From two to three-body scattering in the finite volume: The role of unitarity

Michael Döring The George Washington University





Jefferson Lab

THE GEORGE WASHINGTON UNIVERSITY

WASHINGTON, DC

Scattering Amplitudes and Resonance Properties from Lattice QCD

27-31 August 2018

Work in collaboration with:

Mai, Molina, Hu, Alexandru, Dehua Guo, Hammer, J-Y.Pang, Pilloni, Rusetsky, Szczepaniak et al. <u>Supported by</u>





[Many slides from Maxim Mai]

- Motivation
- Three-body dynamics in infinite volume
- Finite-volume problems (application: 2-body)
- Three-body dynamics in finite volume

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)





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

Isobar formulation

- Understanding of Lattice QCD or experimental searches (BESIII, COMPASS, GlueX) → theory of 3-body scattering problem needed
- Available tools:
 - Faddeev equations (F.E.)
 - F.E. in fixed-center approximation
 - \rightarrow usefull for πd , *Kd* ... systems
 - F.E. in isobar formulation
 - \rightarrow re-parametrization of two-body amplitude

Faddeev(1959)

Brueckner(1953)

Baru et al(2011), Mai et al. (2015)

Omnes(1964), Aaron(1967) Bedaque(1999)



Isobar formulation

- Understanding of Lattice QCD or experimental searches (BESIII, COMPASS, GlueX) → theory of 3-body scattering problem needed
- Available tools:
 - Faddeev equations (F.E.)
 F.E. in fixed-center approximation
 → usefull for πd, Kd ... systems
 Faddeev(1959)
 Baru et al(2011) Mai et al. (2015)
 - F.E. in isobar formulation
 - → re-parametrization of two-body amplitude

Omnes(1964) Aaron(1967) Bedaque(1999)

 T_{12} T_{31} ... (+ 3-body force)

Re-ordering of 3-body amplitude in 2-body sub-amplitudes & spectator \rightarrow Not an approximation up to cut in space of allowed quantum numbers

FADDEEV EQUATIONS WITH ISOBARS

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

Eur. Phys. J. A53 (2017) 177

FE in isobar parametrization

Original study by Amado/Aaron/Young

AAY(1968)

- 3-dimensional integral equation from unitarity constraint & BSE ansatz
- valid below break-up energies (E < 3m) & analyticity constraints unclear

One has to begin with asymptotic states



- *v* a general function <u>without cuts in the phys. region</u>
- two-body interaction is parametrized by an "isobar"

= has definite QN and correct r.h.-singularities w.r.t invariant mass

• S and T are yet unknown functions

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

delta function sets all intermediate particles on-shell

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



General Ansatz for the isobar-spectator interaction

 \rightarrow **B & t** are **new** unknown functions

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





General Ansatz for the isobar-spectator interaction \rightarrow B & τ are new unknown functions











Scattering amplitude

 $3 \rightarrow 3$ scattering amplitude is a 3-dimensional integral equation



– Imaginary parts of **B**, **S** are fixed by **unitarity/matching**

– For simplicity $v=\lambda$ (full relations available)

 $\tau(\sigma(k)) = (2\pi)\delta^+(k^2 - m^2)S(\sigma(k))$

Scattering amplitude

 $3 \rightarrow 3$ scattering amplitude is a 3-dimensional integral equation



• in the rest-frame of isobar (Lorentz invariance!)

Scattering amplitude

 $3 \rightarrow 3$ scattering amplitude is a 3-dimensional integral equation



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

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

• un-subtracted dispersion relation

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

- one- π exchange in TOPT \rightarrow *RESULT, NOT INPUT !*
- One can map to field theory, but does not have to. Result is a-priori dispersive.

Scattering amplitude – analytic expression



From two to three particles in finite volume

Finite-volume & chiral extrapolations



GWU lattice group: the isoscalar sector

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



Chiral extrapolation of σ pole

 $M_{\pi} = 138 \text{ MeV}$

Parametrization	Fitted data	$\operatorname{Re} z^*$	$-\operatorname{Im} z^*$	$\mid g \mid$
chm1	$\sigma_{227,315}$	440_{-90}^{+60}	240^{+20}_{-50}	$3.0^{+0.2}_{-0.6}$
chm2	$\sigma_{227}~ ho_{227}$	430^{+20}_{-30}	250^{+30}_{-30}	$3.0^{+0.1}_{-0.1}$
chm2	$\sigma_{315}~ ho_{315}$	460^{+10}_{-15}	210_{-30}^{+40}	$3.0^{+0.1}_{-0.1}$
chm2	$\sigma_{227,315}~ ho_{227,315}$	440^{+10}_{-16}	240^{+20}_{-20}	$3.0\substack{+0.0\\-0.0}$
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)] 23

Pole trajectory

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



 $\rightarrow \sigma$ becomes a (virtual) bound state @ $M_{\pi} = (345) 415 \text{ MeV}$



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, 2015, 2016, 2017)

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

Kreuzer, Griesshammer(2012), Hammer et al. (2016, 2x)

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

Requirements

- 3-body systems involve (resonant) two-body sub-amplitudes: Construct such that 2body 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.
- Formulation that lattice practice can connect to $\,\rightarrow\,$ isobars
- → This work: Quantization condition from 3-body unitarity in isobar formulation



How to derive the 2-body quantization condition



How to derive the 2-body quantization condition

> Three-body? Analogously!



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 O_h
 - Analogous to radial coordinate in infinite volume
- Find the orthonormal basis for arbitrary functions defined on each point of a given shell.



$$q_i = \frac{2\pi}{L} n_i, \quad n_i \in \mathbb{Z}, \quad i = 1, 2, 3$$
$$\int \frac{d^3 \mathbf{q}}{(2\pi)^3} \to \frac{1}{L^3} \sum_s \sum_{i=1}^{\vartheta(s)} \frac{\vartheta(s)}{i=1}$$

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

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

$$f^{s}(\hat{p}_{j}) = \sqrt{4\pi} \sum_{\Gamma\alpha} \sum_{a} f_{a}^{\Gamma\alpha s} \chi_{a}^{\Gamma\alpha s}(\hat{p}_{j})$$

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

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

Quantization Condition



• 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 MeV, L=3 fm*
- one S-wave isobar \rightarrow two unknowns:
 - vertex(Isobar \rightarrow 2 stable particles)
 - subtraction constant (~mass)
- Project to $\Gamma = A^{1+}$

→ prediction of 3body energy-eigenlevels (C=0)







A physical system: $\pi^+\pi^+\pi^+$

Mai, M.D., arXiv:1807.04746

Three positive pions

- Maximal isospin: $\pi^+\pi^+\pi^+$
 - > LatticeQCD results for ground level available for $\pi^+\pi^+$ & $\pi^+\pi^+\pi^+$
 - > Repulsive channel $\rightarrow Q$: does the "isobar" picture hold?
 - > L=2.5 fm, m_{π} =291/352/491/591 MeV \rightarrow BonusQ: chiral extrapolation in 3body system?

I. 2-body subchannel:

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





- 1) Fix λ , M_{θ} to exp. data
 - \odot incoorrect m_{π} behavior!

2) Chiral NLO & K-matrix

- © works badly for high energies
- 3) Inverse Amplitude
- Truong (1988)
- \odot correct $\sigma \& m_{\pi}$ behavior
- © parameters known

```
Gasser/Leutwyler(1984)
```

Three positive pions

- Maximal isospin: $\pi^+\pi^+\pi^+$
 - > LatticeQCD results for ground level available for $\pi^+\pi^+$ & $\pi^+\pi^+\pi^+$
 - ▶ Repulsive channel $\rightarrow Q$: does the "isobar" picture hold?

- Detmold et al. (2008)
- > $L=2.5 \text{ fm}, m_{\pi}=291/352/491/591 \text{ MeV} \rightarrow BonusQ$: chiral extrapolation in 3body system?

I. 2-body subchannel:

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





- Maximal isospin: $\pi^+\pi^+\pi^+$
 - > LatticeQCD results for ground level available for $\pi^+\pi^+$ & $\pi^+\pi^+\pi^+$
 - > Repulsive channel $\rightarrow Q$: does the "isobar" picture hold? Detmold et al. (2008)
 - > L=2.5 fm, m_{π} =291/352/491/591 MeV \rightarrow BonusQ: chiral extrapolation in 3body system?



- Maximal isospin: $\pi^+\pi^+\pi^+$
 - > LatticeQCD results for ground level available for $\pi^+\pi^+$ & $\pi^+\pi^+\pi^+$
 - > Repulsive channel $\rightarrow Q$: does the "isobar" picture hold? Detmold et al. (2008)
 - > L=2.5 fm, m_{π} =291/352/491/591 MeV \rightarrow BonusQ: chiral extrapolation in 3body system?



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 $\rightarrow Q$: does the "isobar" picture hold?
 - > $L=2.5 \text{ fm}, m_{\pi}=291/352/491/591 \text{ MeV} \rightarrow BonusQ$: chiral extrapolation in 3body system?



Detmold et al. (2008)

Summary

3-body amplitude in infinite volume

- 3-body unitarity dictates on-shell condition (driving term & isobar propagator)
- Result: 3-dim. relativistic integral equations, explicit proof of 3B unitarity above threshold
- Equivalent to Khuri-Treiman equations*

Finite volume investigation:

- On-shell condition dictates leading, power-law finite-volume effects
- Quantization condition
- Bare-bone, stripped-down infinitevolume extrapolation tool (in spirit of Lüscher equation)
- First numerical application to physical system $\pi^+\pi^+\pi^+$

OUTLOOK

- → include spin isobars & multiple isobars
- → unequal masses
- → practical studies: $a_1(1260)$, Roper...

* Ian Aitchison, private communication

SPARES



The Power of Unitarity



The Power of Unitarity



The Power of Unitarity



Residues



Connection to triangle diagrams

Interesting application: a1(1420) – observed in COMPASS – in $f_0(980)\pi$ final state

ONE EXPLANATION:

Log-like behavior of the "triangle-diagram"

Mikhasenko/Ketzer/Sarantsev(2015)

Aceti/Dai/Oset(2016)



– Q: Does such a feature exist in full 3b-unitary FSI?



Connection to triangle diagrams

Interesting application: a1(1420) – observed in COMPASS – in $f_0(980)\pi$ final state

ONE EXPLANATION:

Log-like behavior of the "triangle-diagram"

Mikhasenko/Ketzer/Sarantsev(2015)

Aceti/Dai/Oset(2016)



- Q: Does such a feature exist in full 3b-unitary FSI?



Two-body scattering on lattice

Input for 3-body

The cubic lattice



- Side length L, periodic boundary conditions $\Psi(\vec{x}) \stackrel{!}{=} \Psi(\vec{x} + \hat{\mathbf{e}}_i L)$ \rightarrow finite volume effects \rightarrow Infinite volume $L \rightarrow \infty$ extrapolation
- Lattice spacing a

 → finite size effects
 Modern lattice calculations:
 a ≃ 0.07 fm → p ~ 2.8 GeV
 → (much) larger than typical hadronic scales;

not considered here.

 Unphysically large quark/hadron masses
 → (chiral) extrapolation required.

Two body scattering

In the infinite volume

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



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

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

V: (Pseudo)potential, σ : 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

G, Õ

1

Discretized momenta in the finite volume with periodic boundary conditions

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

 $+\omega_2$

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:

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

• Re-derivation of Lüscher's equation (T determines the phase shift δ):

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

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

Two-body vs. Three-body



Data: HadronSpectrum (Dudek, PRD 2013,Briceño PRL 2016); Analysis: M.D., B. Hu, M. Mai, PLB (2018) See also: Bolton, Briceno, Wilson, Phys.Lett. B757 (2016) 50

Large # of d.o.f. require efficient parametrizations

Example: The coupled-channel $2 \rightarrow 2$, $2 \rightarrow 3$, $3 \rightarrow 3$ meson-baryon system

μ	$J^P =$	$\frac{1}{2}^{-}$	$\frac{1}{2}^{+}$	$\frac{3}{2}^+$	$\frac{3}{2}^{-}$	$\frac{5}{2}^{-}$	$\frac{5}{2}^{+}$	$\frac{7}{2}^+$	$\frac{7}{2}^{-}$	$\frac{9}{2}^{-}$	$\frac{9}{2}^+$
1	πN	S_{11}	<i>P</i> ₁₁	P_{13}	D_{13}	D_{15}	F_{15}	F_{17}	G_{17}	G_{19}	H_{19}
2	$\rho N(S=1/2)$	S_{11}	P_{11}	P_{13}	D_{13}	D_{15}	F_{15}	F_{17}	G_{17}	G_{19}	H_{19}
3	$\rho N(S = 3/2, J - L = 1/2)$	_	P_{11}	P_{13}	D_{13}	D_{15}	F_{15}	F_{17}	G_{17}	G_{19}	H_{19}
4	$\rho N(S = 3/2, J - L = 3/2)$	D_{11}	_	F_{13}	S_{13}	G_{15}	P_{15}	H_{17}	D_{17}	I_{19}	F_{19}
5	ηN	S_{11}	P_{11}	P_{13}	D_{13}	D_{15}	F_{15}	F_{17}	G_{17}	G_{19}	H_{19}
6	$\pi \Delta (J-L = 1/2)$	_	P_{11}	P_{13}	D_{13}	D_{15}	F_{15}	F_{17}	G_{17}	G_{19}	H_{19}
7	$\pi \Delta (J-L = 3/2)$	D_{11}	_	F_{13}	S_{13}	G_{15}	P_{15}	H_{17}	D_{17}	I_{19}	F_{19}
8	σN	P_{11}	S_{11}	D_{13}	P_{13}	F_{15}	D_{15}	G_{17}	F_{17}	H_{19}	G_{19}
9	$K\Lambda$	S_{11}	P_{11}	P_{13}	D_{13}	D_{15}	F_{15}	F_{17}	G_{17}	G_{19}	H_{19}
10	$K\Sigma$	S_{11}	P_{11}	P_{13}	D_{13}	D_{15}	F_{15}	F_{17}	G_{17}	G_{19}	H_{19}

including 3-body dynamics [Julich-Bonn; ANL-Osaka].

Cancellations



Also: all 2^{nd} order singularities in determinant cancel \rightarrow All consequence of Manifest three-body unitarity

Effective method for multi-particle states

The Optical potential [D. Agadjanov, M.D., M. Mai, U.-G. Meißner, A. Rusetsky, JHEP (2016)]

Optical potential in finite volume

- Finite-volume corrections for complex hadronic systems.
- Example: The optical potential on the lattice



• It is not always necessary to explicitly parameterize complicated intermediate states → Absorb all "uninteresting" dynamics in a complex-valued optical potential



$$\begin{array}{l} \text{Minimize:} \quad \chi^{2} = \sum_{k=1}^{m} \frac{\left| \hat{W}^{-1}(E_{k}) - \hat{W}_{L}^{-1}(E_{k}) \right|^{2}}{\sigma_{k}^{2}} + P_{i}(a_{j}, \, b_{j}) \\ P_{1}(a_{j}, \, b_{j}) = \lambda^{4} \int_{E_{\min} + i\varepsilon}^{E_{\max} + i\varepsilon} dE \left| \frac{\partial^{2} \hat{W}^{-1}(E)}{\partial E^{2}} \right| \end{array}$$

The reconstructed infinite-volume limit [LASSO + Cross Validation]



Correct Choice of penalization parameter λ through cross validation:

Fit at finite ϵ , validate at different ϵ' ($E \rightarrow E + i\epsilon$).



Unitarity & Matching

• 3-body Unitarity (normalization condition ↔ phase space integral)

