

# Three-body Interactions in Lattice QCD and Phenomenology

Michael Döring  
Maxim Mai

THE GEORGE  
WASHINGTON  
UNIVERSITY  
WASHINGTON, DC

Jefferson Lab

International Workshop on Partial Wave Analyses and Advanced Tools for Hadron Spectroscopy, PWA11/ATHOS6



Supported by



NSF CAREER grant PHY-1452055

Deutsche  
Forschungsgemeinschaft  
DFG

[Many slides from Maxim Mai]

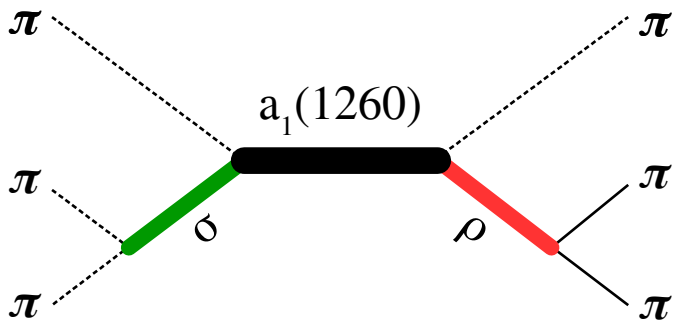
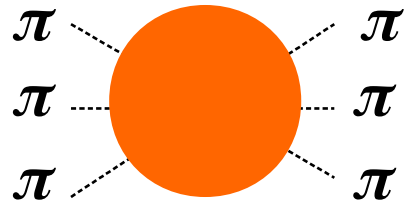
# Outline

---

- Three-body dynamics in infinite volume
- The Finite-volume problems (application: 2-body)
- **Three-body dynamics in finite volume**
  - The 3-pion system at maximal isospin:  
Interpretation of recent lattice QCD data

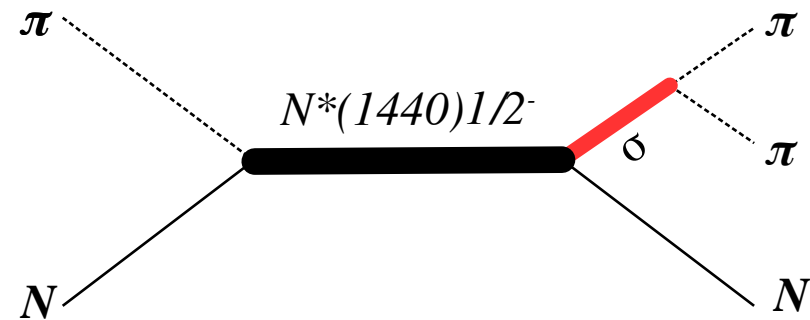
# 3-body dynamics for mesons and baryons

## Light mesons



- Important channel in GlueX @ JLab
- Finite volume spectrum from lattice QCD:  
[Lang, Leskovec, Mohler, Prelovsek \(2014\)](#)  
[Woss, Thomas et al. \[HadronSpectrum\] \(2018\)](#)  
[Hörz, Hanlon \(2019\), ...](#)

## Light baryons



- Roper resonance is debated for ~50 years in experiment. Can only be seen in PWA.
- 1<sup>st</sup> calculation w. meson-baryon operators on the lattice: [Lang et al. \(2017\)](#)

# Three-body Interactions with Isobars

---

**Mai, Hu, M. D., Pilloni, Szczepaniak**

**Eur. Phys. J. A53 (2017) 177**

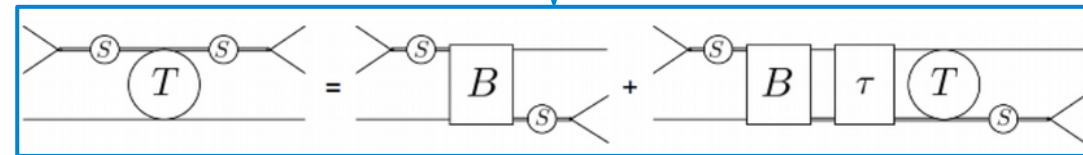
### 3-body Unitarity

$$\begin{aligned} \langle q_1, q_2, q_3 | (\hat{T} - \hat{T}^\dagger) | p_1, p_2, p_3 \rangle &= i \int_P \langle q_1, q_2, q_3 | \hat{T}^\dagger | k_1, k_2, k_3 \rangle \langle k_1, k_2, k_3 | \hat{T} | p_1, p_2, p_3 \rangle \\ &\times \prod_{\ell=1}^3 \left[ \frac{d^4 k_\ell}{(2\pi)^4} (2\pi) \delta^+(k_\ell^2 - m^2) \right] (2\pi)^4 \delta^4 \left( P - \sum_{\ell=1}^3 k_\ell \right) \end{aligned}$$

delta function sets all intermediate particles on-shell

### 3-body Unitarity

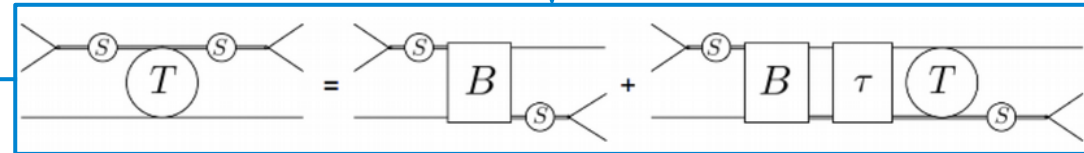
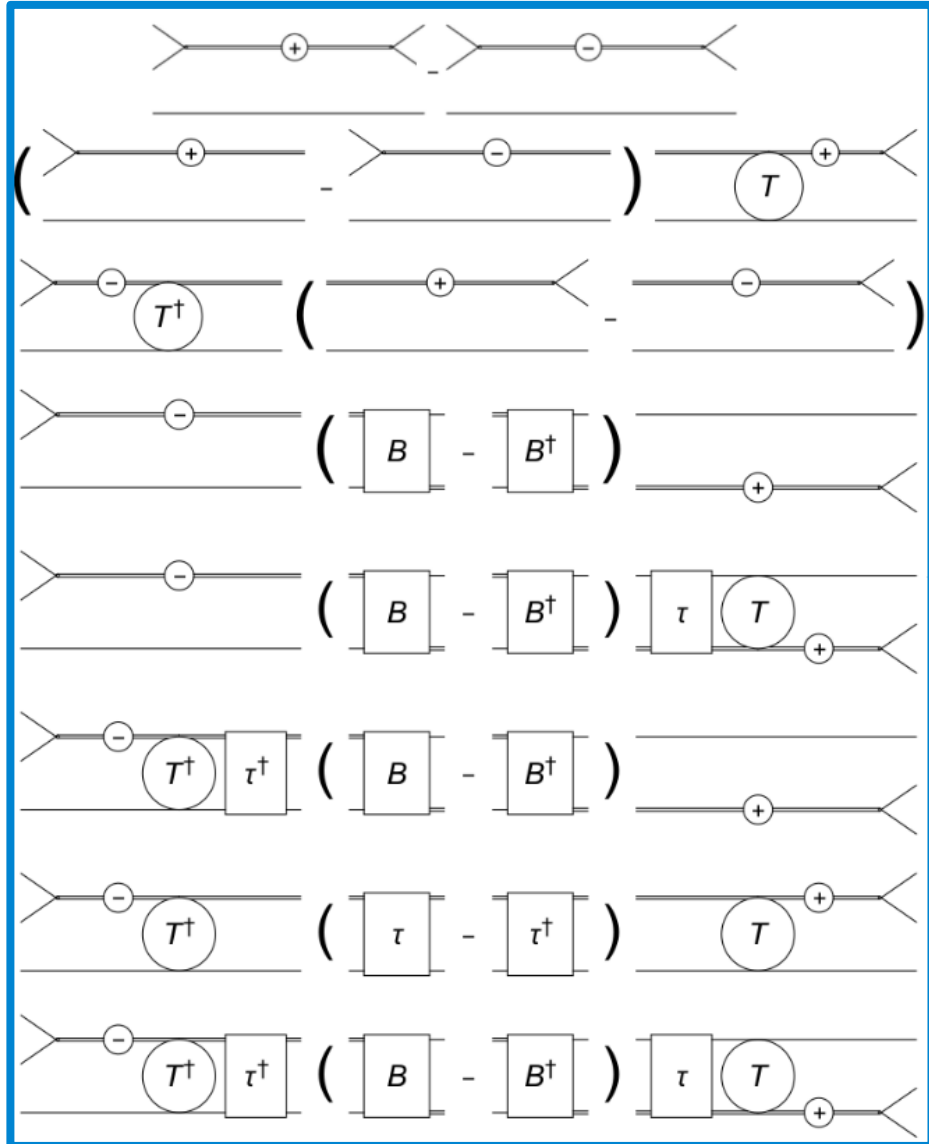
$$\langle q_1, q_2, q_3 | (\hat{T} - \hat{T}^\dagger) | p_1, p_2, p_3 \rangle = i \int_P \langle q_1, q_2, q_3 | \hat{T}^\dagger | k_1, k_2, k_3 \rangle \langle k_1, k_2, k_3 | \hat{T} | p_1, p_2, p_3 \rangle$$



**General Ansatz for the isobar-spectator interaction**  
→ **B &  $\tau$**  are **new** unknown functions

### 3-body Unitarity

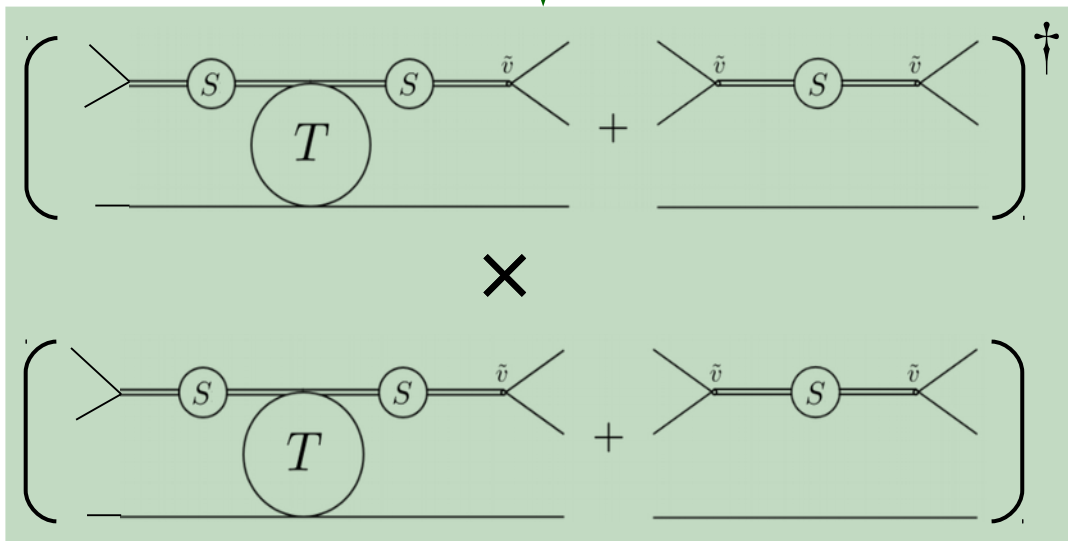
$$\langle q_1, q_2, q_3 | (\hat{T} - \hat{T}^\dagger) | p_1, p_2, p_3 \rangle = i \int_P \langle q_1, q_2, q_3 | \hat{T}^\dagger | k_1, k_2, k_3 \rangle \langle k_1, k_2, k_3 | \hat{T} | p_1, p_2, p_3 \rangle$$



**General Ansatz for the isobar-spectator interaction**  
 → **B &  $\tau$**  are new unknown functions

### 3-body Unitarity

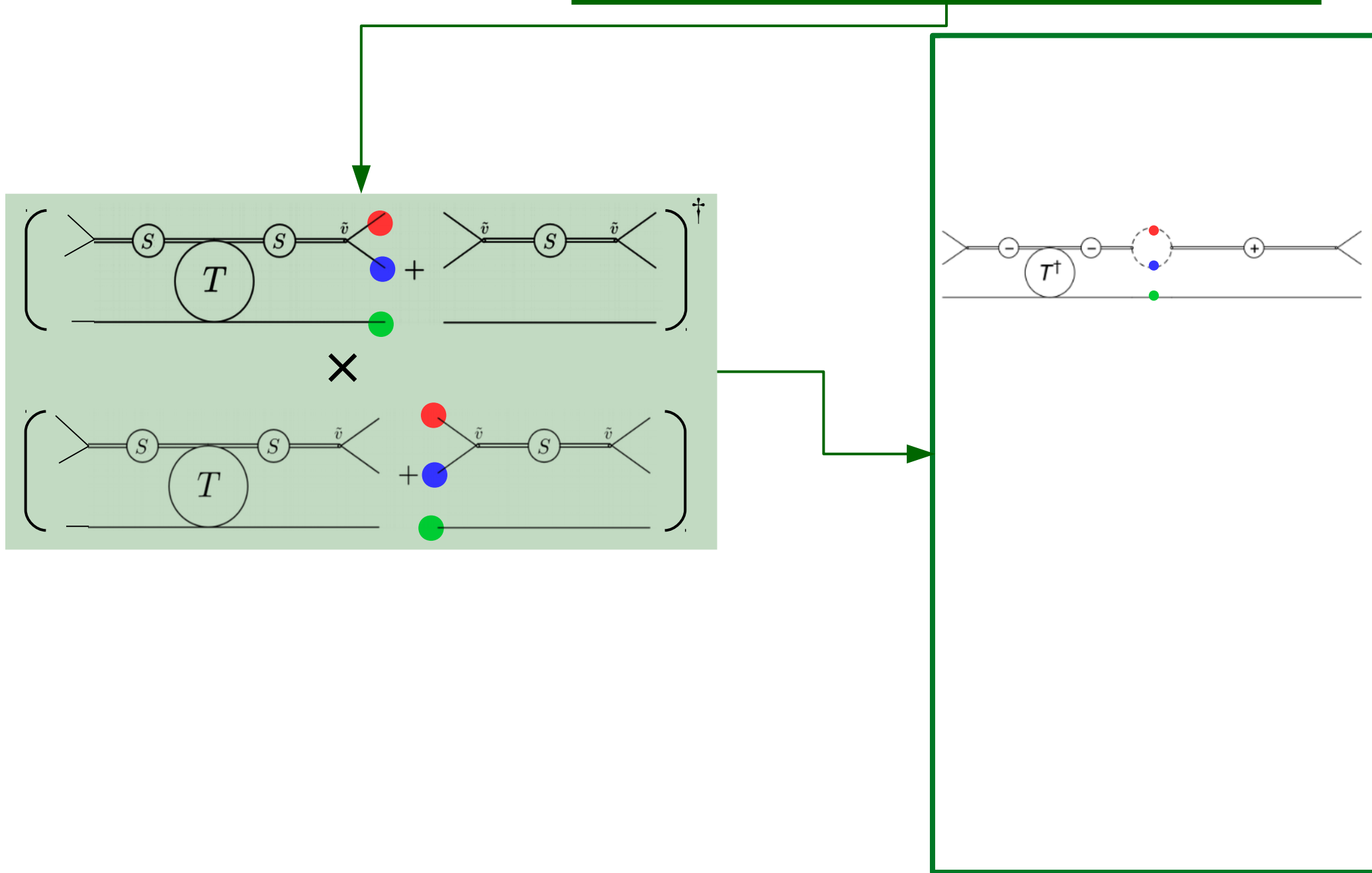
$$\langle q_1, q_2, q_3 | (\hat{T} - \hat{T}^\dagger) | p_1, p_2, p_3 \rangle = i \int_P \langle q_1, q_2, q_3 | \hat{T}^\dagger | k_1, k_2, k_3 \rangle \langle k_1, k_2, k_3 | \hat{T} | p_1, p_2, p_3 \rangle$$





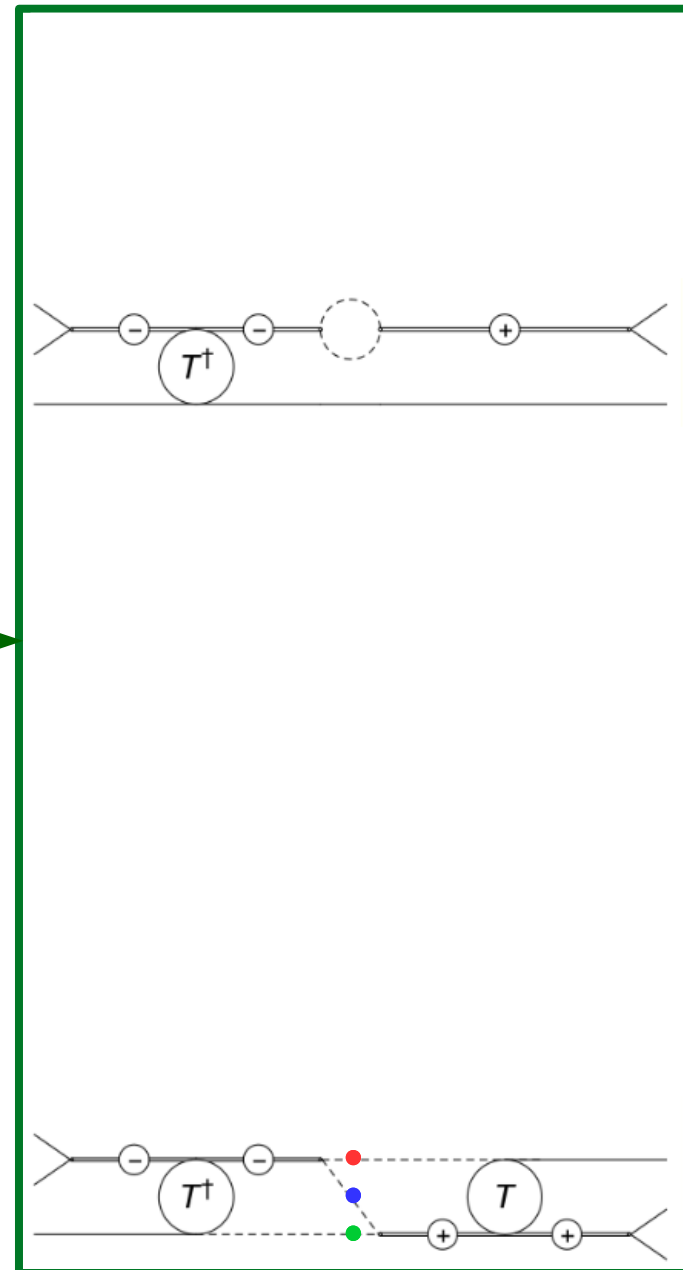
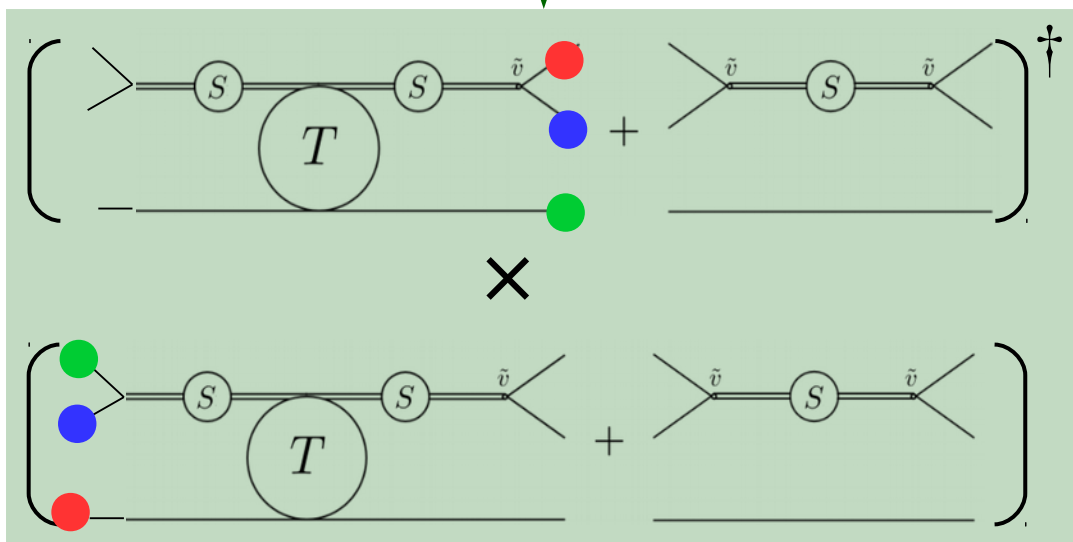
### 3-body Unitarity

$$\langle q_1, q_2, q_3 | (\hat{T} - \hat{T}^\dagger) | p_1, p_2, p_3 \rangle = i \int_P \langle q_1, q_2, q_3 | \hat{T}^\dagger | k_1, k_2, k_3 \rangle \langle k_1, k_2, k_3 | \hat{T} | p_1, p_2, p_3 \rangle$$



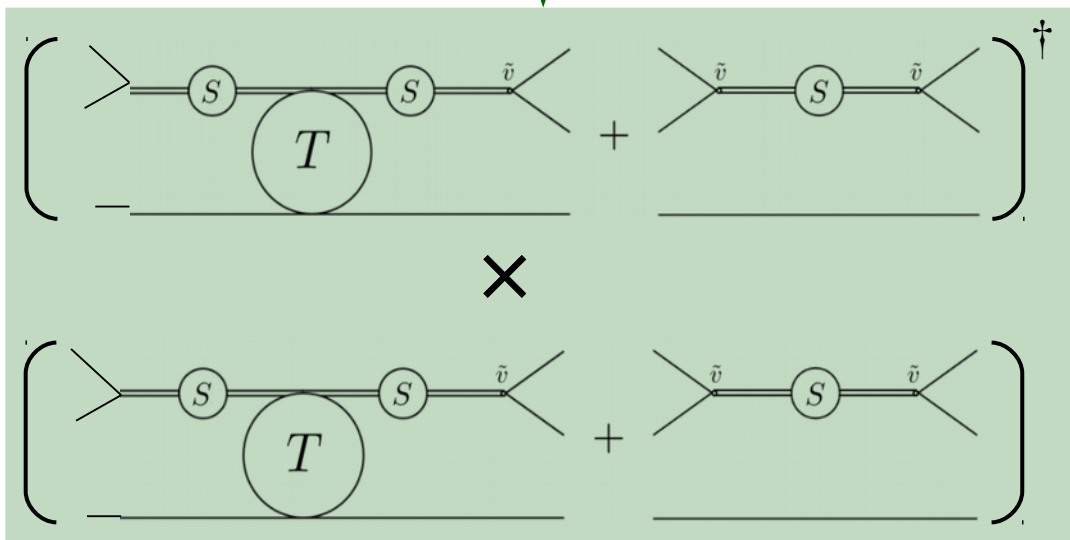
### 3-body Unitarity

$$\langle q_1, q_2, q_3 | (\hat{T} - \hat{T}^\dagger) | p_1, p_2, p_3 \rangle = i \int_P \langle q_1, q_2, q_3 | \hat{T}^\dagger | k_1, k_2, k_3 \rangle \langle k_1, k_2, k_3 | \hat{T} | p_1, p_2, p_3 \rangle$$

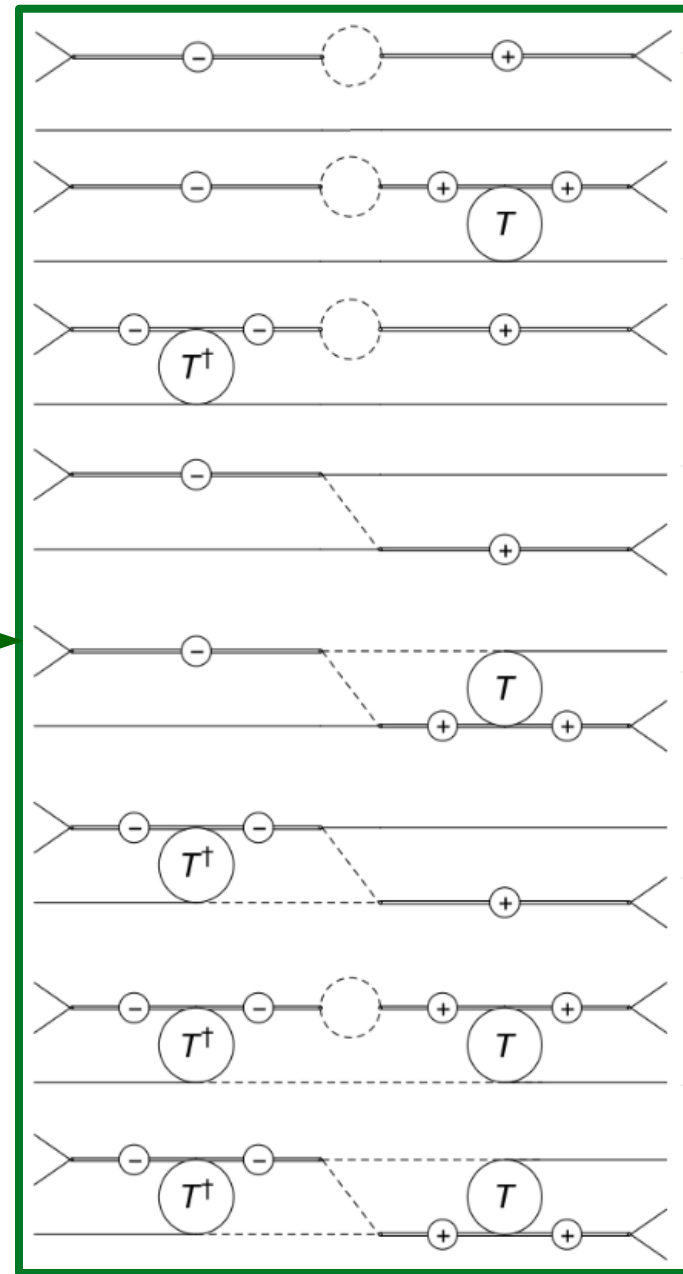


### 3-body Unitarity

$$\langle q_1, q_2, q_3 | (\hat{T} - \hat{T}^\dagger) | p_1, p_2, p_3 \rangle = i \int_P \langle q_1, q_2, q_3 | \hat{T}^\dagger | k_1, k_2, k_3 \rangle \langle k_1, k_2, k_3 | \hat{T} | p_1, p_2, p_3 \rangle$$

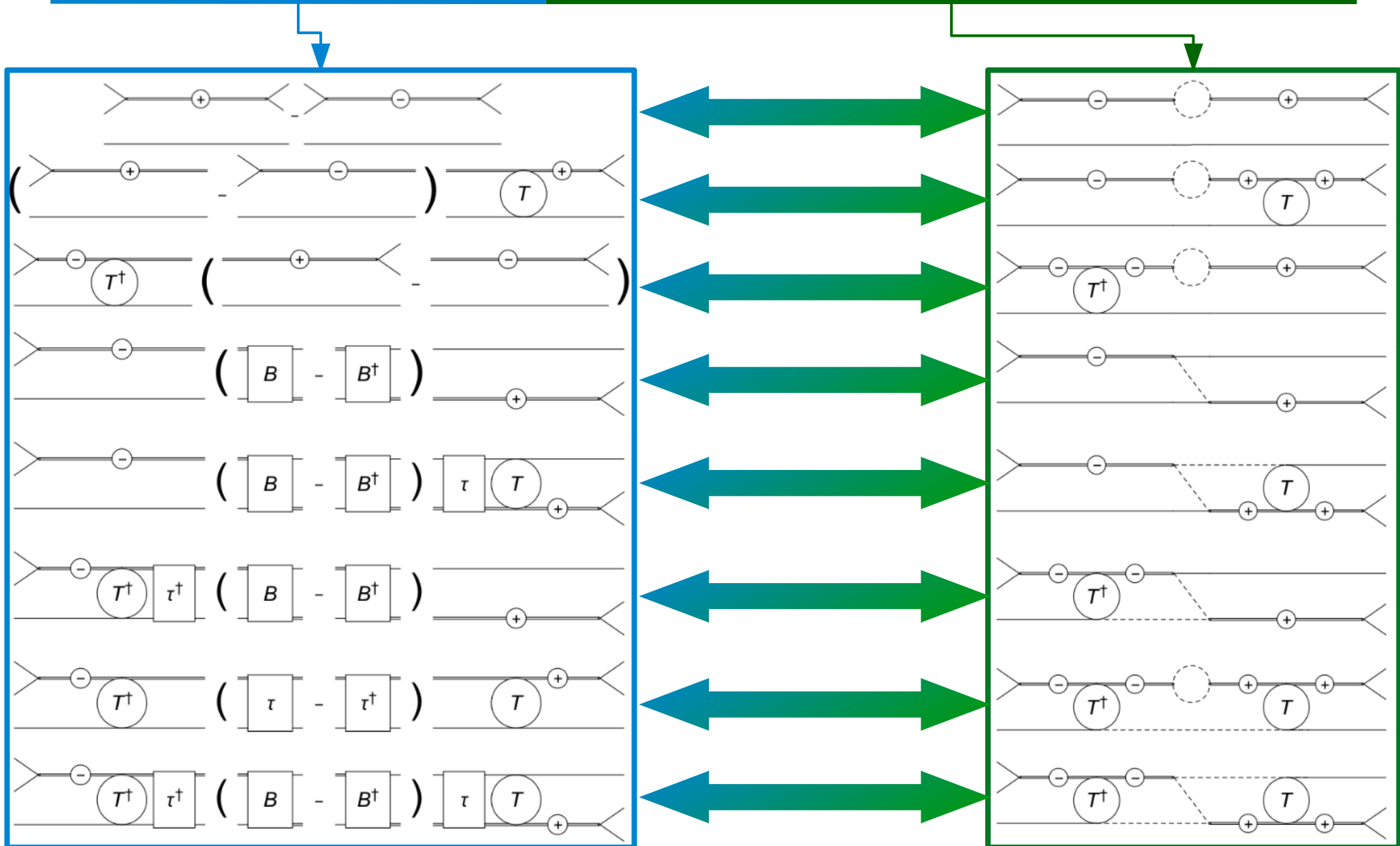


8 top.



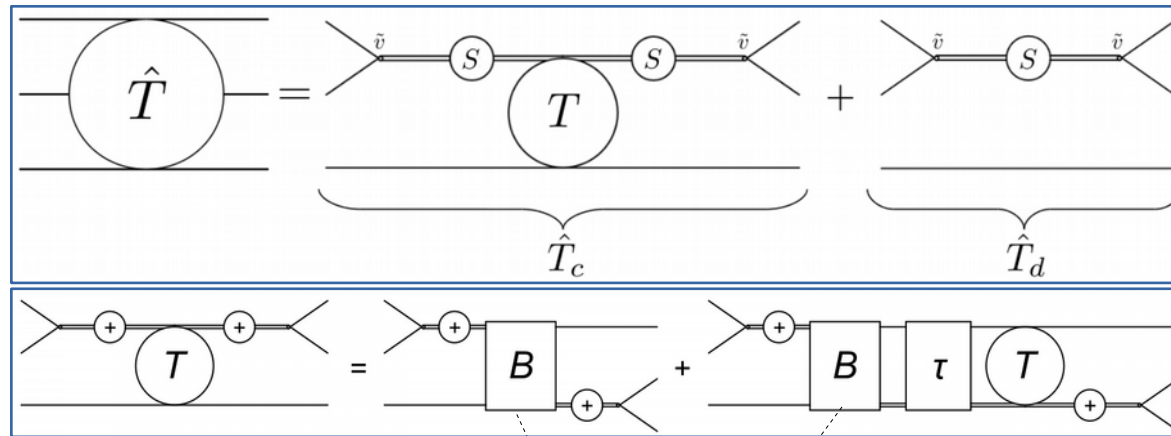
### 3-body Unitarity

$$\langle q_1, q_2, q_3 | (\hat{T} - \hat{T}^\dagger) | p_1, p_2, p_3 \rangle = i \int_P \langle q_1, q_2, q_3 | \hat{T}^\dagger | k_1, k_2, k_3 \rangle \langle k_1, k_2, k_3 | \hat{T} | p_1, p_2, p_3 \rangle$$



# Scattering amplitude

3 → 3 scattering amplitude is a 3-dimensional integral equation



- Imaginary parts of **B**, **S** are fixed by **unitarity/matching**
- For simplicity **v=λ** (full relations available)

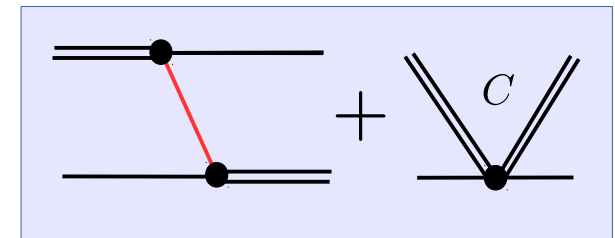
$$\text{Disc } B(u) = 2\pi i \lambda^2 \frac{\delta(E_Q - \sqrt{m^2 + Q^2})}{2\sqrt{m^2 + Q^2}}$$

- un-subtracted dispersion relation

$$\langle q|B(s)|p\rangle = -\frac{\lambda^2}{2\sqrt{m^2 + Q^2} (E_Q - \sqrt{m^2 + Q^2} + i\epsilon)} + C$$

- one- $\pi$  exchange in TOPT → **RESULT, NOT INPUT!**

- One can map to field theory, but does not have to. Result is a-priori dispersive.



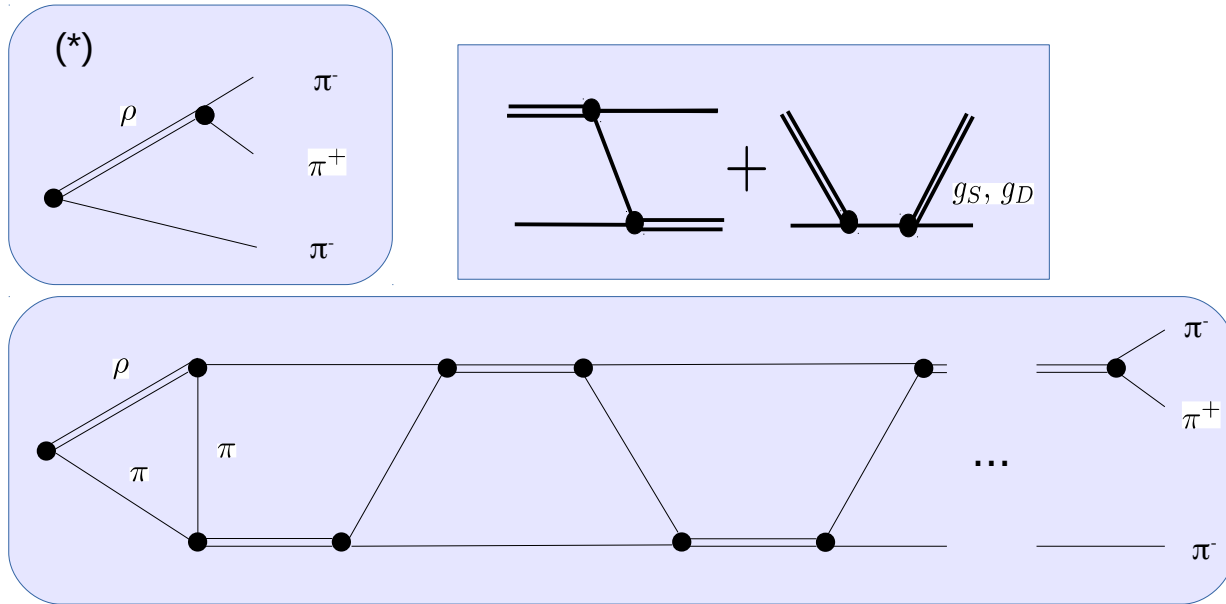
# Application: The $a_1(1260)$ lineshape

Sadasivan, M.D., Mai, in preparation

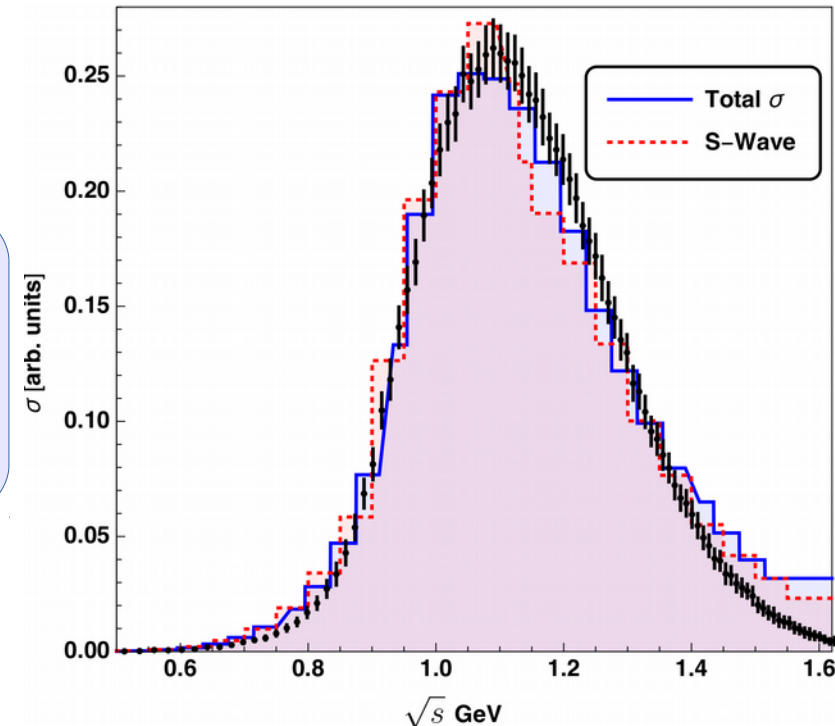
- Recent efforts to study 3-body production beyond the “isobar approximation” (\*)

P. Magalhães, A. C. dos Reis et al., PRD84 (2011); Khmechandani, Martinez, Oset, PRC77 (2008); JPAC: Mikhasenko, Wunderlich et. al., JHEP (2019); Mikhasenko, Pilloni et. al., PRD98 (2018); A. Jackura et al., EPJC79 (2019); Jülich: Janssen et al., PRL (1993)

- Here: Full solution of three-body equation with **exact** three-body unitarity
- S- and D-waves included



+ symmetrization final states



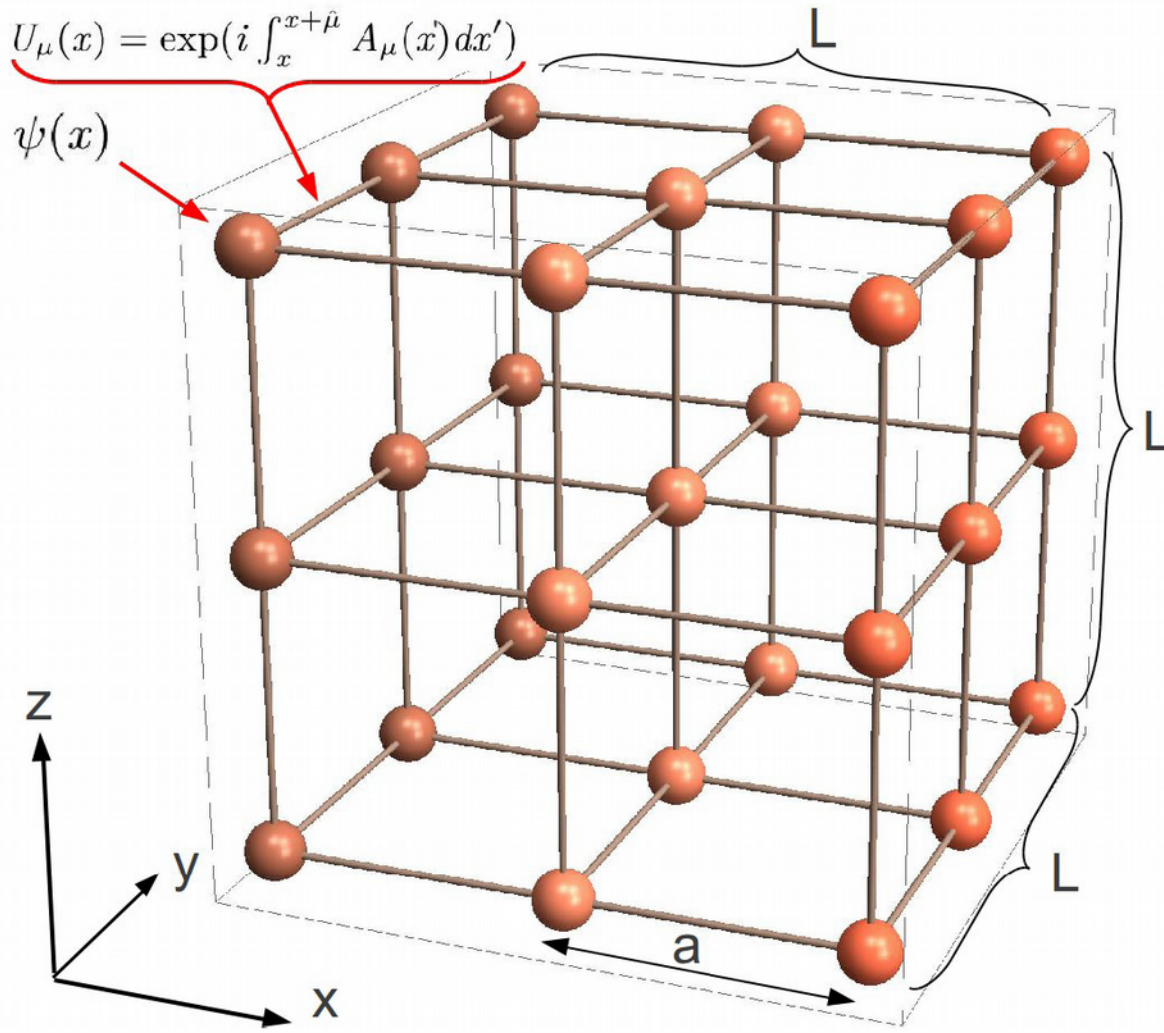
Data: ALEPH coll. hep-ex/0506072

(\*) here meant in the sense of “no rescattering”, “no three-body unitarity”

From two to three particles in finite volume

---

# The cubic lattice



- Side length  $L$ ,  
periodic boundary conditions  
 $\Psi(\vec{x}) \stackrel{!}{=} \Psi(\vec{x} + \hat{e}_i L)$   
 $\rightarrow$  finite volume effects  
 $\rightarrow$  Infinite volume  $L \rightarrow \infty$   
extrapolation
- Lattice spacing  $a$   
 $\rightarrow$  finite size effects  
Modern lattice calculations:  
 $a \simeq 0.07 \text{ fm} \rightarrow p \sim 2.8 \text{ GeV}$   
 $\rightarrow$  (much) larger than typical  
hadronic scales;  
not considered here.
- Unphysically large  
quark/hadron masses  
 $\rightarrow$  (chiral) extrapolation  
required.

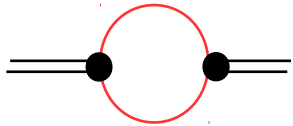


# How to derive the 2-body quantization condition

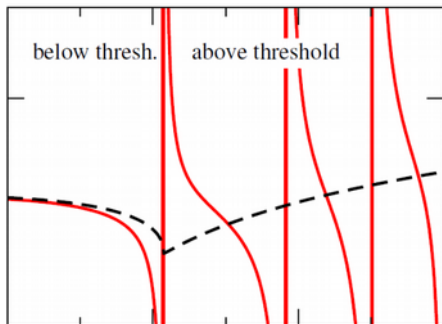
---

Two-body unitarity

On-shell condition



Imaginary parts



Infinite  
→ Fin. Vol

$$\int \frac{d^3 \mathbf{q}}{(2\pi)^3} \rightarrow \frac{1}{L^3} \sum_s \sum_{i=1}^{\vartheta(s)}$$

Power-law fin-vol. effects

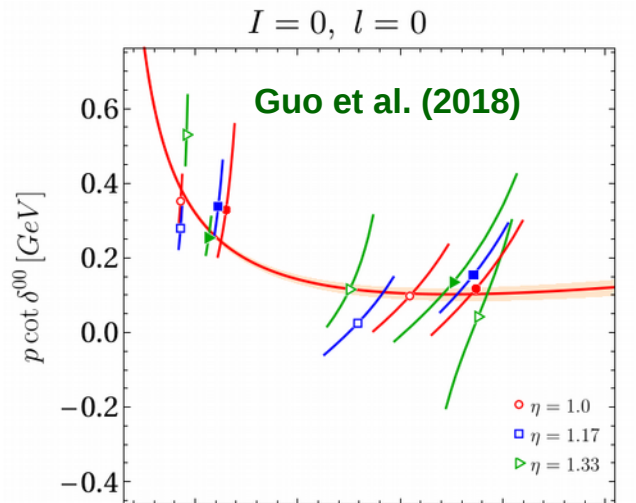
Lüscher

$$p \cot \delta(p) = -8\pi\sqrt{s} \left( \tilde{G}(E) - \text{Re } G(E) \right)$$

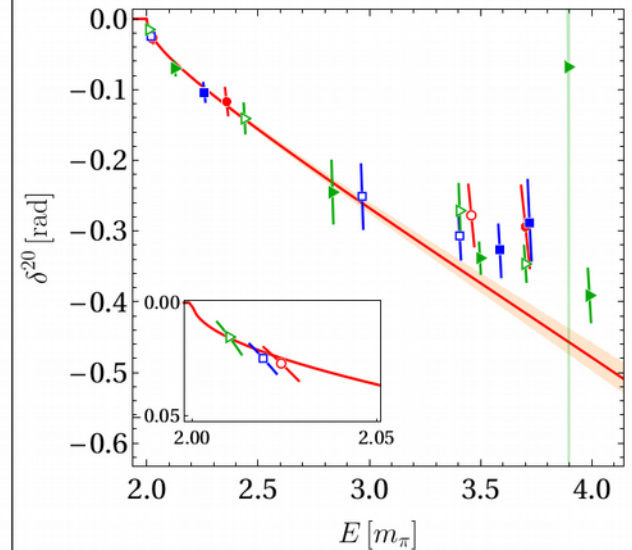
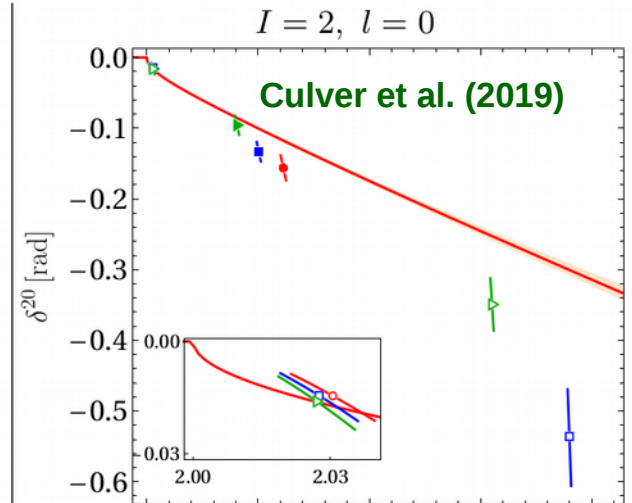
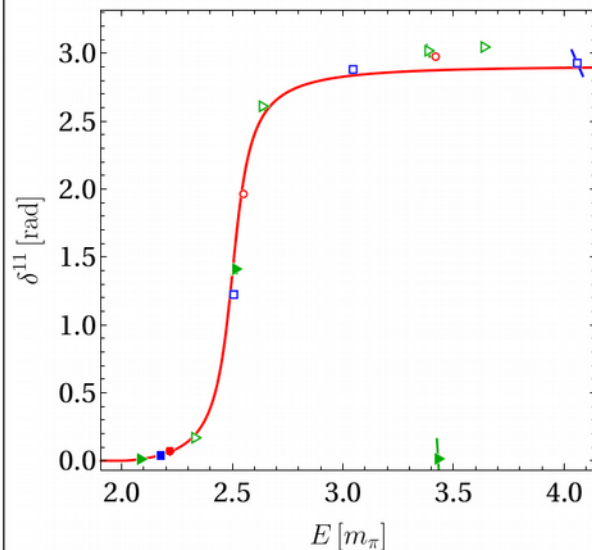
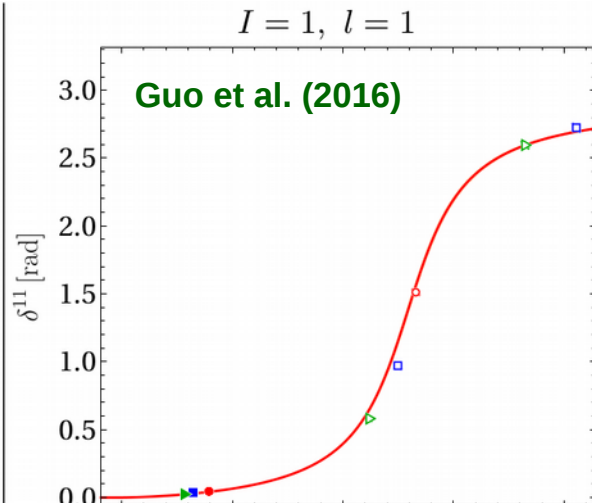
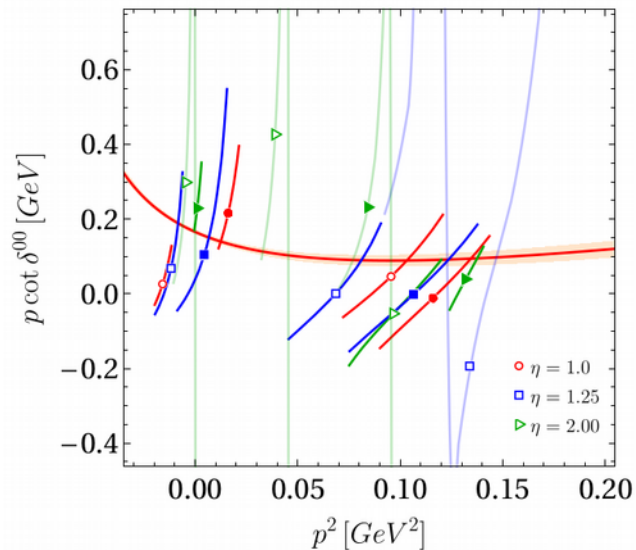
# GWU lattice group: All Isospins

[Culver et al., PRD100 (2019); Mai et al., arXiv:1908.01847 [hep-lat]]

$m_\pi = 224 \text{ MeV}$



$m_\pi = 315 \text{ MeV}$

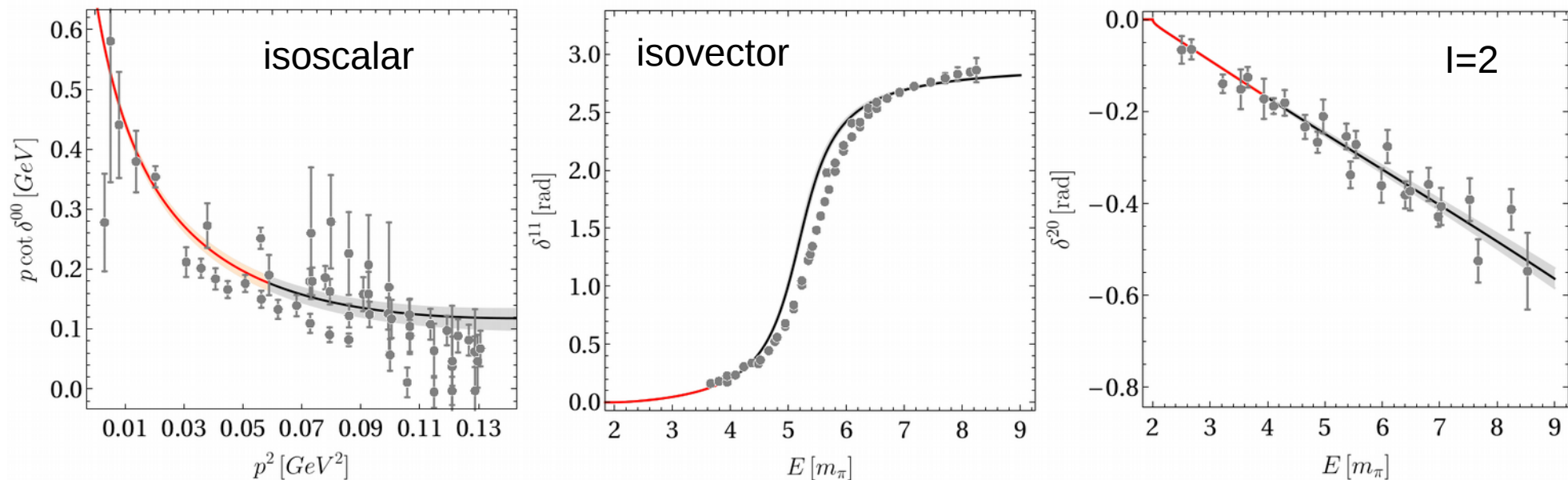


- Simultaneous fit with Inverse Amplitude Method (more later)
- Including correlation between energy eigenvalues, pion masses and pion decay constants
- Including correlations across energy eigenvalues & isospins

# GWU lattice group: Chiral Extrapolation

(Optional & model dependent)

[ Mai et al., arXiv:1908.01847 [hep-lat]]



Scattering lengths and resonance poles:

$m_\pi$ [MeV]		$\sim 315$		$\sim 224$		139
$m_\pi a_0^{I=0}$		$+1.9008^{+0.0521}_{-0.0593}$		$+0.6985^{+0.0010}_{-0.0015}$		$+0.2132^{+0.0008}_{-0.0009}$
$m_\pi a_0^{I=2}$		$-0.1538^{+0.0021}_{-0.0018}$		$-0.0952^{+0.0010}_{-0.0009}$		$-0.0433^{+0.0002}_{-0.0002}$
$m_\sigma$ [MeV]		$+591^{+6}_{-5} - i109^{+4}_{-4}$		$+502^{+4}_{-4} - i175^{+6}_{-5}$		$+443^{+3}_{-3} - i221^{+6}_{-6}$
$g_{\sigma\pi\pi}$ [MeV]		$533^{+2}_{-2}$		$426^{+2}_{-2}$		$397.8^{+0.6}_{-0.6}$
$m_\rho$ [MeV]		$+789^{+1}_{-1} - i20^{+0}_{-0}$		$+738^{+2}_{-1} - i43^{+1}_{-1}$		$+724^{+2}_{-4} - i67^{+1}_{-1}$
$g_{\rho\pi\pi}$ [MeV]		$226^{+2}_{-2}$		$282^{+3}_{-2}$		$323^{+5}_{-3}$



# THREE-BODY AMPLITUDE IN A BOX

---

M. Mai, MD, EPJA 2017 [arXiv: 1709.08222]

# Overview

---

Lüscher-like formalism in  $3 \rightarrow 3$  case is under investigation

Polejaeva/Rusetsky (2012)

Briceño/Hansen/Sharpe (2014-)

Non-relativistic approaches based on dimer picture & effective field theory

Kreuzer, Griesshammer(2012), Hammer et al. (2016)

F. Romero, Rusetsky, Urbach et. al. (2018)

Equivalence of various 3-body formalisms; three-body unitarity for Hansen/Sharpe

Requirements

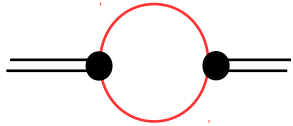
Jackura et al. (2019) [JPAC], Briceño et al. (2019)

- 3-body systems involve (resonant) two-body sub-amplitudes: Construct such that 2-body information can be included
- Need extrapolations between different energies (problem of underdetermination)
- Allow for systematic improvement by allowing more and more quantum numbers as lattice data improve (problem of underdetermination)
- At least, **all** possible intermediate on-shell configurations must be identified and included to ensure all power-law finite-volume effects are taken account of.

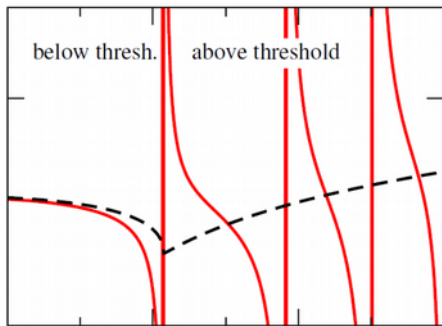
⇒ This work: **Quantization condition from 3-body unitarity in isobar formulation**

Two-body unitarity

On-shell condition



Imaginary parts



Infinite  
→ Fin. Vol

Power-law fin-vol. effects

Lüscher

$$p \cot \delta(p) = -8\pi\sqrt{s} (\tilde{G}(E) - \text{Re } G(E))$$

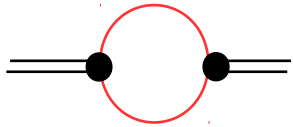
# How to derive the 2-body quantization condition

---

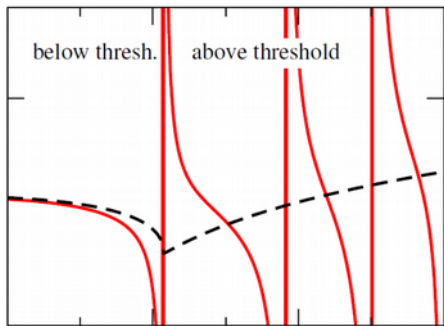
Three-body?  
Analogously!

Two-body unitarity

On-shell condition



Imaginary parts



Infinite  
→ Fin. Vol

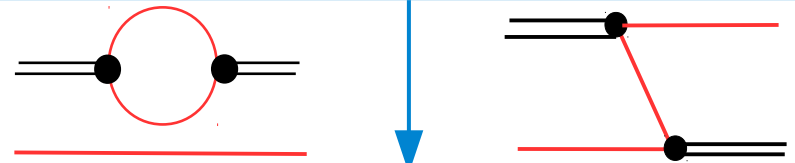
Power-law fin-vol. effects

Lüscher

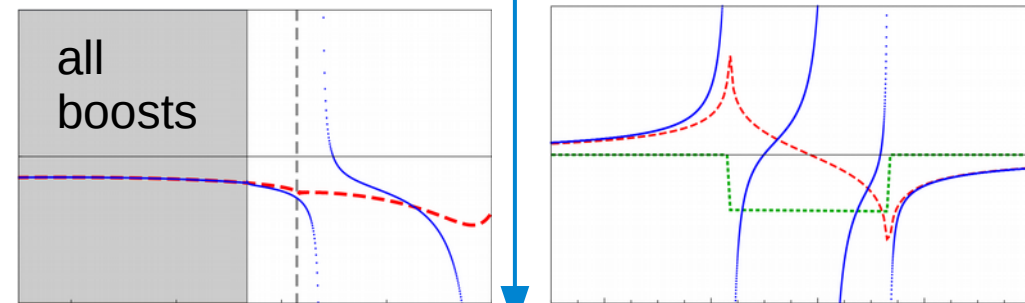
$$p \cot \delta(p) = -8\pi\sqrt{s} \left( \tilde{G}(E) - \text{Re } G(E) \right)$$

Three-body unitarity

On-shell condition



Imaginary parts



Power-law fin-vol. effects

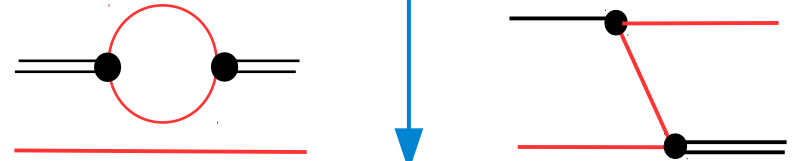
Quantization Condition

$$\text{Det} \left( \mathbf{B}_{\mathbf{u}\mathbf{u}'}^{\Gamma_{\mathbf{s}\mathbf{s}'}}(\mathbf{W}^2) + \frac{2\mathbf{E}_s \mathbf{L}^3}{\vartheta(s)} \tau_s(\mathbf{W}^2)^{-1} \delta_{\mathbf{s}\mathbf{s}'} \delta_{\mathbf{u}\mathbf{u}'} \right) = 0$$

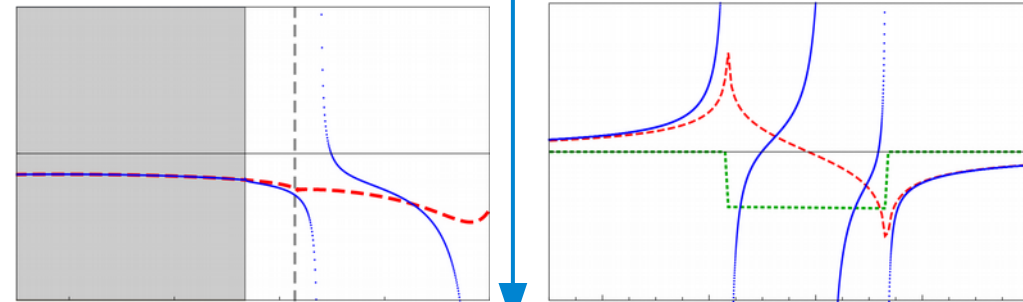
Only exact three-body unitarity guarantees the cancellation of unphysical 1<sup>st</sup> and 2<sup>nd</sup> order poles

Three-body unitarity

On-shell condition



Imaginary parts



Power-law fin-vol. effects

Quantization Condition

$$\text{Det} \left( \mathbf{B}_{\mathbf{u}\mathbf{u}'}^{\Gamma_{\mathbf{s}\mathbf{s}'}}(\mathbf{W}^2) + \frac{2\mathbf{E}_s \mathbf{L}^3}{\vartheta(\mathbf{s})} \tau_{\mathbf{s}}(\mathbf{W}^2)^{-1} \delta_{\mathbf{s}\mathbf{s}'} \delta_{\mathbf{u}\mathbf{u}'} \right) = 0$$





# A physical system:

$$\pi^+ \pi^+ \pi^+$$

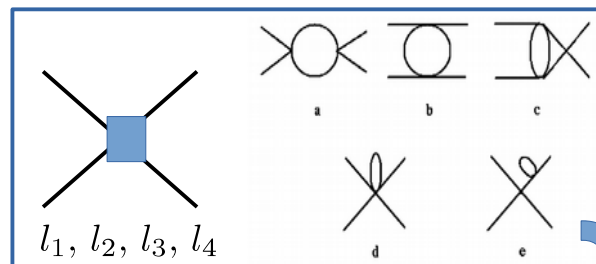
---

Mai, M.D., PRL 122 (2019), 062503

# Three positive pions

- Maximal isospin:  $\pi^+\pi^+\pi^+$ 
  - LatticeQCD results for ground level available for  $\pi^+\pi^+$  &  $\pi^+\pi^+\pi^+$
  - Repulsive channel
  - $L=2.5\text{ fm}$ ,  $m_\pi=291/352/491/591\text{ MeV}$

NPLQCD, Detmold et al. (2008)



Inverse Amplitude method

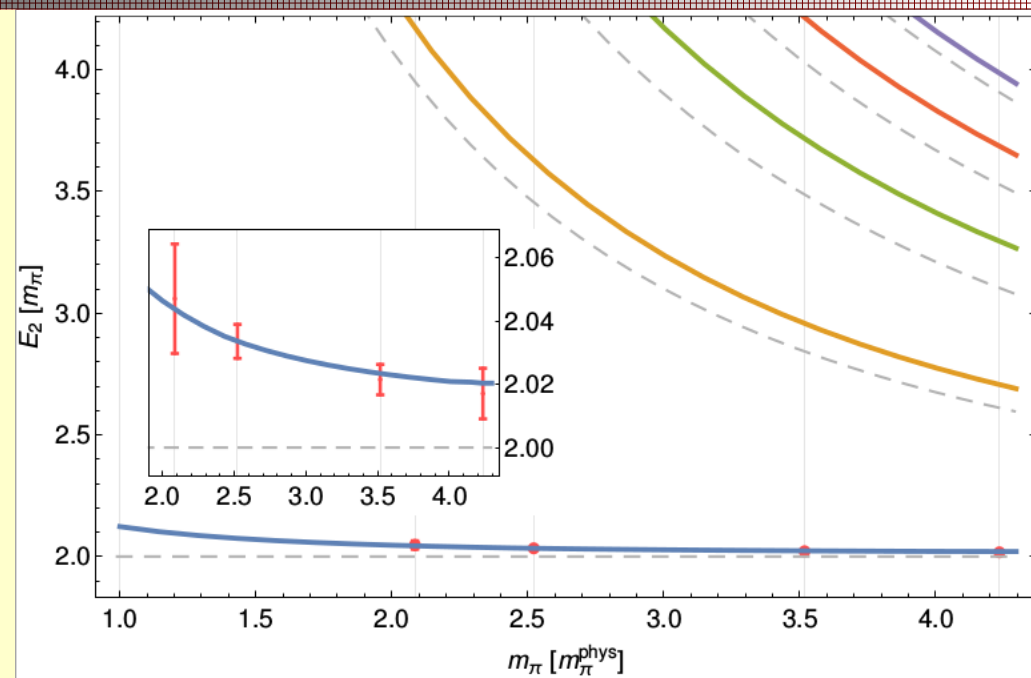
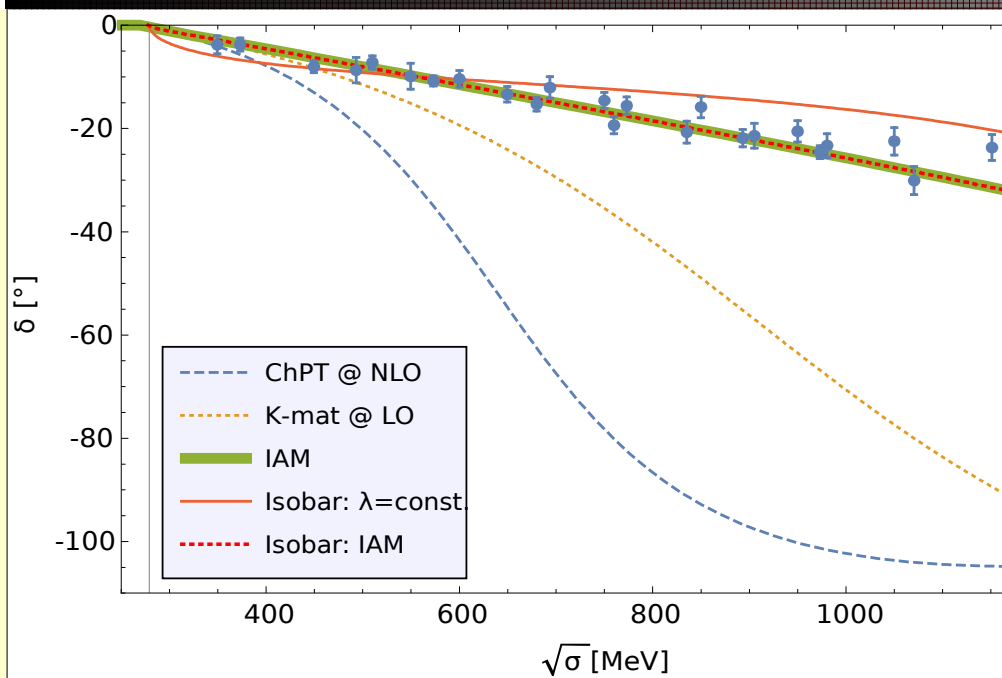
Truong (1988), Peláez (1999),  
Gómez Nicola, Peláez (2002), ...

## I. 2-body subchannel:

- one-channel problem:  $\pi\pi$ -system in S-wave,  $I=2$
- 2-body amplitude consistent with 3-body one

$$\frac{T_{\text{LO}}^2}{T_{\text{LO}} - T_{\text{NLO}}}$$

discretize (Lüscher)  $\rightarrow$  predicted fin-vol. spectrum



- Maximal isospin:  $\pi^+\pi^+\pi^+$ 
  - LatticeQCD results for ground level available for  $\pi^+\pi^+$  &  $\pi^+\pi^+\pi^+$
  - Repulsive channel
  - $L=2.5 \text{ fm}, m_\pi=291/352/491/591 \text{ MeV}$

NPLQCD, Detmold et al. (2008)

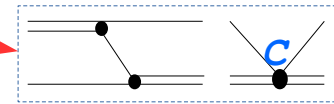
## II. 3-body spectrum

Remaining unknown:  $C$

- *genuine (momenta-dependent) 3-body “force”*
- *simplest case:*  $C_{qp} = c \delta^{(3)}(\mathbf{p}-\mathbf{q})$

QUANTIZATION CONDITION

$$\text{Det} \left( \mathbf{B}_{\mathbf{u}\mathbf{u}'}^{\Gamma_{\mathbf{s}\mathbf{s}'}}(\mathbf{W}^2) + \frac{2\mathbf{E}_s \mathbf{L}^3}{\vartheta(\mathbf{s})} \tau_{\mathbf{s}}(\mathbf{W}^2)^{-1} \delta_{\mathbf{s}\mathbf{s}'} \delta_{\mathbf{u}\mathbf{u}'} \right) = 0$$



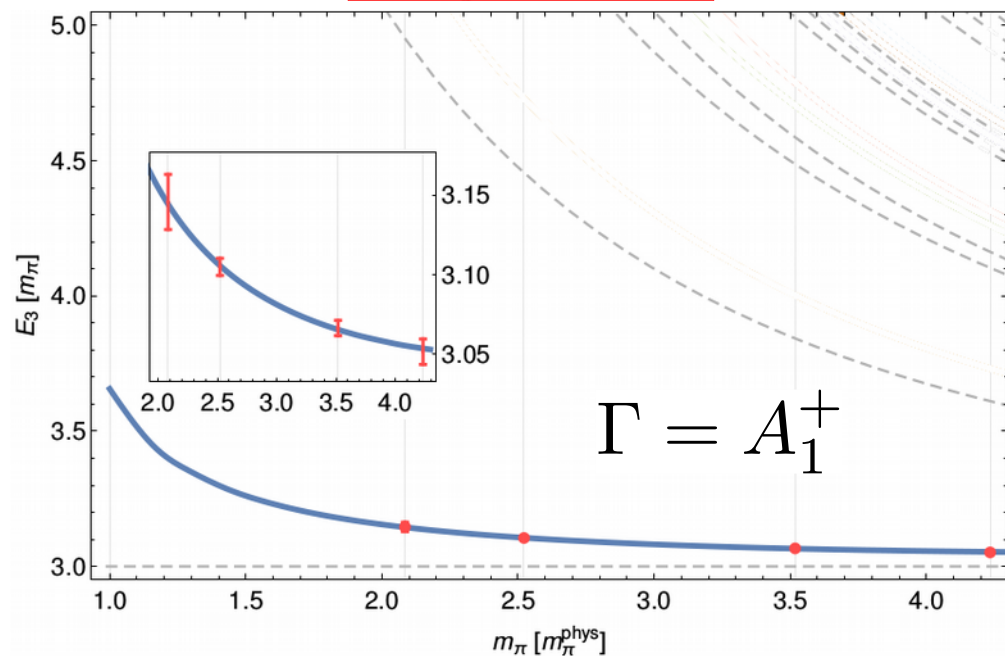
- Maximal isospin:  $\pi^+\pi^+\pi^+$ 
  - LatticeQCD results for ground level available for  $\pi^+\pi^+$  &  $\pi^+\pi^+\pi^+$
  - Repulsive channel
  - $L=2.5 \text{ fm}, m_\pi=291/352/491/591 \text{ MeV}$

NPLQCD, Detmold et al. (2008)

## II. 3-body spectrum

Remaining unknown:  $C$

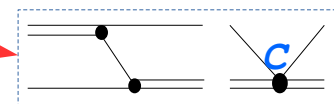
- *genuine (momenta-dependent) 3-body “force”*
- *simplest case:*  $C_{qp} = c \delta^{(3)}(\mathbf{p}-\mathbf{q})$



**Fit  $C$**  to NPLQCD ground state level  
 $\rightarrow C = (0.2 \pm 1.5) \cdot 10^{-10}$

QUANTIZATION CONDITION

$$\text{Det} \left( \mathbf{B}_{\mathbf{u}\mathbf{u}'}^{\Gamma_{\mathbf{s}\mathbf{s}'}}(\mathbf{W}^2) + \frac{2\mathbf{E}_s \mathbf{L}^3}{\vartheta(\mathbf{s})} \tau_{\mathbf{s}}(\mathbf{W}^2)^{-1} \delta_{\mathbf{s}\mathbf{s}'} \delta_{\mathbf{u}\mathbf{u}'} \right) = 0$$



# First prediction of excited levels for physical system

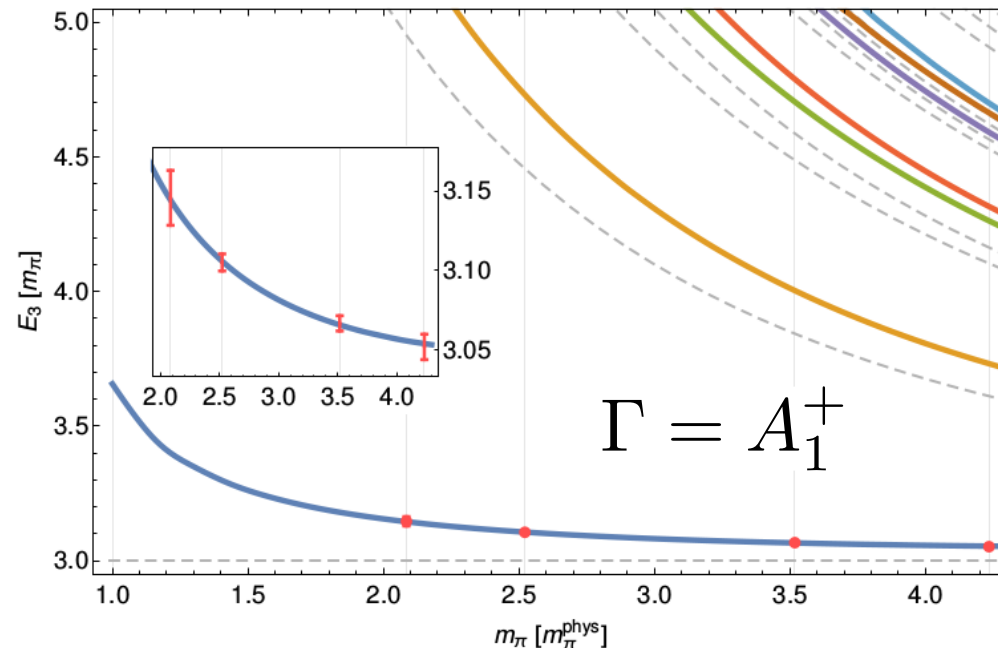
- Maximal isospin:  $\pi^+\pi^+\pi^+$ 
  - LatticeQCD results for ground level available for  $\pi^+\pi^+$  &  $\pi^+\pi^+\pi^+$
  - Repulsive channel
  - $L=2.5 \text{ fm}, m_\pi=291/352/491/591 \text{ MeV}$

NPLQCD, Detmold et al. (2008)

## II. 3-body spectrum

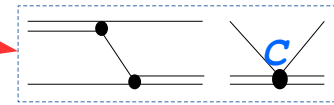
Remaining unknown:  $C$

- *genuine (momenta-dependent) 3-body “force”*
- *simplest case:*  $C_{qp} = c \delta^{(3)}(\mathbf{p}-\mathbf{q})$



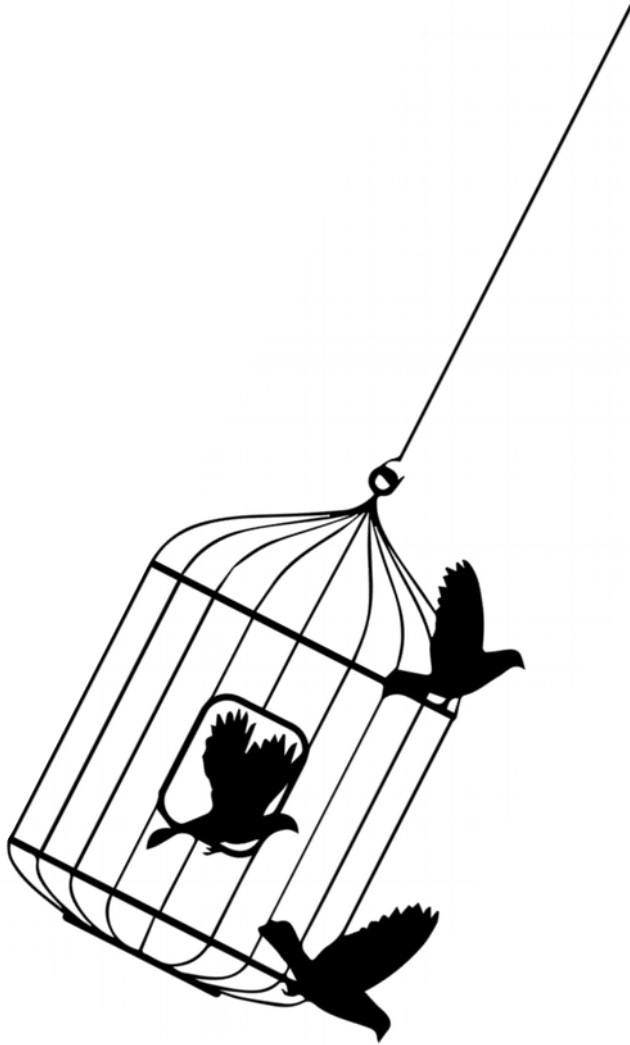
QUANTIZATION CONDITION

$$\text{Det} \left( \mathbf{B}_{\mathbf{u}\mathbf{u}'}^{\Gamma_{\mathbf{s}\mathbf{s}'}}(\mathbf{W}^2) + \frac{2\mathbf{E}_s \mathbf{L}^3}{\vartheta(\mathbf{s})} \tau_{\mathbf{s}}(\mathbf{W}^2)^{-1} \delta_{\mathbf{s}\mathbf{s}'} \delta_{\mathbf{u}\mathbf{u}'} \right) = 0$$



**Predict excited spectrum:**

- novel pattern
  - 1/1 of interacting/non-interacting lvl
- all QC-poles are simple
- chiral extrapolation to phys point  
(under assumptions)



# The Moving $\pi^+ \pi^+ \pi^+$ System

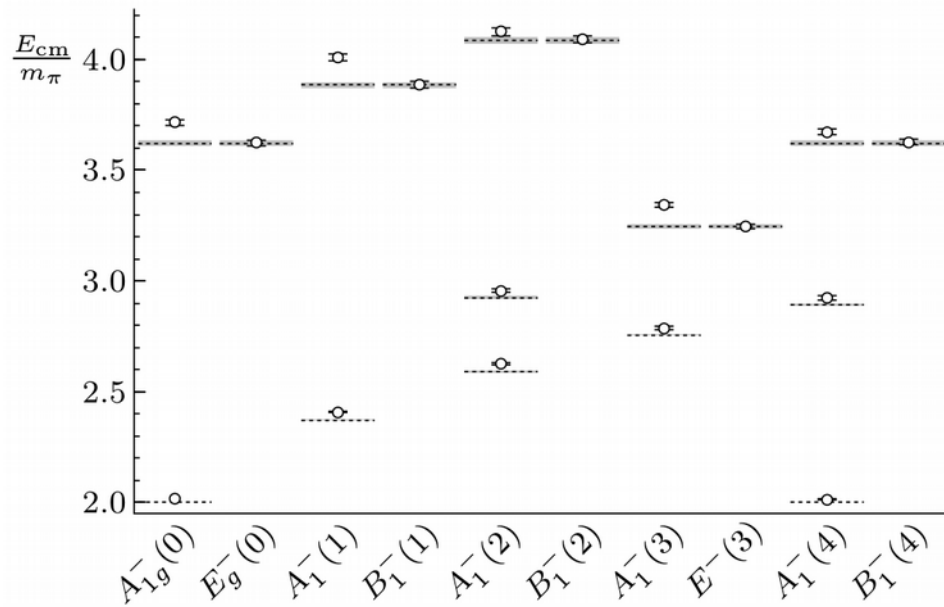
---

Mai, M.D., Alexandru, Culver  
(in preparation)

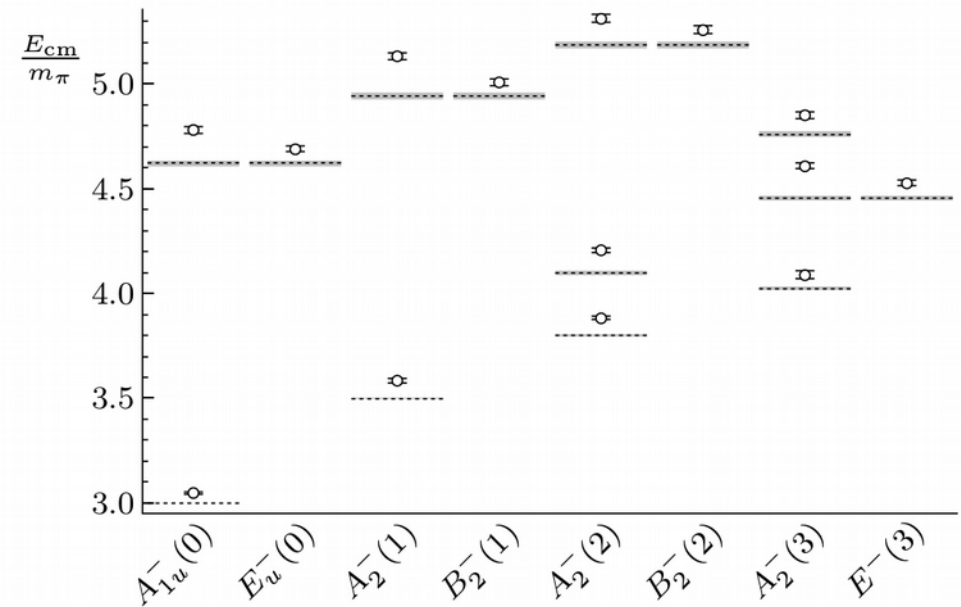
# New Lattice Data

Hörz, Hanlon, arXiv:1905.04277 [hep-lat]

Two-body spectrum  $\pi^+\pi^+$



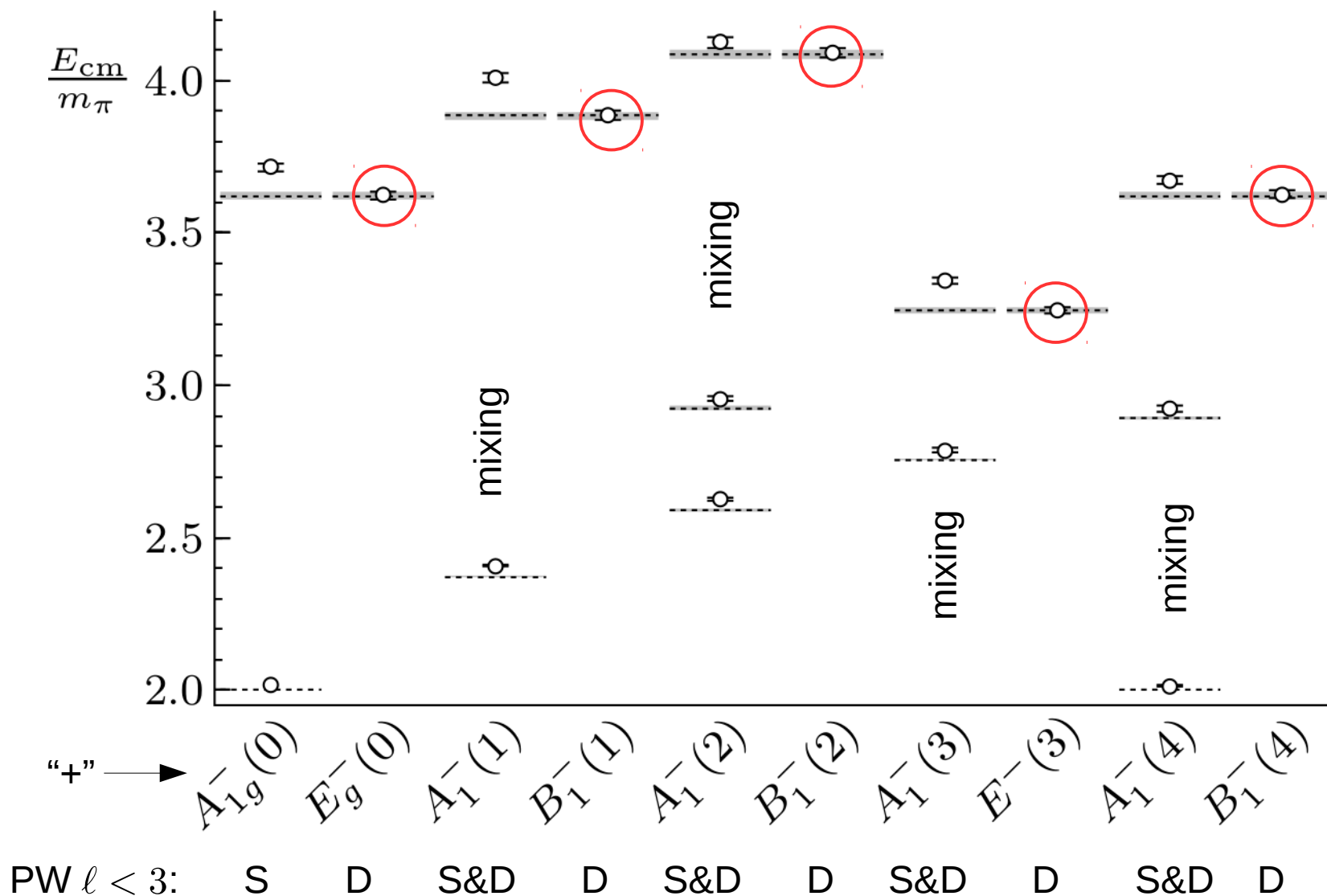
Three-body spectrum  $\pi^+\pi^+\pi^+$



- **First lattice data on excited energy eigenvalues** from multi-pion operators  
→ More reliable extraction of scattering eigenvalues
- D200 CLS ensemble (2+1) with improved Wilson fermions and tree-level Lüscher–Weisz gauge action; stochastic LapH method;  $m_\pi=200$  MeV;  $L=4.1$  fm
- High number of Wick contraction (20,679,840 diagrams) managed with novel method from quantum chemistry

# Two-body spectrum: D-wave (I)

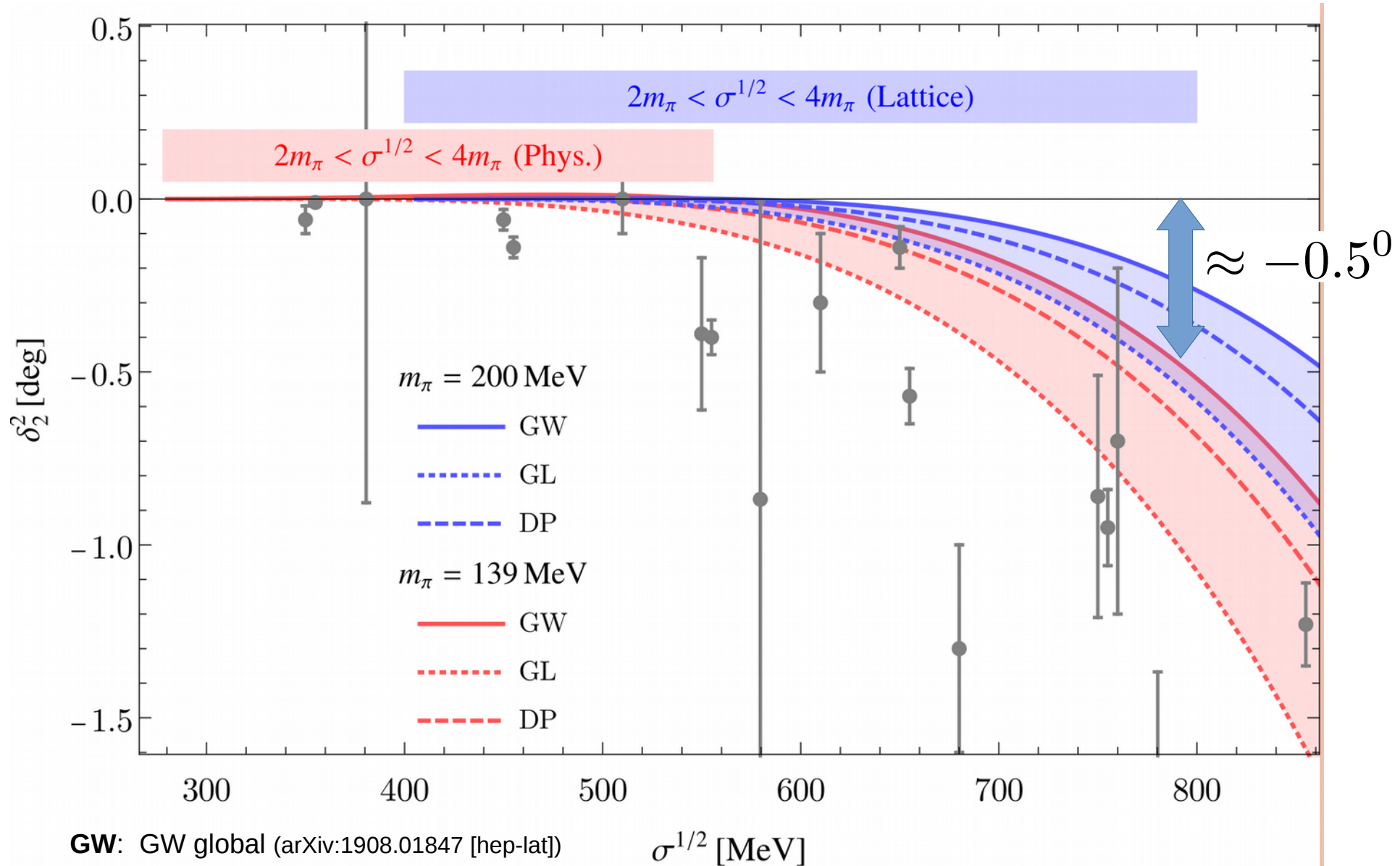
Hörz, Hanlon, arXiv:1905.04277 [hep-lat]



→ I=2 D-wave vanishes within uncertainties – what does IAM predict?



# D-wave (II): prediction



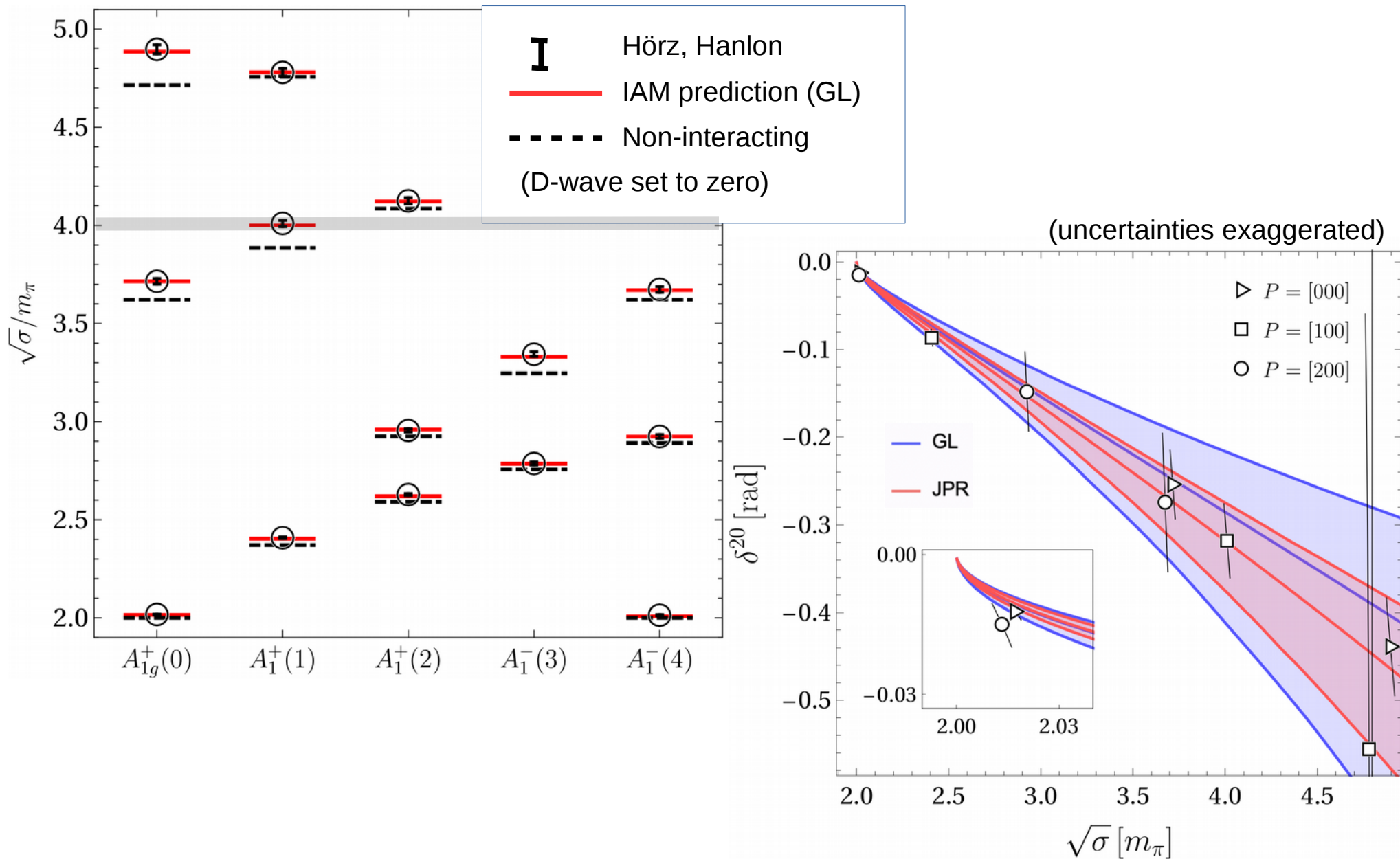
**GW:** GW global (arXiv:1908.01847 [hep-lat])

**GL:** Gasser, Leutwyler (Annals Phys. 158, 1984)

**DP:** Dobado, Peláez (PRD 56 (1997))

See also [Nebreda, Peláez, Ríos, PRD83 (2011)]

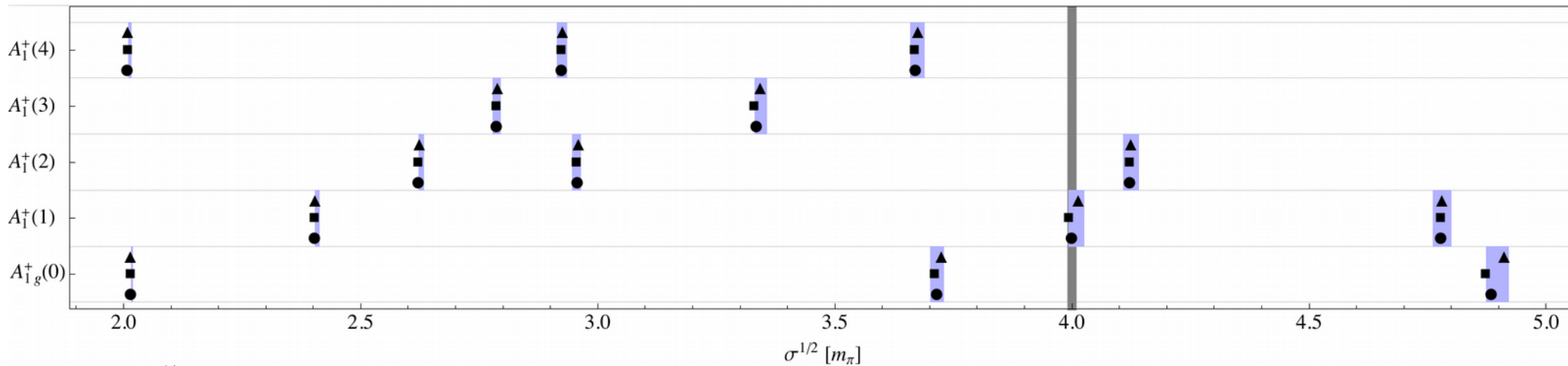
# IAM predictions 2-body spectrum



→ We may consider this as *any* suitable 2-body Parametrization (like, e.g., K-matrix with conformal mapping)

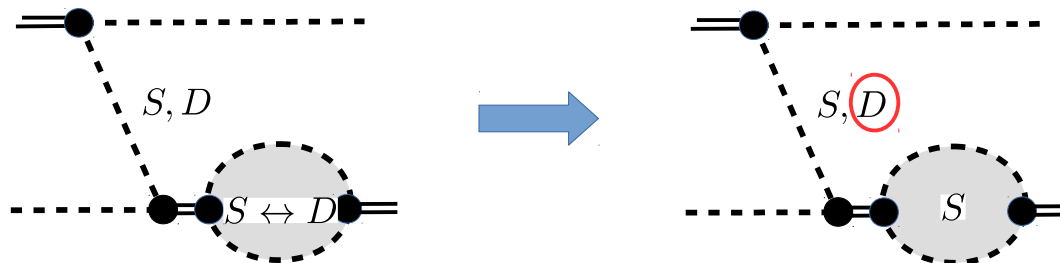
# IAM predictions: Different LECs

(D-wave set to zero)



- ▲ Nebraska, Peláez, Rios (PRD88, 2013)
- GW global (arXiv:1908.01847 [hep-lat])
- Gasser, Leutwyler (Annals Phys. 158, 1984)

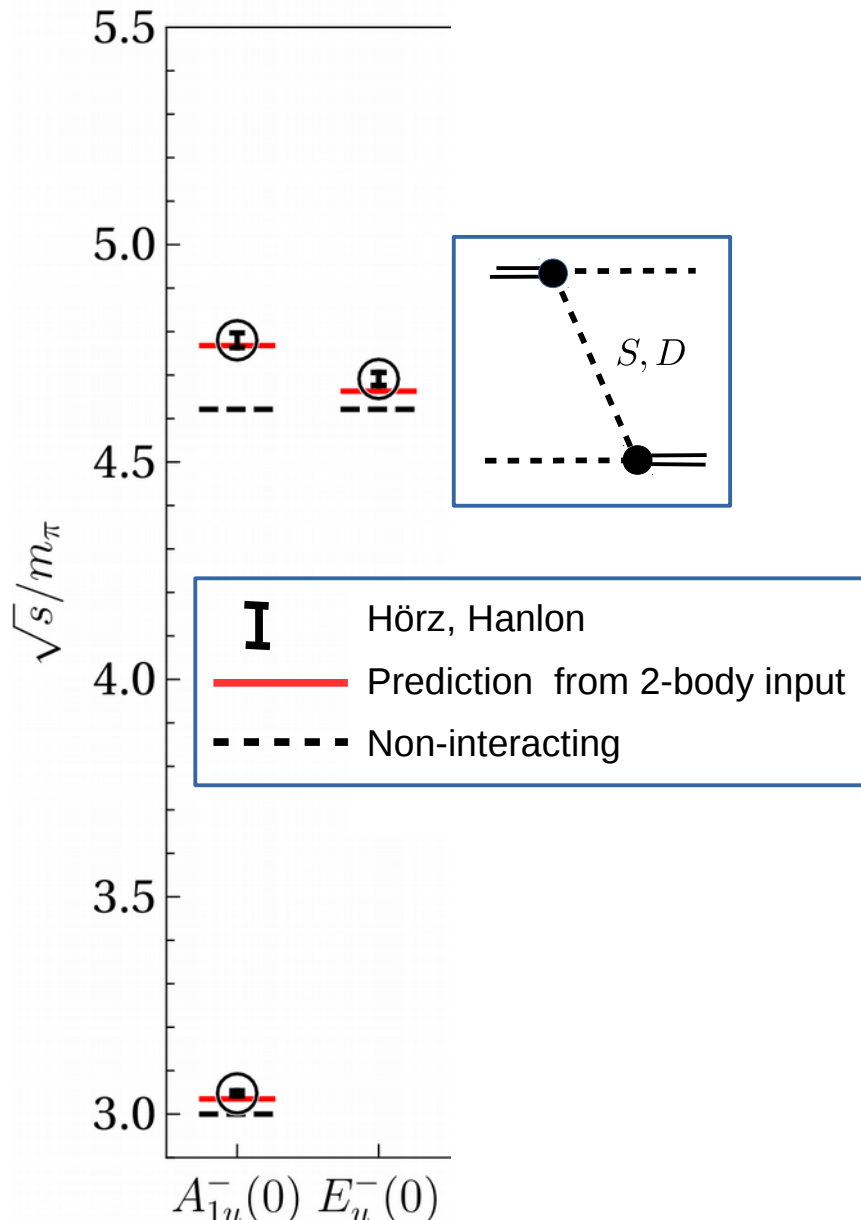
- Robust predictions of the 2-body spectrum irrespective of used LECs
- No sign of D-wave up to very high energies in irreps with S&D-wave mixing
- Ignore the vanishing  $\pi^+\pi^+ - D$ -wave, but keep the important  $\pi^+ -$  isobar D-wave



"in-flight transitions"

# 3-body Spectrum: Predictions (I)

Data: Hörz, Hanlon, arXiv:1905.04277 [hep-lat]



**S** **D** (lowest participating wave)

- S-wave prediction good at threshold (like for NPLQCD data)
- S-wave prediction good at high energies  
→ **Energy dependence matched**
- No sign of 3-body force (like for NPLQCD data)
- D-wave prediction qualitatively good  
→ **Relative\* strength between S- and D-wave matched**  
→ **Consequence that 3-body interaction dominated by exchange**  
→ **Consequence of 3-body Unitarity**

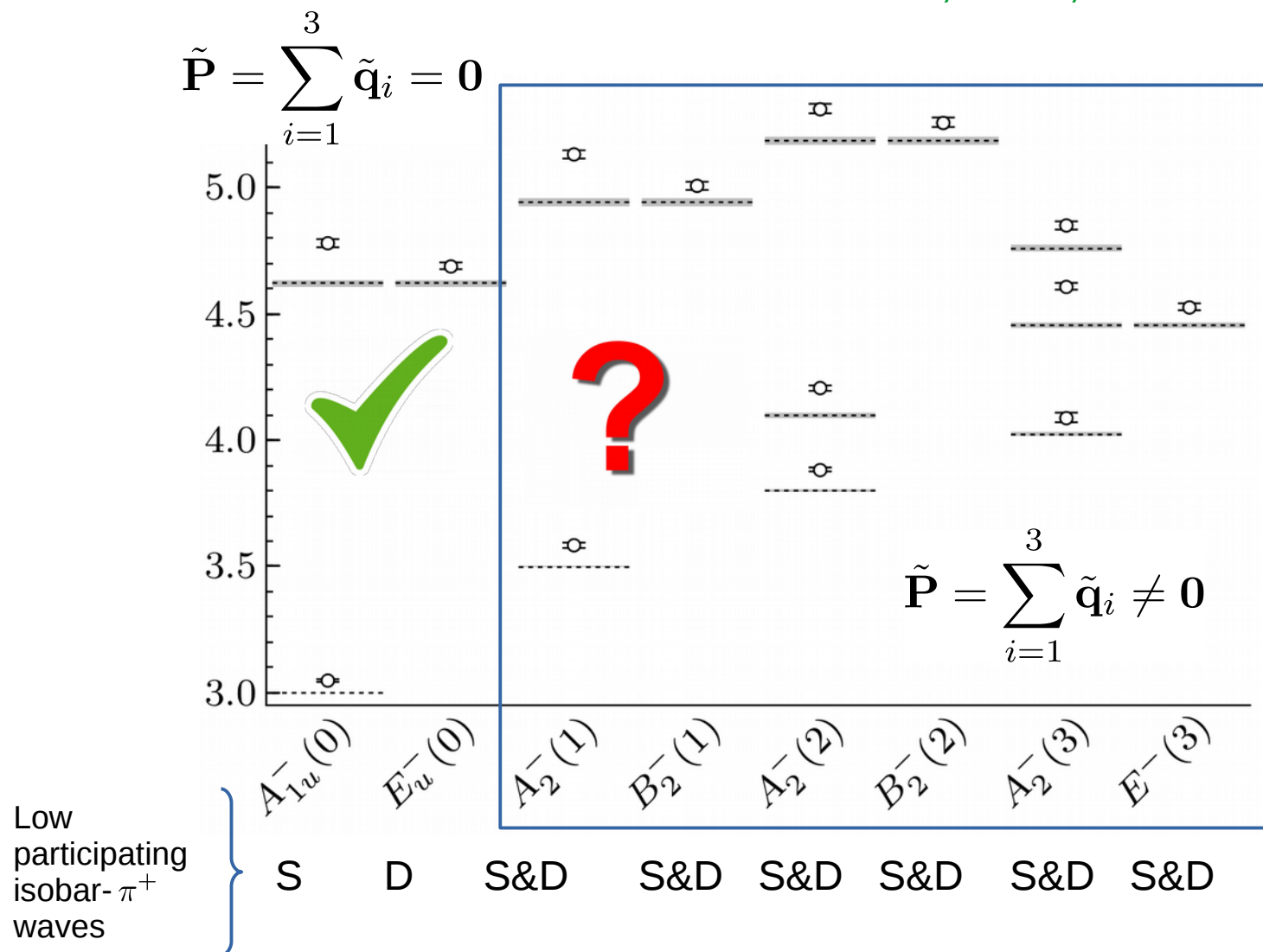
• **Three-body unitarity directly visible in the eigenvalue spectrum of lattice QCD**

\*and absolute

Technical note: Projection technique for 3-body systems to irreps from M.D., Hammer, Mai, Pang, Rusetsky, Wu PRD97 (2018)

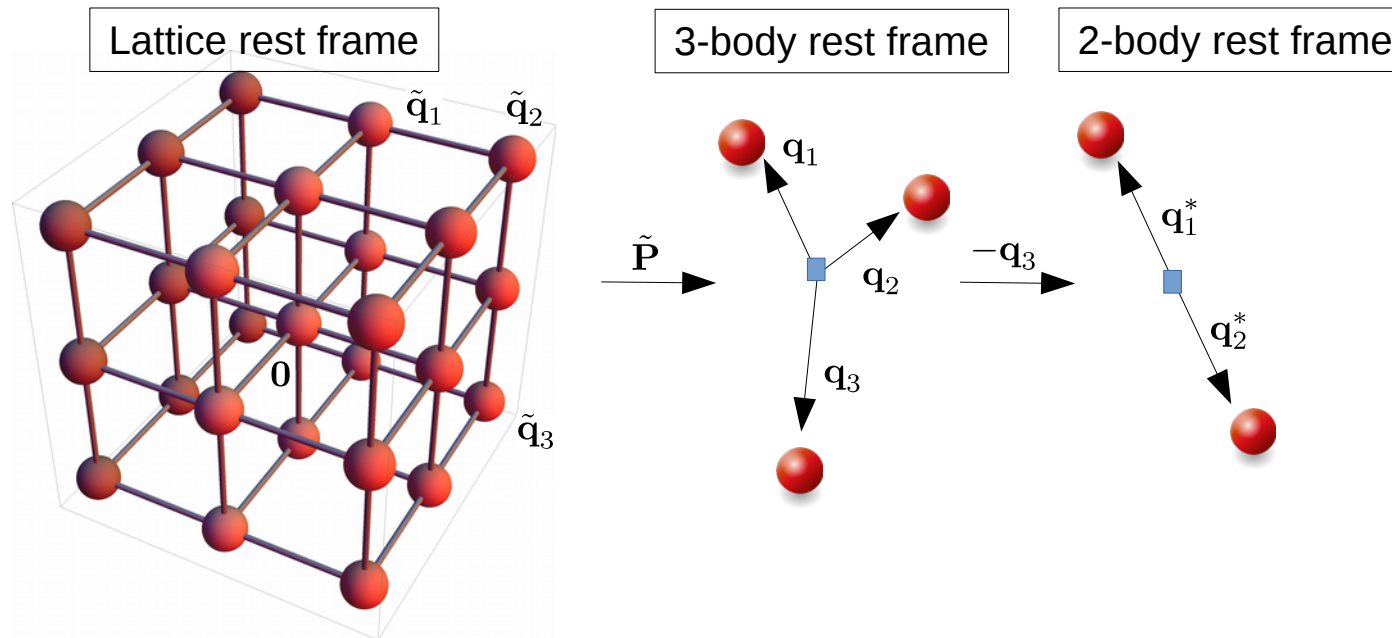
# 3-body spectrum: Moving frames

Data: Hörz, Hanlon, arXiv:1905.04277 [hep-lat]



→ Need to develop a framework for moving 3-body systems!

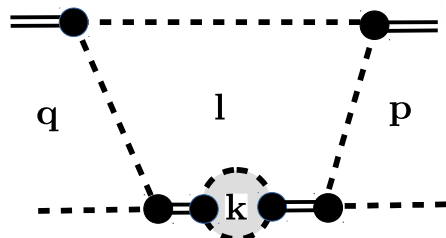
# Moving frames for 3-body systems



**Usually:** Explicit S- and D-wave projected parameterizations in coupled channels  
**Here:** Boost of unprojected 3-body amplitude. A-posteriori projections with suitable Clebsch-Gordan coefficients → Requires plane-wave solution of scattering

$$\left. \begin{aligned} \tilde{\mathbf{P}} &= \tilde{\mathbf{q}}_1 + \tilde{\mathbf{q}}_2 + \tilde{\mathbf{q}}_3 = \tilde{\mathbf{p}}_1 + \tilde{\mathbf{p}}_2 + \tilde{\mathbf{p}}_3 \\ (L/2\pi)\tilde{\mathbf{P}} &\in \{(0, 0, 1), (0, 1, 1), (1, 1, 1)\} \end{aligned} \right\} \mathbf{q} = \tilde{\mathbf{q}} + \left[ \left( \frac{\tilde{P}^0}{\sqrt{s}} - 1 \right) \frac{\tilde{\mathbf{q}}\tilde{\mathbf{P}}}{|\tilde{\mathbf{P}}^2|} - \frac{\tilde{q}^0}{\sqrt{s}} \right] \tilde{\mathbf{P}}$$

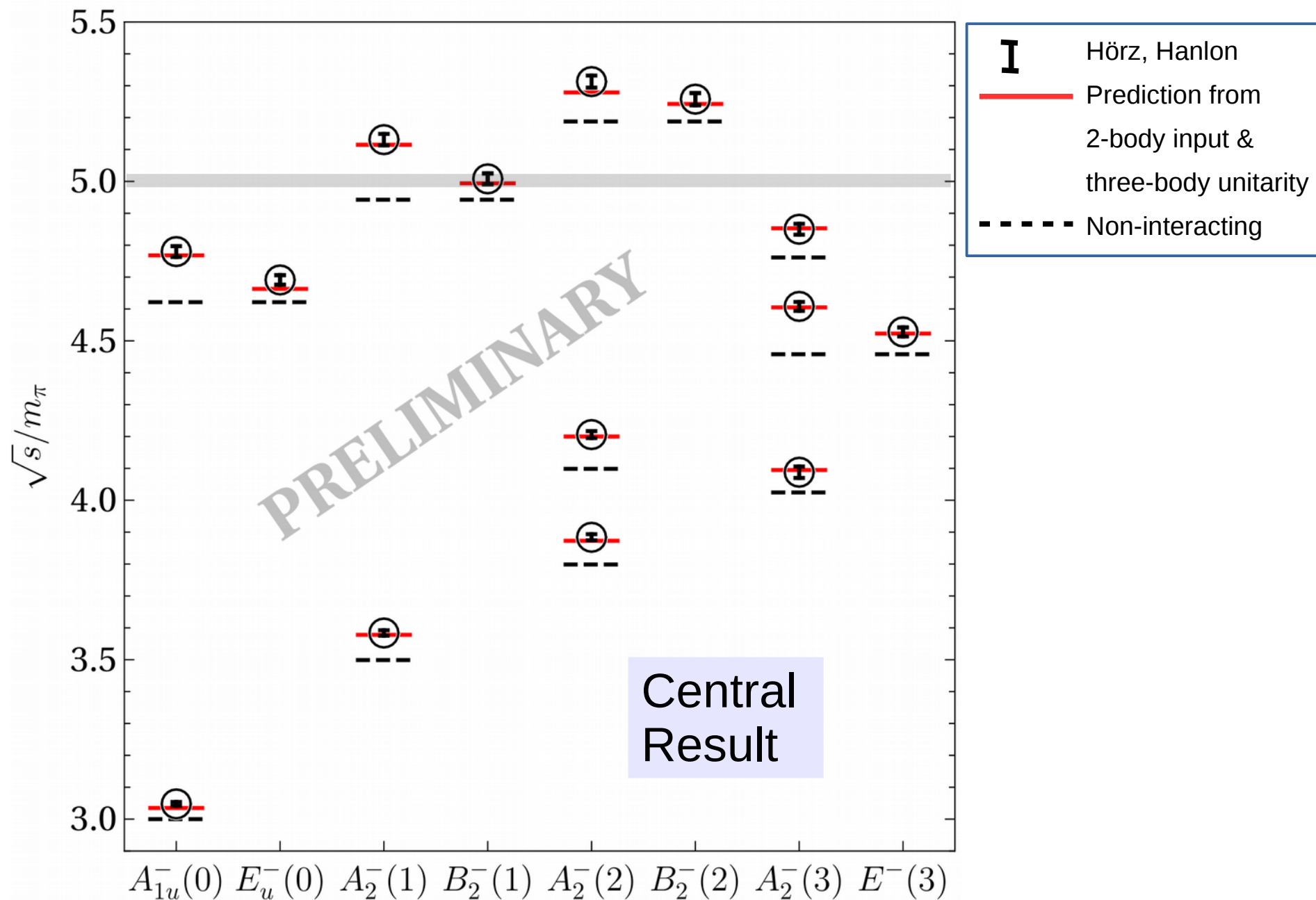
3-body summation:  $\int \frac{d^3\mathbf{l}}{(2\pi)^3} g(\mathbf{l}) \rightarrow \int \frac{d^3\tilde{\mathbf{l}}}{(2\pi)^3} g(\mathbf{l}(\tilde{\mathbf{l}})) \tilde{J}(\tilde{\mathbf{l}}) \rightarrow \frac{1}{L^3} \sum_{\mathbf{n}} g(\mathbf{l}(\tilde{\mathbf{l}})) \tilde{J}(\tilde{\mathbf{l}})$



→  $\hat{T}(\mathbf{q}(\tilde{\mathbf{q}}), \mathbf{p}(\tilde{\mathbf{p}}))$  3 → 3 boosted plane-wave amplitude  
 Poles → Eigenvalues

# 3-body spectrum: Complete Predictions

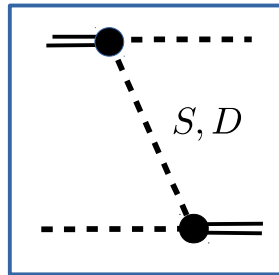
Data: Hörz, Hanlon, arXiv:1905.04277 [hep-lat]



# Summary

## 3-body Unitarity

- 3-body unitarity dictates on-shell condition (exchange term & isobar propagator)
- On-shell condition dictates leading, power-law finite-volume effects
- “Bare-bone” infinite-volume extrapolation tool (in spirit of Lüscher equation)
- Optional: Pion-mass extrapolation



## The $\pi^+\pi^+\pi^+$ System

- First application to physical 3-body system [PRL 2019]
- NPLQCD threshold data well predicted, excited levels predicted
- First explanation of excited 3-body levels (data from Hörz/Hanlon)
- Consequences of three-body unitarity directly visible in data (S vs. D waves)
- First development and application of moving frames for 3-body systems

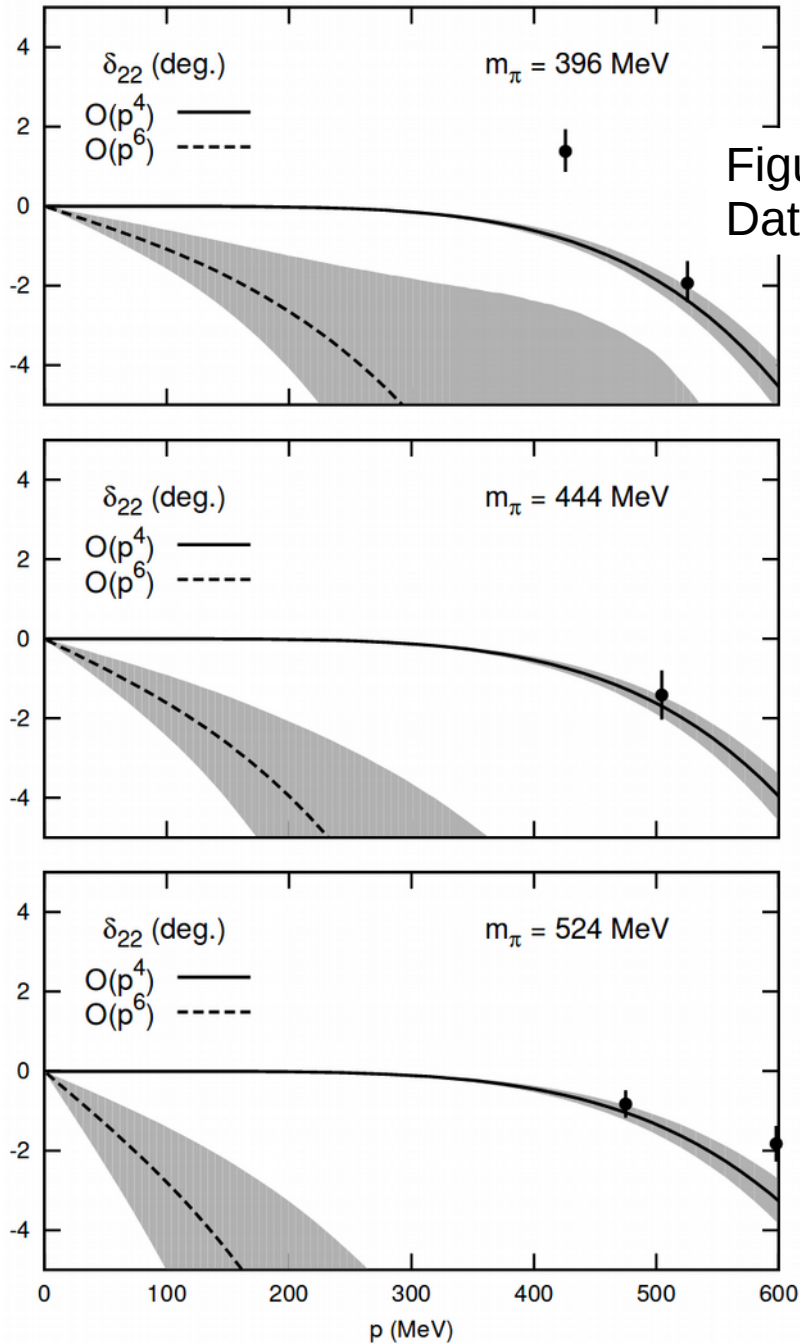
## OUTLOOK

- Implementation of spin isobars & multiple isobars
- unequal masses
- practical studies:  $a_1(1260)$ , Roper, exotics...



**SPARES**

# I=2 D-wave at HadSpec Pion Masses



Perturbative  $O(p^4)$ ,  $O(p^6)$  calculation

Figure from [Nebreda, Peláez, Ríos, PRD83 (2011)]

Data: [Dudek, Edwards, Peardon, Richards, Thomas, PRD83 (2011)]

# Scattering amplitude – analytic expression

$$\langle q_1, q_2, q_3 | \hat{T}_c(s) | p_1, p_2, p_3 \rangle = \frac{1}{3!} \sum_{n=1}^3 \sum_{m=1}^3 T_{22}(\sigma(q_n)) \langle q_n | T(s) | p_m \rangle T_{22}(\sigma(p_m))$$

External on-shell  
2-body interaction

Recasting in on-shell  
2 → 2 amplitudes +  
real 3-body forces

with

$$\begin{aligned} \langle q | T(s) | p \rangle = & \langle q | C(s) | p \rangle + \frac{1}{m^2 - (P - p - q)^2 - i\epsilon} \\ & - \int \frac{d^3\ell}{(2\pi)^3} \frac{1}{2E_\ell} T_{22}(\sigma(\ell)) \left( \langle \ell | C(s) | q \rangle \right. \\ & \left. + \frac{1}{m^2 - (P - p - \ell)^2 - i\epsilon} \right) \langle \ell | T(s) | p \rangle \end{aligned}$$

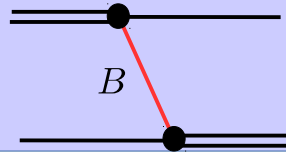
Real three-body force

Exchange force

On-shell 2 → 2 interaction  
(even within integral, but  
without left-hand cuts)

# The Power of Unitarity

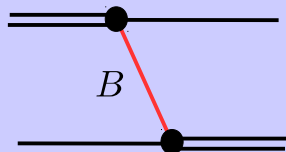
Question: Does



provide full imaginary part of all possible  $3 \rightarrow 3$  transitions?

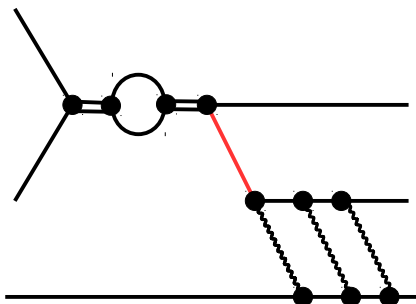
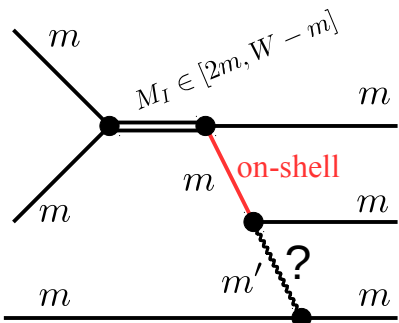
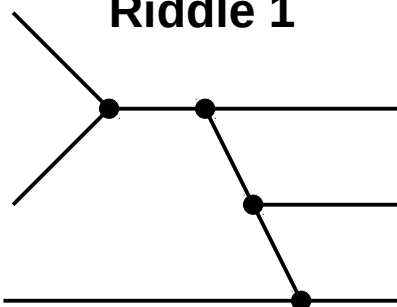
# The Power of Unitarity

Question: Does

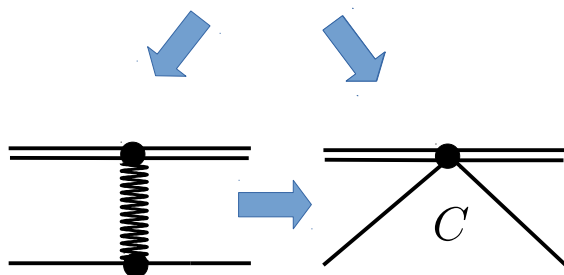
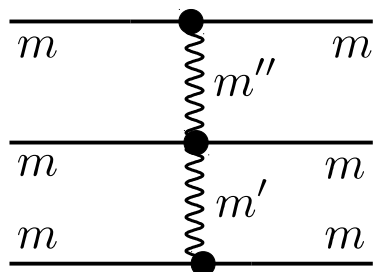


provide full imaginary part of all possible  $3 \rightarrow 3$  transitions?

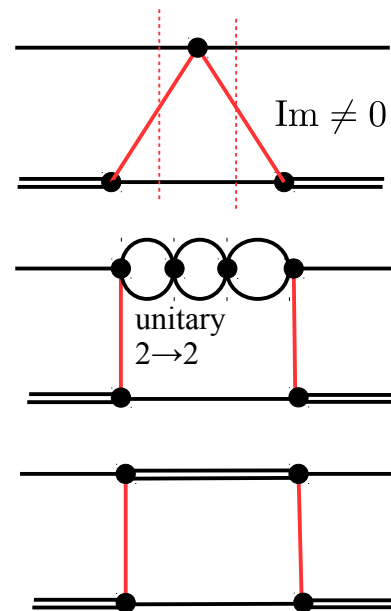
**Riddle 1**



**Riddle 2**



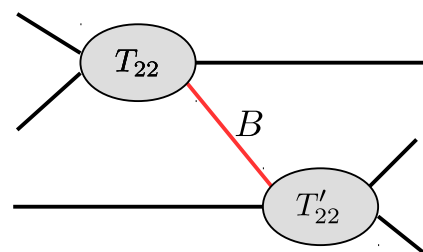
**Riddle 3**



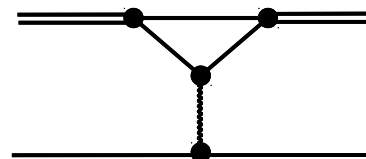
$$p_2^2 \neq m^2 \quad p_3^2 = m^2$$

$$t \leq 0 < m'^2$$

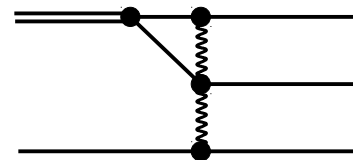
$$p_1^2 = m^2 \quad p_4^2 = m^2$$



**Riddle 4**

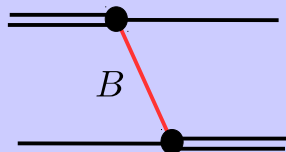


**Riddle 5**



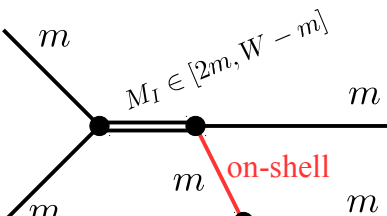
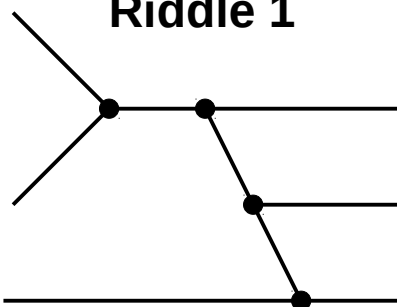
# The Power of Unitarity

Question: Does

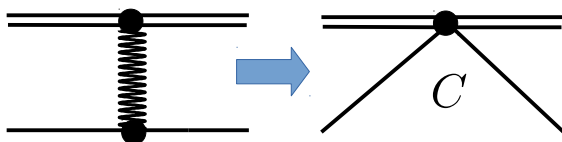
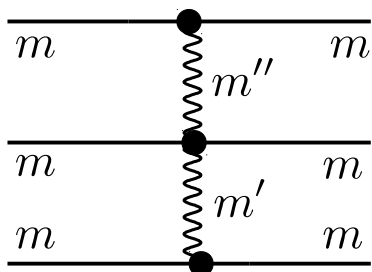


provide full imaginary part of all possible  $3 \rightarrow 3$  transitions?

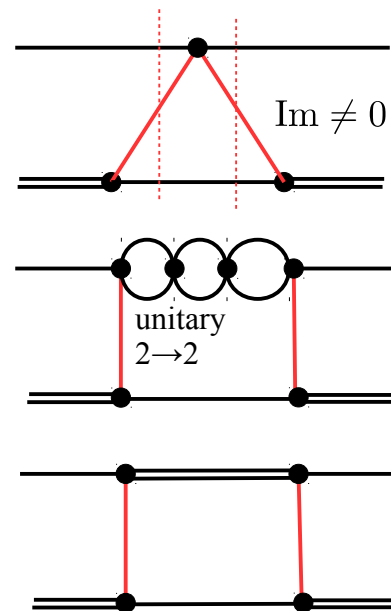
**Riddle 1**



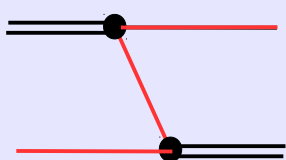
**Riddle 2**



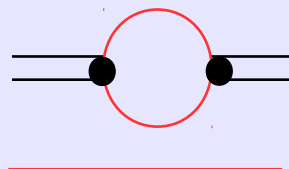
**Riddle 3**



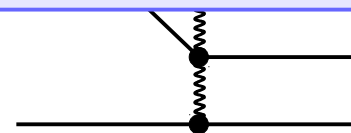
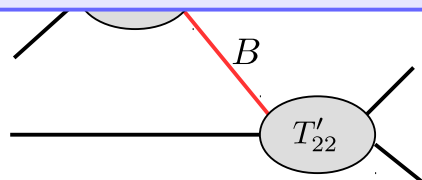
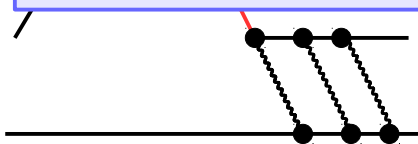
**Answer: Yes.**



and



are the only on-shell configurations in physical region. Three-body unitarity avoids many artificial complications of diagrammatic expansions.

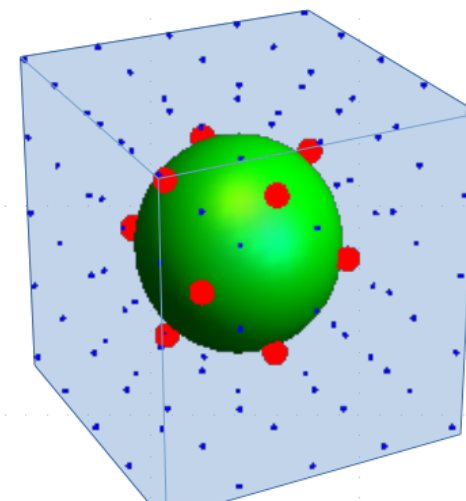


**Riddle 5**

# Projection to irreps

[M. D. , Hammer, Mai, Pang, Rusetsky, Wu (2018) ]

- **Lüscher formalism relies on regular  $2 \rightarrow 2$  potentials**
  - Now: manifestly singular interactions
  - Find generalization that projects also the interactions to the irreps of cubic symmetry, not only propagation
- **Separation of variables**
  - shells = sets of points related by  $\mathbf{O}_h$
  - Analogous to radial coordinate in infinite volume
- **Find the orthonormal basis for arbitrary functions defined on each point of a given shell.**



$$q_i = \frac{2\pi}{L} n_i, \quad n_i \in \mathbb{Z}, \quad i = 1, 2, 3$$

$$\int \frac{d^3 \mathbf{q}}{(2\pi)^3} \rightarrow \frac{1}{L^3} \sum_s \sum_{i=1}^{\vartheta(s)}$$

- **J (inf. volume)  $\rightarrow$  irreps (finite volume):**  $\Gamma \in \{A_1^\pm, A_2^\pm, E^\pm, T_1^\pm, T_2^\pm\}$
- **Partial wave projection (inf. Volume)  $\rightarrow$  Irrep. projection (fin.)**

$$f(\mathbf{p}) = \sqrt{4\pi} \sum_{\ell m} Y_{\ell m}(\hat{\mathbf{p}}) f_{\ell m}(p)$$

$$f_{\ell m}(p) = \frac{1}{\sqrt{4\pi}} \int d\Omega Y_{\ell m}^*(\hat{\mathbf{p}}) f(\mathbf{p})$$



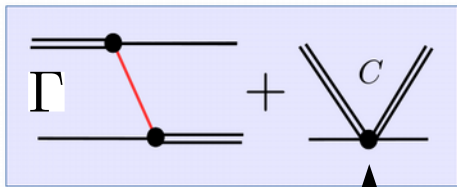
$$f^s(\hat{\mathbf{p}}_j) = \sqrt{4\pi} \sum_{\Gamma\alpha} \sum_a f_a^{\Gamma\alpha s} \chi_a^{\Gamma\alpha s}(\hat{\mathbf{p}}_j)$$

$$f_a^{\Gamma\alpha s} = \frac{\sqrt{4\pi}}{\vartheta(s)} \sum_{j=1}^{\vartheta(s)} f^s(\hat{\mathbf{p}}_j) \chi_a^{\Gamma\alpha s}(\hat{\mathbf{p}}_j)$$

(a is index u in quantization condition; Quantization condition has projection in incoming AND outgoing basis states with indices u, u')

# Quantization Condition

$$\text{Det} \left( \mathbf{B}_{\mathbf{uu}'}^{\Gamma \mathbf{ss}'} (W^2) + \frac{2E_s L^3}{\vartheta(s)} \tau_s (W^2)^{-1} \delta_{\mathbf{ss}'} \delta_{\mathbf{uu}'} \right) = 0$$



Fix to 3 → 3 data

$W$  – total energy

$s/s'$  - shell index

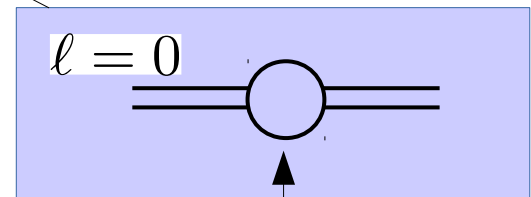
$u/u'$  - basis index

Determinant of  $(s,u) \times (s',u')$  matrix  
at fixed  $W, \Gamma, L$

$\vartheta$  – multiplicity

$L$  – lattice volume

$E_s$  – spect. energy



Fix to 2 → 2 data:

$$T_{22} = \nu \tau \nu$$

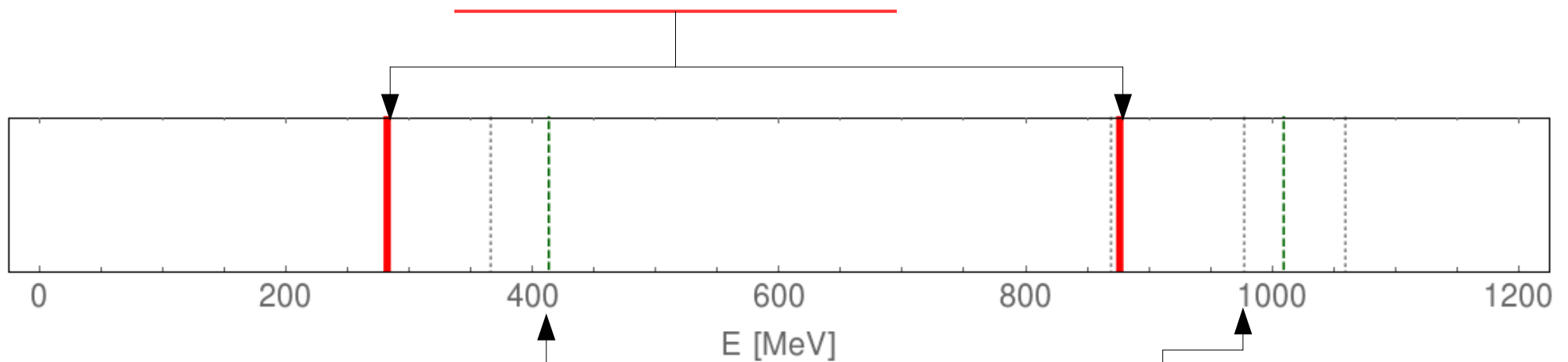
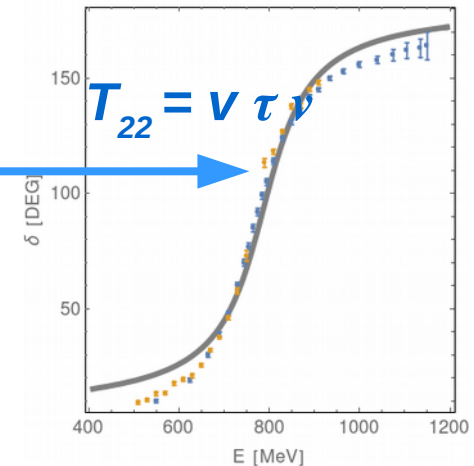
- Not a Lüscher-like equation (“left”: infinite volume, “right”: finite volume)
- Instead: Fix parameters to lattice eigenvalues
- With parameters fixed, evaluate infinite-volume amplitude
- Same workflow as in many 2-body coupled-channel fits (see, e.g.,  
M.D., Meißner, Oset, Rusetsky, EPJA (2012))



# Numerical demonstration

[M. Mai, MD, EPJA 2017 [arXiv: 1709.08222]]

- Numerical demonstration of three-body finite volume formalism
- 3 particles in finite volume:  $m=138 \text{ MeV}$ ,  $L=3 \text{ fm}$
- one S-wave isobar  $\rightarrow$  two unknowns:
  - vertex(Isobar  $\rightarrow$  2 stable particles)
  - subtraction constant ( $\sim$ mass)
- Project to  $\Gamma = A^{1+}$ 
  - $\rightarrow$  prediction of 3body energy-eigenlevels ( $C=0$ )



unphysical lvls cancel out (exact proof available)

# Two-body scattering on lattice

---

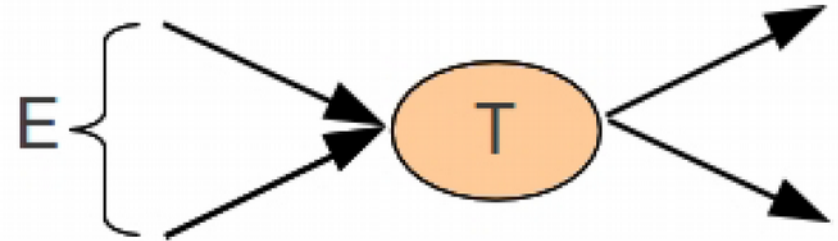
Input for 3-body

# Two body scattering

In the infinite volume

- Unitarity of the scattering matrix  $S$ :  $SS^\dagger = \mathbb{1}$        $[S = \mathbb{1} - i \frac{p}{4\pi E} T]$ .

$$\text{Im } T^{-1}(E) = \sigma \equiv \frac{p}{8\pi E}$$



- $\rightarrow$  Generic (Lippman-Schwinger) equation for unitarizing the  $T$ -matrix:

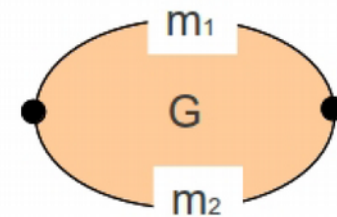
$$T = V + V G T \quad \text{Im } G = -\sigma$$

$V$ : (Pseudo)potential,  $\sigma$ : phase space.

- $G$ : Green's function:

$$G = \int \frac{d^3 \vec{q}}{(2\pi)^3} \frac{f(|\vec{q}|)}{E^2 - (\omega_1 + \omega_2)^2 + i\epsilon},$$

$$\omega_{1,2}^2 = m_{1,2}^2 + \vec{q}^2$$



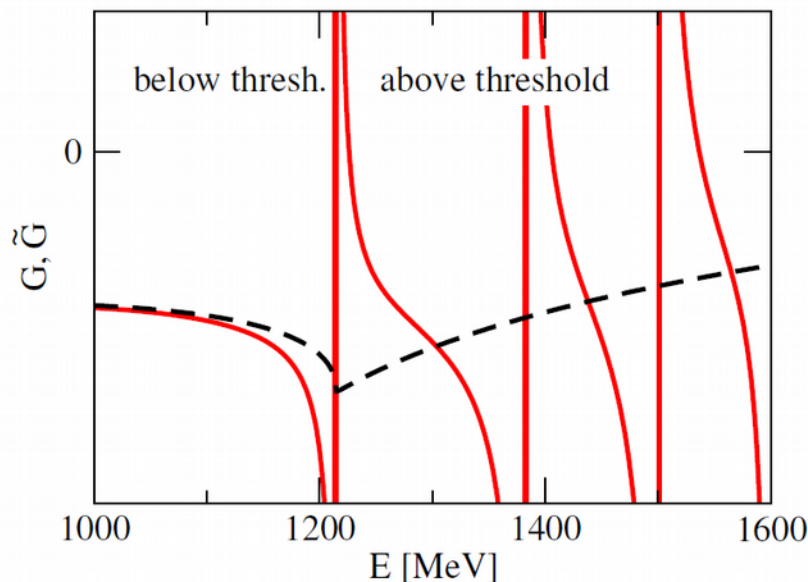
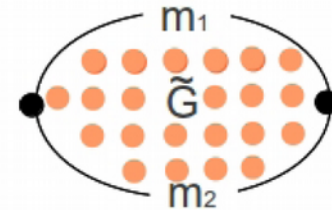
# Discretization

Discretized momenta in the finite volume with periodic boundary conditions

$$\Psi(\vec{x}) \stackrel{!}{=} \Psi(\vec{x} + \hat{e}_i L) = \exp(i L q_i) \Psi(\vec{x}) \implies q_i = \frac{2\pi}{L} n_i, \quad n_i \in \mathbb{Z}, \quad i = 1, 2, 3$$

$$\int \frac{d^3 \vec{q}}{(2\pi)^3} g(|\vec{q}|^2) \rightarrow \frac{1}{L^3} \sum_{\vec{n}} g\left(\left|\frac{2\pi}{L} \vec{n}\right|^2\right), \quad \vec{q} = \frac{2\pi}{L} \vec{n}, \quad \vec{n} \in \mathbb{Z}^3$$

$$G \rightarrow \tilde{G} = \frac{1}{L^3} \sum_{\vec{q}} \frac{f(|\vec{q}|)}{E^2 - (\omega_1 + \omega_2)^2}$$



- $E > m_1 + m_2$ :  $\tilde{G}$  has poles at free energies in the box,  $E = \omega_1 + \omega_2$
- $E < m_1 + m_2$ :  $\tilde{G} \rightarrow G$  exponentially with  $L$  (regular summation theorem).

# Finite $\rightarrow$ infinite volume: the Lüscher equation

Warning: rather crude re-derivation

- Measured eigenvalues of the Hamiltonian (tower of *lattice levels*  $E(L)$ )  
 $\rightarrow$  Poles of scattering equation  $\tilde{T}$  in the finite volume  $\rightarrow$  determines  $V$ :

$$\tilde{T} = (1 - V\tilde{G})^{-1} V \rightarrow V^{-1} - \tilde{G} \stackrel{!}{=} 0 \rightarrow V^{-1} = \tilde{G}$$

- The interaction  $V$  determines the  $T$ -matrix in the infinite volume limit:

$$T = (V^{-1} - G)^{-1} = (\tilde{G} - G)^{-1}$$

- Re-derivation of Lüscher's equation ( $T$  determines the phase shift  $\delta$ ):

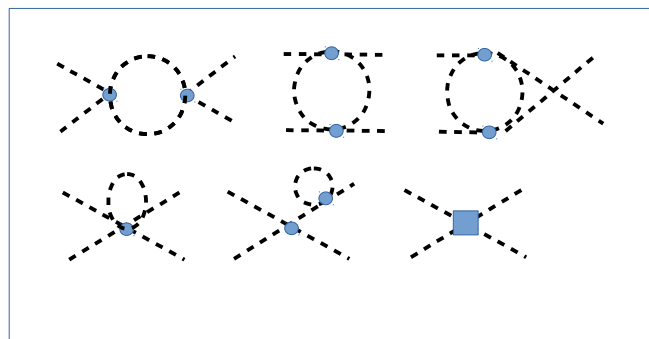
$$p \cot \delta(p) = -8\pi\sqrt{s} (\tilde{G}(E) - \text{Re } G(E))$$

- $V$  and dependence on renormalization have disappeared (!)
- $p$ : c.m. momentum
- $E$ : scattering energy
- $\tilde{G} - \text{Re } G$ : known kinematical function  
( $\simeq \mathcal{Z}_{00}$  up to exponentially suppressed contributions)
- **One phase at one energy.**

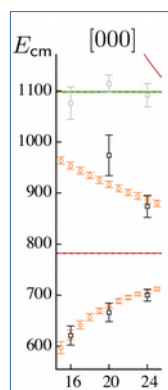
# Finite-volume & chiral extrapolations

## QCD calculations in finite volume

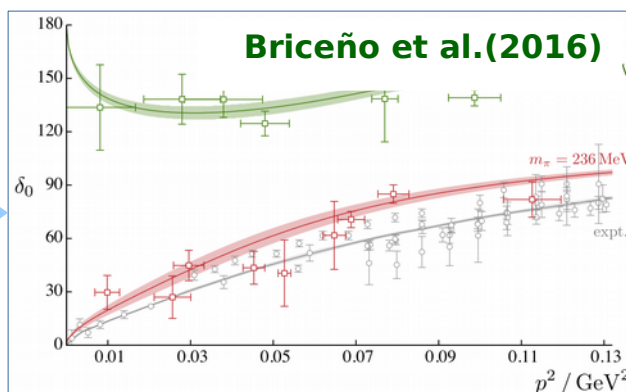
- unphysical pion mass
- (periodic) boundary conditions  
→ discrete momenta & discrete spectrum



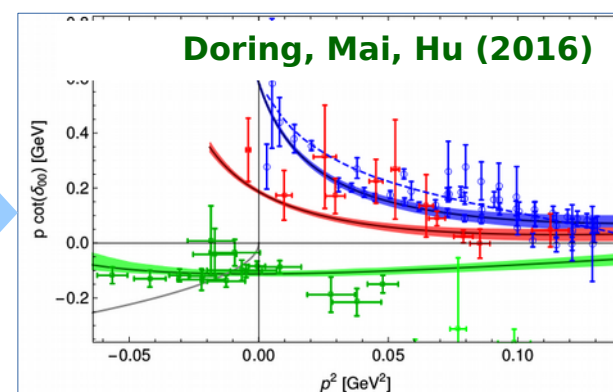
## Recipe for 2 → 2 scattering (e.g. $I=J=0$ $\pi\pi$ scattering)



HSC(2016)



(This step can be skipped)



### LÜSCHER(1986)

- 1 eigenenergy  $\leftrightarrow$  1 phase-shift in infinite volume
- also with coupled channels  
**He et al. (2005)**  
**Doring, Prelovsek, HSC**

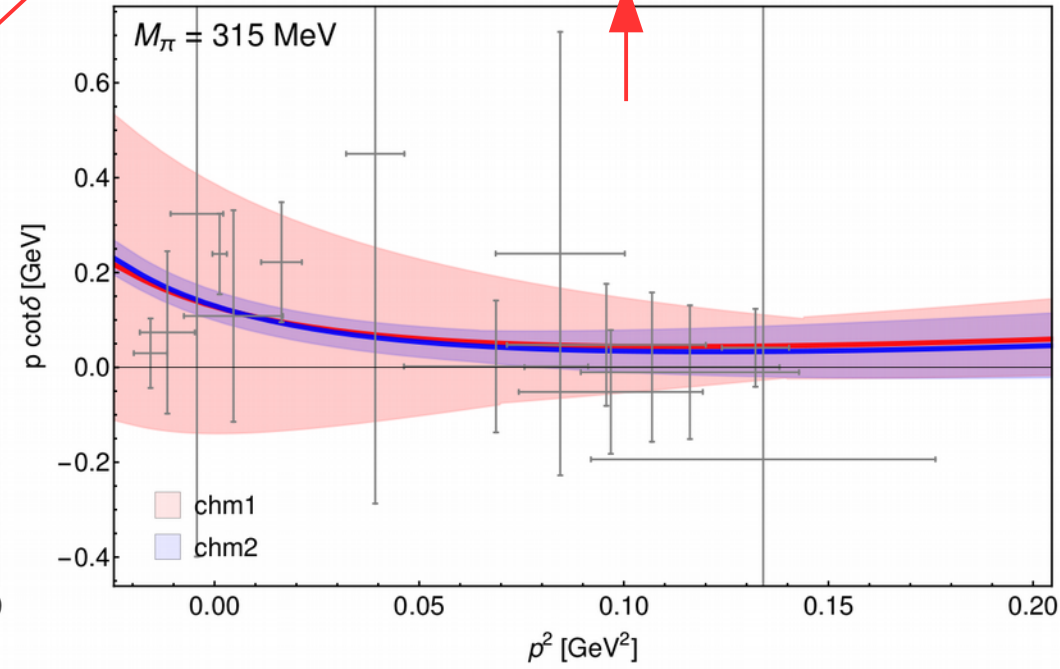
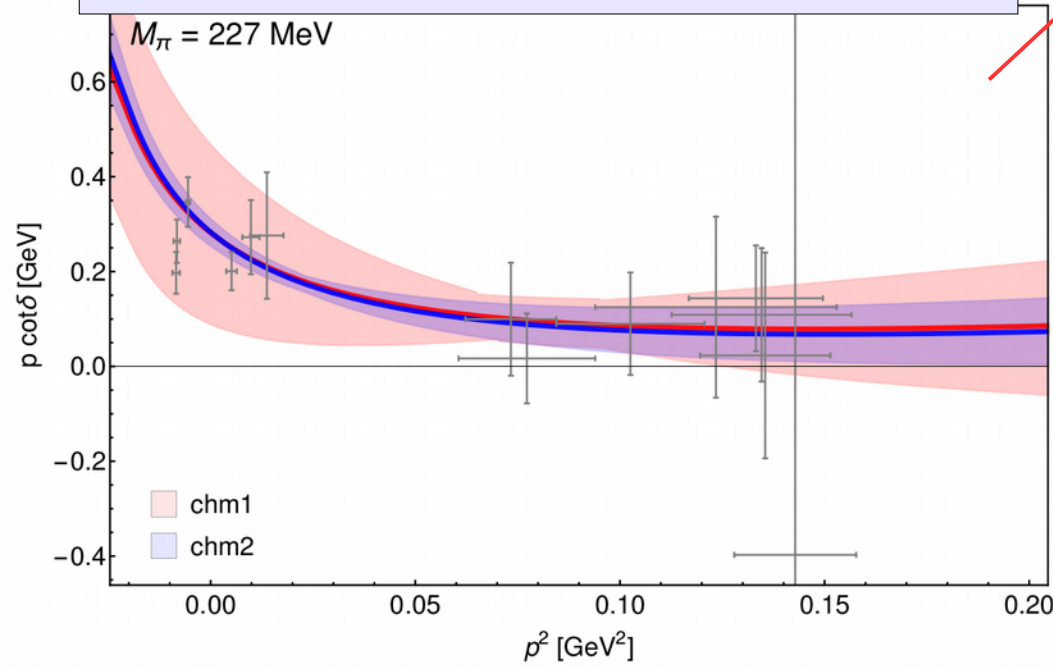
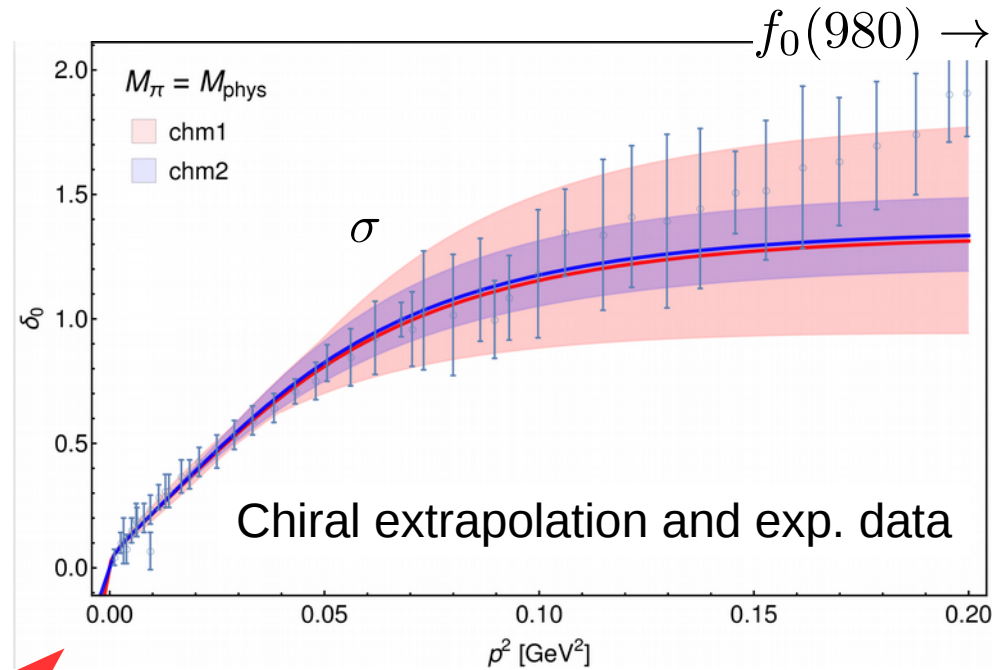
### CHIRAL EXTRAPOLATIONS

- $M_\pi$  dependence from NLO ChPT (IAM)  
**Gasser, Leutwyler(1981)**  
**Dobado, Pelaez (1997)**
- Extrapolation in flavor  
**B. Hu, MD, R. Molina M. Mai et al. (2016)**

# GWU lattice group: the isoscalar sector

[Guo, Alexandru, Molina, M.D., M. Mai, PRD (2018) ]

- nHYP-smearred clover fermions with mass-degenerate quark flavors ( $N_f = 2$ )
- $M_\pi = 227$  MeV and 315 MeV
- 3 elongated boxes
- Large variational basis including several meson-meson operators
- Moving frames
- Conformal mapping for  $\sigma$  pole extraction
- Unitarized Chiral Perturbation Theory fits for chiral extrapolation:  
**chm1:**  $I = L = 0, M_\pi = 227, 315$  MeV  
**chm2:**  $I = L = 0, 1, M_\pi = 227, 315$  MeV



# Chiral extrapolation of $\sigma$ pole

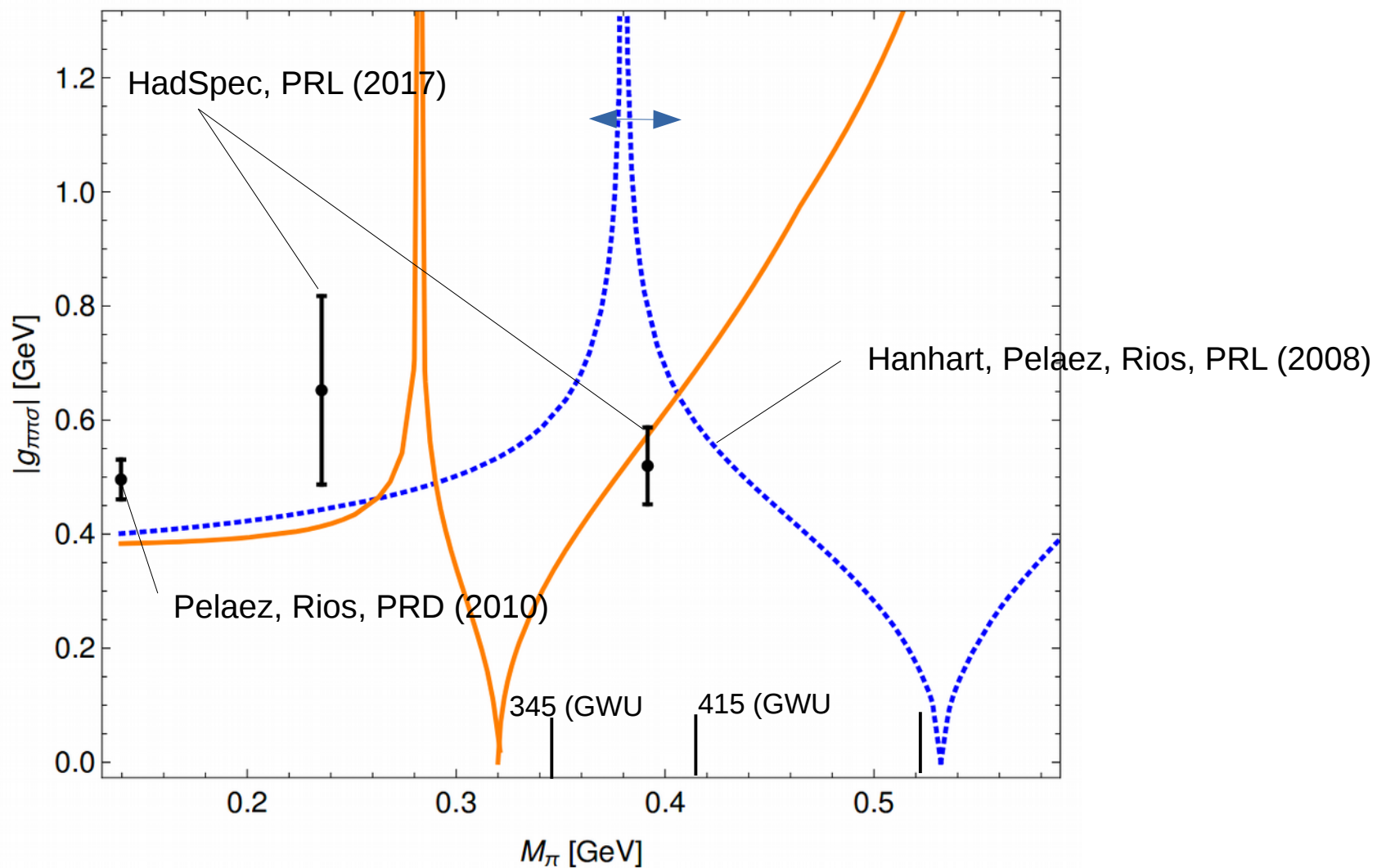
Parametrization	Fitted data	$M_\pi = 138 \text{ MeV}$		
		$\text{Re } z^*$	$-\text{Im } z^*$	$ g $
chm1	$\sigma_{227,315}$	$440^{+60}_{-90}$	$240^{+20}_{-50}$	$3.0^{+0.2}_{-0.6}$
chm2	$\sigma_{227} \rho_{227}$	$430^{+20}_{-30}$	$250^{+30}_{-30}$	$3.0^{+0.1}_{-0.1}$
chm2	$\sigma_{315} \rho_{315}$	$460^{+10}_{-15}$	$210^{+40}_{-30}$	$3.0^{+0.1}_{-0.1}$
chm2	$\sigma_{227,315} \rho_{227,315}$	$440^{+10}_{-16}$	$240^{+20}_{-20}$	$3.0^{+0.0}_{-0.0}$
Ref. [1]	experimental	$449^{+22}_{-16}$	$275^{+12}_{-12}$	$3.5^{+0.3}_{-0.2}$

[1] J. R. Pelaez, [Phys. Rept. \*\*658\*\*, 1 \(2016\), arXiv:1510.00653 \[hep-ph\]](#).

[Consistent with conformal-mapping amplitude parametrization (model-independent, not shown)]

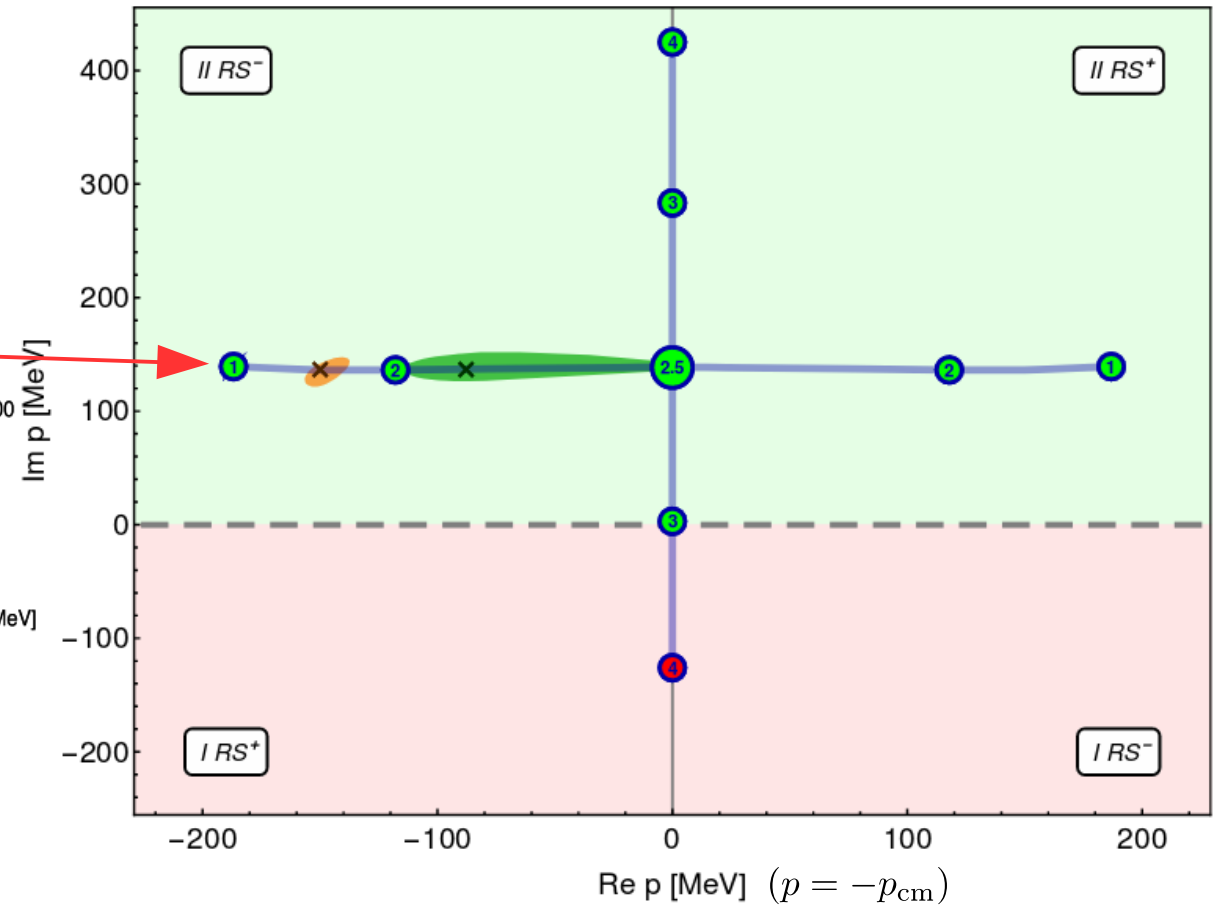
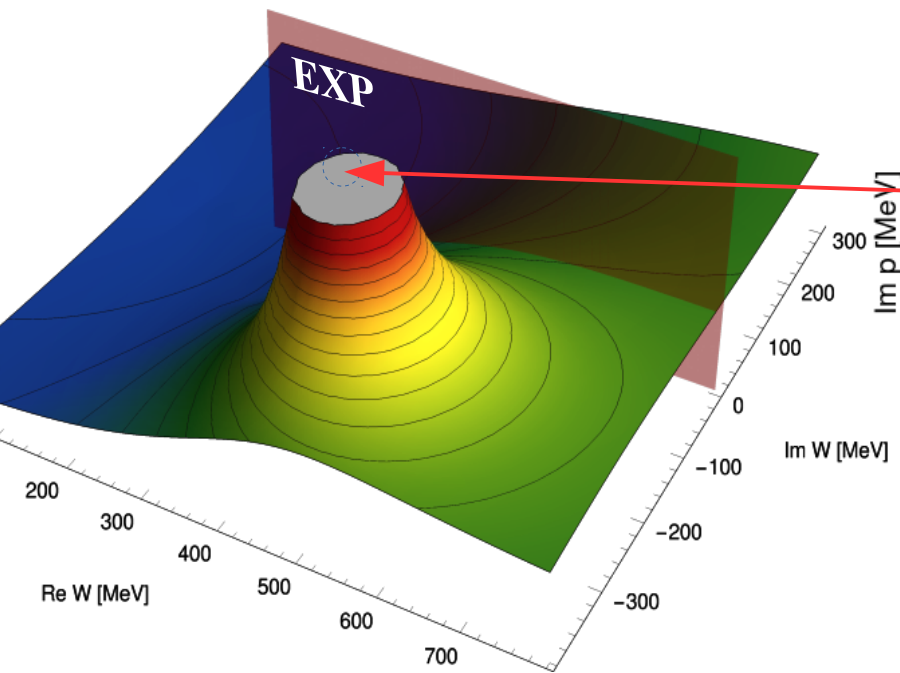


# Residues



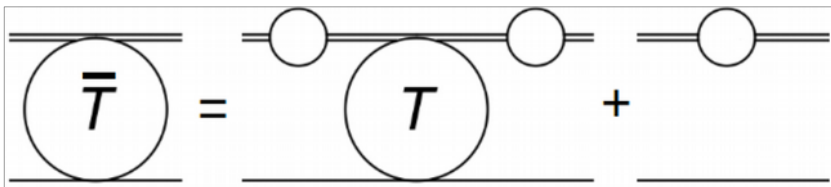
# Pole trajectory

First prediction: Hanhart, Pealez, Rios, PRL (2008)



→  $\sigma$  becomes a (virtual) bound state @  $M_\pi = (345) 415$  MeV

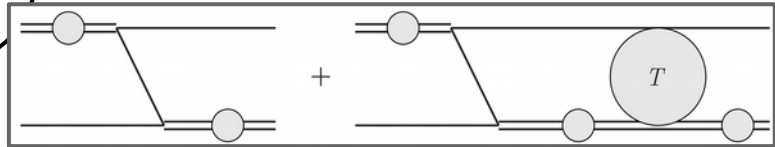
# Cancellations



→ fin. vol. normalization of  $\delta$ -distribution!

$$\bar{T}_{nm}^{A_1^+}(s) = \tau_n(s) T_{nm}^{A_1^+}(s) \tau_m(s) - 2E_n \tau_n(s) \frac{L^3}{\vartheta(n)} \delta_{nm}$$

$$T_{nm}^{A_1^+}(s) = B_{nm}^{A_1^+}(s) - \frac{1}{L^3} \sum_{x \in \text{sets}_8} \vartheta(x) B_{nx}^{A_1^+}(s) \frac{\tau_x(s)}{2E_x} T_{xm}^{A_1^+}(s)$$



$B^{A_1^+}$  singular at  $W^+ = E_m + E_n + E(\mathbf{q}_{nj} + \mathbf{p}_{mi})$

$\tau_m^{-1}$  singular at  $W^{\pm\pm} = E_m \pm E((2\pi/L)\mathbf{y}) \pm E((2\pi/L)\mathbf{y} + \mathbf{p}_{mi})$  for  $\mathbf{y} \in \mathbb{Z}^3$

– when isobar-momenta are discretized in the 3-body cms momenta

$$\tau = \sigma(k) - M_0^2 - \frac{1}{(2\pi)^3} \int d^3\ell \frac{\lambda^2}{2E_\ell(\sigma(k) - 4E_\ell^2 + i\epsilon)}$$

Also: all 2<sup>nd</sup> order singularities in determinant cancel → All consequence of Manifest three-body unitarity