

$\pi^+\pi^+K^+$ and $K^+K^+\pi^+$ Interactions From Lattice QCD

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Outline

Overview of 3-particle quantization condition

2+1 particle systems

Energy spectra from lattice QCD

Fitting procedure

Fitting to energy shifts

Parametrizing $\mathcal{K}_2$ and $\mathcal{K}_{\text{df},3}$

Finding zeros

Fit results

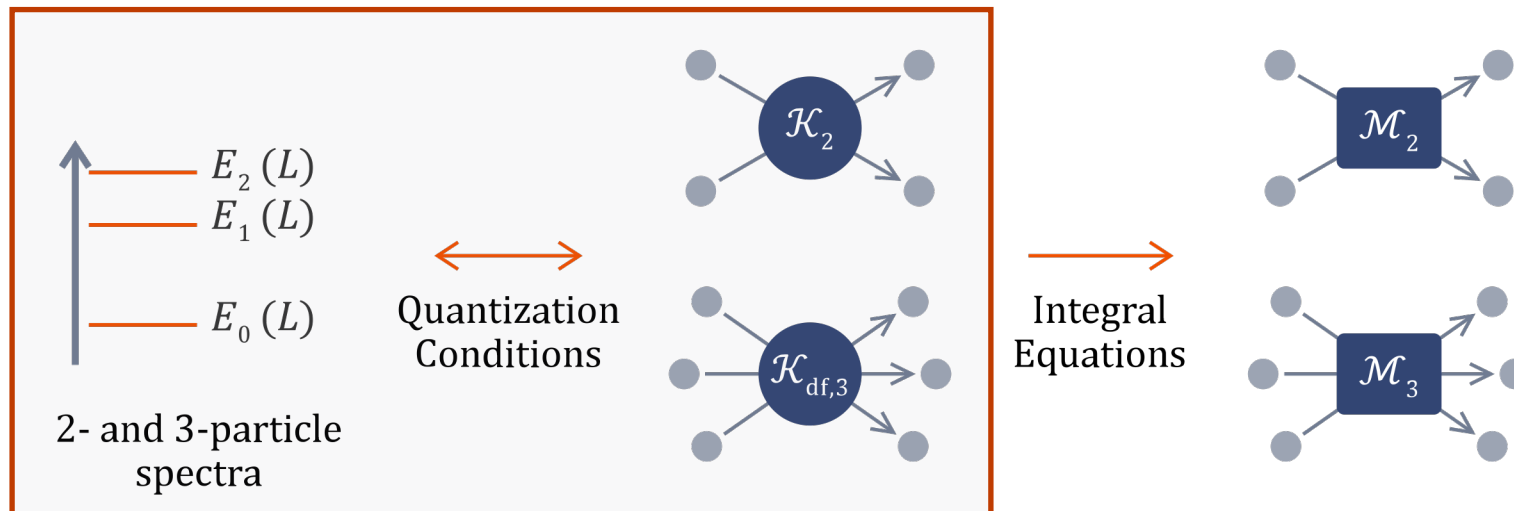
Comparison with χPT

Summary and future work

Based on work with Drew Hanlon, Ben Hörz, Colin Morningstar, Fernando Romero-López, and Steve Sharpe

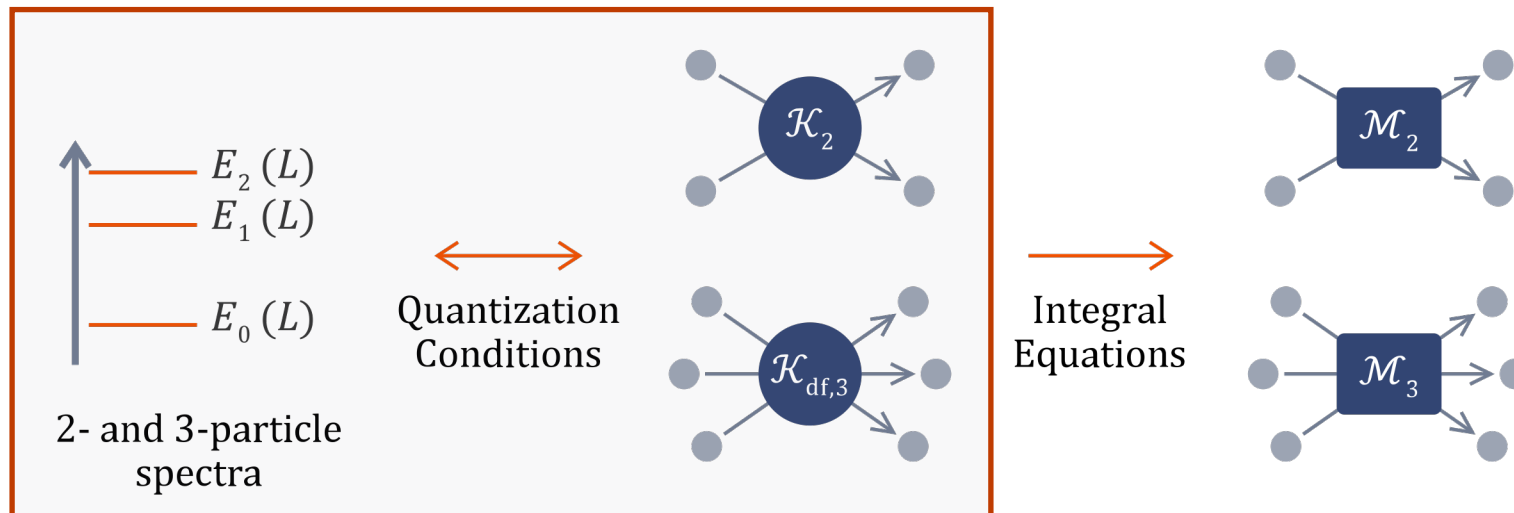
Overview

- Use finite-volume 2- and 3-particle spectra, obtained with lattice QCD, to determine 2- and 3-particle scattering amplitudes
 - Formalism exists for arbitrary choice of spinless particles
 - Has been implemented for three identical scalars:
 - $3\pi^+$, $3K^+$, 3π ($I = 1$), and ϕ^4 theory (See talks by A. Hanlon and M. Garofalo)



Overview

- Many systems of interest involve nondegenerate particles, e.g. $\pi\pi N$ (See talk by D. Severt)
- First step is to consider “2+1” systems: $\pi^+\pi^+K^+$ and $K^+K^+\pi^+$ (See talk by S. Sharpe)
 - Dominant s-wave interactions mildly repulsive—no resonance in 2-particle subchannels or overall system
 - Expect most levels to be slightly above corresponding free energies



Workflow: The Quantization Condition

- $\mathcal{K}_{\text{df},3}$ is a real, infinite-volume (but scheme-dependent) K matrix
 - Smooth apart from possible 3-particle resonance poles
 - Integral equations ensure unitarity of $\mathcal{M}_3$
- Parametrize $\mathcal{K}_2$ and $\mathcal{K}_{\text{df},3}$ in an effective-range-like expansion about threshold
 - Determine parameters by fitting spectrum
- With multiple frames and waves, no 1-to-1 relation between energies and phase shifts
 - A global fit is required



New for 2+1 Particle Systems

$$\det[\hat{F}_3^{-1}(E, \mathbf{P}, L) + \mathcal{K}_{\text{df},3}(E^*)] = 0$$

- QC3 involves matrices with an additional spectator-flavor index: $klmi$
 - E.g. for $\pi^+\pi^+K^+$
 - Spectator π^+ : $i = 1 \Rightarrow \pi^+K^+$ scattering
 - Spectator K^+ : $i = 2 \Rightarrow \pi^+\pi^+$ scattering
 - All partial waves contribute to π^+K^+ scattering; only even waves contribute to $\pi^+\pi^+$
 - In practice, set $l_{\text{max}} = 1$ to avoid too many parameters, particularly in $\mathcal{K}_{\text{df},3}$
- Cut-off function H , must be chosen to avoid left-handed cuts
 - These occur when $s_2 = |m_1^2 - m_2^2|$ in a subchannel with particle masses m_1 and m_2
- Python implementation of QC3 available on GitHub: https://github.com/ferolo2/QC3_release

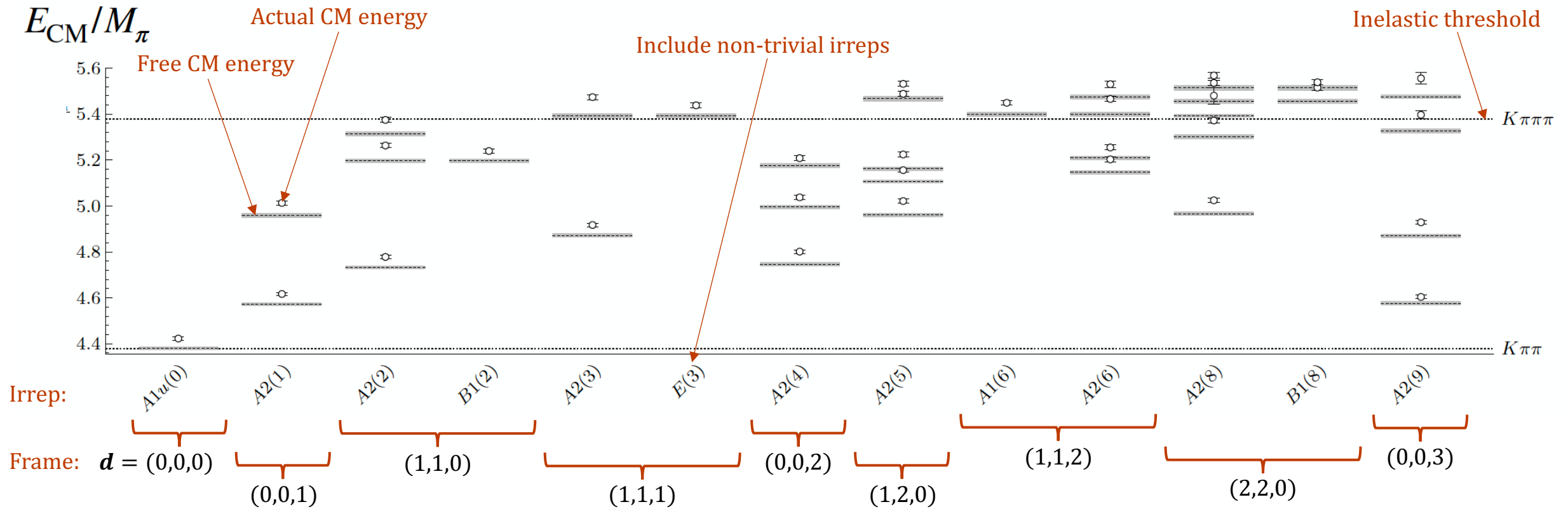
LQCD details

- Methods similar to those used for $3\pi^+$ and $3K^+$ ^[1] (See talk by A. Hanlon)
- Use CLS ensembles D200 and N203 (open BCs in time)
- Use stochastic LapH & contraction tricks to obtain multiple levels for $2\pi^+$, π^+K^+ , $2K^+$, $\pi^+\pi^+K^+$, and $\pi^+K^+K^+$
 - Use frames up to $d^2 = 9$ where ($\mathbf{P} = (2\pi/L)\mathbf{d}$)
 - Projected onto irreps of finite-volume little groups
- Fit to correlator ratios to directly obtain shifts from free energies in lab frame, ΔE_{lab}

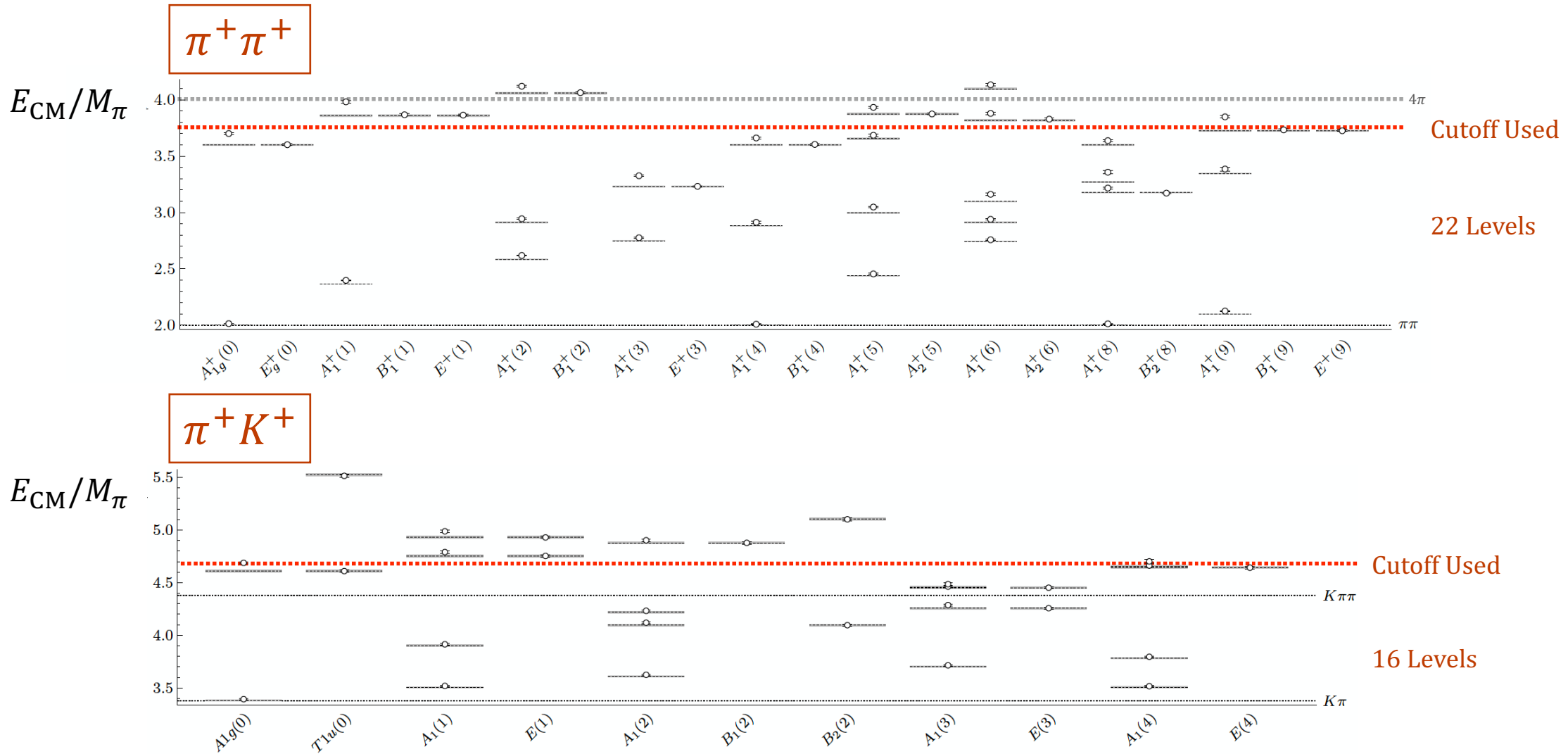
	$(L/a)^3 \times (T/a)$	M_π [MeV]	M_K [MeV]	N_{cfg}	Bin Size	$M_\pi L$
N203	$48^3 \times 128$	340	440	771	1	5.4
D200	$64^3 \times 128$	200	480	2000	3	4.2

[1] Blanton, Hanlon, Hörz, Morningstar, Romero-López, Sharpe, 2106.05590 (JHEP)

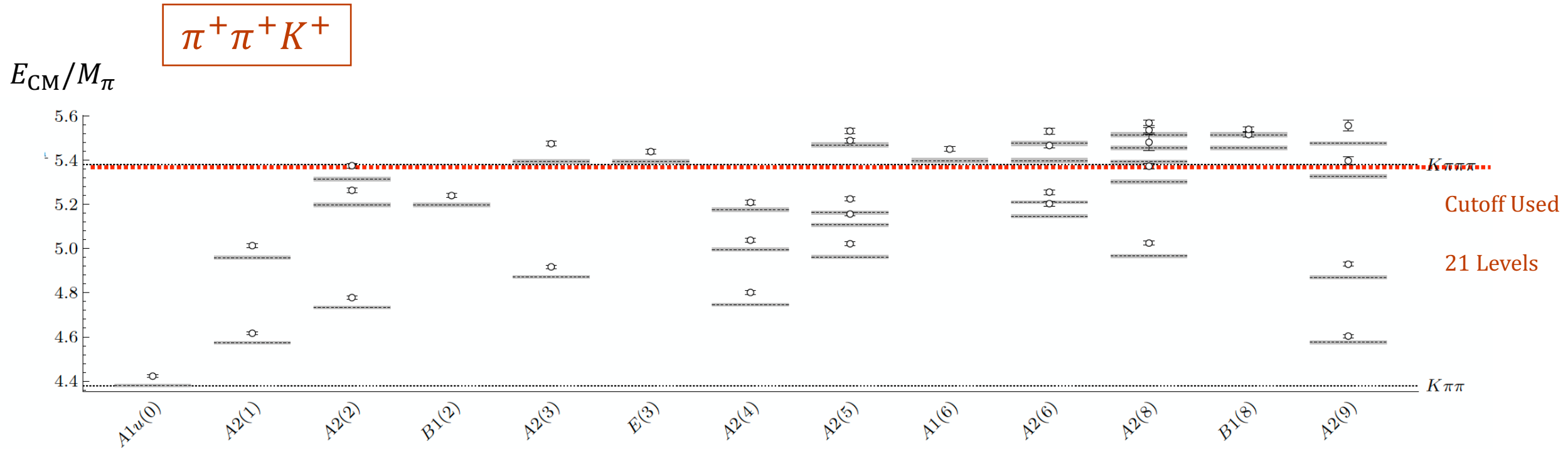
Examples of Levels: D200 $\pi^+\pi^+K^+$



Examples of Levels: D200 $\pi^+\pi^+K^+$



Examples of Levels: D200 $\pi^+\pi^+K^+$



Fitting to Energy Shifts

- Previously converted energy shifts ΔE_{lab} to E_{CM} using M_π and M_K ^[1]
 - Determined at rest on given jackknife sample, assuming continuum dispersion relation
 - Then fit QCs to E_{CM}
 - Leads to increased errors in E_{CM} so that fits that seem better than they really are
- Here we fit QCs directly to ΔE_{lab}
 - ΔE_{lab} is the direct output of ratio fits
 - Using the new method, we find larger, more realistic χ^2

[1] Blanton, Hanlon, Hörz, Morningstar, Romero-López, Sharpe, 2106.05590 (JHEP)

Fitting to Energy Shifts— $\pi\pi\pi$ fit Comparison

Ensemble	D200 (orig)	D200 (new)
Cutoffs	3.74, 4.74	3.74, 4.74
χ^2	73.6	73.7
DOFs	22+19-4 = 37	22+19-4 = 37
p-value	0.00032	0.00031
B_0^{pp}	-11.6(6)	-11.5(6)
B_1^{pp}	-2.49(42)	-2.38(38)
$2z_{pp}^2$	$2M_\pi^2$ (fixed)	$2M_\pi^2$ (fixed)
$\mathcal{K}_0$	-150(190)	-130(190)
$\mathcal{K}_1$	20(180)	41(170)

- χ^2 almost identical for the two fits
- Significance of nonzero $\mathcal{K}_{\text{df},3}$ is 1.4σ (original fit), 1.0σ (new fit).
- Difference between fits is 0.5σ

Ensemble	N203 (orig)	N203 (new)
Cutoffs	3.46, 4.46	3.46, 4.46
χ^2	93.7	129.7
DOFs	27+27-4 = 50	27+27-4 = 50
p-value	1.8×10^{-4}	5.3×10^{-9}
B_0^{pp}	-4.88(9)	-4.87(9)
B_1^{pp}	-2.27(11)	-1.90(9)
$2z_{pp}^2$	$2M_\pi^2$ (fixed)	$2M_\pi^2$ (fixed)
$\mathcal{K}_0$	240(220)	500(210)
$\mathcal{K}_1$	-1700(330)	-1400(340)

- χ^2 significantly larger for new fit
- Significance of nonzero $\mathcal{K}_{\text{df},3}$ is 7.0σ (original fit), 4.4σ (new fit)
- Difference between fits is 3.4σ

Threshold Expansion For $\mathcal{K}_2$

- Work to linear order in q^2 expansion, dropping $\mathcal{O}(q^4)$ terms
 - Implies that we keep s- and p-wave terms in $\pi^+ K^+$ channel
 - Only s waves for identical pairs
- Previously found that d-wave terms needed for good description of $\pi^+ \pi^+$ and $K^+ K^+$ levels^[1]
 - Here, d-wave description requires too many parameters
 - Thus, we expect and find poorer fits
- We use form with an Adler zero rather than effective-range expansion
 - Previous work found former to provide better fits for $2\pi^+/3\pi^+$ system

[1] Blanton, Hanlon, Hörz, Morningstar, Romero-López, Sharpe, 2106.05590 (JHEP)

Threshold Expansion For $\mathcal{K}_2$

- Adler zero threshold expansions:

- For $2\pi^+$ and $2K^+$:
$$q \cot \delta_0^{\pi\pi} = \frac{M^2 \sqrt{s_2}}{s_2 - 2Z^2 M^2} (B_0^{\pi\pi} + B_1^{\pi\pi} q^2)$$
- For $\pi^+ K^+$ s-wave:
$$q \cot \delta_0^{\pi K} = \frac{M_\pi^2 \sqrt{s_2}}{s_2 - M_\pi^2 - M_K^2} (B_0^{\pi K} + B_1^{\pi K} q^2)$$
- For $\pi^+ K^+$ p-wave:
$$q^3 \cot \delta_1^{\pi K} = \frac{M_\pi^3 \sqrt{s_2}}{M_\pi + M_K} \frac{1}{P_0^{\pi K}}$$

Threshold Expansion For $\mathcal{K}_{\text{df},3}$

- Work to linear order in 3-particle Mandelstam variables, dropping $\mathcal{O}(\Delta^2)$ terms
- Four terms allowed by symmetries (Lorentz, $1 \leftrightarrow 1'$, time reversal, parity)

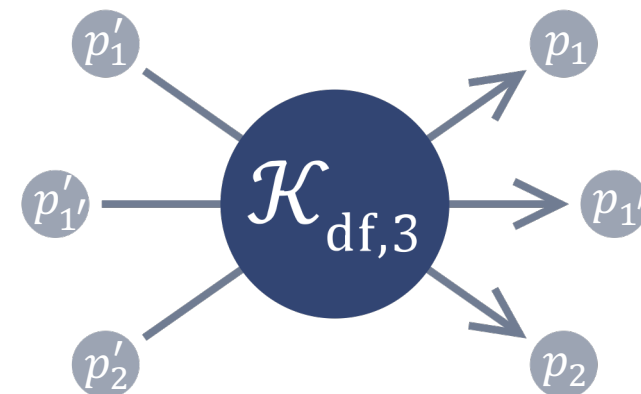
$$\mathcal{K}_{\text{df},3} = \mathcal{K}_{\text{df},3}^{\text{iso},0} + \mathcal{K}_{\text{df},3}^{\text{iso},1} \Delta + \mathcal{K}_{\text{df},3}^{\text{B},1} \Delta_2^S + \mathcal{K}_{\text{df},3}^{\text{E},1} \tilde{t}_{22}$$

- Only $\mathcal{K}^E$ couples to nontrivial irreps: contains $J = 0, 1$ while other terms only have $J = 0$

$$\Delta = \frac{s - M}{M^2} \text{ where } s = (p_1 + p_{1'} + p_2)^2 = P^2 \text{ and } M = 2m_1 + m_2$$

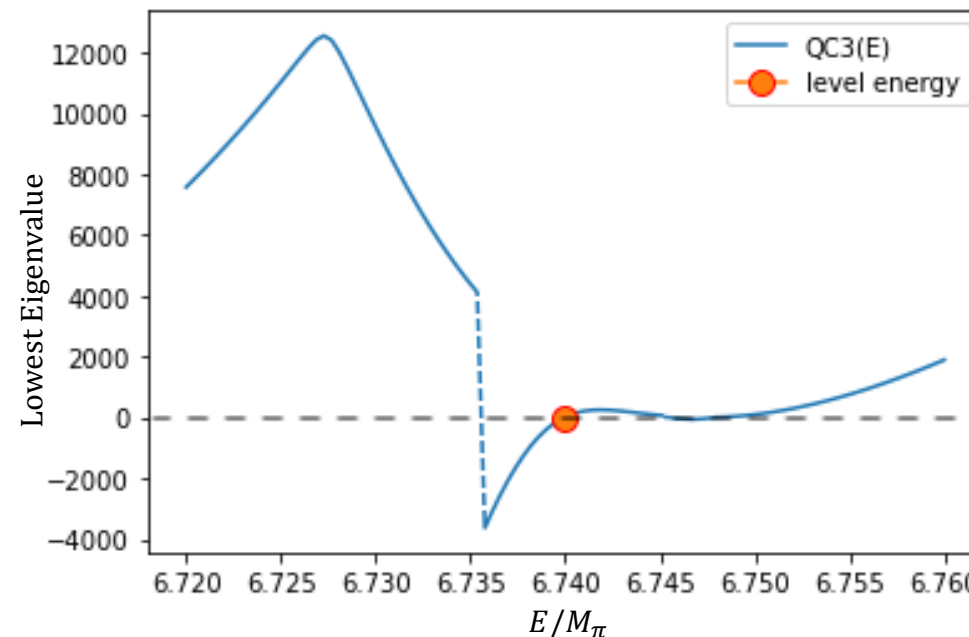
$$\Delta_2^S = \Delta_2 + \Delta'_2 \text{ where } \Delta_2 = \frac{(p_1 + p_{1'})^2 - 4m_1^2}{M^2} \text{ and } \Delta'_2 = \frac{(p_{1'} + p_{1'})^2 - 4m_1^2}{M^2}$$

$$\tilde{t}_{22} = \frac{t_{22}}{M^2} = \frac{(p_2 - p'_2)^2}{M^2}$$



Fitting With QC3

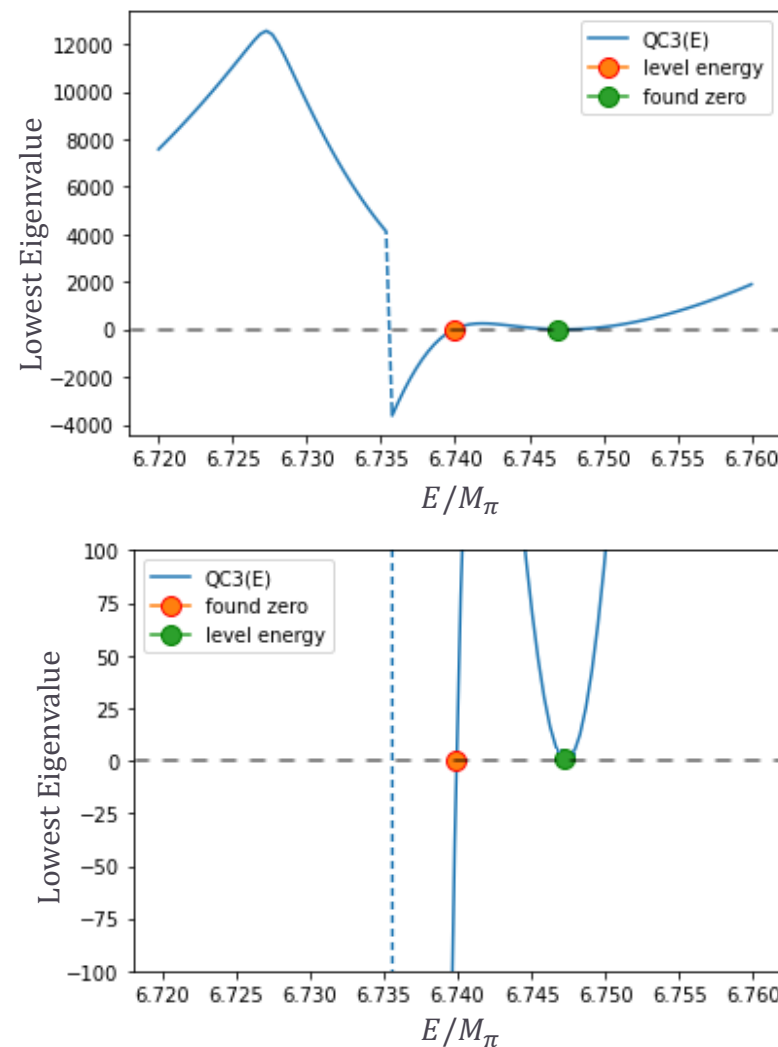
- Want to find zeros of $\det[\hat{F}_3^{-1}(E, \mathbf{P}, L) + \mathcal{K}_{\text{df},3}(E^*)]$
 - For given set of $\mathcal{K}_2$ and $\mathcal{K}_{\text{df},3}$ parameters, and for a given level, find zero near the input energy
 - Plot shows lowest eigenvalue as a function of E_{CM}
 - Repeat for each energy level in 2- and 3-particle spectra



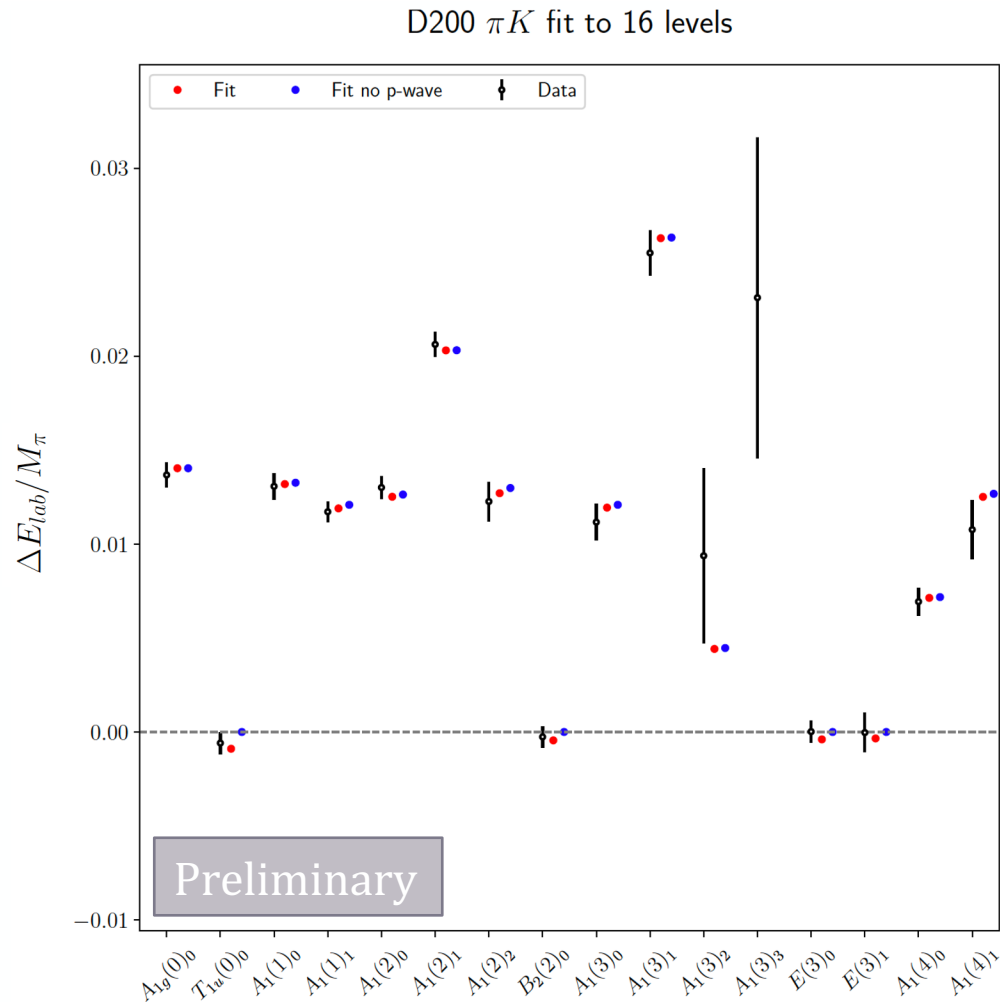
- By comparing the energy spectra to the zeros for both QC2 and QC3, compute χ^2
- Update the $\mathcal{K}_2$ and $\mathcal{K}_{\text{df},3}$ parameters and repeat, looking for the lowest χ^2
- Use Nelder-Mead to update parameters, minimizing χ^2 until acceptable tolerance reached

Implementation challenges

- Can be difficult to find *correct* zeros
 - Avoid double zeros corresponding to free energies (see plot)
 - For physical solutions, the lowest eigenvalue crosses from negative to positive
 - Have encountered no unphysical solutions
 - Zeros can be close together, making determination difficult as K-matrix parameters are varied



Preliminary Results

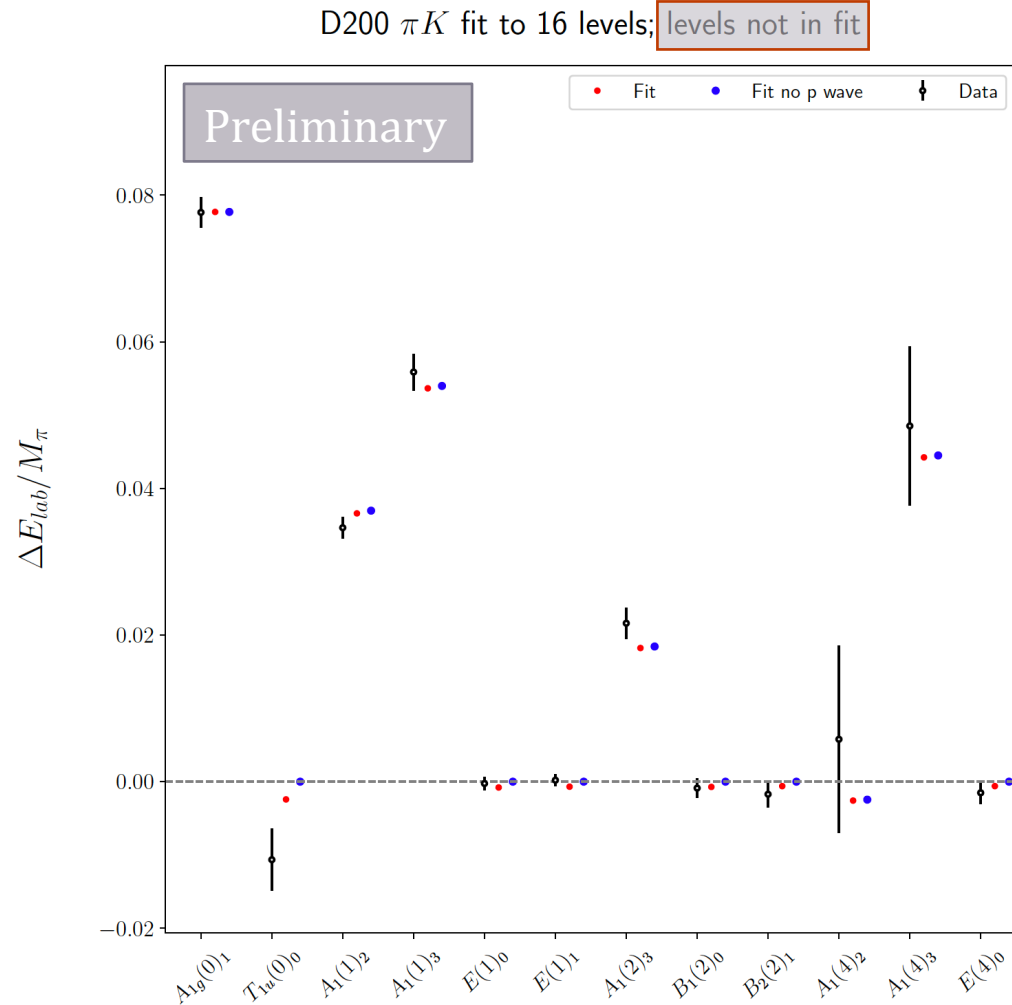


3-parameter fit to 16 $\pi^+ K^+$ levels on D200

$\chi^2/\text{dof} = 15.5/13$

1.7 σ significance of attractive p-wave interaction

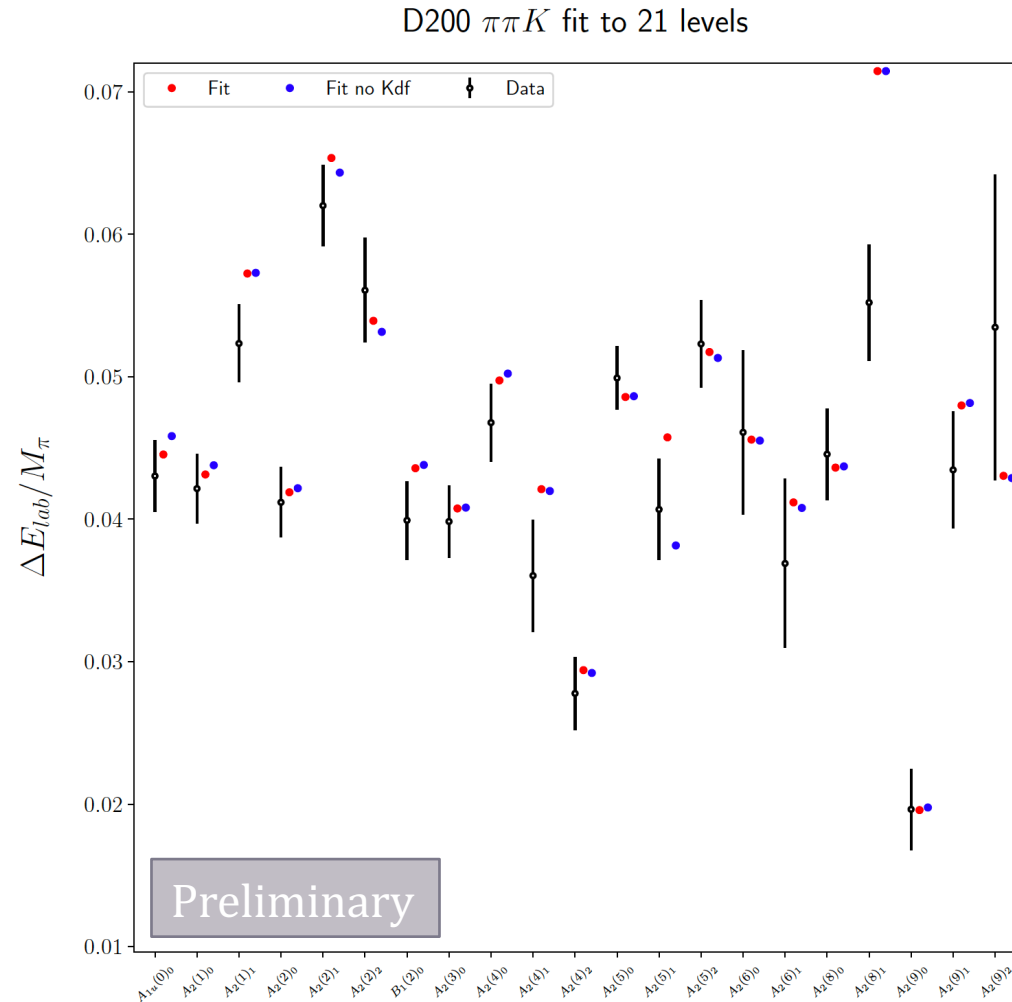
Preliminary Results



Plot shows fit to levels above the inelastic threshold

Still find reasonably good agreement between data and fits

Preliminary Results



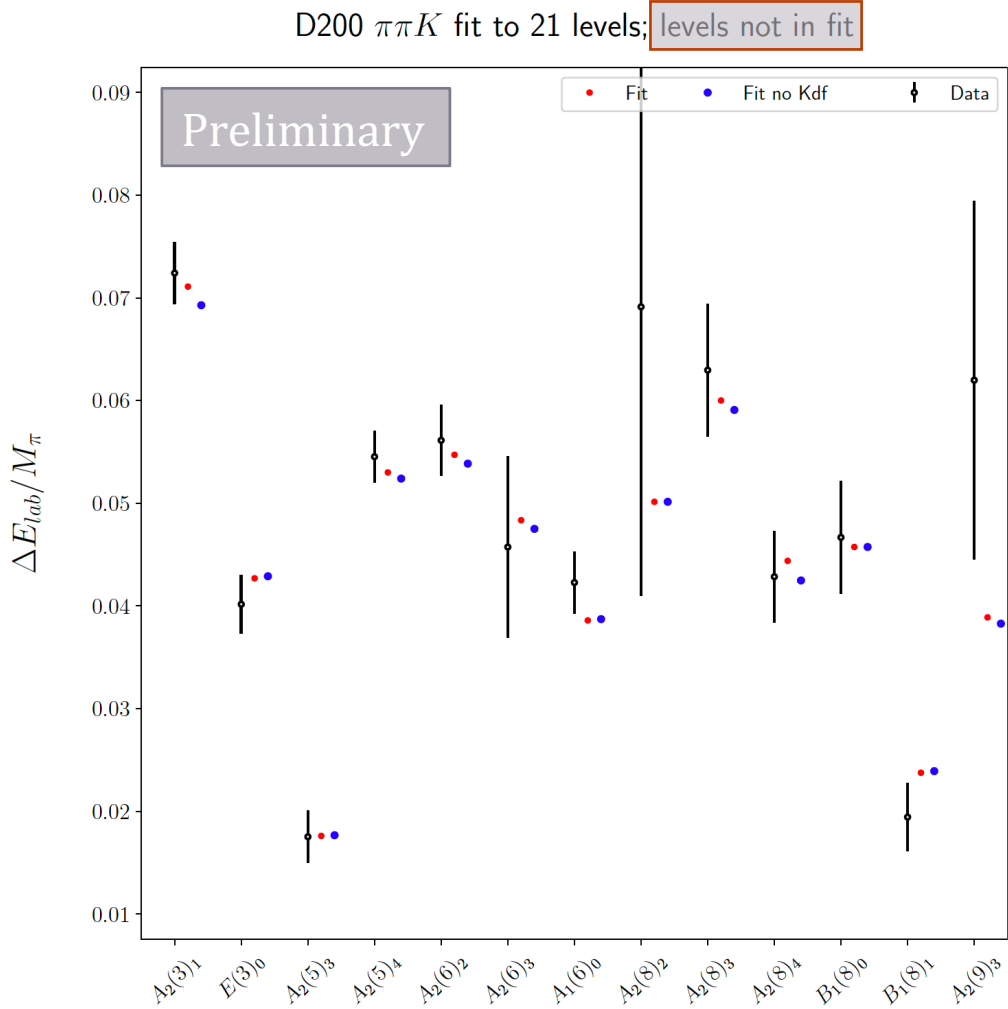
$B_0^{\pi\pi}$	-11.5(6)
$B_1^{\pi\pi}$	-2.5(4)
$Z_{\pi\pi}^2$	1 (fixed)
$B_0^{\pi K}$	-12.9(4)
$B_1^{\pi K}$	-2.8(3)
$Z_{\pi K}^2$	1 (fixed)
$P_0^{\pi K}$	0.0007(6)
$\mathcal{K}_0$	190(80)
$\mathcal{K}_1$	-690(340)
$\mathcal{K}_B$	160(650)
$\mathcal{K}_E$	170(420)

9-parameter fit to 59 $\pi^+\pi^+$, π^+K^+ , $\pi^+\pi^+K^+$ levels

$\chi^2/\text{dof} = 112/50$

Significance of non-zero $\mathcal{K}_{\text{df},3}$ is 3.2σ

Preliminary Results



$B_0^{\pi\pi}$	-11.5(6)
$B_1^{\pi\pi}$	-2.5(4)
$Z_{\pi\pi}^2$	1 (fixed)
$B_0^{\pi K}$	-12.9(4)
$B_1^{\pi K}$	-2.8(3)
$Z_{\pi K}^2$	1 (fixed)
$P_0^{\pi K}$	0.0007(6)
$\mathcal{K}_0$	190(80)
$\mathcal{K}_1$	-690(340)
$\mathcal{K}_B$	160(650)
$\mathcal{K}_E$	170(420)

Plot shows fit to levels above the inelastic threshold

Still find reasonably good agreement between data and fits

Comparing 2- and (3+2)-Particle Fits

$\pi\pi K + \pi\pi + \pi K$

D200

$KK\pi + KK + \pi K$

N203

Fit	$B_0^{\pi K}$	$B_1^{\pi K}$	$P_0^{\pi K}$	χ^2/dof	$M_\pi a_0^{\pi K}$
$\pi\pi K$	-12.9(4)	-2.8(3)	0.0007(6)	N/A	0.109(3)
$KK\pi$	-13.8(4)	-2.2(3)	0.0020(6)	N/A	0.102(3)
πK (16)	-13.1(5)	-2.5(3)	0.0012(7)	15.5/13	0.108(4)
πK (26)	-13.1(5)	-2.4(2)	0.0013(6)	31.0/23	0.108(4)
πK (28)	-13.3(5)	-2.3(2)	0.0017(6)	34.4/25	0.106(4)
πK (thr)	N/A	N/A	N/A	N/A	0.106(5)

Fit	$B_0^{\pi K}$	$B_1^{\pi K}$	$P_0^{\pi K}$	χ^2/dof	$M_\pi a_0^{\pi K}$
$\pi\pi K$	-5.39(11)	-1.89(17)	0.006(4)	N/A	0.208(4)
$KK\pi$	-5.31(13)	-2.17(19)	0.009(4)	N/A	0.211(5)
πK (19)	-5.42(15)	-2.07(21)	0.004(4)	21.1/16	0.207(6)
πK (36)	-5.45(15)	-2.02(21)	0.002(3)	36.1/33	0.206(6)
πK (thr)	N/A	N/A	N/A	N/A	0.213(7)

- Two particle fit parameters extracted from simultaneous 2- and 3- particle fits consistent with 2-particle fits alone
- Find slightly smaller errors when fits include both 2- and 3-particle levels
 - Result holds for D200 and N203
 - Result holds for other scattering channels

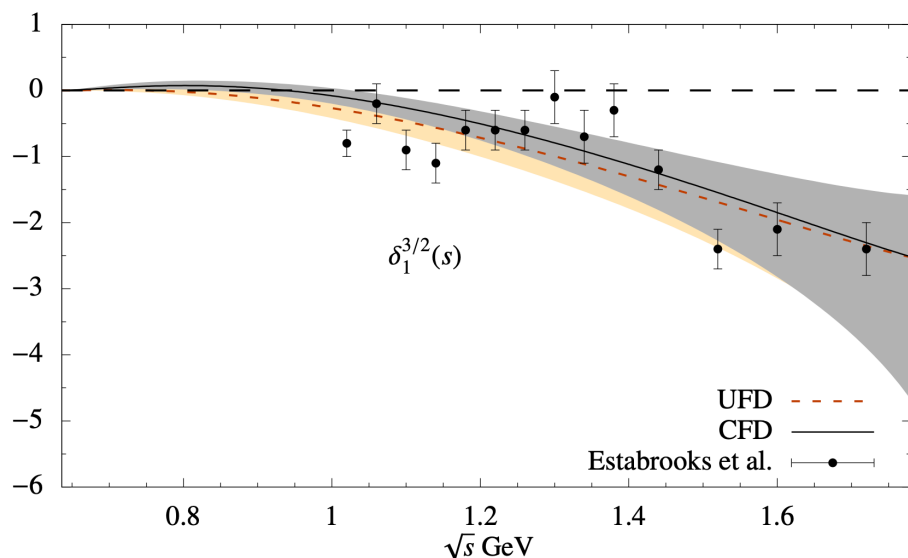
Conclusions from fits

- Working to linear order in threshold expansion (s and p waves) gives reasonable description of energy levels
 - Significantly worse than that obtained for identical particles with d waves included^[1]
- Obtain 1-2% precision in s-wave scattering length for all channels
- Fits continue to predict levels with good accuracy above inelastic threshold
 - Threshold expansions are not breaking down
- Simultaneous fits to 2- and 3-particle spectra lead to somewhat smaller errors in 2-particle parameters compared to 2-particle fits alone

[1] Blanton, Hanlon, Hörz, Morningstar, Romero-López, Sharpe, 2106.05590 (JHEP)

Conclusions from fits

- Find attractive p-wave $\pi^+ K^+$ scattering length, but only with 1.7σ significance

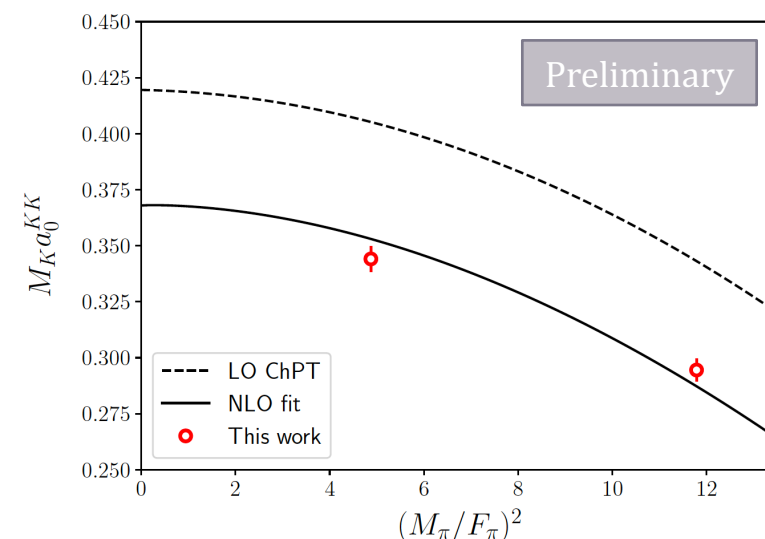
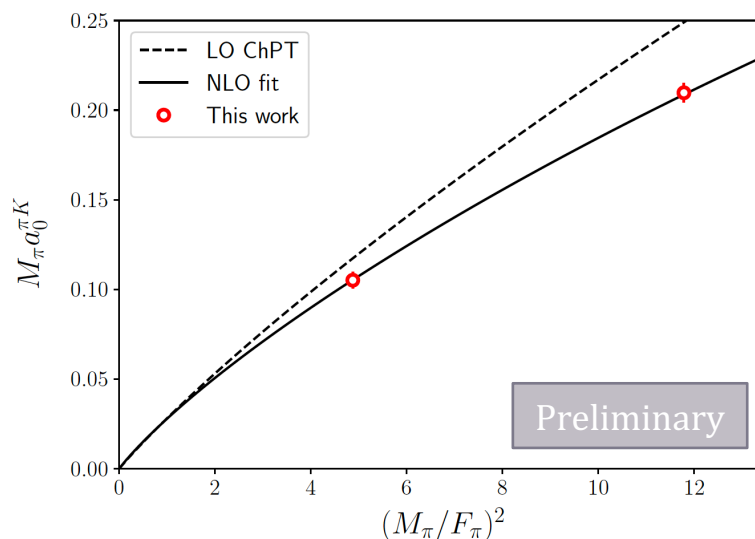
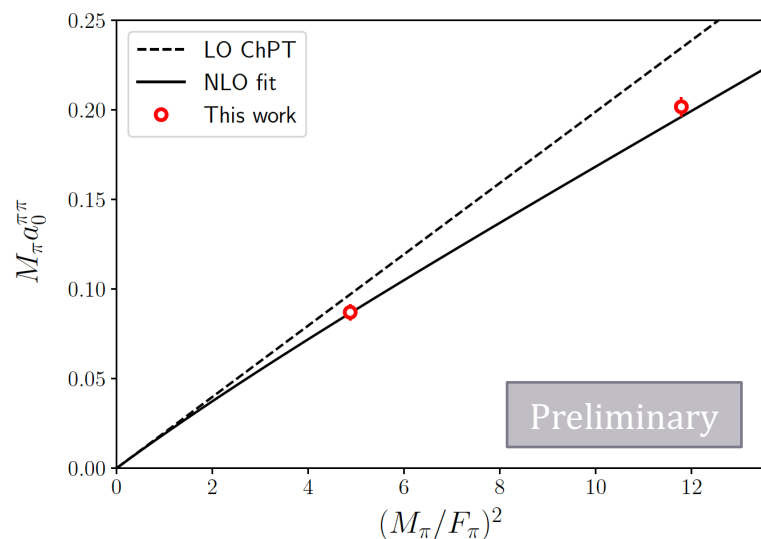


- Opposite sign to (very weakly) repulsive experimental result
- Sign of the phase shift consistent with dispersive analysis [\[1\]](#) at energies we consider, below ~ 1 GeV
- Experimental data above 1 GeV; lattice data allows access to lower energies

- We find non-zero $\mathcal{K}_{\text{df},3}$ with 3–5 σ significance for $\pi^+ \pi^+ K^+$ and $\pi^+ K^+ K^+$
 - To improve would require a reduction in the $\sim 10\%$ errors in ΔE_{lab}

[1] J. R. Peláez and A. Rodas, Phys. Rept. 969, 1 (2022), arXiv:2010.11222 [hep-ph].

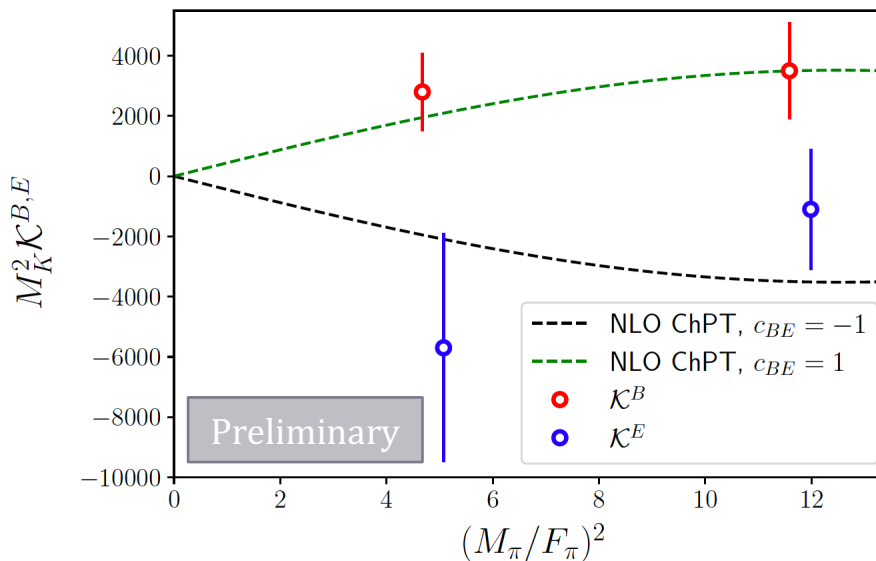
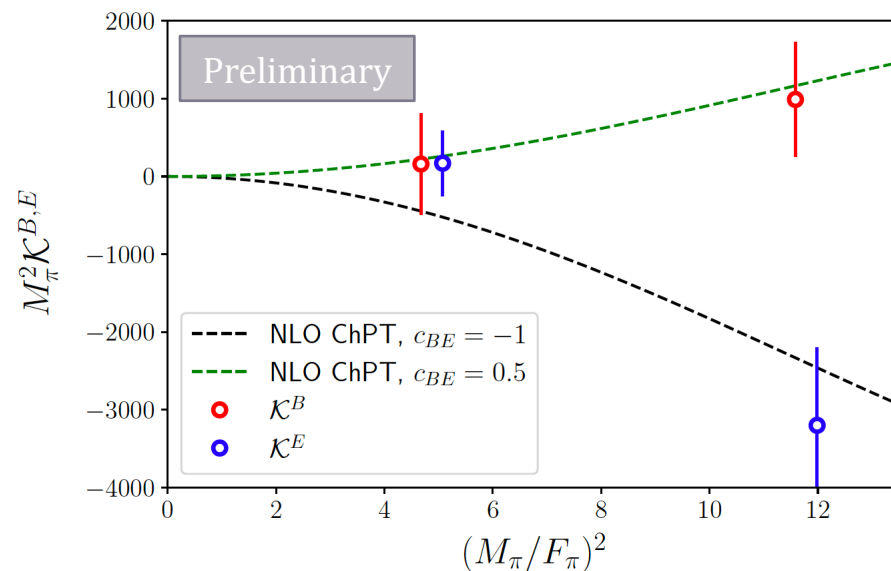
Comparison with χPT



χ^2/dof	$L_{\pi\pi}$	L_5
5.5/4	-0.00089(3)	-0.00050(8)

- Plots show simultaneous fits to $a_0^{\pi\pi}$, $a_0^{\pi K}$, a_0^{KK} using NLO SU(3) χPT
- Running L_5 FLAG value from $\mu = 770$ MeV to our scale, $4\pi F_\pi \approx 1160$ MeV, the quoted result of 0.00095(41) runs to -0.00001(41)
 - Result agrees at $\sim 1\sigma$

$\mathcal{K}^B$ and $\mathcal{K}^E$ Compared to χPT Form



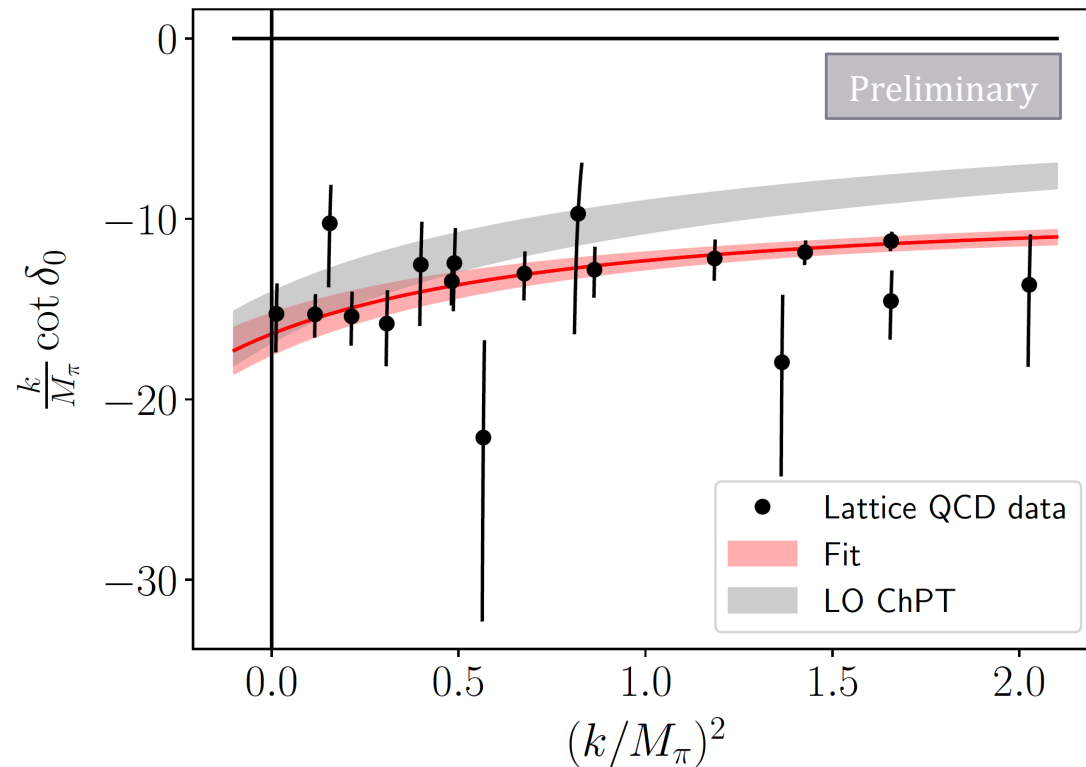
- Note that these plots do not show fits
- Results for $\mathcal{K}^B$ and $\mathcal{K}^E$ are consistent with NLO χPT forms and expectation that $c_{BE} \sim \mathcal{O}(1)$ ^[1]
- Generic NLO χPT forms:

$$M_\pi^2 \mathcal{K}_{\text{df},3}^{B,E}(\pi\pi K) = c_{BE} r_\pi^4 r_K^2 \quad \text{and} \quad M_\pi^2 \mathcal{K}_{\text{df},3}^{B,E}(KK\pi) = c_{BE} r_K^4 r_\pi^2$$

$$\text{where } r_\pi = M_\pi/F_\pi \quad \text{and} \quad r_K = M_K/F_\pi$$

[1] Blanton, Hanlon, Hörz, Morningstar, Romero-López, Sharpe, 2106.05590 (JHEP)

Physical-Point Ensembles Next



2-Particle πK Fit Parameters

$B_0^{\pi K}$	-25.8(1.7)
$B_1^{\pi K}$	-4.3(1.0)
$z_{\pi K}^2$	1 (fixed)
$p_0^{\pi K}$	0.0003(10)
χ^2/dof	19.6/(23-3)

- Preliminary analysis for CLS E250 physical-point ensembles has just begun!

Summary and Outlook

- First step of 3-particle formalism successfully applied to 2+1 systems
 - We encountered no problems with unphysical solutions in applying the QC3
 - Enlarged matrices in QC3 require small clusters to perform fits in a few days
- Determining 3-particle interaction ($\mathcal{K}_{\text{df},3}$) remains challenging
- Current and future work:
 - Analysis should be extended to chiral behavior of effective range
 - Physical-point ensembles
 - Solving integral equations (second step of formalism)
 - Extend to systems with 2- and 3-particle resonant behavior (e.g. $3\pi(I = 0,1)$, $\pi\pi N$)
 - Hoping to extend to 3 neutrons someday

$\pi^+\pi^+K^+$ and $K^+K^+\pi^+$ Interactions From The Lattice

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