# Progress in calculating multiparticle amplitudes from lattice QCD



#### Steve Sharpe University of Washington

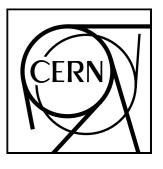


# Dreams of a lattice theorist

### Testing the SM with D decays



# Observation of *CP* violation in charm decays



CERN-EP-2019-042 13 March 2019

LHCb collaboration<sup>†</sup>

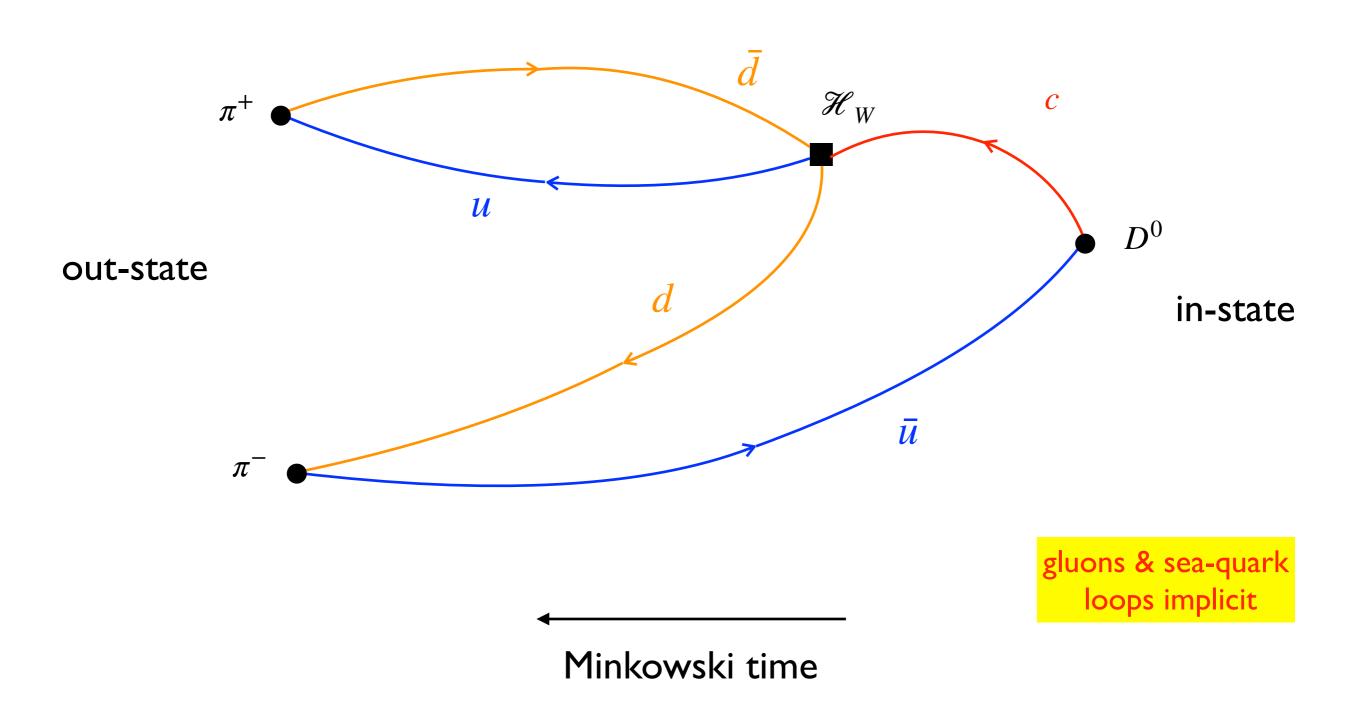
#### Abstract

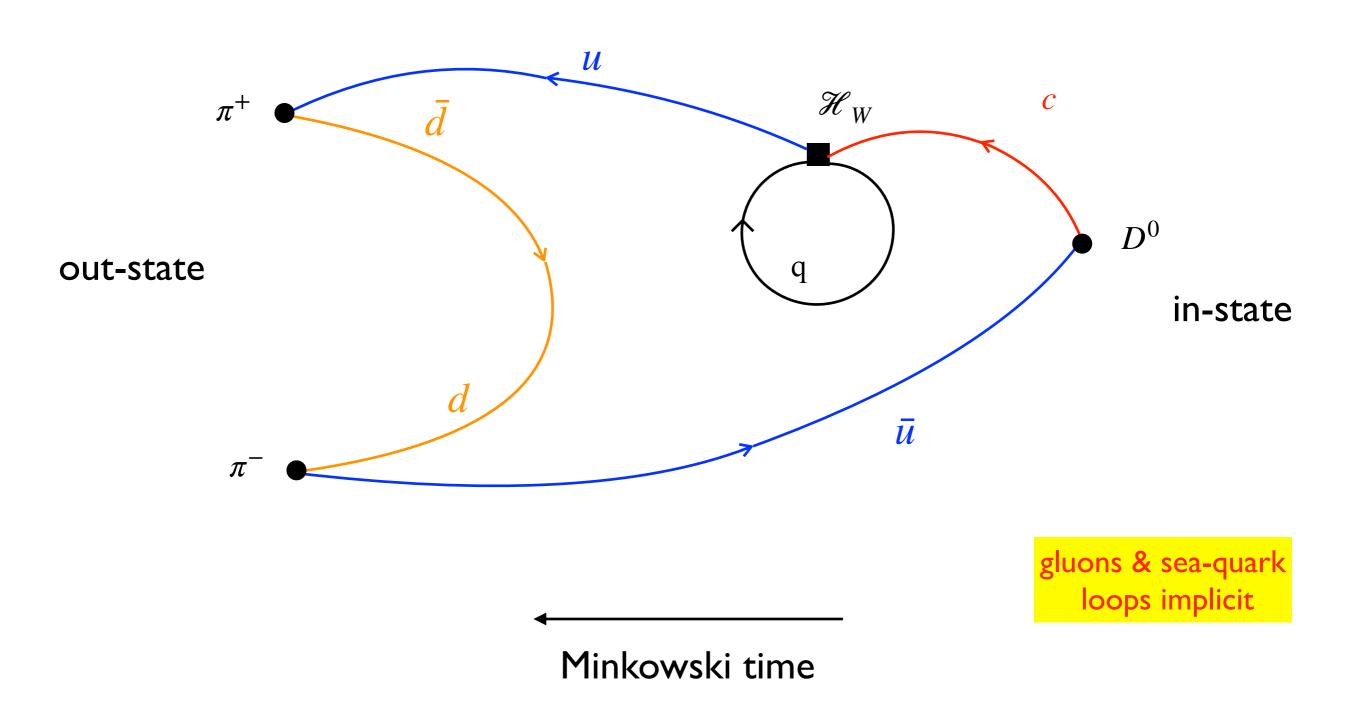
A search for charge-parity (CP) violation in  $D^0 \to K^- K^+$  and  $D^0 \to \pi^- \pi^+$  decays is reported, using pp collision data corresponding to an integrated luminosity of 6 fb<sup>-1</sup> collected at a center-of-mass energy of 13 TeV with the LHCb detector. The flavor of the charm meson is inferred from the charge of the pion in  $D^*(2010)^+ \to D^0\pi^+$  decays or from the charge of the muon in  $\overline{B} \to D^0\mu^-\bar{\nu}_{\mu}X$  decays. The difference between the CP asymmetries in  $D^0 \to K^- K^+$  and  $D^0 \to \pi^- \pi^+$  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

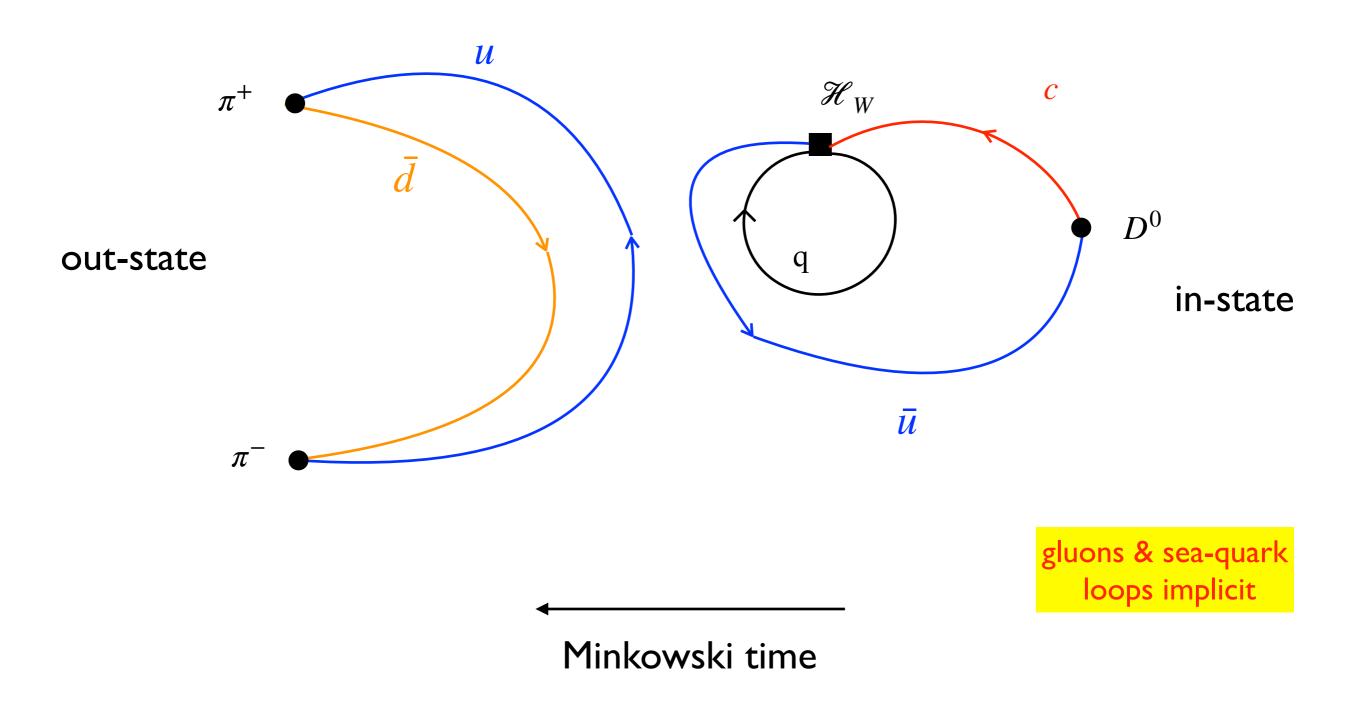
#### $\Delta A_{CP} = (-15.4 \pm 2.9) \times 10^{-4},$

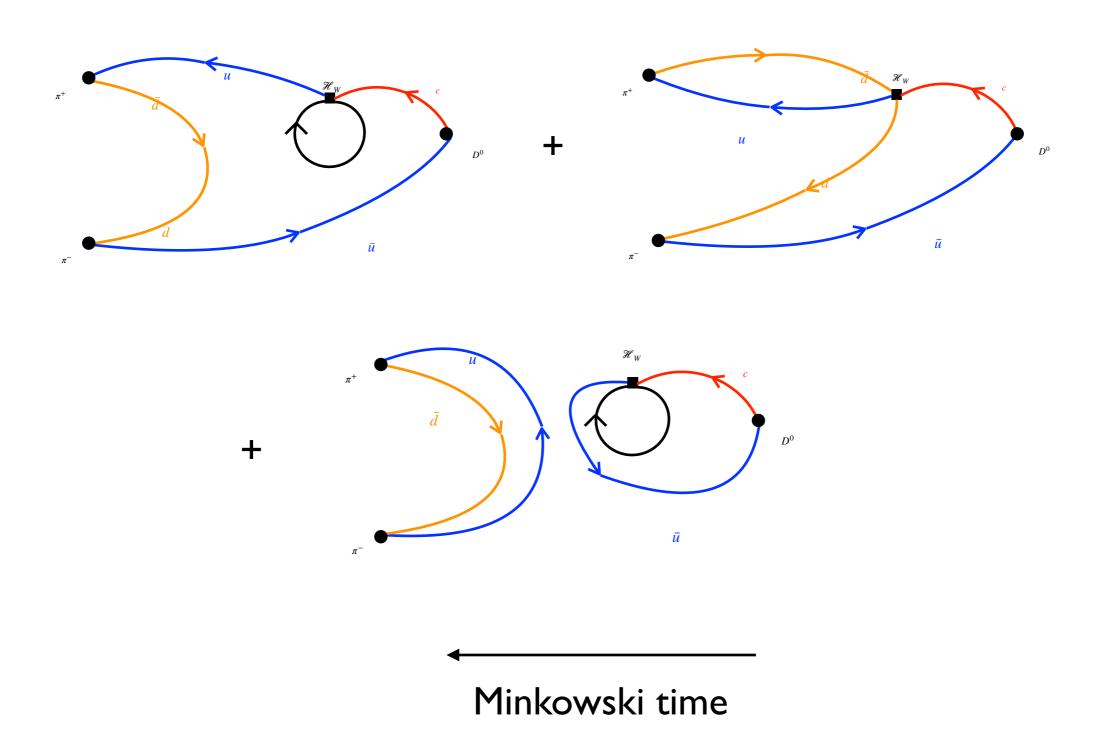
 $5.3\sigma$  effect

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.

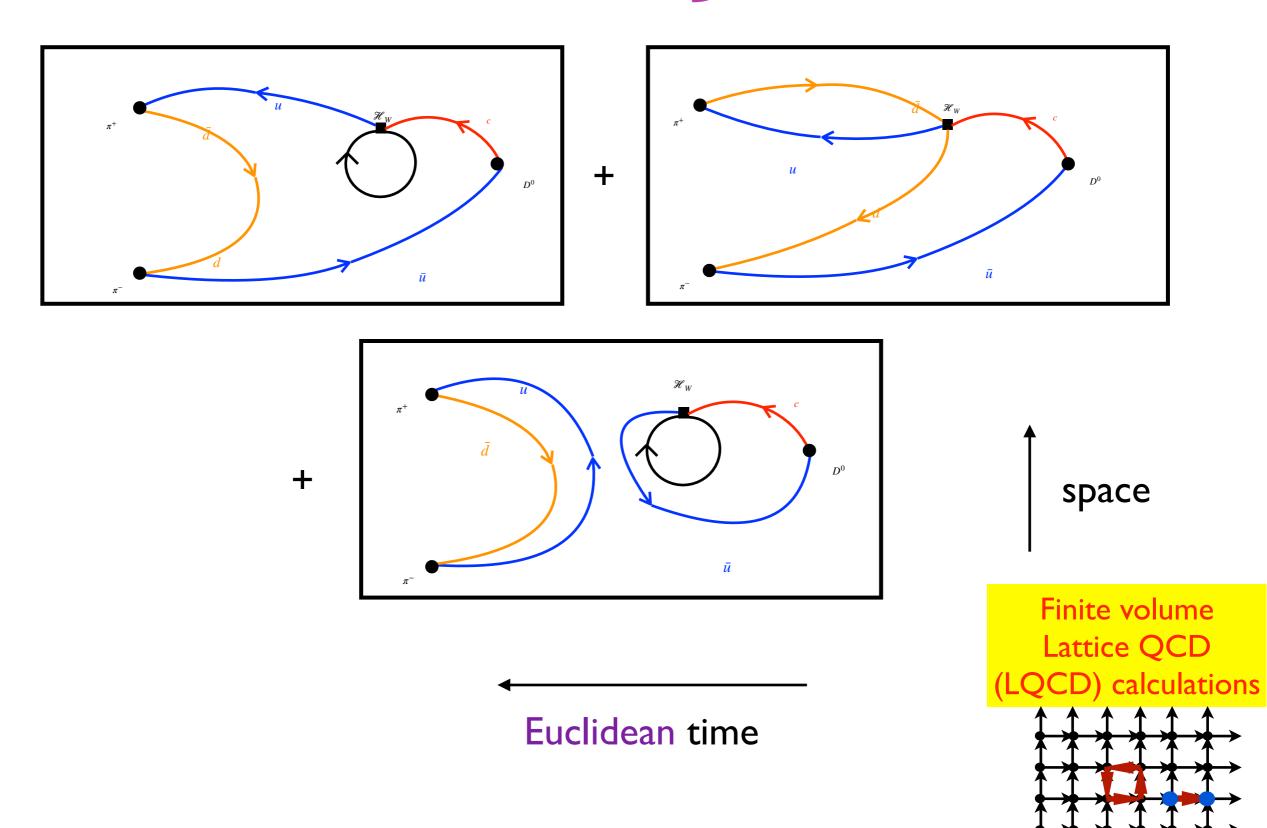




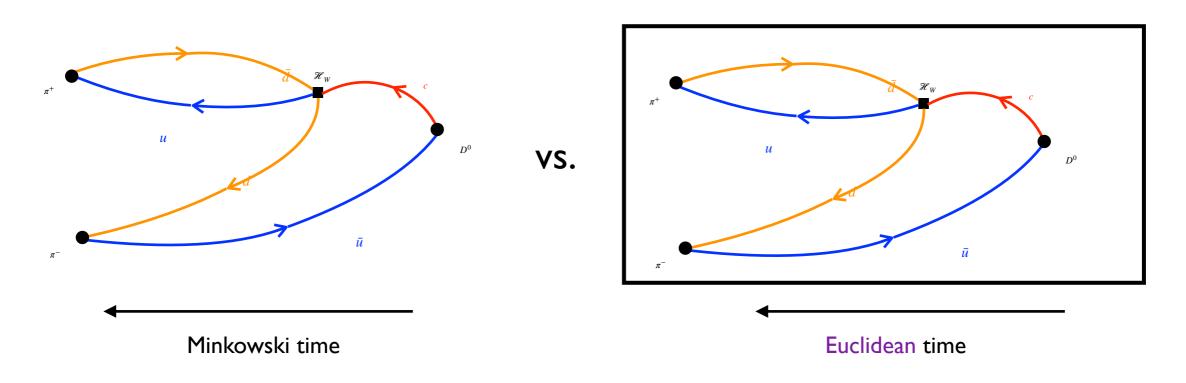




## ...what we might achieve

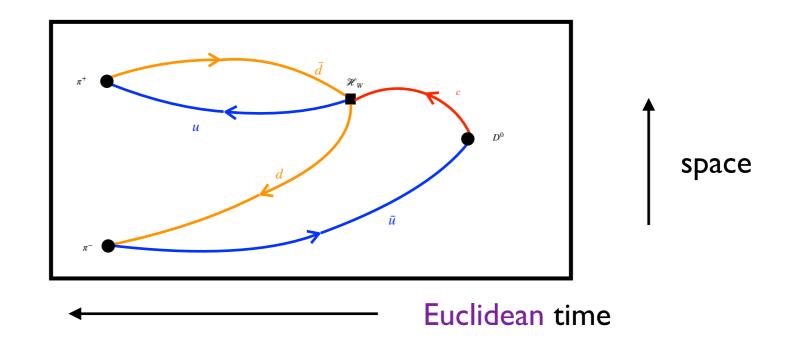


### Problems

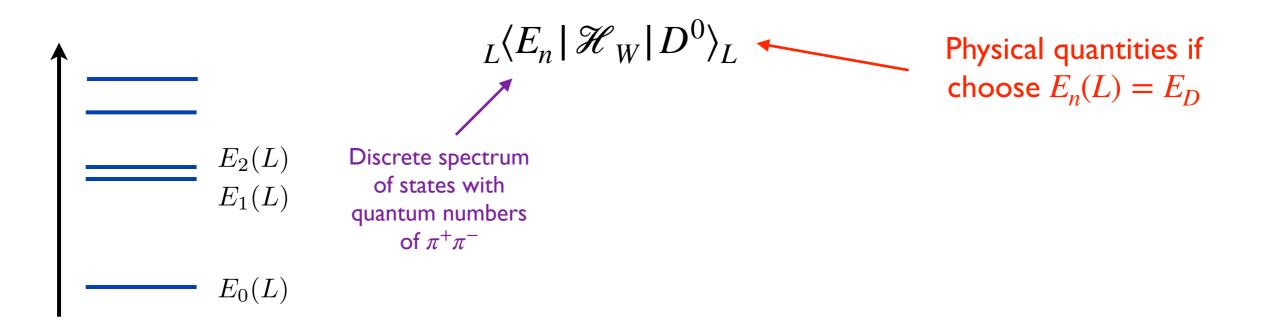


- No in- and out-states in finite volume
  - Cannot separate final-state particles
- Need to analytically continue from Euclidian to Minkowski momenta
  - Ill-posed problem given discrete momenta in finite volume

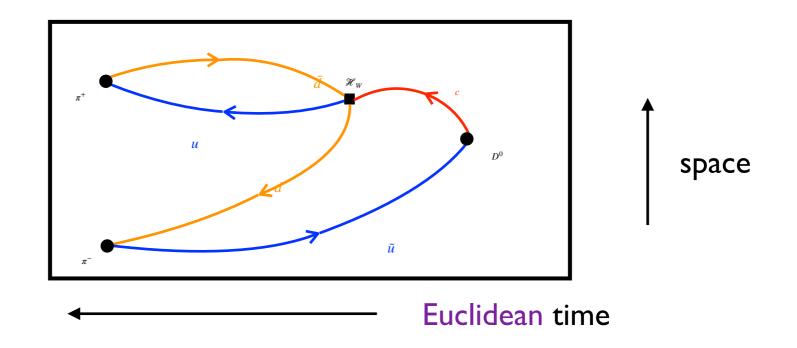
# Rephrasing



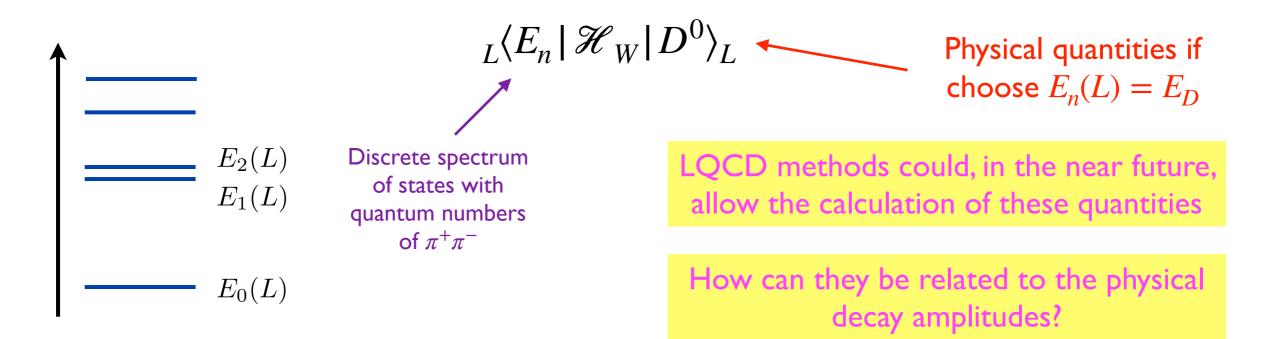
What LQCD can determine are finite-volume matrix elements:



# Rephrasing



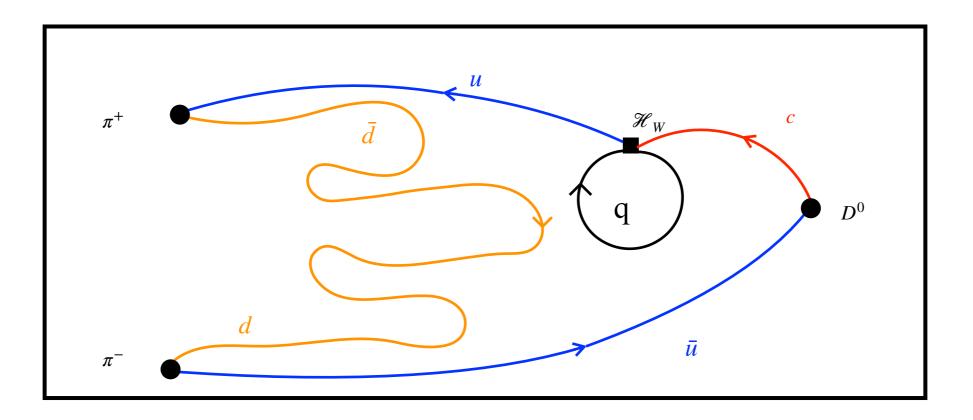
What LQCD can determine are finite-volume matrix elements:



### The fundamental issue

$$_L \langle E_n | \mathscr{H}_W | D^0 \rangle_L \longrightarrow {}_{out} \langle \pi^+ \pi^- | \mathscr{H}_W | D^0 \rangle_{in}$$

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



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  - 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

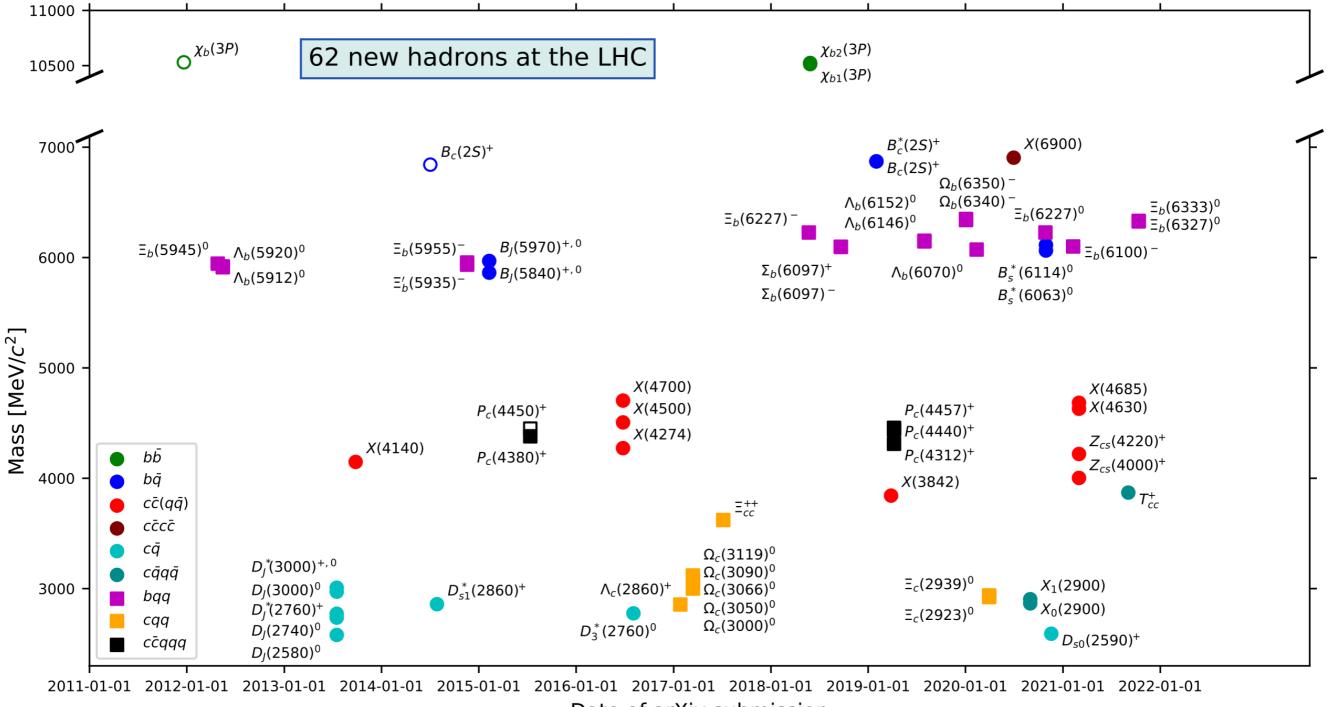
Today I will briefly summarize the status, and describe examples of recent work

### 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**



Date of arXiv submission

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

+ data from Babar, Belle, COMPASS, ...

### Motivations

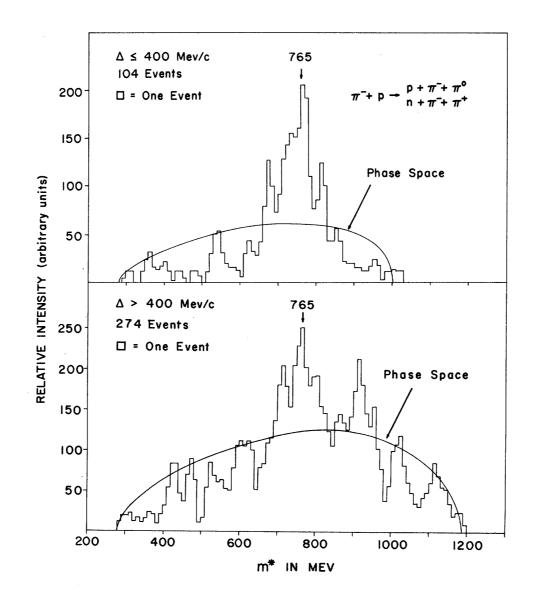
- Most resonances have 3 (or more) particle decay channels
  - $\omega(782, I^G J^{PC} = 0^{-1^{--}}) \rightarrow 3\pi$
  - $N(1440, J^P = \frac{1}{2}^+) \to N\pi, N\pi\pi$
  - $T_{cc}(3875, I = 0, J^P = 1^+?) \rightarrow D^0 D^0 \pi^+$
- Determining 3-body "forces"
  - NNN interactions needed as input for EFT treatments of large nuclei, and for the neutron-star equation of state
  - $\pi\pi\pi, \pi K\bar{K}, \dots$  interactions needed as input to study pion & kaon condensation

# History & status of finite-volume formalism for 2 particles

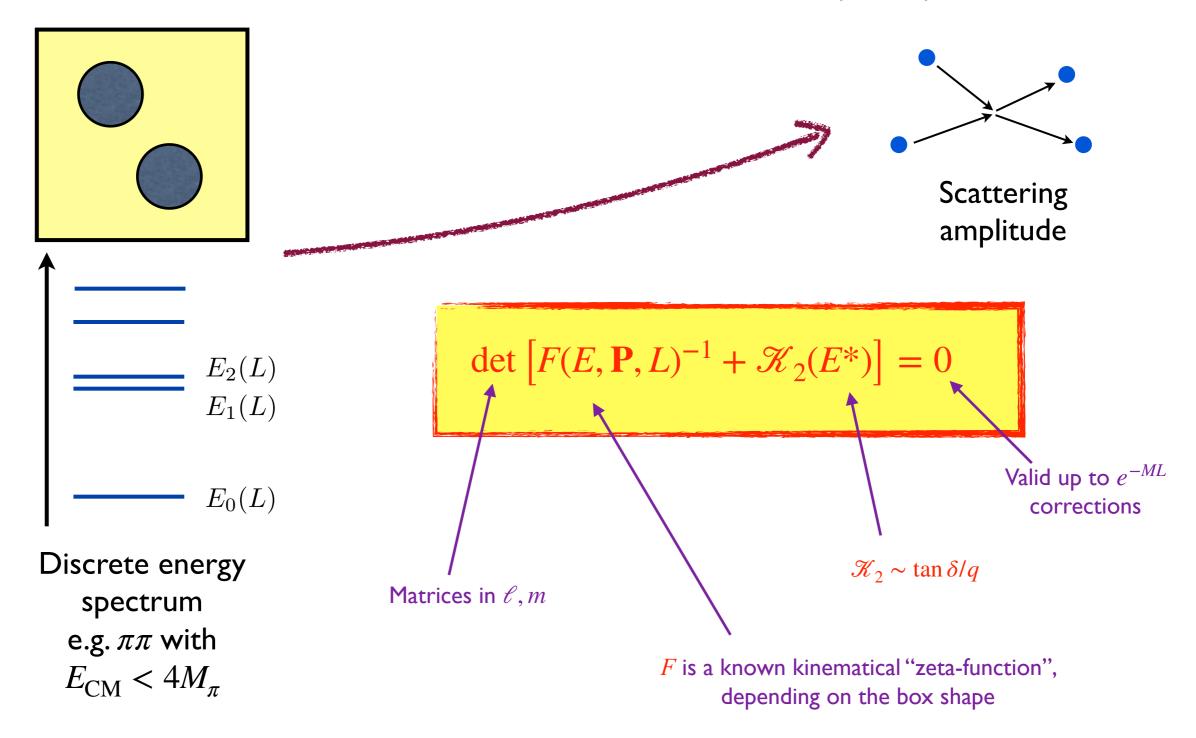
#### • **1961**: Discovery of the $\rho$ meson

EVIDENCE FOR A  $\pi$ - $\pi$  RESONANCE IN THE I=1, J=1 STATE\*

A. R. Erwin, R. March, W. D. Walker, and E. West Brookhaven National Laboratory, Upton, New York and University of Wisconsin, Madison, Wisconsin (Received May 11, 1961)



- **I96I**: Discovery of the  $\rho$  meson
- 1986/91: Lüscher derived "two-particle quantization condition" (QC2)



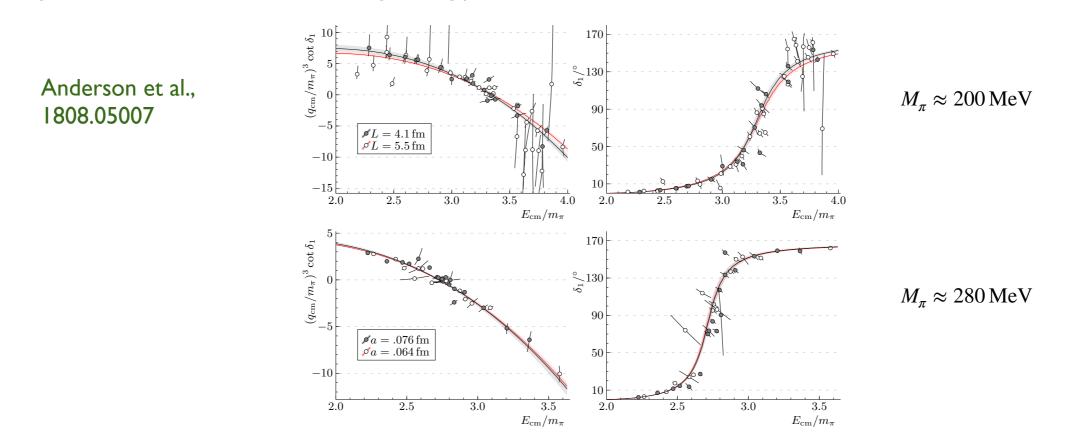
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  - 2005: Kim, Sachrajda & SRS alternate derivation, basis for many subsequent generalizations
- 1999: Measurement of  $\varepsilon'/\varepsilon = 16.1(2.3)10^{-4}$  by KTeV/NA48 direct CPV in  $K \rightarrow \pi\pi$



NA48 @ CERN: Cern website

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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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- 2014 2019: LQCD implementation of QC2 for the  $\rho$  resonance in  $\pi\pi$  scattering
- 2020: LQCD calculation of  $\varepsilon'/\varepsilon = 21.7(8.4)10^{-4}$  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,<sup>1</sup> T. Blum,<sup>2,3</sup> P. A. Boyle,<sup>4,5</sup> M. Bruno,<sup>6</sup> N. H. Christ,<sup>1</sup> D. Hoying,<sup>3,2</sup> C. Jung,<sup>4</sup> C. Kelly<sup>®</sup>,<sup>4</sup> C. Lehner,<sup>7,4</sup> R. D. Mawhinney,<sup>1</sup> D. J. Murphy,<sup>8</sup> C. T. Sachrajda,<sup>9</sup> A. Soni,<sup>4</sup> M. Tomii,<sup>2</sup> and T. Wang<sup>1</sup>

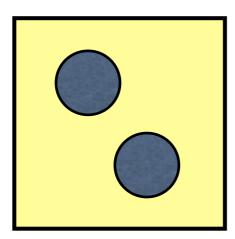
(RBC and UKQCD Collaborations)

# History & status of finite-volume formalism for 3 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

VS



e.g.  $2\pi$  with  $E_{\rm CM} < 4M_\pi$ 

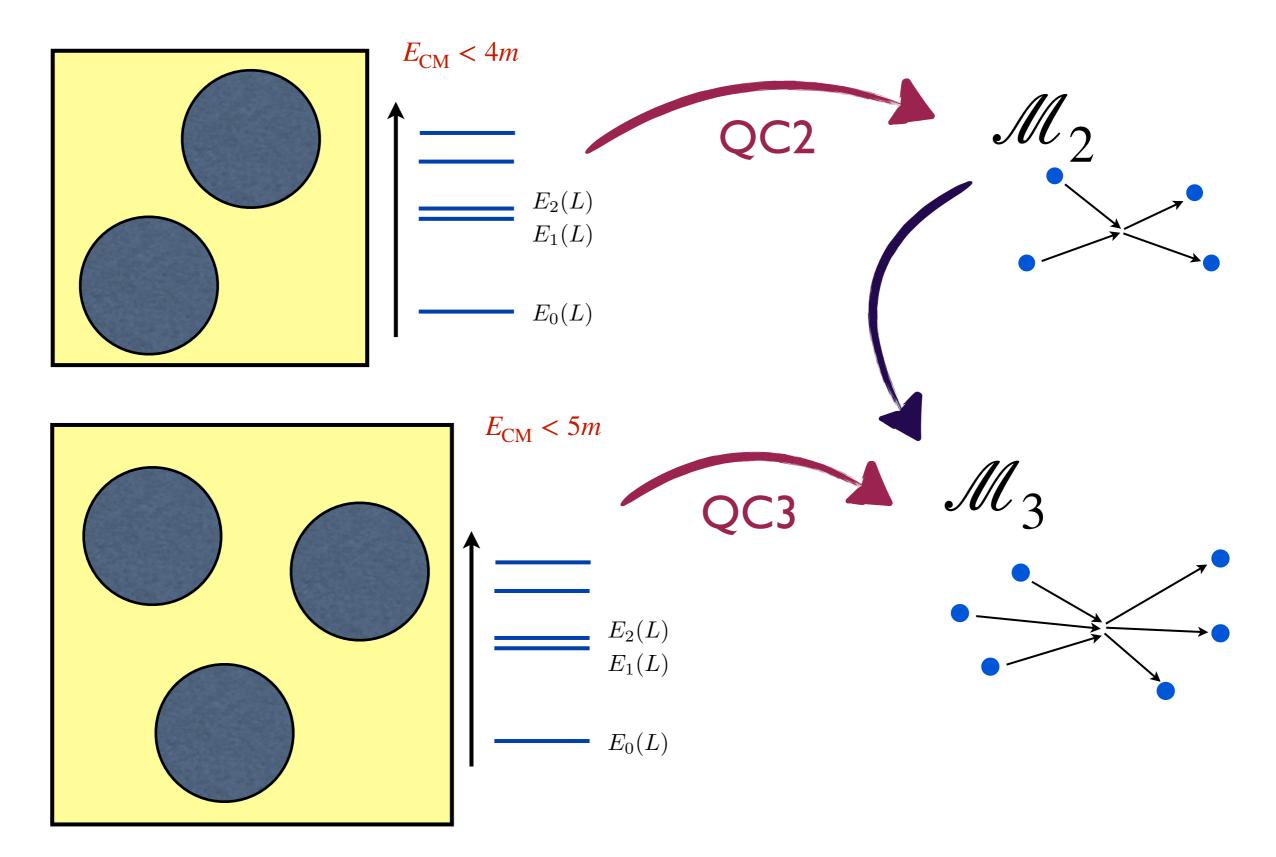
e.g.  $3\pi$  with  $E_{\rm CM} < 5M_\pi$ 

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

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

- Dominant contribution from pairwise interactions,  $\Delta E_n \sim 1/L^3$
- 3-particle interactions give subleading contributions  $\propto 1/L^6$
- Scattering amplitude  $\mathcal{M}_3$  at given  $E_{\rm CM}$ , is a (complex) function of Dalitz-plot variables, and incorporates final-state interactions
- $\mathcal{M}_3$  has divergences for physical momenta

#### Structure of the result (Z<sub>2</sub> symmetry)



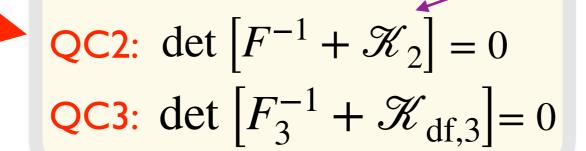
S. Sharpe, ``Progress in multiparticle amplitudes from the lattice," BAPTS, 10/13/23

### Two-step method

#### 2 & 3 particle Spectra from LQCD

L

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



Quantization conditions

[These are the RFT forms, and assume  $\mathbb{Z}_2$  symmetry]

Integral equations in infinite volume

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

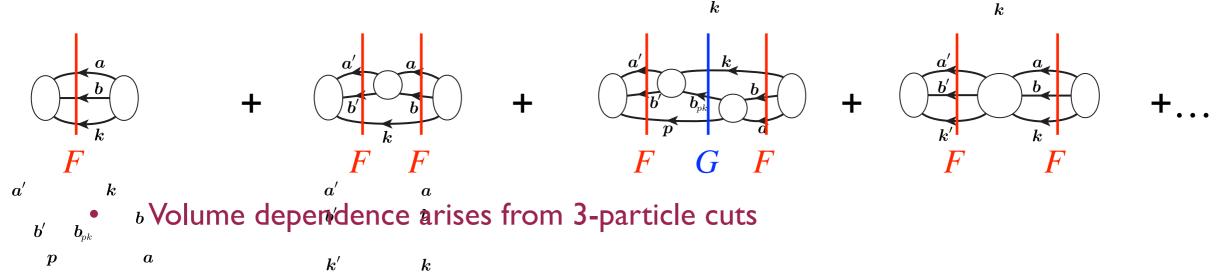


Incorporates initial- and final-state interactions

#### Further details of QC3

$$\det \left[ F_3^{-1} + \mathscr{K}_{df,3} \right] = 0$$

 Derived by determining power-law volume dependence of finite-volume<sup>3</sup>-particle correlation functions to all orders in a skeleton expansion in a generic relativistic EF<sub>0</sub> b



•  $F_3$  contains two-particle interactions ( $\mathscr{K}_2$ ) and kinematic functions (F & G)

$$F_3 = \frac{1}{2\omega L^3} \left[ \frac{F}{3} - F \frac{1}{\mathscr{K}_2^{-1} + F + G} F \right]$$

#### Status: formalism

[Full references at end of slides]

- 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-1/2 particles, e.g. 3 neutrons [Draper, Hansen, Romero-López, SRS]

#### Many resonances can now be studied!

Resonance	$I_{\pi\pi\pi}$	$J^P$	Decays
$\omega(782)$	0	1-	$\pi^+\pi^0\pi^-$
$h_1(1170)$	0	1+	$\rho\pi \to 3\pi$
$\omega_3(1670)$	0	3-	$3\pi, 5\pi$
$\pi(1300)$	1	0-	$\rho\pi \to 3\pi$
$a_1(1260)$	1	1+	$3\pi, K\bar{K}\pi$
$\pi_1(1400)$	1	1-	$\eta\pi, 3\pi?$
$\pi_2(1670)$	1	$2^{-}$	$3\pi, K\bar{K}\pi$
$a_2(1320)$	1	$2^{+}$	$3\pi, K\bar{K}, 5\pi, \eta\pi$
$a_4(1970)$	1	$4^{+}$	$3\pi, K\bar{K}, 5\pi, \eta\pi$

### Status: applications

#### [References at end of slides]

- $3\pi^+$ : determined parameters in threshold expansion of  $\mathscr{K}_{df,3}$ , including pair interactions in sand d-waves; integral equations solved for s-wave interactions only
- $3K^+$ : determined s- and d-wave parameters in  $\mathscr{K}_{\mathrm{df},3}$
- $\phi^4$ : extracted  $\mathscr{K}_{df,3}$  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  $\mathscr{K}_{df,3}$ ; found evidence for small discretization effects
- Integral equations solved for complex energies for simple system with near-unitary twoparticle 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

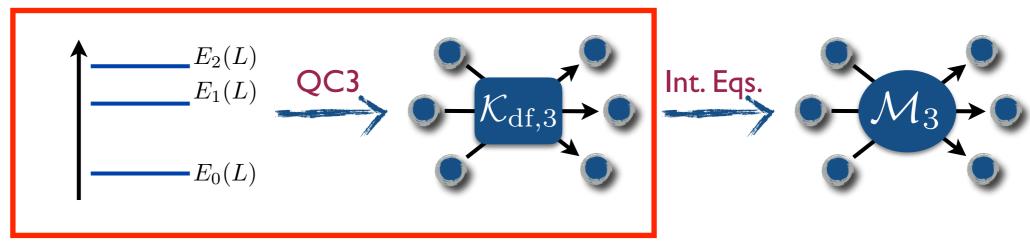
# $\pi^+\pi^+K^+$ and $K^+K^+\pi^+$ amplitudes using LQCP

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

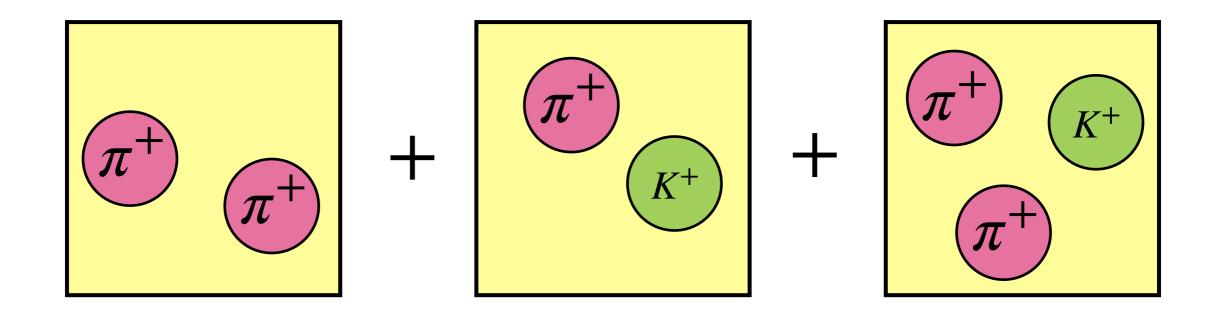
#### A step on the way to $T_{cc} \rightarrow DD\pi$ , etc.



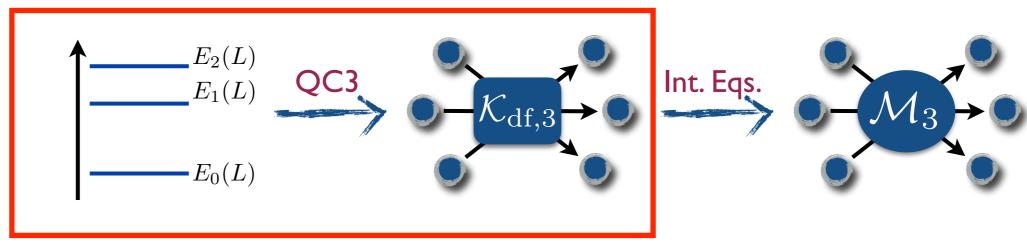
#### Strategy



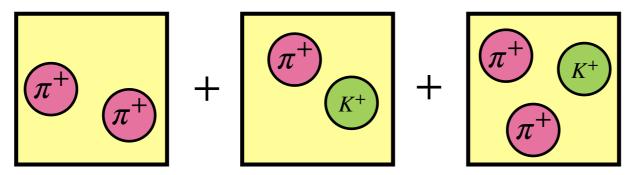
- Consider multiparticle system with weakly repulsive interactions—pions and kaons at maximal isospin  $(2\pi^+/3\pi^+, 2K^+/3K^+, 2\pi^+/\pi^+K^+/3K^+, 2K^+/\pi^+K^+/3K^+)$ 
  - No resonances in two-particle subchannels or in three-particle system
  - Simultaneously fit to several spectra,; for example,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



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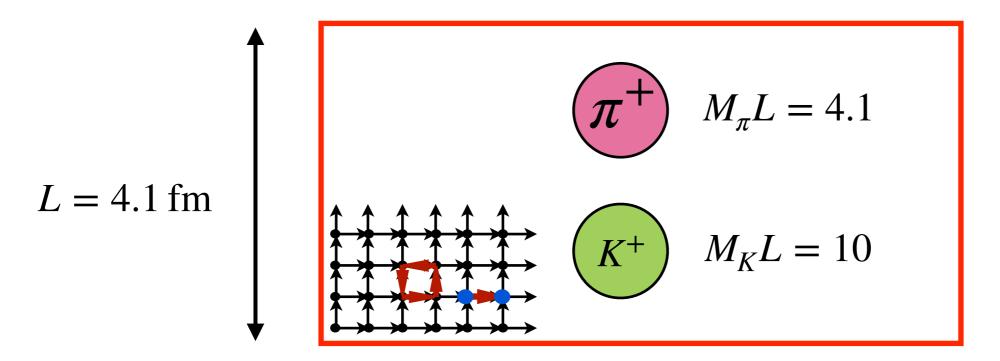
- Parametrize  $\mathscr{K}_{df,3}$  (and  $\mathscr{K}_2$ ) as the most general smooth function consistent with particle interchange, time-reversal and parity symmetries, using an expansion about threshold
  - Generalization of the effective-range expansion for  $\mathcal{K}_2$ ; here keep first two 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

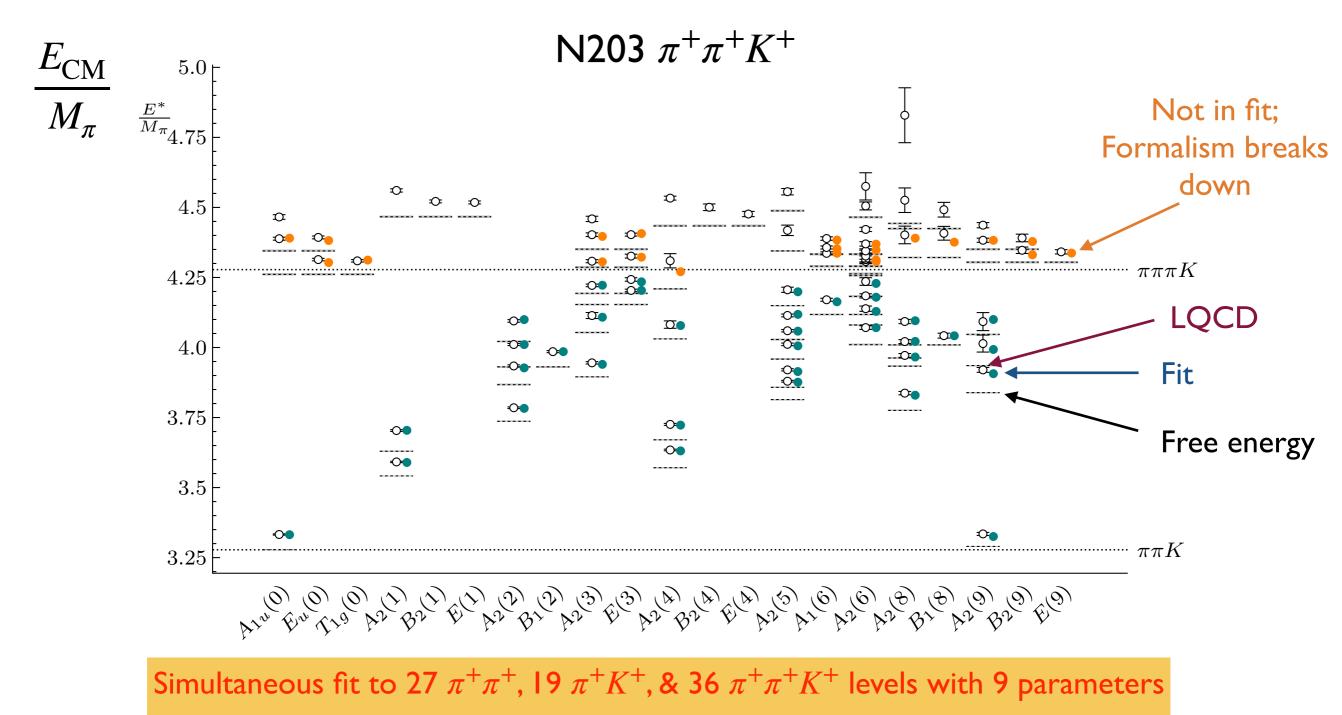
• Improved Wilson fermions at a = 0.064 fm (CLS lattices)

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

D200 configurations

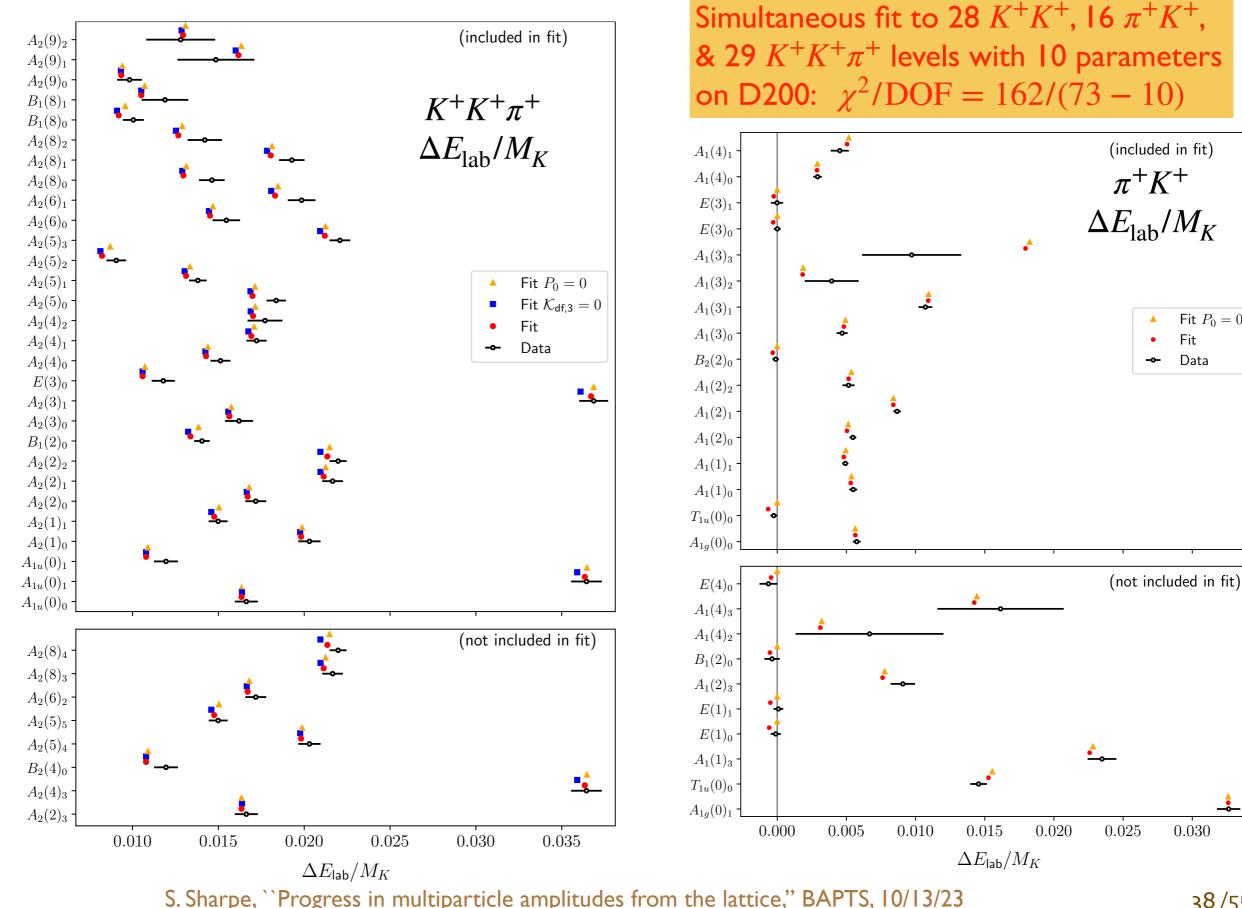


## Example of fit



 $\chi^2$ /DOF = 119/(82 - 9)

## Fit is to lab-frame shifts



38/55

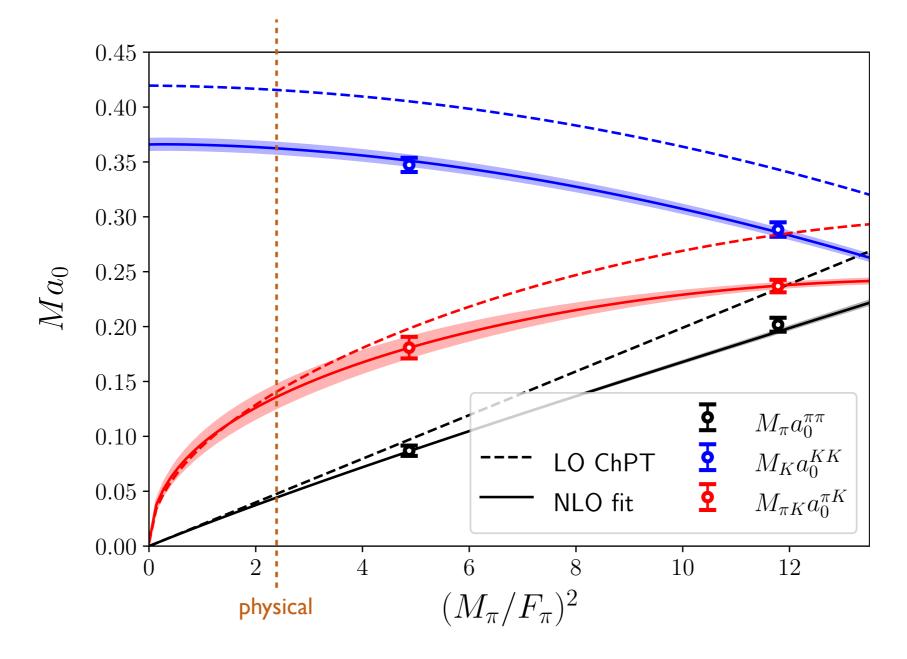
0.030

Fit  $P_0 = 0$ 

Fit

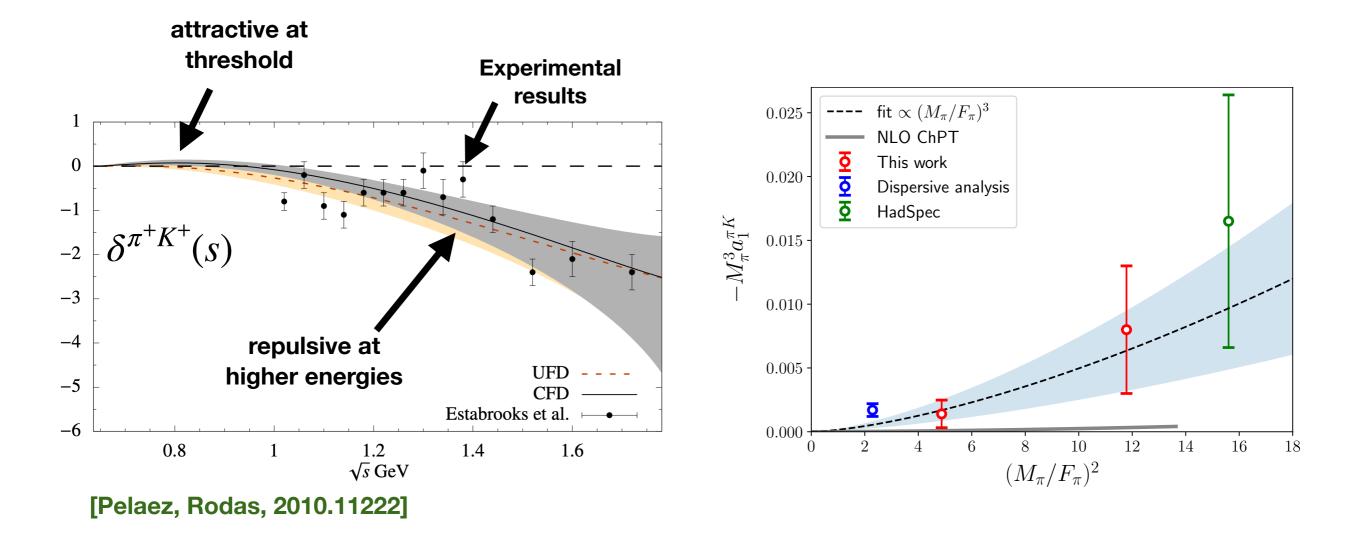
Data

## Results: scattering lengths



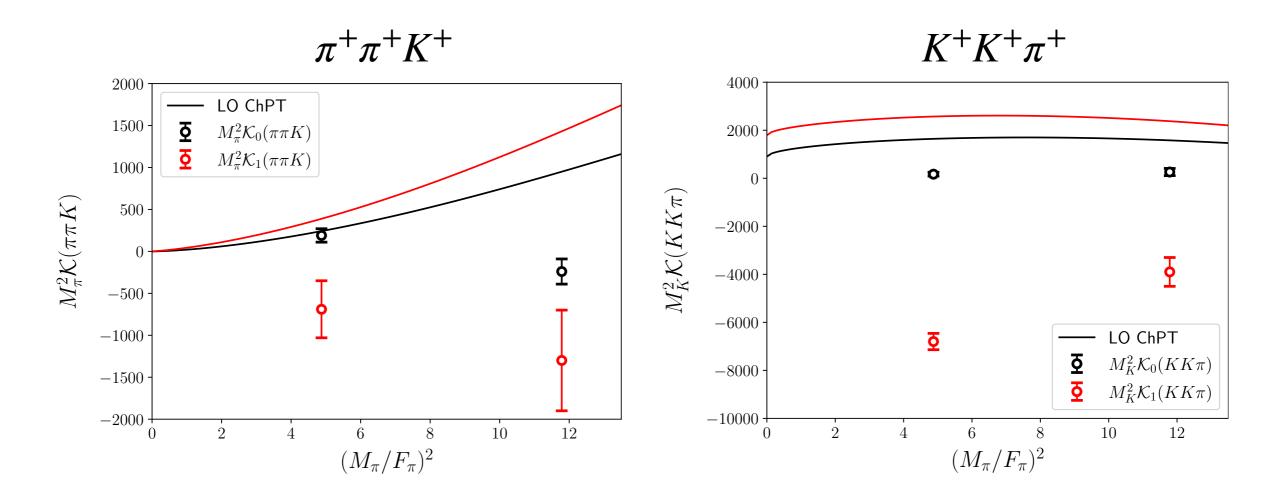
- 2-particle s-wave scattering lengths are well determined
- All are repulsive and consistent with ChPT
  - Evidence for small discretization errors

## P-wave $\pi^+ K^+$ scatt. Length

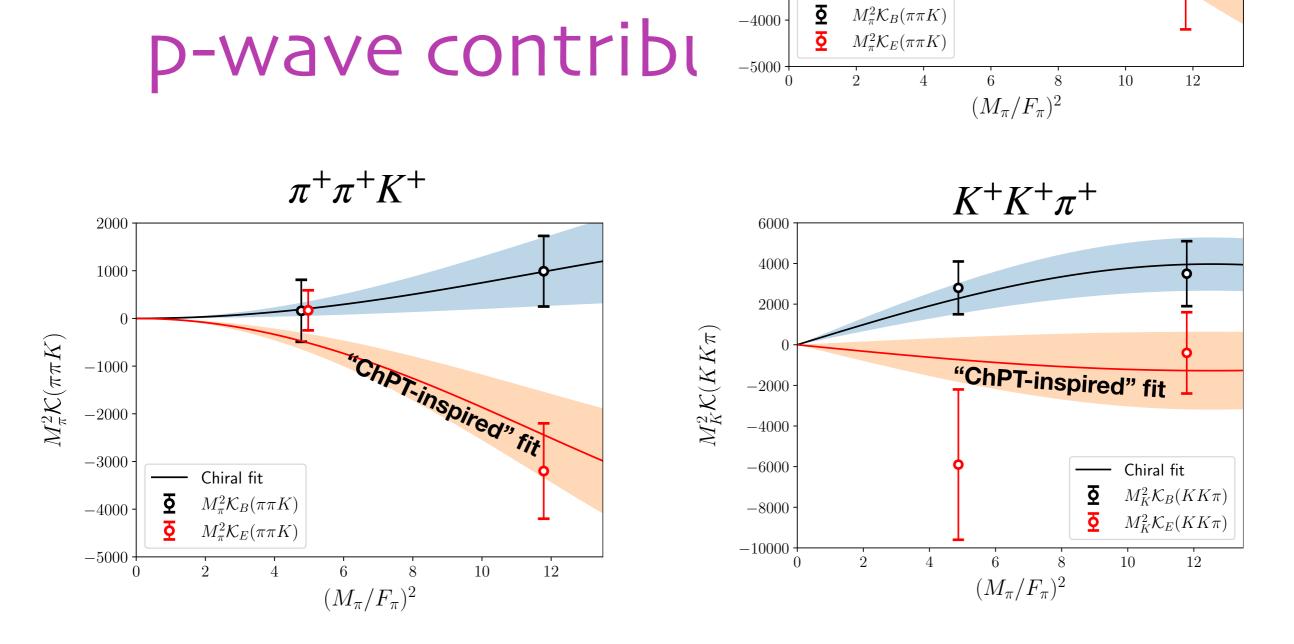


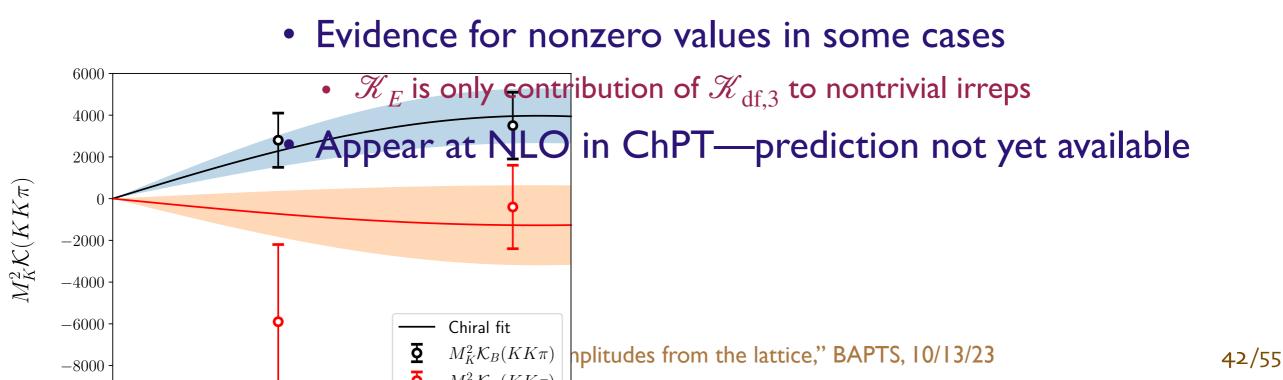
- Find evidence for **attractive** p-wave scattering length
  - Consistent with dispersive analysis

## s-wave contributions to $\mathcal{K}_{df,3}$



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



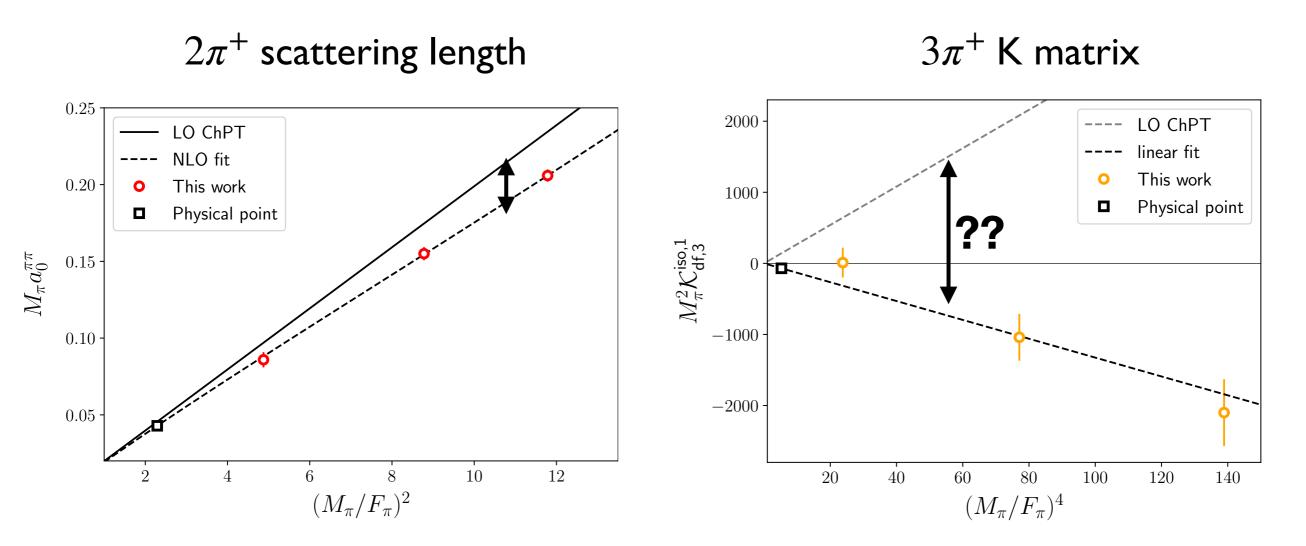


# NLO ChPT results for $\mathscr{K}_{df,3}$ for $3\pi^+ \rightarrow 3\pi^+$

[Baeza-Ballesteros, Bijnens, Husek, Romero-López, SRS, Sjö, 2303.13206]



### $2\pi/3\pi$ K matrices vs ChPT



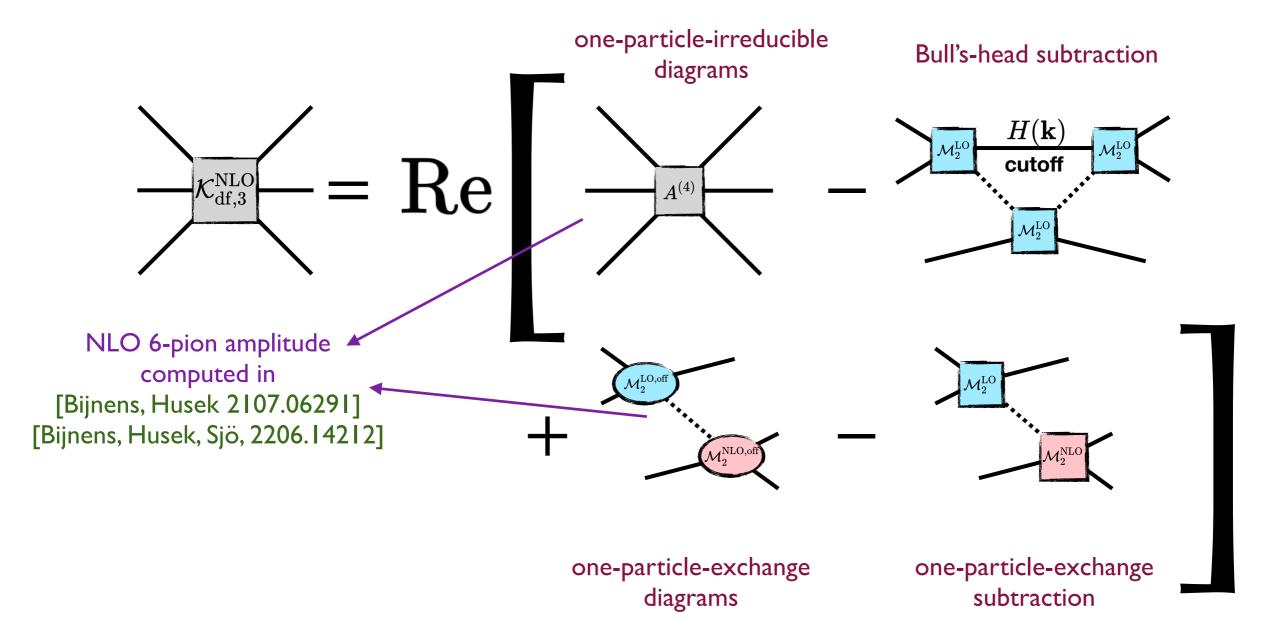
[Results from Blanton, Hanlon, Hörz, Morningstar, Romero-López, SRS, 2106.05590 (JHEP)]

- LO ChPT describes 2-pion sector well
- Large discrepancy in 3-pion sector!

## NLO ChPT for $\mathscr{K}_{df,3}$

• Integral equations simplify to:

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



Threshold expansion for 
$$\mathcal{K}_{df,3}$$

- $\mathscr{K}_{df,3}$  is a real, smooth function which is Lorentz, P and T invariant
- Expand about threshold in powers of  $\Delta = (s 9M_{\pi}^2)/9M_{\pi}^2$ ,  $\tilde{t}_{ij} = (p'_i p_j)^2/9M_{\pi}^2$ , ...

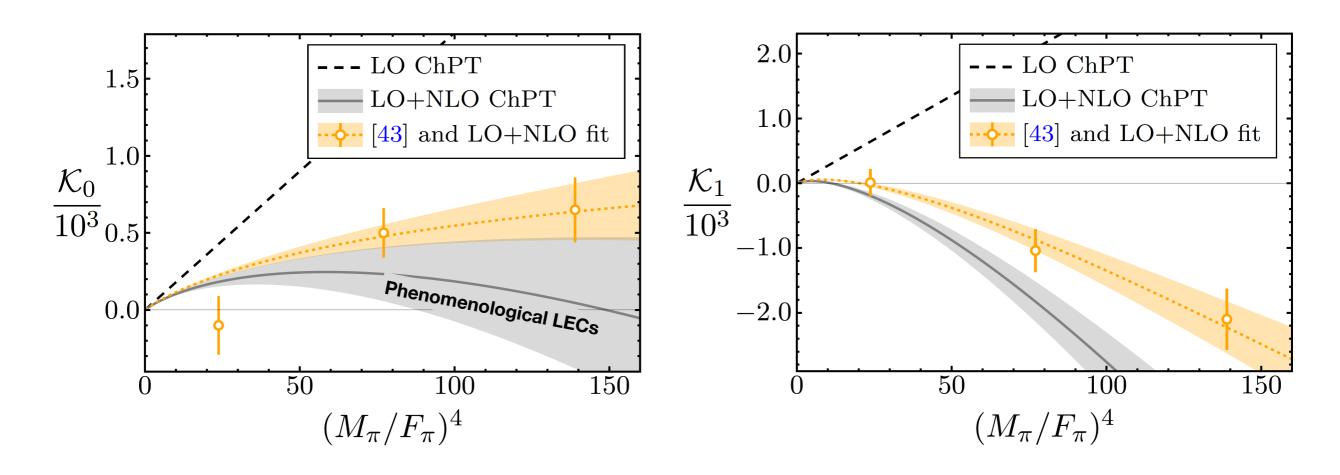
$$\mathcal{K}_{\mathrm{df},3} = \begin{array}{c} \begin{array}{c} \mathsf{Depend on CM energy} \\ \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},0} + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},1}\Delta + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},2}\Delta^{2} \\ \end{array} + \begin{array}{c} \begin{array}{c} \mathsf{Angular dependence} \\ \mathcal{K}_{A}\Delta_{A} + \mathcal{K}_{B}\Delta_{B} \\ \end{array} + \mathcal{O}(\Delta^{3}) \\ \end{array} \\ \Delta_{B} = \sum_{i,j=1}^{3} \tilde{t}_{ij}^{2} - \Delta^{2}, \end{array}$$

- Can separate terms in fit based on dependence on energy and rotational properties
  - E.g. only  $\mathcal{K}_B$  contributes to nontrivial irreps

## NLO ChPT results for $\mathscr{K}_{df,3}$

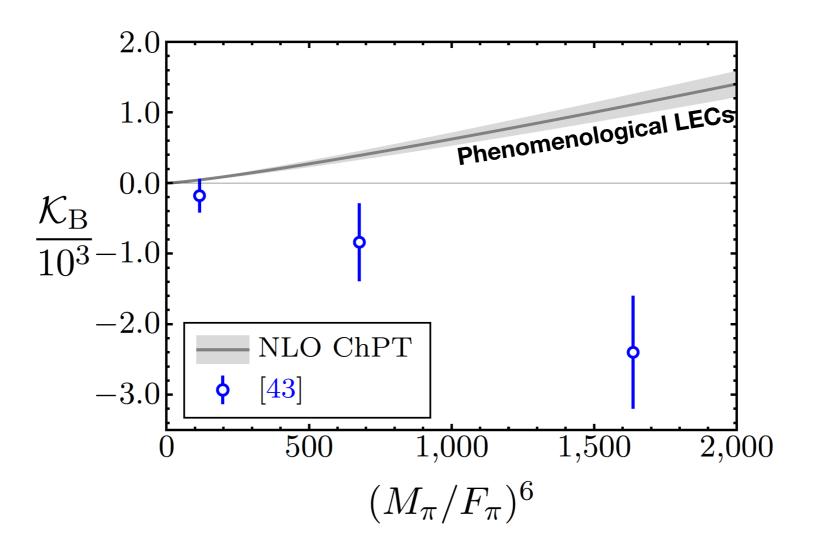
$$\begin{split} \kappa &= 1/(16\pi^2) \\ \mathcal{K}_0 &= \left(\frac{M_{\pi}}{F_{\pi}}\right)^4 18 + \left(\frac{M_{\pi}}{F_{\pi}}\right)^6 \left[-3\kappa(35+12\log 3) - \mathcal{D}_0 + 111L + \ell_{(0)}^r\right], \\ \mathcal{K}_1 &= \left(\frac{M_{\pi}}{F_{\pi}}\right)^4 27 + \left(\frac{M_{\pi}}{F_{\pi}}\right)^6 \left[-\frac{\kappa}{20}(1999+1920\log 3) - \mathcal{D}_1 + 384L + \ell_{(1)}^r\right], \\ \mathcal{K}_2 &= \left(\frac{M_{\pi}}{F_{\pi}}\right)^6 \left[\frac{207\kappa}{1400}(2923 - 420\log 3) - \mathcal{D}_2 + 360L + \ell_{(2)}^r\right], \\ \mathcal{K}_A &= \left(\frac{M_{\pi}}{F_{\pi}}\right)^6 \left[\frac{9\kappa}{560}(21809 - 1050\log 3) - \mathcal{D}_A - 9L + \ell_{(A)}^r\right], \\ \mathcal{K}_B &= \left(\frac{M_{\pi}}{F_{\pi}}\right)^6 \left[\frac{27\kappa}{1400}(6698 - 245\log 3) - \mathcal{D}_B + 54L + \ell_{(B)}^r\right]. \\ \mathcal{L} &= \kappa \log(M_{\pi}^2/\mu^2) \quad \text{LECs} \\ & \text{Numerical coefficients} \\ & \text{Dependence cancels} \\ & \text{Dependence cancels} \\ \end{aligned}$$

### Comparison to LQCD



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

### Comparison to LQCD

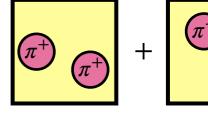


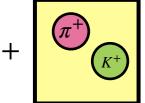
- $\mathcal{K}_B$  first appears at NLO in ChPT
- Discrepancy may be resolved by NNLO terms?

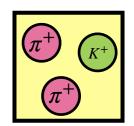
# Summary & Outlook

### 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  $K \rightarrow 3\pi$  decay amplitudes is now open







### Outlook

- Generalize formalism to broaden applications
  - 3 nucleons with  $I = \frac{1}{2}$  (nnp & ppn)
  - $T_{cc}(3875, I = 0, J^P = 1^+?) \rightarrow D^0 D^0 \pi^+, D^+ D^0 \pi^0, D^+ D^+ \pi^-$
  - Accessing the WZW term:  $K\bar{K} \leftrightarrow \pi^+\pi^0\pi^-(I=0)$
  - $N(1440, J^P = \frac{1}{2}^+) \to N\pi, N\pi\pi$
  - $J^{PC}, I^G = 1^{-+}, 1^-: \pi_1(1600) \to \eta \pi, 3\pi, KK\pi\pi, \eta \pi \pi \pi, 5\pi$
- Extend implementations using LQCD simulations
  - $3\pi^+$ ,  $3K^+$ ,  $\pi^+\pi^+K^+$ ,  $K^+K^+\pi^+$  at physical quark masses
  - I=0, I three-particle resonances ( $\omega$ ,  $a_1$ , ...)
- Extend applications of integral equations in the presence of three-particle resonances, e.g.  $T_{cc}$
- Move on to 4 particles!

### ExoHad collaboration

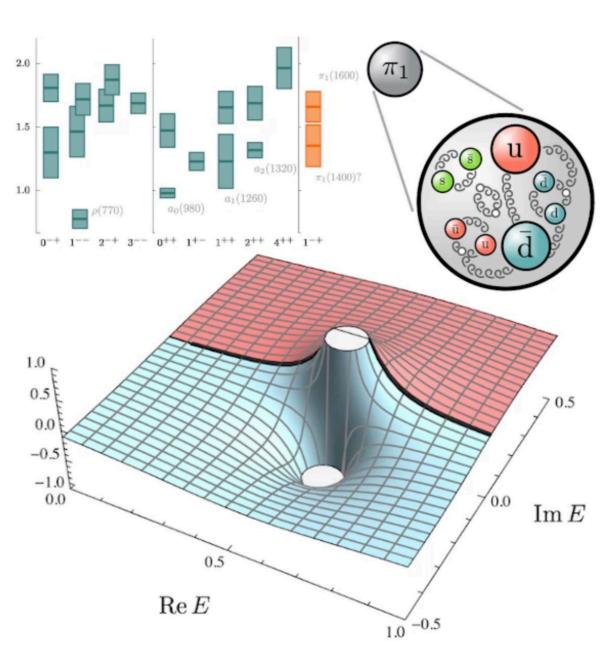
ExoHad Collaboration

exohad.org

People Events Talks Publications



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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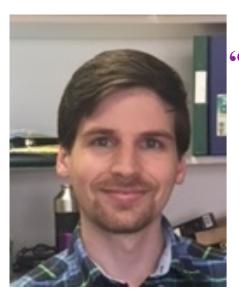


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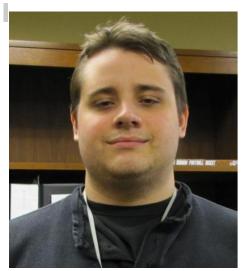


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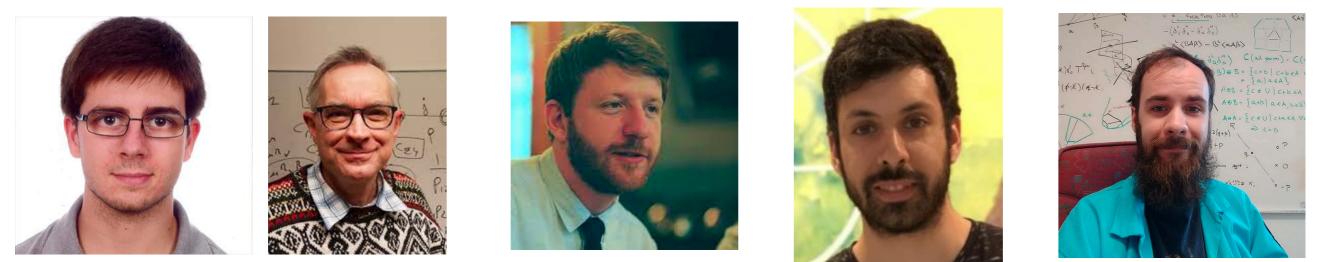
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