!
Lattice Techniques for $K \to \pi \pi$ Calculation

- $M_W \ll$ hadronic scale (1 GeV): use Weak effective theory
- $\Delta S = 1$ effective operator: CPV : $\tau = -V_{ts}^* V_{td} / (V_{ud} V_{us}^*)$

$$H_W^{\text{eff}} = \frac{G_F}{\sqrt{2}} V_{us}^* V_{ud} \sum_{i=1}^{10} \left[ z_i(\mu) + \tau y_i(\mu) \right] Q_i(\mu)$$

Wilson coefficients $y_i$ and $z_i$ calculated in perturbative regime.

- On lattice use low-energy operator: $\langle \pi \pi | Q_i | K \rangle$
- Non-perturbatively renormalize at high energy scale $\mu$
Finite-Volume Effects

- Lattice has finite size \( \sim (3 \text{ fm})^3 \) : finite-volume effects play large role: allowed energy states discretized. State normalization differs. Continuous pion FSI.
- Finite-volume lattice decay amplitudes are related to those in the infinite-volume by the ”Lellouch-Luscher” formula.
- This requires physical kinematics - \( E_{\pi\pi} = m_K \)
- \( m_\pi = 135 \text{ MeV} \) and \( m_K = 500 \text{ MeV} \) : need moving pions
- However ground state (easiest and cleanest state to isolate on lattice) comprises stationary pions. How can we solve this?
Workaround for $\Delta I = 3/2$ calculation

- On the lattice we have the freedom to choose boundary conditions imposed when calculating quark propagators.
- Typically use periodic BCs: $\psi(x + L) = \psi(x) \Rightarrow p = 2\pi n/L$
- Applying antiperiodic BCs on just d-quark prop:
  \[ d(x + L) = -d(x) \Rightarrow p_d = (2n + 1)\pi/L \]
- Charged pion $(u\bar{d})(x + L) = -(u\bar{d})(x)$: ground state $p_{\pi^\pm} = \pm\pi/L$
- Problem: we need $\pi^+\pi^0$ but $(d\bar{d})(x + L) = +(d\bar{d})(x)$
  i.e. periodic BCs with minimum momentum 0. However...
- Wigner-Eckart theorem (in SU(2) isospin):
  \[ \langle (\pi^+\pi^0)_{I=2} | Q^{\Delta I_z=1/2} | K^+ \rangle = \frac{\sqrt{3}}{2} \langle (\pi^+\pi^+)_{I=2} | Q^{\Delta I_z=3/2} | K^+ \rangle \]
- APBCs on d-quark break isospin symmetry allowing mixing between isospin states: however $\pi^+\pi^+$ is the only charge-2 state hence it cannot mix.
Results

- RBC & UKQCD recently published (arXiv:1111.1699) calculation of $\Delta I = 3/2$ decay using:
  - 2+1f domain wall fermions on a $32^3 \times 64 \times 32$ lattice with $a^{-1} = 1.37(1)$ GeV.
  - Near physical pions: $m^{PQ}_\pi \sim 140$ MeV, $m^{uni}_\pi \sim 170$ MeV
  - (Nearly) energy conserving decays: $p = \sqrt{2\pi}/L$ gave $E_{\pi\pi} = 486$ MeV vs. $m_K = 506$ MeV
- Determined
  \[
  \text{Re}A_2 = \left[1.436(62)_{\text{stat}}(258)_{\text{sys}}\right] \times 10^{-8} \text{ GeV}
  \]
  \[
  \text{Im}A_2 = -\left[6.83(51)_{\text{stat}}(1.30)_{\text{sys}}\right] \times 10^{-8} \text{ GeV}
  \]
- Large systematic error: 15% discretization error: continuum limit needed. 7% FV corrections, 6% renormalization and 8% from PT truncation of Wilson coeffs.
- New ensembles have since been generated which will substantially reduce systematics.
Computational challenges of $\Delta I = 1/2$ calculation

- Measuring $A_0$ is considerably more challenging.
- Measure both $K^0 \rightarrow \pi^+ \pi^-$ and $K^0 \rightarrow \pi^0 \pi^0$.
- $\pi\pi$ state has vacuum quantum numbers, hence there are disconnected diagrams:

```
  1  2  3  4
  0  D  t  4

  1  2  3  4
  0  C  t  4

  1  2  3  4
  0  R  t  4

  1  2  3  4
  0  V  t  4
```

- Need large statistics and many source positions but with modern hardware (e.g. IBM BlueGene/Q machines codeveloped with members of RBC/UKQCD) we can now perform such calculations with large enough physical volumes.
**Obtaining physical kinematics in the \( \Delta I = 1/2 \) calculation**

- Must measure \( K^0 \rightarrow \pi^+\pi^- \) and \( K^0 \rightarrow \pi^0\pi^0 \)
- Wigner-Eckart trick cannot be used for \( I = 0 \) final state
- If we stay with APBC on d-quarks, isospin-breaking would allow mixing between \( I = 0 \) and \( I = 2 \) final states.
- Require moving \( \pi^0 \), but momentum cancels in \( \bar{d}d \)
- Need to apply BCs that commute with isospin and produce moving \( \pi^0 \) as well as \( \pi^+ \) and \( \pi^- \).
- G-parity boundary conditions satisfy these criteria.
**G-Parity Boundary Conditions**

- G-parity is a charge conjugation followed by a 180 degree isospin rotation about the y-axis:
  \[ \hat{G} = \hat{C} e^{i \pi \hat{I}_y} : \quad \hat{G} |\pi^{\pm}\rangle = -|\pi^{\pm}\rangle \]
  \[ \hat{G} |\pi^0\rangle = -|\pi^0\rangle \]

- Pions are all eigenstates with e-val -1, hence G-parity BCs make pion wavefunctions antiperiodic, with minimum momentum \( \pi/L \).

- G-parity commutes with isospin.

- At the quark level:
  \[ \hat{G} \begin{pmatrix} u \\ d \end{pmatrix} = \begin{pmatrix} -Cd^T \\ C\bar{u}^T \end{pmatrix} \quad \text{where} \quad C = \gamma^2 \gamma^4. \]

- Requires extensive code modifications to treat two flavours that mix at the boundary.

References:
Gauge Field Boundary Conditions

- Dirac operator for $C\bar{U}^T$ field involves conjugate links $U^*$.
- As this field transitions seamlessly to the $d$-field at the boundary, the links must also transition from $U$ to $U^*$, i.e. links obey complex conjugate BCs (equiv to charge conjugation BCs).
- Boundary link gauge transformation is unusual:
  \[ U_\mu(L - 1) \rightarrow V^\dagger(L - 1)U_\mu(L - 1)V^*(0) \]
- Necessitates generation of new ensemble of gauge links satisfying these BCs.

(Note: for other choices of BC, e.g. APBC, new ensembles would still need to be generated, but due to presence of disconnected diagrams)
**Unusual Contractions**

- Flavor mixing at boundary allows contraction of up and down fields:
  \[ g_{y,x}^{(2,1)} = C \bar{u}_y^T d_x , \]
  \[ g_{x,y}^{(1,2)} = -d_x u_y^T C^T \]

- Interpret as boundary creating/destroying flavor (violating baryon number)

- More Wick contractions to evaluate.

- Some states mix at the boundary, e.g.
  \[ uud \leftrightarrow \bar{d}d\bar{u} \]

  hence the proton is not an eigenstate.
Kaons

- $K \rightarrow \pi \pi$ calculation needs stationary $K^0$.
- Need an eigenstate with e-val +1 for periodic BCs and hence $p_{\text{min}} = 0$.
- $K^0 = \bar{s}d$ is not a G-parity eigenstate: $\bar{s}d \leftrightarrow \bar{s}u$
- Introduce 'strange isospin' ($I'$): s-quark in doublet
- Can now form an eigenstate:
  \[ K^g_0 = \frac{1}{\sqrt{2}}(\bar{s}d + \bar{u}s') = \frac{1}{\sqrt{2}}(K_0 + K'_0) \]
  with e-val +1.
- Unphysical partner $K'_0$ mixes with physical state $K_0$. For a physical operator, e.g. $A_\mu = \bar{s}\gamma^5\gamma^\mu d$, $K'_0$ only contributes after propagating through the boundary: suppressed like $e^{-m_K L}$, a sub-% effect.
- Up to these effects, only change is a normalization factor.
Locality

- Theory has one too many flavors. Must take square-root of \( s'/s \) determinant in evolution to revert to 3 flavors.
- Determinant becomes non-local, violating a necessary condition for formal analytic continuation of Euclidean results to Minkowski (Osterwalder-Schrader theorem).
- Non-locality is however only a boundary effect that vanishes as \( L \to \infty \). With sufficiently large volumes the effect should be benign.
- Estimate size of effect: Staggered ChPT?
Results: Pion Dispersion Relation

- Generated $16^3 \times 32$ fully dynamical test ensembles with $G$-parity BCs in 0,1,2 directions.

\[ a^{-1} = 1.73(3) \text{ GeV} \]

\[ m_\pi \sim 420 \text{ MeV} \]
**Results: Kaon Dispersion Relation**

- Stationary kaon states demonstrated:
Results: $B_K$

- $\bar{K}^0 \leftrightarrow K^0$ mixing amplitude shown to be independent as expected. These 4-quark effective vertices are similar to those used in $K \rightarrow \pi\pi$ calculation, hence this is a valuable demonstration.
**Ensemble for physical $K \to (\pi\pi)_{I=0}$ calculation**

- Evolution code (CPS+BFM) for Mobius DW and Iwasaki+DSDR gauge action with G-parity BCs is now complete.

- Generation of $32^3 \times 64 \times 16$ configurations has been underway for over a month on the USQCD BGQ half-rack at BNL. Will soon have enough thermalized configurations to begin testing.

- Parameters are the same as the ensemble used for the $\Delta I = 3/2$ calculation: $\beta = 1.75$ ($a^{-1} = 1.37(1) \text{ GeV}$) and $m_\pi = 143(1) \text{ MeV}$ (PQ), $171(1) \text{ MeV}$ (unitary)

- Mobius parameters tuned to match to regular DWF, allows factor of 2 reduction in Ls for same physics.

- Dirac matrix is intrinsically 2-flavor, hence $\det(M^\dagger M)$ contains 4 flavors: must use RHMC even for light quarks.

- RHMC cost overhead (no chronological inverter) makes using multiple Hasenbusch steps more expensive. Ensemble is more difficult to tune.
More precise measurements of $\Delta I = 3/2$ amplitude will soon be completed.

Substantial progress has been made in the march towards calculating the $\Delta I = 1/2$ amplitude.

Further investigation of systematic errors associated with G-parity technique is required. However all tests to date have not indicated any sicknesses with the approach.

Work still to be done in deciding best technique for measuring disconnected diagrams in the more complex environment of the calculation with G-parity.

G-parity techniques may be useful for controlling errors in other frontier calculations performed by RBC & UKQCD, e.g. $K_L - K_S$ mass difference.
Extra Slides
Layout of the Problem

- Two fermion fields on each site indexed by flavor index:
  \[ \psi^{(1)}(x) = d(x), \quad \psi^{(2)}(x) = C\bar{u}^T(x) \]
- BCs are:
  \[ \psi^{(1)}(x + L\hat{y}) = \psi^{(2)}(x), \]
  \[ \psi^{(2)}(x + L\hat{y}) = -\psi^{(1)}(x), \]
- Periodic BCs in other dirs.
- Single U-field shared by both flavors, with complex conj BCs.
- Dirac op for \( \psi^{(2)} \) uses \( U^*_\mu \).
Exploiting the Gauge-Field Symmetry

- Quark fields interact with the same gauge fields. Suggests propagators are related in some way.

- In fact, we find that:
  \[ G_{x,z}^{(2,2)} = -\gamma^5 C \left[ G_{x,z}^{(1,1)} \right]^\dagger C \gamma^5 \]
  \[ G_{x,z}^{(1,2)} = +\gamma^5 C \left[ G_{x,z}^{(2,1)} \right]^\dagger C \gamma^5 \]

- Relative sign due to \(-\) sign at boundary between \(u\) and \(d\).

- Can be rewritten \( G_{x,z} = \gamma^5 C \sigma_1 \sigma_3 [G_{x,z}]^\dagger \sigma_3 \sigma_1 C^\dagger \gamma^5 \) where are 2x2 flavour (also spin/colour) matrices.

- Substantially simplifies contractions: form is often identical to standard form up to additional flavour matrices: e.g.

  \[ \langle \pi(x) | \pi(y) \rangle = \text{tr} \ G_{x,y} \sigma_3 G_{x,y}^\dagger \] (in large time limit)

  \[ F_1 = \frac{1}{2} (1 - \sigma_3) \]

  Usually \( \text{tr} \ G_{x,y} G_{x,y}^\dagger \)
The One-Flavor Method

- Obtain equivalent formulation by unwrapping flavor indices onto two halves of doubled lattice:
  - Antiperiodic boundary conditions in G-parity direction.
  - $U$ -field on first half and $U^*$-field on second half.
Choosing an Approach

- One flavor setup is much easier to implement.
- However recall that we needed APBC in 2 directions for physical kinematics in $\Delta I = 3/2$ calculation.
- $G$-parity in >1 dir using one-flavor method requires doubling the lattice again, which is highly inefficient.
- A second approach requires non-nearest neighbour communication:
  - Also inefficient depending on machine architecture.
  - Choose to implement two-flavor method.
K $\rightarrow \pi \pi$ Decays on the Lattice

- Energies are discretized in finite-volume.
- For two non-interacting pions $E_{\pi\pi} = 2\sqrt{m_\pi^2 + k_\pi^2}$, where components of $k_\pi$ discretized in units of $2\pi/L$ assuming periodic BCs.
- Interactions shift the allowed energies such that $k_\pi$ are not known a priori and must be measured.
- Allowed $k_\pi$ are quantized by Luscher condition $\delta(k_\pi) + \phi(k_\pi) = n\pi$, hence we can determine the scattering phase shifts $\delta(k_\pi)$ once $k_\pi$ is measured.
- Switching on effective weak interaction $H_W$, allowed energies are further modified:

$$k - k_\pi = \Delta k = \pm \frac{m_K}{4k_\pi} |M| + O(|M|^2)$$

- Note this uses degenerate PT, thus requires $E_{\pi\pi} = m_K$.
Decays on the Lattice

- Switching on $H_W$ induces corresponding change in infinite-volume scattering lengths:

$$\Delta \delta_0 = \pm \frac{k_\pi |A|^2}{32\pi m^2 K |M|} + O(H^2_W)$$

- Imposing Luscher factor allows us to combine equations for $\Delta \delta_0$ and $\Delta k$, giving the Lellouch-Luscher formula:

$$|A|^2 = 8\pi \left\{ q \frac{\partial \phi}{\partial q} + k \frac{\partial \delta_0}{\partial k} \right\}_{k=k_\pi} \left( \frac{m_K}{k_\pi} \right)^3 |M|^2$$

where $q = kL/2\pi$

- As $\phi$ is analytic, only unknown is $\partial \delta_0 / \partial k$. We measure this from the phenomenological curve at the measured $k_\pi$. 
\(K \rightarrow \pi\pi\) Decays on the Lattice

- Infinite-volume S-matrix \(\langle \pi\pi|L_W|K\rangle = Ae^{i\delta_0}\) final state scattering induces dependence on s-wave scattering length \(\delta_0\).

- Finite-volume matrix element: \(M = \langle \pi\pi|H_W|K\rangle\) where \(H_W\) is effective weak vertex.

- Using degenerate PT (requires \(E_{\pi\pi} = m_K\), weak effective theory and Luscher's quantization condition
  \[\delta(k_\pi) + \phi(k_\pi) = n\pi\]
  \[E_{\pi\pi} = 2\sqrt{m_\pi^2 + k_\pi^2}\]
  one obtains the Lellouch-Luscher formula relating them:
  \[|A|^2 = 8\pi \left\{ q \frac{\partial \phi}{\partial q} + k \frac{\partial \delta_0}{\partial k} \right\}_{k = k_\pi} \left( \frac{m_K}{k_\pi} \right)^3 |M|^2\]
  where \(q = kL/2\pi\)

- As \(\phi\) is analytic, only unknown is \(\partial \delta_0/\partial k\). We measure this from the phenomenological curve at the measured \(k_{\pi}\)
Moving kaon?

- One possibility is to consider a moving kaon $K(p_K)$ decaying to $\pi(p_\pi)\pi(0)$. Need\[ \sqrt{m_K^2 + p_K^2} \approx \sqrt{m_\pi^2 + p_\pi^2} + m_\pi \]
- $\sim 780$ MeV energy required.
- SNR decreases exponentially in the energy difference between the state energy and the pion mass: this will be too noisy.
Finite-volume lattice decay amplitudes are related to those in the infinite-volume by the "Lellouch-Luscher" formula.

This requires physical kinematics and need moving pions. However ground state comprises stationary pions.

Could attempt to tune L such that first excited state energy matches kaon mass.

This will be extremely noisy, and, especially when there are disconnected diagrams, it is highly unlikely that a decent signal could be extracted.
Force Histogram

- Example force histogram produced during evolution tuning