Progress in calculating multiparticle amplitudes from lattice QCD

Steve Sharpe
University of Washington
Dreams of a lattice theorist
Observation of $CP$ violation in charm decays

LHCb collaboration

Abstract

A search for charge-parity $CP$ violation in $D^0 \rightarrow K^- K^+$ and $D^0 \rightarrow \pi^- \pi^+$ decays is reported, using $pp$ collision data corresponding to an integrated luminosity of 6 fb$^{-1}$ collected at a center-of-mass energy of 13 TeV with the LHCb detector. The flavor of the charm meson is inferred from the charge of the pion in $D^*(2010)^+ \rightarrow D^0 \pi^+$ decays or from the charge of the muon in $B \rightarrow D^0 \mu^- \bar{\nu}_\mu X$ decays. The difference between the $CP$ asymmetries in $D^0 \rightarrow K^- K^+$ and $D^0 \rightarrow \pi^- \pi^+$ decays is measured to be $\Delta A_{CP} = [-18.2 \pm 3.2 \text{ (stat.)} \pm 0.9 \text{ (syst.)}] \times 10^{-4}$ for $\pi$-tagged and $\Delta A_{CP} = [-9 \pm 8 \text{ (stat.)} \pm 5 \text{ (syst.)}] \times 10^{-4}$ for $\mu$-tagged $D^0$ mesons. Combining these with previous LHCb results leads to

$$\Delta A_{CP} = (-15.4 \pm 2.9) \times 10^{-4},$$

where the uncertainty includes both statistical and systematic contributions. The measured value differs from zero by more than five standard deviations. This is the first observation of $CP$ violation in the decay of charm hadrons.

5.3σ effect
What we want...

\[ \pi^+ \rightarrow u \rightarrow \bar{d} \rightarrow \mathcal{H}_W \rightarrow c \rightarrow D^0 \]

out-state \hspace{1.5cm} in-state

\[ \pi^- \rightarrow \bar{d} \rightarrow d \rightarrow u \rightarrow \bar{u} \]

Minkowski time

gluons & sea-quark loops implicit
What we want...

out-state

\[ \pi^+ \quad \bar{d} \quad u \]

\[ \pi^- \quad d \quad \bar{u} \]

in-state

\[ \mathcal{H}_W \quad c \quad D^0 \]

Minkowski time

gluons & sea-quark loops implicit
What we want…

\[
\begin{align*}
\pi^+ & \rightarrow u \\
\bar{d} & \rightarrow \pi^-
\end{align*}
\]

\[
\begin{align*}
q & \rightarrow \mathcal{H}_W \\
\bar{u} & \rightarrow c \\
D^0 & \rightarrow \text{in-state}
\end{align*}
\]

Minkowski time

S. Sharpe, "Progress in multiparticle amplitudes from the lattice," LNS colloquium, MIT, 5/8/23
What we want...

\[
\pi^+ \rightarrow u \rightarrow \pi^- + \bar{d} \rightarrow \pi^+ - \bar{u} + \bar{d} + \bar{u} \rightarrow \pi^- + \bar{d} - \bar{u} + \bar{d} - \bar{u} \rightarrow \pi^+ - \bar{d} + \bar{u} - \bar{d} + \bar{u} \rightarrow \pi^- + \bar{d} - \bar{u} + \bar{d} - \bar{u} \rightarrow \pi^+ - \bar{d} + \bar{u} - \bar{d} + \bar{u} \]

Minkowski time
…what we might achieve

Finite volume
Lattice QCD
(LQCD) calculations

S. Sharpe, "Progress in multiparticle amplitudes from the lattice," LNS colloquium, MIT, 5/8/23
Problems

- No in- and out-states in finite volume
  - Cannot separate final-state particles
- Need to analytically continue from Euclidian to Minkowski momenta
  - Ill-posed problem given discrete momenta in finite volume
What LQCD can determine are finite-volume matrix elements:

\[ L \langle E_n | \mathcal{H}_W | D_0 \rangle_L \]

Physical quantities if choose \( E_n(L) = E_D \)

Discrete spectrum of states with quantum numbers of \( \pi^+ \pi^- \)
Rephrasing

What LQCD can determine are finite-volume matrix elements:

$L \langle E_n | \mathcal{H}_W | D^0 \rangle_L$

Physical quantities if choose $E_n(L) = E_D$

LQCD methods could, in the near future, allow the calculation of these quantities

How can they be related to the physical decay amplitudes?
The fundamental issue

\[ L\langle E_n | \mathcal{H}_W | D^0 \rangle_L \rightarrow_{\text{out}} \langle \pi^+ \pi^- | \mathcal{H}_W | D^0 \rangle_{\text{in}} \]

- This is a nontrivial (and so-far unsolved) QFT problem because \(|E_n\rangle_L\) are composed of contributions from \(\pi\pi, 4\pi, K\bar{K}, 6\pi, \ldots\) with \(j = 0, 2, \ldots\)
  - Even if you use a two-pion operator, the strong interactions unavoidably lead to mixing with other states
  - Solution will require amplitudes for \(\pi\pi \rightarrow \pi\pi, 3\pi \rightarrow 3\pi, \pi\pi \rightarrow 4\pi, \ldots\), which will need to be determined from the energies \(E_n(L)\)
The fundamental issue

\[ L\langle E_n | \mathcal{H}_W | D^0 \rangle_L \longrightarrow \text{out} \langle \pi^+ \pi^- | \mathcal{H}_W | D^0 \rangle_{\text{in}} \]

- This is a nontrivial (and so-far unsolved) QFT problem because \( |E_n\rangle_L \) is composed of contributions from \( \pi\pi, 4\pi, K\bar{K}, 6\pi, \ldots \) with \( j = 0, 2, \ldots \)

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  - A solution will require amplitudes for \( \pi\pi \rightarrow \pi\pi, 3\pi \rightarrow 3\pi, \pi\pi \rightarrow 4\pi, \ldots \), which will need to be determined from the energies \( E_n(L) \)

  - A side benefit of any solution will be the ability to use LQCD results for \( E_n(L) \) to study resonances with decays into multiple two-, three- and four-particle channels

Over the last 10 years, the corresponding issues for three particles have been solved, and are beginning to be implemented in LQCD simulations

Today I will briefly summarize the status, and describe examples of recent work
Outline

• Further motivation for studying 3-particle resonances & decays

• History and status of finite-volume formalism for 2 & 3 particles

• Examples of recent work
  • Extraction of $\pi^+\pi^+K^+ \rightarrow \pi^+\pi^+K^+$ and $K^+K^+\pi^+ \rightarrow K^+K^+\pi^+$ K-matrices using LQCD with close to physical quark masses
  • NLO Chiral PT calculation of three-particle K matrix

• Summary & Outlook
Motivations for studying three particles using LQCD
Cornucopia of exotics

62 new hadrons at the LHC

[I. Danilkin, talk at INT workshop, March 23]

+ data from Babar, Belle, COMPASS, …

S. Sharpe, "Progress in multiparticle amplitudes from the lattice," LNS colloquium, MIT, 5/8/23
Motivations

- Most resonances have 3 (or more) particle decay channels
  - $\omega(782, I^GJ^{PC} = 0^-1^{--}) \rightarrow 3\pi$
  - $N(1440, J^P = \frac{1^+}{2}) \rightarrow N\pi, N\pi\pi$
  - $T_{cc}(3875, I = 0, J^P = 1^+?) \rightarrow D^0D^0\pi^+$

- Determining 3-body “forces”
  - NNN interactions needed as input for EFT treatments of large nuclei, and for the neutron-star equation of state
  - $\pi\pi\pi, \pi K\bar{K}, \ldots$ interactions needed as input to study pion & kaon condensation
History & status of finite-volume formalism for 2 particles
Sketch of history for two particles

- 1961: Discovery of the $\rho$ meson
Sketch of history for two particles

- 1961: Discovery of the $\rho$ meson
- 1986/91: Lüscher derived “two-particle quantization condition” (QC2)

$F$ is a known kinematical “zeta-function”, depending on the box shape

$\mathcal{H}_2 \sim \tan \delta / q$

Valid up to $e^{-ML}$ corrections

$\det \left[ F(E, P, L)^{-1} + \mathcal{H}_2(E^*) \right] = 0$

Matrices in $\ell, m$

Discrete energy spectrum
- e.g. $\pi \pi$ with $E_{CM} < 4M_\pi$

Scattering amplitude
Sketch of history for two particles

- **1961**: Discovery of the $\rho$ meson
- **1986/91**: Lüscher derived “two-particle quantization condition” (QC2)
  - 2005: Kim, Sachrajda & SRS — alternate derivation, basis for many subsequent generalizations
- **1999**: Measurement of $\varepsilon' / \varepsilon = 16.1(2.3) \times 10^{-4}$ by KTeV/NA48 — direct CPV in $K \rightarrow \pi\pi$

NA48 @ CERN: Cern website
Sketch of history for two particles

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• 2001: Lellouch & Lüscher (LL): relation between $L\langle E_n(\pi\pi) | \mathcal{H}_W | K \rangle_L$ and $\mathcal{A}(K \to \pi\pi)$
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- 2014 - 2019: LQCD implementation of QC2 for the $\rho$ resonance in $\pi\pi$ scattering (and many other resonances subsequently)

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**Figure 2**: Top row: Comparison of $\sim K \to \pi\pi$ between the C101 and D101 ensembles, which have the same parameters but different physical volumes.

Bottom row: The same comparison for the $N_{200}$ and $N_{401}$ ensembles (white and gray markers respectively), which have (approximately) the same quark masses but different lattice spacings.

Anderson et al., 1808.05007

$M_\rho \approx 200$ MeV

$M_\rho \approx 280$ MeV
Sketch of history for two particles

- 1961: Discovery of the $\rho$ meson
- 1986/91: Lüscher derived “two-particle quantization condition” (QC2)
  - 2005: Kim, Sachrajda & SRS — alternate derivation, basis for many subsequent generalizations
- 1999: Measurement of $\epsilon'/\epsilon = 16.1(2.3)10^{-4}$ by KTeV/NA48 — direct CP in $K \rightarrow \pi\pi$
- 2001: Lellouch & Lüscher (LL): relation between $L\langle E_n(\pi\pi) | H_W | K\rangle_L$ and $A(K \rightarrow \pi\pi)$
- 2014 - 2019: LQCD implementation of QC2 for the $\rho$ resonance in $\pi\pi$ scattering
- 2020: LQCD calculation of $\epsilon'/\epsilon = 21.7(8.4)10^{-4}$ in the standard model using LL method with physical quark masses and (almost) all errors controlled

Direct CP violation and the $\Delta I = 1/2$ rule in $K \rightarrow \pi\pi$ decay from the standard model

R. Abbott,¹ T. Blum,² ³ P. A. Boyle,⁴ ⁵ M. Bruno,⁶ N. H. Christ,¹ D. Hoying,³ ² C. Jung,⁴ C. Kelly,⁶ ⁴ C. Lehner,⁷ ⁴ R. D. Mawhinney,¹ D. J. Murphy,⁸ C. T. Sachrajda,⁹ A. Soni,⁴ M. Tomii,⁷ and T. Wang¹

(RBC and UKQCD Collaborations)

S. Sharpe, “Progress in multiparticle amplitudes from the lattice,” LNS colloquium, MIT, 5/8/23
History & status of finite-volume formalism for 3 particles
Sketch of history for three particles

- [Beane, Detmold, Savage et al. 07-11] studied ground state energies of $N\pi^+, MK^+, N\pi^+ + MK^+$ systems, and determined 3-particle interactions for particles at rest

- [Polejaeva & Rusetsky 12] showed in NREFT that 3 body spectrum determined by $2 \rightarrow 2 \& 3 \rightarrow 3$ infinite-volume scattering amplitudes

- [Hansen & SRS 14, 15] derived quantization condition (QC3) for 3 identical scalars in generic, relativistic EFT, working to all orders in Feynman-diagram expansion, keeping all angular momenta—“RFT approach”

- [Hammer & Rusetsky 17] derived QC3 using NREFT—greatly simplified derivation

- [Mai & Döring 17] obtained QC3 using unitary, relativistic representation of $3 \rightarrow 3$ amplitude—“FVU approach”

- [Blanton & SRS 20] showed equivalence of RFT & FVU approaches

- [Hansen, Romero-López, SRS 21] derived formalism for determining $K \rightarrow 3\pi$ amplitude
Additional issues with 3 particles

- Energy shifts $\Delta E_n = E_n - E_{n,\text{free}} \sim 1/L^3$
- Scattering amplitude in each partial wave, at given $E_{\text{CM}}$, is a (complex) number

(For simplicity, assume G-parity-like $Z_2$ symmetry, so no $2 \leftrightarrow 3$ transitions; formalism can be generalized)

- Dominant contribution from pairwise interactions, $\Delta E_n \sim 1/L^3$
- 3-particle interactions give subleading contributions $\propto 1/L^6$
- Scattering amplitude $M_3$ at given $E_{\text{CM}}$, is a (complex) function of Dalitz-plot variables, and incorporates final-state interactions
- $M_3$ has divergences for physical momenta
Structure of the result \((Z_2\) symmetry)
Two-step method

2 & 3 particle Spectra from LQCD

Quantization conditions

\[ QC2: \det \left[ F^{-1} + \mathcal{K}_2 \right] = 0 \]
\[ QC3: \det \left[ F_3^{-1} + \mathcal{K}_{df,3} \right] = 0 \]

Integral equations in infinite volume

Incorporates initial- and final-state interactions

Intermediate infinite-volume K matrix:
A short-distance, real, three-particle interaction free of unitary cuts, and with physical divergences subtracted; unphysical since depends on cutoff

Scattering amplitude \( M_3 \)

Infinite-volume K matrix:
Obtained from Feynman diagrams using PV prescription for poles; Real, free of unitary cuts

[These are the RFT forms, and assume \( \mathbb{Z}_2 \) symmetry]
Further details of QC3

\[ \text{det} \left[ F^{-1}_3 + \mathcal{H}_{df,3} \right] = 0 \]

- Derived by determining power-law volume dependence of finite-volume 3-particle correlation functions to all orders in a skeleton expansion in a generic relativistic EFT

- Volume dependence arises from 3-particle cuts

- \( F_3 \) contains two-particle interactions (\( \mathcal{H}_2 \)) and kinematic functions (F & G)

\[
F_3 = \frac{1}{2\omega L^3} \left[ \frac{F}{3} - F \frac{1}{\mathcal{H}_2^{-1}} + F + G \right]
\]
Status: formalism

- 3 identical spinless particles [Hansen, SRS; Hammer, Pang, Rusetsky; Mai, Döring]
- Mixing of two- and three-particle channels for identical spinless particles [Briceño, Hansen, SRS]
- 3 degenerate but distinguishable particles, e.g. 3\pi with isospin 0, 1, 2, 3 [Hansen, Romero-López, SRS]
- 3 nondegenerate particles, e.g. \( D^+_s D^0 \pi^- \) [Blanton, SRS]
- (Single-channel) 2+1 systems, e.g. \( \pi^+ \pi^+ K^+ \) [Blanton, SRS]
- 3 identical spin-\( \frac{1}{2} \) particles, e.g. 3 neutrons [Draper, Hansen, Romero-López, SRS]

<table>
<thead>
<tr>
<th>Resonance</th>
<th>( I_{\pi\pi} )</th>
<th>( J^P )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \omega(782) )</td>
<td>0</td>
<td>1^-</td>
</tr>
<tr>
<td>( h_1(1170) )</td>
<td>0</td>
<td>1^+</td>
</tr>
<tr>
<td>( \omega_3(1670) )</td>
<td>0</td>
<td>3^-</td>
</tr>
<tr>
<td>( \pi(1300) )</td>
<td>1</td>
<td>0^-</td>
</tr>
<tr>
<td>( a_1(1260) )</td>
<td>1</td>
<td>1^+</td>
</tr>
<tr>
<td>( \pi_1(1400) )</td>
<td>1</td>
<td>1^-</td>
</tr>
<tr>
<td>( \pi_2(1670) )</td>
<td>1</td>
<td>2^-</td>
</tr>
<tr>
<td>( a_2(1320) )</td>
<td>1</td>
<td>2^+</td>
</tr>
<tr>
<td>( a_4(1970) )</td>
<td>1</td>
<td>4^+</td>
</tr>
</tbody>
</table>

Many resonances can now be studied!
Status: applications

[References at end of slides]

- $3\pi^+$: determined parameters in threshold expansion of $\mathcal{H}_{df,3}$, including pair interactions in s- and d-waves; integral equations solved for s-wave interactions only

- $3K^+$: determined s- and d-wave parameters in $\mathcal{H}_{df,3}$

- $\phi^4$: extracted $\mathcal{H}_{df,3}$ in single-scalar theory; extracted 3-particle resonance parameters in two-scalar theory, using RFT and FVU approaches

- $3\pi$ with $I = 1$: first study of $a_1(1260)$ with formalism based on 2 levels; solved integral equations in FVU approach

- $\pi^+\pi^+K^+$ & $K^+K^+\pi^+$: determined s- and p-wave parameters in $\mathcal{H}_{df,3}$; found evidence for small discretization effects

- Integral equations solved for complex energies for simple system with near-unitary two-particle interactions and Efimov states (bound or resonant)

- ChPT: LO results for $3\pi^+$, $\pi^+\pi^+K^+$, $K^+K^+\pi^+$, $3K^+$, including $a^2$ effects: agree in rough magnitude but not in detail with results from LQCD calculations

- ChPT: NLO result for $3\pi^+$; greatly improves agreement with LQCD results

S. Sharpe, “Progress in multiparticle amplitudes from the lattice,” LNS colloquium, MIT, 5/8/23
\[ \pi^+ \pi^+ K^+ \text{ and } K^+K^+\pi^+ \]

amplitudes using LQCD

[Draper, Hanlon, Hörz, Morningstar, Romero-López & SRS, 2302.13587 (JHEP)]

A step on the way to \( T_{cc} \rightarrow DD\pi, \) etc.
Consider multiparticle system with weakly repulsive interactions—pions and kaons at maximal isospin ($2\pi^+/3\pi^+$, $2K^+/3K^+$, $2\pi^+/\pi^+K^+/3K^+$, $2K^+/\pi^+K^+/3K^+$)

- No resonances in two-particle subchannels or in three-particle system
- Simultaneously fit to several spectra; for example, to obtain the $\pi^+\pi^+K^+$ interaction need:
Consider multiparticle system with weakly repulsive interactions—pions and kaons at maximal isospin ($2\pi^+/3\pi^+, 2K^+/3K^+, 2\pi^+\pi^+K^+/3K^+, 2K^+\pi^+K^+/3K^+$)

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$$2\pi^+ + \pi^+ + \pi^+ + K^+ + K^+ + \pi^+ + K^+ + K^+ + \pi^+ + K^+ + K^+ + \pi^+$$

- Parametrize $\mathcal{K}_{df,3}$ (and $\mathcal{K}_2$) as the most general smooth function consistent with particle interchange, time-reversal and parity symmetries, using an expansion about threshold
  - Generalization of the effective-range expansion for $\mathcal{K}_2$; here keep first two terms
  - $s$-wave interactions in $\pi^+\pi^+$ (sub)channel, $s$- and $p$-wave in $\pi^+K^+$; 9 or 10 parameters in all
Lattices used in pilot calculation

- Improved Wilson fermions at $a = 0.064$ fm (CLS lattices)

<table>
<thead>
<tr>
<th></th>
<th>$(L/a)^3 \times (T/a)$</th>
<th>$M_\pi$ [MeV]</th>
<th>$M_K$ [MeV]</th>
<th>$N_{cfg}$</th>
<th>$t_{src}/a$</th>
<th>$N_{ev}$</th>
<th>dilution</th>
<th>$N_r(\ell/s)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>N203</td>
<td>$48^3 \times 128$</td>
<td>340</td>
<td>440</td>
<td>771</td>
<td>32, 52</td>
<td>192</td>
<td>(LI12, SF)</td>
<td>6/3</td>
</tr>
<tr>
<td>D200</td>
<td>$64^3 \times 128$</td>
<td>200</td>
<td>480</td>
<td>2000</td>
<td>35, 92</td>
<td>448</td>
<td>(LI16, SF)</td>
<td>6/3</td>
</tr>
</tbody>
</table>

D200 configurations

$L = 4.1$ fm

$M_\pi L = 4.1$

$M_K L = 10$
Example of fit

\[ \frac{E_{\text{CM}}}{M_{\pi}} \]

\[ \frac{E^*}{M_{\pi}} \]

N203 \( \pi^+ \pi^+ K^+ \)

Simultaneous fit to 27 \( \pi^+ \pi^+ \), 19 \( \pi^+ K^+ \), & 36 \( \pi^+ \pi^+ K^+ \) levels with 9 parameters

\[ \chi^2/\text{DOF} = 119/(82 - 9) \]
Fit is to lab-frame shifts

Simultaneous fit to 28 $K^+K^+$, 16 $\pi^+K^+$, & 29 $K^+K^+\pi^+$ levels with 10 parameters on D200: $\chi^2$/DOF = 162/(73 – 10)
Results: scattering lengths

\begin{equation}
L_{ri}(\mu^2) = L_{ri}(\mu_1) + i \frac{16}{\pi^2} \ln \left( \frac{\mu_1}{\mu_2} \right), \tag{5.2}
\end{equation}

with \(5 = 3/8\), we find that the result from our fit yields \(L_5(770 \text{ MeV}) = 1.0(1.5) \cdot 10^{-3}\). Varying the choice of \(F_{fi}\) to take for the initial scale (using the physical value of \(F_{fi}\), or the value on either of the ensembles) leads to changes in \(L_5\) that are significantly smaller than the error. Our result for \(L_5\) is in agreement with all values in the literature, although we note that our error is much larger than that in the other values.

![Graph showing results for \(M_{fi}a_{fi}fifi\), \(M_{fi}K_{a}fiK\), and \(M_{K}a_{0}KK\) as a function of \((M_{\pi}/F_{\pi})^2\), with shaded bands showing the uncertainties in the fit.](image)

- 2-particle s-wave scattering lengths are well determined
- All are repulsive and consistent with ChPT
  - Evidence for small discretization errors
Find evidence for attractive p-wave scattering length
- Consistent with dispersive analysis
s-wave contributions to $\mathcal{H}_{\text{df,3}}$

- Evidence for nonzero values ($2 - 5\sigma$)
- Overall effect of $\mathcal{H}_{\text{df,3}}$ is repulsive
- LO ChPT predicts opposite sign (but see later)

S. Sharpe, ``Progress in multiparticle amplitudes from the lattice,” LNS colloquium, MIT, 5/8/23
p-wave contributions to $\mathcal{H}_{df,3}$

- Evidence for nonzero values in some cases
  - $\mathcal{H}_E$ is only contribution of $\mathcal{H}_{df,3}$ to nontrivial irreps
- Appear at NLO in ChPT—prediction not yet available
NLO ChPT results for \( K_{df,3} \) for \( 3\pi^+ \rightarrow 3\pi^+ \)

[Baeza-Ballesteros, Bijnens, Husek, Romero-López, SRS, Sjö, 2303.13206]
2\pi^+/3\pi^+ K matrices vs ChPT

2\pi^+ scattering length

\[ M_{\pi\pi} a_{\pi}^0 \]

\[ (M_\pi/F_\pi)^2 \]

LO ChPT

NLO fit

This work

Physical point

[Results from Blanton, Hanlon, Hörz, Morningstar, Romero-López, SRS, 2106.05590 (JHEP)]

- LO ChPT describes 2-pion sector well
- Large discrepancy in 3-pion sector!
NLO ChPT for $\mathcal{K}_{df,3}$

- Integral equations simplify to:

$$\mathcal{K}_{df,3}^{NLO} = \text{Re} \mathcal{M}_{df,3}^{NLO}$$

- NLO 6-pion amplitude computed in
  - [Bijnens, Husek 2107.06291]
  - [Bijnens, Husek, Sjö, 2206.14212]

- Integral equations simplify to:

$$\mathcal{K}_{df,3}^{NLO} = \text{Re} \mathcal{M}_{df,3}^{NLO}$$

- Bull's-head subtraction

- One-particle-exchange subtraction

- One-particle-irreducible diagrams

- One-particle-exchange diagrams
Threshold expansion for $\mathcal{K}_{df,3}$

- $\mathcal{K}_{df,3}$ is a real, smooth function which is Lorentz, P and T invariant

- Expand about threshold in powers of $\Delta = (s - 9M_\pi^2)/9M_\pi^2$, $\tilde{t}_{ij} = (p'_i - p_j)^2/9M_\pi^2$, ... 

\[
\mathcal{K}_{df,3} = \mathcal{K}_{df,3}^{\text{iso,0}} + \mathcal{K}_{df,3}^{\text{iso,1}} \Delta + \mathcal{K}_{df,3}^{\text{iso,2}} \Delta^2 + \mathcal{K}_A \Delta_A + \mathcal{K}_B \Delta_B + \mathcal{O}(\Delta^3)
\]

- Can separate terms in fit based on dependence on energy and rotational properties

  - E.g. only $\mathcal{K}_B$ contributes to nontrivial irreps

\[
\Delta_B = \sum_{i,j=1}^{3} \tilde{t}_{ij}^2 - \Delta^2
\]
NLO ChPT results for $\mathcal{K}_{df,3}$

\[ \kappa = 1/(16\pi^2) \]

\[
\mathcal{K}_0 = \left( \frac{M_\pi}{F_\pi} \right)^4 18 + \left( \frac{M_\pi}{F_\pi} \right)^6 \left[ -3\kappa(35 + 12 \log 3) - \mathcal{D}_0 + 111L + \ell_{(0)}^r \right], \\
\mathcal{K}_1 = \left( \frac{M_\pi}{F_\pi} \right)^4 27 + \left( \frac{M_\pi}{F_\pi} \right)^6 \left[ -\frac{\kappa}{20}(1999 + 1920 \log 3) - \mathcal{D}_1 + 384L + \ell_{(1)}^r \right], \\
\mathcal{K}_2 = \left( \frac{M_\pi}{F_\pi} \right)^6 \left[ \frac{207\kappa}{1400} (2923 - 420 \log 3) - \mathcal{D}_2 + 360L + \ell_{(2)}^r \right], \\
\mathcal{K}_A = \left( \frac{M_\pi}{F_\pi} \right)^6 \left[ \frac{9\kappa}{560} (21809 - 1050 \log 3) - \mathcal{D}_A - 9L + \ell_{(A)}^r \right], \\
\mathcal{K}_B = \left( \frac{M_\pi}{F_\pi} \right)^6 \left[ \frac{27\kappa}{1400} (6698 - 245 \log 3) - \mathcal{D}_B + 54L + \ell_{(B)}^r \right].
\]

Numerical coefficients depend on cutoff $H(\mathbf{k})$.

$\mu$-dependence cancels.

LECs

$L \equiv \kappa \log (M_\pi^2 / \mu^2)$
Comparison to LQCD

- (Very) large NLO corrections
- Discrepancy with LO ChPT resolved!
- ChPT not trustworthy for $\mathcal{K}_1$
Comparison to LQCD

• $\mathcal{K}_B$ first appears at NLO in ChPT
• Discrepancy may be resolved by NNLO terms?
Summary & Outlook
Summary

- Two-particle sector is entering precision phase
  - Frontier is two nucleons, which are more challenging for LQCD
- Major steps have been taken in the three-particle sector
  - Formalism well established & cross checked, and almost complete
  - Several applications to three-particle spectra from LQCD
  - Initial discrepancy with LO ChPT explained by large NLO contributions
  - Integral equations solved in several cases
  - Path to a calculation of $K \to 3\pi$ decay amplitudes is now open
Example of complete application

\[ M_\pi \approx 390 \text{ MeV}, \quad a \approx 0.12 \text{ fm}, \quad L \approx 2.5 \text{ & } 2.9 \text{ fm} \]

---

\[ E_2(L) \quad E_1(L) \quad E_0(L) \]

\[ \mathcal{K}_{df,3} \quad \mathcal{M}_3 \]

[Hansen, Briceño, Dudek, Edwards, Wilson (HADSPEC collaboration) 2009.04931 PRL 21]

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**FIG. 3.** Top: Dalitz-like plot of \( m_{13}^4 |\mathcal{M}_3|^2 \) for \( \sqrt{s_3} = 3.7m \) with final kinematics fixed to \( \{ p_1'^2, p_2'^2 \} = \{ 0.01 m_\pi^2, 0.7 m_\pi^2 \} \Rightarrow \{ m_{12}', m_{13}' \} = \{ 2.1 m_\pi, 2.25 m_\pi \} \). Bottom: Same total energy, now with incoming and outgoing kinematics set equal, as discussed in the text.
Outlook

- Generalize formalism to broaden applications
  - 3 nucleons with $I = \frac{1}{2}$ (nnp & ppn)
  - $T_{cc}(3875, I = 0, J^P = 1^+?) \rightarrow D^0D^0\pi^+, D^+D^0\pi^0, D^+D^+\pi^-$
  - Accessing the WZW term: $K\bar{K} \leftrightarrow \pi^+\pi^0\pi^-(I = 0)$
  - $N(1440, J^P = \frac{1}{2}^+ ) \rightarrow N\pi, N\pi\pi$
  - $J^{PC}, I^G = 1^{-+}, 1^- : \pi_1(1600) \rightarrow \eta\pi, 3\pi, KK\pi\pi, \eta\pi\pi\pi, 5\pi$

- Extend implementations using LQCD simulations
  - $3\pi^+, 3K^+, \pi^+\pi^+K^+, K^+K^+\pi^+$ at physical quark masses
  - $I=0,1$ three-particle resonances ($\omega, a_1, \ldots$)

- Extend applications of integral equations in the presence of three-particle resonances, e.g. $T_{cc}$

- Move on to 4 particles!
The Exo(tic) Had(ron) Collaboration started in 2023 to explore all aspects of exotic hadron physics, from predictions within lattice QCD, through reliable extraction of their existence and properties from experimental data, to descriptions of their structure within phenomenological models.
Thank you!

Questions?
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Alternate 3-particle approaches

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Formalism to determine $K \to 3\pi$ amplitudes using LQCD

[Hanson, Romero-López & SRS, 2101.10246 (JHEP)]
A much simpler case

\[ L\langle E_n | \mathcal{H}_W | \bar{K}^0 \rangle_L \longrightarrow \text{out} \langle \pi^+ \pi^- | \mathcal{H}_W | \bar{K}^0 \rangle_{\text{in}} \]

- This is a nontrivial (but solved) QFT problem; \( |E_n\rangle_L \) are composed of contributions from \( \pi \pi \) states alone (with \( j > 0 \) highly suppressed) [Lellouch & Lüscher, 01]

- LL formalism shows how to include the effects of final-state interactions that are absent in the finite-volume matrix element
A much simpler case

\[ L \langle E_n | \mathcal{H}_W | \bar{K}^0 \rangle_L \rightarrow \text{out} \langle \pi^+ \pi^- | \mathcal{H}_W | \bar{K}^0 \rangle_{\text{in}} \]

- Alternative form of LL result valid if only s-wave interactions (based on approach of [Briceño, Hansen, Walker-Loud])

\[
\left| \text{out} \langle \pi^+ \pi^- | \mathcal{H}_W | \bar{K}^0 \rangle_{\text{in}} \right|^2 = 2M_K L^6 \left| L \langle E_n | \mathcal{H}_W | \bar{K}^0 \rangle_L \right|^2 \\
\times \left| \frac{1}{1 - i \mathcal{K}_2(E) \rho(E)} \right|^2 \left( \frac{\partial F(E, L)^{-1}}{\partial E} + \frac{\partial \mathcal{K}_2(E)}{\partial E} \right)
\]

- Includes Watson phase
- Known kinematic function
- Determine using QC2 for range of E

S. Sharpe, "Progress in multiparticle amplitudes from the lattice," LNS colloquium, MIT, 5/8/23
Generalization to $K \rightarrow 3\pi$

\[ L\langle E_n \mid \mathcal{H}_W \mid K \rangle_L \rightarrow \text{out} \langle 3\pi \mid \mathcal{H}_W \mid K \rangle_{\text{in}} \]

finite-volume $3\pi$ states

- Needed to allow LQCD calculations of $K \rightarrow 3\pi$ amplitudes, including CP parts
- Important milestone on way to $D \rightarrow \pi\pi, K\bar{K}$
- Method also applies to $\gamma^* \rightarrow 3\pi$ and $\eta \rightarrow 3\pi$
- Piggybacks on our earlier work generalizing QC3 to $3\pi$ states of arbitrary isospin [Hansen, Romero-López & SRS, 2003.10974 (JHEP)]
- Addresses one of the challenges of $D \rightarrow \pi\pi, K\bar{K}$: the incorporation of final-state interactions that rearrange the distribution in the Dalitz plot
Ingredients from LQCD

(1) Finite-volume matrix element: $L\langle E_n | \mathcal{H}_W | K \rangle_L$

(2) $\mathcal{H}_2$ and $\mathcal{H}_{df,3}$ from 2- and 3-particle spectrum for total isospin 0,1,2

Technology exists to calculate in near future
Sketch of method

- Recall two-step method for applying QC3

\[ E_2(L) \quad E_1(L) \quad E_0(L) \]

\[ QC3 \rightarrow K_{df,3} \rightarrow \text{Int. Eqs.} \rightarrow M_3 \]
Sketch of method

- Recall two-step method for applying QC3

\[ E_2(L) \rightarrow QC3 \rightarrow K_{df,3} \rightarrow \text{Int. Eqs.} \rightarrow M_3 \]

- Similar two-step method needed here

\[ L\langle E_n | H_W | K \rangle_L \]
finite-volume matrix element from LQCD

Intermediate infinite-volume, but unphysical, decay amplitude: short-distance quantity free of unitary cusps

\[ \text{out}\langle 3\pi | H_W | K \rangle_{\text{in}} \]

Constraint conditions

\[ A_{PV}^{K3\pi} \]
Infinite-volume integral eqs.

Parametrize enforcing smoothness and symmetries, similarly to \( K_{df,3} \)
Isotropic approximation

- $A_{K3\pi}^{PV}$ and $\mathcal{H}_{df,3}$ are independent of momenta, and $\mathcal{H}_2$ is pure s-wave
  
  - Only a single finite-volume matrix element from LQCD is needed to determine $A_{K3\pi}^{PV}$
  
  - Integral equations still needed, but simplify considerably
  
  - Can combine two steps & give single expression (ignoring isospin)

\[
|T_{K3\pi}^{iso}(E^*, m_{12}^2, m_{23}^2)|^2 = 2E_K(P)L^6 \langle E_n, P, A_1, L | \mathcal{H}_W(0) | K, P, L \rangle^2 \\
\times \left| L^{iso}(E^*, m_{12}^2, m_{23}^2) \frac{1}{1 + \mathcal{H}_{df,3}^{iso}(E^*) F_{3}^{\infty,iso}(E^*)} \right|^2 \left( \frac{\partial F_{3}^{iso}(E, P, L)}{\partial E} \right)^{-1} + \frac{\partial \mathcal{H}_{df,3}^{iso}(E^*)}{\partial E} \right)
\]

Obtain by solving single integral equation involving $\mathcal{H}_2$; incorporates two-particle final-state interactions

Incorporates three-particle final-state interactions

Analog of factor in Lellouch-Lüscher result

Analogous to expression obtained using leading-order non relativistic effective field theory in [Müller & Rusetsky, 2012.13957]

S. Sharpe, “Progress in multiparticle amplitudes from the lattice,” LNS colloquium, MIT, 5/8/23