Resonance extraction from the finite Volume

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- 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  $a \rightarrow finite size effects$ 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
 → (chiral) extrapolation required. Eigenvalues in the finite 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:

$$T = V + V G T$$
 Im  $G = -\sigma$ 

G

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

• G: Green's function:

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

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

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

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

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





- $E > m_1 + m_2$ :  $\tilde{G}$  has poles at free energies in the box,  $E = \omega_1 + \omega_2$
- E < m<sub>1</sub> + m<sub>2</sub>: G̃ → G exponentially with L (regular summation theorem).

Measured eigenvalues of the Hamiltonian (tower of *lattice levels* E(L))
 → Poles of scattering equation T̃ in the finite volume → determines V:

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

• 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  $\delta$ ):

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

- 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.

Energy interpolations to relate eigenvalues:

Unitarized CHPT in one- and two-channel scattering.

Unitary extension of ChPT, can be matched to ChPT order-by-order:

$$T_{\ell} = V_{\ell}^{\text{IAM}} + V_{\ell}^{\text{IAM}} G T_{\ell} \qquad V_{\ell}^{\text{IAM}} = \left(1 - V_{\ell}^{[4]} (V_{\ell}^{[2]})^{-1}\right)^{-1} V_{\ell}^{[2]}$$
$$V_{\ell}^{[2]} \equiv V_{\ell}^{[2]}(p, M_{\pi}, M_{K}, M_{\eta_{8}}, f), \qquad V_{\ell}^{[4]} \equiv V_{\ell}^{[4]}(p, M_{\pi}, M_{K}, M_{\eta_{8}}, f, L_{i})$$

Table :  $L_i$  [×10<sup>3</sup>] fitted to meson-meson scattering data

$ \begin{array}{c} L_1 \\ 0.873^{+0.017}_{-0.028} \end{array} $	$L_2 \\ 0.627^{+0.028}_{-0.014}$	$L_3$ -3.5 [fixed]	${}^{L_4}_{-0.710^{+0.022}_{-0.026}}$
$ \begin{array}{c} L_5 \\ 2.937^{+0.048}_{-0.094} \end{array} $	$L_6 + L_8 \\ 1.386^{+0.026}_{-0.050}$	$ L_7 \\ 0.749^{+0.106}_{-0.074} $	$q_{\max}$ [MeV] 981 [fixed]

Fit to meson-meson PW data using unitary ChPT with NLO terms [M.D., Meißner, JHEP (2012)] using IAM [Oller, Oset, Peláez, PRC (1999)]



• A resonance is characterized by its (complex) pole position and residues, corresponding to resonance mass, width, and branching ratio.







Ι	L	S	Resonance	sheet	$z_0 \; [MeV]$	$a_{-1}  [M_{\pi}]$	$a_{-1}  [M_{\pi}]$
0	0	0	$\sigma(600)$	pu	$434 {+}i261$	$-31 - i  19  (\bar{K}K)$	$-30+i86(\pi\pi)$
0	0	0	$f_0(980)$	pu	$1003 {+} i15$	$16 - i79(\bar{K}K)$	$-12+i4(\pi\pi)$
1/2	0	$^{-1}$	$\kappa(800)$	pu	$815 {+}i226$	$-36+i39(\eta K)$	$-30+i57(\pi K)$
1	0	0	$a_0(980)$	pu	1019 - i4	$-10 - i107(\bar{K}K)$	$21\!-\!i31(\pi\eta)$
0	1	0	$\phi(1020)$	p	976 + i0	$-2+i0(\bar{K}K)$	—
1/2	1	$^{-1}$	$K^{*}(892)$	pu	889 + i25	$-10+i0.1(\eta K)$	$14 + i 4 (\pi K)$
1	1	0	$\rho(770)$	pu	$755 \! + \! i  95$	$-11+i2(\bar{K}K)$	$33+i17(\pi\pi)$

- Pole positions  $z_0$  [MeV] ( $\sim$  masses and widths)
- Residues  $a_{-1}[M_{\pi}]$  (~ branching ratios)
- I, L, S: isospin, angular momentum, strangeness.



[M.D., Meißner, JHEP (2012)] Loops in *t*- and *u*-channel (1-loop calculation): [Albaladejo, Oller, Oset, Rios, Roca, JHEP (2013)]

## Reconstruction of the $\kappa(800)$ stabilized by ChPT

Fit potential

$$V^{\text{fit}} = \left(\frac{V_2 - V_4^{\text{fit}}}{V_2^2}\right)^{-1}, \quad V_4^{\text{fit}} = a + b(s - s_0) + c(s - s_0)^2 + d(s - s_0)^3 + \cdots$$

 $[V_2 \equiv V_{\rm LO} \text{ from } f_{\pi}, f_K, f_{\eta}, M_{\pi}, M_K, M_{\eta}; s \equiv E^2]$ 



Figure : Pseudo lattice-data and  $(s^0, s^1, s^2)$  fit to those data with uncertainties (bands).

Figure : Solid line: Actual phase shift. Error bands of the  $(s^0, s^1), (s^0, s^1, s^2)$ , and  $(s^0, s^1, s^2, s^3)$  fits.

[see also: HadronSpectrum; Dudek, Wilson et al., 1406.4158]

## The $\kappa(800)$ pole



Convergence of results determines degrees of freedom (more formal: F-test).

## Avoided level crossing in the energy levels



Using Unitarized Chiral Perturbation Theory to produce energy levels

[M. D., Meißner, Oset, Rusetsky, EPJA (2011)]

## Changing the input ...



- Weaker coupling to the  $K\bar{K}$  channel,  $f_0(980)$  disappears
- Avoided level crossing still occurs at the same place: threshold!
- The threshold can be moved by using twisted b.c.!

#### Need for an interpolation in energy (coupled channels) Twisting the boundary conditions [Bernard, Lage, Meißner, Rusetsky, JHEP (2011), M.D., Meißner, Oset, Rusetsky, EPJA (2011)]

- S-wave, coupled-channels  $\pi\pi$ ,  $\bar{K}K \rightarrow f_0(980)$ .
- Three unknown transitions
  - $V(\pi\pi \to \pi\pi)$ •  $V(\pi\pi \to \bar{K}K)$ •  $V(\bar{K}K \to \bar{K}K)$



• Twisted B.C. for the *s*-quark:  $u(\vec{x} + \hat{\mathbf{e}}_i L) = u(\vec{x})$   $d(\vec{x} + \hat{\mathbf{e}}_i L) = d(\vec{x})$  $s(\vec{x} + \hat{\mathbf{e}}_i L) = e^{i\theta_i}s(\vec{x})$ 

- Periodic B.C.:  $\Psi(\vec{x} + \hat{\mathbf{e}}_i L) = \Psi(\vec{x})$
- Periodic in 2 dim.:

- Twisted B.C.:  $\Psi(\vec{x} + \hat{\mathbf{e}}_i L) = e^{i\theta_i} \Psi(\vec{x})$
- Periodic/antiperiodic:



 $\theta_2 = \pi$ 

#### Coupled-channel systems with thresholds [M.D., Meißner, Oset/Rusetsky, EPJA 47 (2011)]

- $\bullet$  Need for an interpolation in energy (  $\rightarrow$  Unitarized ChPT,... )
- Expand a two-channel transition V in energy  $(i, j: \pi\pi, \overline{K}K)$ :

$$V_{ij}(E) = a_{ij} + b_{ij}(E^2 - 4M_K^2)$$

- Include model-independently known LO contribution in *a*, *b*.
- Or even NLO contributions (7 LECs: more fit parameters).



Moving frames and coupled channels:

Scanning resonance lineshapes.

• Resonance scan needed because Lüscher method is modulus  $\pi$ .



• Operators with non-zero momentum of the center-of-mass:  $\vec{P} = \vec{p}_1 + \vec{p}_2 \neq 0$  Rummukainen, Gottlieb, NPB (1995)

## Breaking of cubic symmetry through boost Example: Lattice points $\vec{q}^*$ boosted with $P = (0, 0, 0) \rightarrow \frac{2\pi}{L} (0, 0, 2)$ :

#### • Infinite volume limit: Rotational symmetry



$$\int \frac{d^3 \vec{q}}{(2\pi)^3} g(|\vec{q}|) Y_{\ell m}(\theta,\phi) Y^*_{\ell' m'}(\theta,\phi) \sim \delta_{\ell \ell'} \delta_{mm'}.$$

S→S	0	0	0
0	$P_{\text{-}1}\toP_{\text{-}1}$	0	0
0	0	$P_0\toP_0$	0
0	0	0	$P_1 \to P_1$

#### • Infinite volume limit: Rotational symmetry



• Wigner-Eckart theorem:



• Finite volume: Rotational symmetry  $\rightarrow$  Cubic symmetry



• S - G-wave mixing, but S - P waves still orthogonal:

S→S	0	0	0
0	$P_{\text{-}1}\toP_{\text{-}1}$	0	0
0	0	$P_0\toP_0$	0
0	0	0	$P_1\toP_1$

 $\bullet$  Finite volume & boost: Cubic symmetry  $\rightarrow$  subgroups of cubic symmetry



$$\frac{1}{L^3} \sum_{\vec{n}} g(|\vec{q}|) Y_{\ell m}(\theta, \phi) Y^*_{\ell' m'}(\theta, \phi) \sim A_{\ell \ell' m m'}.$$

• For boost 
$$P = \frac{2\pi}{L}$$
 (0,1,1):

$$S \rightarrow S$$
 $0$  $S \rightarrow P_0$  $0$  $0$  $P_{-1} \rightarrow P_{-1}$  $0$  $P_{-1} \rightarrow P_1$  $P_0 \rightarrow S$  $0$  $P_0 \rightarrow P_0$  $0$  $0$  $P_1 \rightarrow P_{-1}$  $0$  $P_1 \rightarrow P_1$ 

• Finite volume & boost: Cubic symmetry  $\rightarrow$  subgroups of cubic symmetry



More complicated boosts:

$$\begin{array}{lll} S \rightarrow S & S \rightarrow P_{-1} & S \rightarrow P_{0} & S \rightarrow P_{1} \\ P_{-1} \rightarrow S & P_{-1} \rightarrow P_{-1} & P_{-1} \rightarrow P_{0} & P_{-1} \rightarrow P_{1} \\ P_{0} \rightarrow S & P_{0} \rightarrow P_{-1} & P_{0} \rightarrow P_{0} & P_{0} \rightarrow P_{1} \\ P_{1} \rightarrow S & P_{1} \rightarrow P_{-1} & P_{1} \rightarrow P_{0} & P_{1} \rightarrow P_{1} \end{array}$$

**Disentanglement of partial waves** [M.D., Meißner, Oset, Rusetsky, EPJA (2012)] Example: *S*- and *P*-waves for the  $\kappa(800)/K^*(892)$  system

Knowledge of P-wave (from separate analysis of lattice data) allows to disentangle the S-wave:

$$p \cot \delta_S = -8\pi E \frac{p \cot \delta_P \hat{G}_{SS} - 8\pi E (\hat{G}_{SP}^2 - \hat{G}_{SS} \hat{G}_{PP})}{p \cot \delta_P + 8\pi E \hat{G}_{PP}}$$



- $\delta_S \equiv \delta^0_{1/2}(\pi K \to \pi K)$
- Red solid: Actual *S*-wave phase shift.
- Dash-dotted: Reconstructed S-wave phase shift, PW-mixing ignored.
- Dashed: Reconstructed *S*-wave phase shift, PW-mixing disentangled.
- small *p*-wave: Level shift  $\Delta E \simeq -\frac{6\pi E_S \delta_P}{L^3 p \omega_1 \omega_2}$

See also: Rummukainen, Gottlieb, NPB (1995); Kim, Sachrajda, Sharpe, NPB (2005); Davoudi, Savage, PRD (2011), Z. Fu, PRD (2012); Leskovec, Prelovsek, PRD (2012); Dudek, Edwards, Thomas, PRD (2012); Hansen, Sharpe, PRD 86 (2012); Briceño, Davoudi, PRD 88 (2013); Göckeler, Horsley, Lage, Meißner, Rakow, Rusetsky, Schierholz, Zanotti, PRD (2012)

#### Asymmetric boxes & boosts M.D., R. Molina, GWU Lattice Group [A. Alexandru et al.]



- $L_x = x L, L_y = L, L_z = L$ x = 1, 1.26, 2.04
- $\frac{L}{2\pi} \vec{P} = (1, 1, 0), x = 1$ : irreps  $A_1, B_1, B_2$
- $\frac{L}{2\pi} \vec{P} = (1, 1, 0), x \neq 1$ : irreps  $A_1, B_1$  (!) pure p-wave level survives!



Chiral extrapolations and coupled channels:

Baryons.

 $J^P = 1/2^-$  in the finite volume [M.D., Mai, Meißner, EPJA (2013)

Unitarized chiral interaction with NLO contact terms in BSE



Data: SAID (2006); Extension of SAID analysis framework itself to finite volume in progress.

## Chiral extrapolation to a QCDSF lattice setup



## Prediction of the lattice spectrum



 No one-to-one mapping of levels to resonances → coupled channel analysis needed; hidden poles appear.

# $N\pi$ (1/2<sup>-</sup>) channel

 $m_{\pi}$ =266 MeV; distillation method; variational analysis using a basis of N (3 quarks) and N $\pi$  (5 quarks) interpolators;



C.B. Lang and V. Verduci,

2.0

1.8

Phys.Rev. D 87, 054502 (2013)

Thursday, August 1, 13

#### Chiral extrapolation from dynamical coupled channels approaches based on Jülich solution NPA 829, 170 (2009)

- Larger theoretical uncertainties.
- Quark mass dependence of effective  $2\pi N$  channels is intricate.
- Finite-volume effects of 3-body channels unexplored.
- Accessing the Roper puzzle.





# First prediction of the $\Lambda(1405)$ in the finite volume [M. D./Haidenbauer/Meißner/Rusetsky, EPJA 47 (2011)]

(Non-factorizing/off-shell) Lippman-Schwinger equation in the finite volume,

$$T^{(\mathrm{P})}(q'',q') = V(q'',q') + \frac{2\pi^2}{L^3} \sum_{i=0}^{\infty} \vartheta^{(\mathrm{P})}(i) \frac{V(q'',q_i) T^{(\mathrm{P})}(q_i,q')}{\sqrt{s} - E_a(q_i) - E_b(q_i)}, \quad q_i = \frac{2\pi}{L} \sqrt{i} \;.$$



- Access to sub-KN-threshold dynamics:
- Discrepancies of lowest levels: levels sensitive to different  $\Lambda(1405)$  dynamics.
- One- or two-pole structure:
  - Will NOT lead to additional level.
  - but shifted threshold levels.

See also Martinez, Bayar, Jido, Oset, PRC 86 (2012).

#### The $\Lambda(1405)$ : Predictions from Unitarized CHPT Raguel Molina, M.D., preliminary



Finite volume spectrum

- Coupled channels  $\pi\Sigma, \ \bar{K}N, \ \eta\Lambda, K\Xi$
- Unitarized LO  $\chi$  potential V in T = V + VGT
- No freedom at this order  $\rightarrow$  full prediction.
- UCHPT has two poles for the  $\Lambda(1405)$ .
- $\rightarrow$  new data not in conflict with two-pole structure of a molecular  $\Lambda(1405)$  (but not yet a proof thereof).
- $\label{eq:loss} \bullet \to \mathsf{needed: Statistical} \\ \mathsf{NLO analysis in} \\ \mathsf{combination with more} \\ \mathsf{accurate data.} \\ \end{split}$

#### The $\Lambda(1405)$ : Predictions from Unitarized CHPT Raquel Molina, M.D., preliminary



Two-pole structure in the infinite volume

- Coupled channels  $\pi\Sigma, \ \bar{K}N, \ \eta\Lambda, K\Xi$
- Unitarized LO  $\chi$  potential V in T = V + VGT
- No freedom at this order  $\rightarrow$  full prediction.
- UCHPT has two poles for the  $\Lambda(1405)$ .
- $\rightarrow$  new data not in conflict with two-pole structure of a molecular  $\Lambda(1405)$  (but not yet a proof thereof).
- → needed: Statistical NLO analysis in combination with more accurate data.

#### The $\Lambda(1405)$ : Predictions from Unitarized CHPT Raguel Molina, M.D., preliminary



Residues at eigenvalues (Overlap)

- Coupled channels  $\pi\Sigma, \ \bar{K}N, \ \eta\Lambda, K\Xi$
- Unitarized LO  $\chi$  potential V in T = V + VGT
- No freedom at this order  $\rightarrow$  full prediction.
- UCHPT has two poles for the  $\Lambda(1405).$
- $\rightarrow$  new data not in conflict with two-pole structure of a molecular  $\Lambda(1405)$  (but not yet a proof thereof).
- $\label{eq:linear} \bullet \to \mathsf{needed: Statistical} \\ \mathsf{NLO analysis in} \\ \mathsf{combination with more} \\ \mathsf{accurate data.} \\ \end{cases}$

Three particles:

New finite volume methods.

#### Three-particle intermediate states See also: Hansen/Sharpe (2014), Grießhammer/Kreuzer (2013), Roca/Oset (2013),...



- $\pi N$  scattering: Known large inelasticities  $\pi\pi N \ [\pi\Delta, \ \sigma N, \ \rho N, \dots]$
- $\pi\pi/\pi N$  boosted subsystems.
- Is it enough to include (boosted) 2-particle subsystems in the propagator?
   No.
- Three-body s-channel dynamics requires particle exchange transitions. ⇒ Three-body unitarity

[Aaron, Almado, Young, PR 174 (1968) 2022, Aitchison, Brehm, PLB 84 (1979) 349, PRD 25 (1982) 3069,...]

#### Three-body unitarity Aaron, Almado, Young, PR 174 (1968) 2022



- (a, b) Unitarity relation and particle exchange.
- (c) Amplitude at one loop.
- (d) Contact interactions: unitarity preserved.

### Consequence: Threshold openings in the complex plane Existence shown model-independently in [S. Ceci, M.D., C. Hanhart *et. al.*, PRC 84 (2011)]







## Applications to: Roper $N(1440)1/2^+$ , $a_1(1260)$ , X(3872),...

[Mahbub, Kamleh et al., PLB 693]

- open: quenched
- filled: full dynamical



[Data: SAID 2006; Fit: Jülich 2012]

- Earliest onset of inelasticity into  $\pi\pi N$  (all particles in S-wave)
- Entanglement of Roper pole and complex  $\pi\Delta$  branch point
- Strong pion mass dependence expected
- Unknown, large 3-body finite-volume effects

- Rapid progress in the actual ab-initio calculations of resonances/phase shifts:  $\rho(770)$ ,  $a_0(980)$ ,  $K^*(s, p, d)$ ,  $[N(1535), \Lambda(1405)]$ , ....
- Structure of  $\Lambda(1405)$  from first principles comes into reach.
- Close to the physical point, finite volume effects dominate the spectrum.
- Use finite volume effects in your favor: Lüscher & extensions (coupled channels, moving frames, twisted boundary conditions,...)
- Energy interpolation needed in many aspects —Unitarized ChPT & coupled-channel approaches can provide a framework.
  - Prediction of levels & Chiral extrapolation
    - $\rightarrow$  find suitable lattice setups to cover resonance region with eigenstates.
  - Provide lattice setups that are maximally sensitive to resonances.
  - Analysis of lattice data.
- Three-particle interaction bears new conceptual challenges and opportunities. [funded through NSF Career grant 2015-2020]

## Phase shifts from a moving frame: the $\sigma(600)$

Comparison: Variation of L vs moving frames





#### Mixing of partial waves in boosted multiple channels: $\sigma(600)$ [M.D., E. Oset, A. Rusetsky, EPJA (2012)]



Solid: Levels from  $A_1^+$ . Non-solid: Neglecting the *D*-wave.

- $\pi\pi$  &  $\bar{K}K$  in S-wave,  $\pi\pi$  in D-wave.
- Organization in Matrices  $(A_1^+)$ , e.g.  $\vec{P} = (2\pi/L)(0,0,1), (2\pi/L)(1,1,1),$ and  $(2\pi/L)(0,0,2)$ :



 Phase extraction: Expand and fit V<sub>S</sub>, V<sub>D</sub> simultaneously to different representations, as in case of multi-channels (reduction of error).

# Kπ scattering and K\* width in moving frames

Prelovsek, Leskovec, <u>Lang</u>, Mohler, this conf. and *arXiv: 1307.0736* 

p-wave, coupled system of 5 q $\bar{q}$  and 3 K $\pi$  operators, total momentum P=(000),(001),(011)



## The $a_0(980)$



- $M_{\pi} \sim 300$  MeV, no singly disconnected diagrams.
- Operators:  $\overline{K}K$  molecular, diquark-antidiquark, meson-meson.
- Two low-lying states, large overlap with meson-meson.

- $M_{\pi} \sim 300$  MeV, singly disconnected diagrams included.
- Operators:  $q\bar{q}$ ,  $\bar{K}K$  molecular.
- Again, two low lying states, no information on additional state.



## Three particles in a finite volume



- In case of 2 particles:  $r \gg R$ , when particles are near the walls
- In case of 3 particles: it may happen that  $r \gg R$ ,  $r_1 \simeq R$ , when the particles are near the walls

The problem with the disconnected contributions: is the finite-volume spectrum in the 3-particle case determined solely through the on-shell scattering matrix?

• Despite the presence of the disconnected contributions, the energy spectrum of the 3-particle system in a finite box is still determined by the <u>on-shell</u> scattering matrix elements in the infinite volume

[Polejaeva, Rusetski, EPJA (2012)]