Three-particle dynamics in a finite volume

Akaki Rusetsky, University of Bonn

In collaboration with M. Döring, H.-W. Hammer, M. Mai, J.-Y. Pang, F. Romero-López, C. Urbach and J. Wu

arXiv:1706.07700, arXiv:1707.02176 + ongoing work

INT Workshop “Multi-Hadron Systems from Lattice QCD,” February 6, 2018, Seattle

Plan

- Introduction
- Formalism:
  - Non-relativistic EFT and dimer picture
  - Independence from the off-shell effects
  - Quantization condition
- Comparison with other approaches
- Symmetries of the box and reduction of the quantization condition
- The finite volume spectrum: bound and scattering states
- The shift of the ground state
- Conclusions, outlook

Extracting three-particle observables from the lattice

K. Polejaeva and AR, EPJA 48 (2012) 67
Finite volume energy levels determined solely by the S-matrix

M. Hansen and S. Sharpe, PRD 90 (2014) 116003; PRD 92 (2015) 114509
Quantization condition

R. Briceno and Z. Davoudi, PRD 87 (2013) 094507
Dimer formalism, quantization condition

P. Guo, PRD 95 (2017) 054508
Quantization condition in the 1+1-dimensional case

S. Kreuzer and H.-W. Hammer, PLB 694 (2011) 424; EPJA 43 (2010) 229; PLB 673 (2009) 260; S. Kreuzer and H. W. Grießhammer, EPJA 48 (2012) 93
Dimer formalism, numerical solution

M. Mai and M. Döring, EPJA 53 (2017) 240
Three-body unitarity + analyticity (similar in spirit to the present approach)

Alternative approach: HAL QCD

$\hookrightarrow$ Is the finite-volume spectrum determined solely by the three-body S-matrix elements in the infinite volume?

The strategy

☹ Quantization condition very complicated, involves "unconventional" scattering amplitudes...

$\hookrightarrow$ Do not try to extract the amplitudes directly from data, in analogy to Lüscher's formula!

$\hookrightarrow$ Extract low-energy couplings, get amplitudes by solving scattering equations in the infinite volume!

- NREFT: relativistic kinematics will be included later
- Effective couplings: only exponentially suppressed effects at large volumes!

? Is the information about the S-matrix sufficient to uniquely determine the spectrum? Do the *off-shell couplings,* which are not fixed from matching to the S-matrix, contribute to the finite-volume energies?

NREFT: dimer picture in the two-particle sector

$$\mathcal{L} = \psi^\dagger \left(i\partial_0 - \frac{\nabla^2}{2m} \right) \psi + \mathcal{L}_2$$

$$\mathcal{L}_2 = -\frac{C_0}{2}\,\psi^\dagger\psi^\dagger\psi\psi - \frac{C_2}{4}\,(\psi^\dagger\nabla^2\psi^\dagger\psi\psi + \text{h.c.}) + \cdots$$

$C_0, C_2, \ldots$ matched to $p\cot\delta(p) = -\frac{1}{a} + \frac{r}{2}\,p^2 + \cdots$

dimer:

$$\mathcal{L}_2 \to \mathcal{L}_2^{\text{dimer}} = \sigma T^\dagger T + \left(T^\dagger \left[f_0\psi\psi + f_1\psi\nabla^2\psi + \cdots \right] + \text{h.c.} \right)$$

- Dimer framework algebraically equivalent to the three-particle framework
- Higher partial waves can be included: dimers with arbitrary spin
- Can be generalized to the non-rest frames

Off-shell term, two particle sector

$$\langle \mathbf{p}|\mathcal{L}_2|\mathbf{q}\rangle = -2C_0 - C_2(\mathbf{p}^2+\mathbf{q}^2) - C_4(\mathbf{p}^2+\mathbf{q}^2)^2 - C_4'(\mathbf{p}^2-\mathbf{q}^2)^2 + \cdots$$

Off-shell term can be eliminated with the use of EOM

$$-\frac{C_4'}{4}\left(\psi^\dagger\nabla^4\psi^\dagger\psi\psi - \psi^\dagger\nabla^2\psi^\dagger\psi\nabla^2\psi + h.c\right) = \frac{C_4'}{4}\,m^2\partial_t^2(\psi^\dagger\psi^\dagger\psi\psi)$$

Insertions of the off-shell term vanish on shell (dim.reg., no scale)

$$\int\frac{d^d\mathbf{k}}{(2\pi)^d}\,(\mathbf{p}^2-\mathbf{k}^2)^2\frac{1}{\mathbf{k}^2-q_0^2}\,f(\mathbf{k}) \quad = \quad (\mathbf{p}^2-q_0^2)^2\int\frac{d^d\mathbf{k}}{(2\pi)^d}\,\frac{1}{\mathbf{k}^2-q_0^2}\,f(\mathbf{k})$$

$$+ \quad \text{no scale integrals}$$

- The result does not depend on the regularization
- No off-shell term in the dimer formulation: one coupling at each order

Off-shell term in the three-particle sector

$$\mathcal{L}_3^{(4)} = \frac{D_4''}{12}\,(\psi^\dagger\psi^\dagger\nabla^4\psi^\dagger\,\psi\psi\psi + 2\psi^\dagger\nabla^2\psi^\dagger\nabla^2\psi^\dagger\,\psi\psi\psi - 3\psi^\dagger\psi^\dagger\nabla^2\psi^\dagger\,\psi\psi\nabla^2\psi + \text{h.c.}) + \cdots$$

- Off-shell term proportional to D_4'' can be eliminated using EOM
- In the momentum space, the potential is proportional to

$$V^{\text{off}-\text{shell}} \propto D_4''(E(\mathbf{p}) - E(\mathbf{q}))^2\,, \quad E(\mathbf{p}) = \frac{1}{2m}\,(\mathbf{p}_1^2 + \mathbf{p}_2^2 + \mathbf{p}_3^2)$$

All insertions of this potential vanish on shell (no-scale integrals)

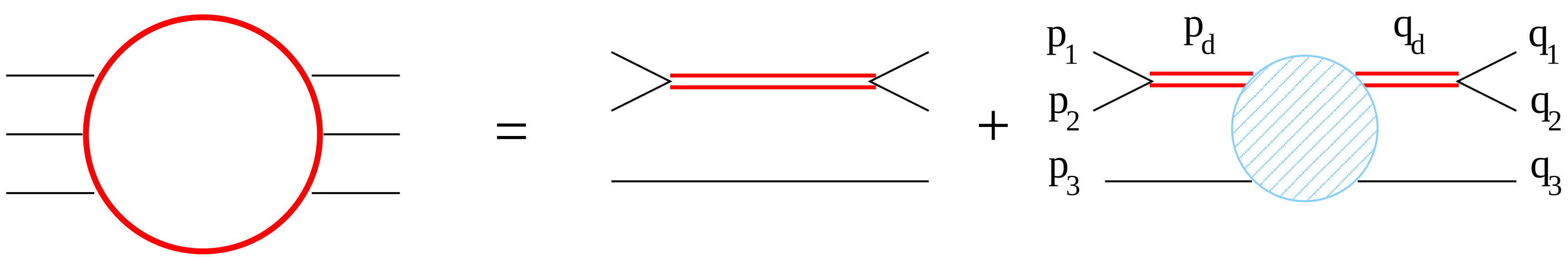
$\hookrightarrow$ The S-matrix does not depend on D_4''!

$$\begin{aligned}\mathcal{L}_3^{\text{dimer}} &= h_0 T^\dagger T\psi^\dagger\psi + h_2 T^\dagger T(\psi^\dagger\nabla^2\psi + \text{h.c.}) \\ &+ h_4 T^\dagger T(\psi^\dagger\nabla^4\psi + \text{h.c.}) + h_4' T^\dagger T\nabla^2\psi^\dagger\nabla^2\psi + \cdots\end{aligned}$$

- Two couplings h_4, h_4': off-shell coupling D_4'' can be eliminated!

Why are there no off-shell terms in the dimer picture

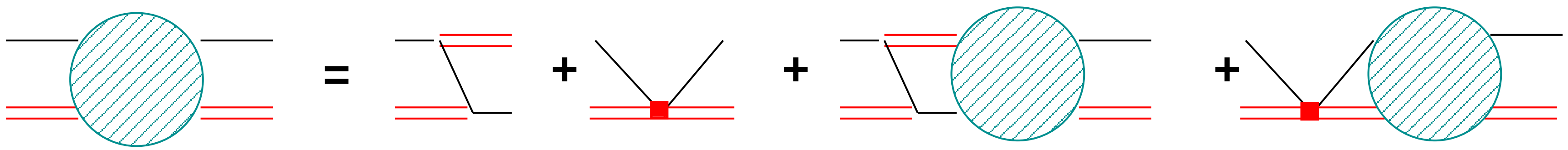
Off-shell dimers are physical:



$$\mathbf{p}_d^2 = (\mathbf{p}_1 + \mathbf{p}_2)^2 \,, \qquad \mathbf{q}_d^2 = (\mathbf{q}_1 + \mathbf{q}_2)^2$$

$$\mathbf{p}_d^2 \neq \mathbf{q}_d^2$$

The scattering equation



$$\mathcal{M}(\mathbf{p},\mathbf{q};E) = Z(\mathbf{p},\mathbf{q};E) + \int_{\mathbf{k}}^{\Lambda} Z(\mathbf{p},\mathbf{k};E)\tau(\mathbf{k};E)\mathcal{M}(\mathbf{k},\mathbf{q};E)$$

$$Z(\mathbf{p},\mathbf{q};E) = \frac{1}{\mathbf{p}^2+\mathbf{q}^2+\mathbf{pq}-mE} + H_0 + H_2(\mathbf{p}^2+\mathbf{q}^2) + \cdots$$

$H_0, H_2, \ldots$ are related to the couplings $h_0, h_2, \ldots$

$$\tau^{-1}(\mathbf{k};E) = k^*\cot\delta(k^*) + \underbrace{\sqrt{\frac{3}{4}\mathbf{k}^2 - mE}}_{=k^*}$$

Finite volume

$$\mathbf{k} = \frac{2\pi}{L}\,\mathbf{n}\,, \quad \mathbf{n} \in \mathbb{Z}^3\,, \qquad\qquad \int_{\mathbf{k}}^{\Lambda} \to \frac{1}{L^3}\sum_{\mathbf{k}}^{\Lambda}$$

$$\mathcal{M}_L(\mathbf{p},\mathbf{q};E) = Z(\mathbf{p},\mathbf{q};E) + \frac{8\pi}{L^3}\sum_{\mathbf{k}}^{\Lambda} Z(\mathbf{p},\mathbf{q};E)\tau_L(\mathbf{k};E)\mathcal{M}_L(\mathbf{k},\mathbf{q};E)$$

$$\tau_L^{-1}(\mathbf{k};E) = k^*\cot\delta(k^*) - \frac{4\pi}{L^3}\sum_{\mathbf{l}} \frac{1}{\mathbf{k}^2+\mathbf{l}^2+\mathbf{kl}-mE}$$

- Poles in the amplitude $\rightarrow$ finite-volume energy spectrum
- $k^*\cot\delta(k^*)$ fitted in the two-particle sector;
  $H_0, H_2, \ldots$ should be fitted to the three-particle energies
- S-matrix in the infinite volume $\rightarrow$ equation with $H_0, H_2, \ldots$
- No-scale arguments apply in the finite volume as well:
  no off-shell effects in the finite volume spectrum!

Quantization condition

The particle-dimer scattering amplitude:

$$\mathcal{M}_L = Z + Z\tau_L\mathcal{M}_L$$

The three-particle scattering amplitude:

$$T_L^{(3)} = \tau_L + \tau_L\mathcal{M}_L\tau_L = (\tau_L^{-1} - Z)^{-1}$$

The quantization condition:
the three-body energy levels coinside with the poles of $T_L^{(3)}$:

$$\det(\tau_L^{-1} - Z) = 0$$

- The spectrum is determined only by the on-shell input!
- Compare with:
  Polejaeva and AR, Hansen and Sharpe, Briceno and Davoudi, Mai and Döring!

Comparison with Hansen & Sharpe

Relativistic vs. non-relativistic:

- Dynamics: No particle creation/annihilation, except Briceno, Hansen and Sharpe, PRD 95 (2017) 074510: connecting the 2- and 3-particle channels

  (not needed for the energies below higher (4-particle) threshold)

- Kinematics: Can be taken into account via covariant NREFT: Colangelo, Gasser, Kubis and AR, PLB 638 (2006) 187 (work in progress)

Introducing smooth cutoff $H(\mathbf{q})$ on the spectator momentum $\mathbf{q}$:

- Above a given spectator momentum $\mathbf{q}$, the kernel is no more singular, the regular summation theorem applies
- “Unconventional” scattering amplitude in the limit $L \to \infty$
- Similar in Polejaeva and AR, the smooth cutoff moved to zero!

“Unconventional” scattering amplitude

- If no $2 \to 3$ transitions present, both approaches contain identical sets of diagrams
- Particle-dimer formalism is algebraically equivalent to the three-particle formalism

The role of the cutoff:

$$\mathcal{M}_L = Z + \sum_{\mathbf{q}} H(\mathbf{q}) Z \tau_L \mathcal{M}_L + \sum_{\mathbf{q}} (1 - H(\mathbf{q})) Z \tau_L \mathcal{M}_L$$

$$\mathcal{M}_L = \mathcal{M}_H + \sum_{\mathbf{q}} H(\mathbf{q}) \mathcal{M}_H \tau_L \mathcal{M}_L \,, \quad \mathcal{M}_H = Z + \int_{\mathbf{q}} (1 - H(\mathbf{q})) Z \tau \mathcal{M}_H$$

- $\mathcal{M}_H$ related to the “unconventional” HS amplitude $\mathcal{K}_{3,df}$
- If cutoff $H(\mathbf{q})$ is removed for $|\mathbf{q}| < \Lambda$, then $\mathcal{K}_{3,df} \to H_0(\Lambda) + \ldots$

Comparison to Briceno & Davoudi

- Both approaches contain identical sets of diagrams
- In BD approach, dimers are characterized in terms of poles and residues (both volume dependent)
- A cutoff emerges effectively: the highest pole in the dimer propagator
- Relation of the *energy spectrum* to the *three-particle amplitude* is algebraically rather complicated

Comparison with Döring and Mai

- Relativistic approach based on the two- and three-particle unitarity and analyticity

(suffices for the energies below the higher (4-particle) threshold)

- Isobar picture used: equivalent to the particle-dimer framework. Not a model. The actual existence of the two-body resonance is not required
- The quantization condition is identical to ours, except relativistic kinematics
- Lagrangian is not specified. Fixing the Lagrangian would be equivalent to the choice of parameterization of the two-body scattering amplitude and the three-body force

See more in Maxim Mai's talk!

Reduction of the quantization condition: the symmetries

- Symmetry in a finite volume: octahedral group O_h, including inversions (rest frame), little groups (moving frames)
- Reduction: an analog of the partial-wave expansion in a finite volume
- Analog for a sphere $|\mathbf{k}| = \text{const}$ for a cube: *shells*

$$s = \left\{ \mathbf{k} \ : \quad \mathbf{k} = g\mathbf{k}_0 \, , \quad g \in O_h \right\}$$

- Each shell s is characterized by the *reference momentum* $\mathbf{k}_0$
- Shells are counted by increasing $|\mathbf{k}|$
- The momenta, unrelated by the O_h, but having $|\mathbf{k}| = |\mathbf{k}'|$, belong to the different shells

The expansion in the basis of irreps

For an arbitrary function of the momentum $\mathbf{p}$, belonging to a shell s,

$$f(\mathbf{p}) = f(g\mathbf{p}_0) = \sum_{\Gamma}\sum_{ij} T_{ij}^{(\Gamma)}(g) f_{ji}^{(\Gamma)}(\mathbf{p}_0)\,, \qquad \Gamma = A_1^{\pm}, A_2^{\pm}, E^{\pm}, T_1^{\pm}, T_2^{\pm}$$

Projecting back the components:

$$\frac{G}{s_\Gamma}\, f_{ji}^{(\Gamma)}(\mathbf{p}_0) = \sum_{g\in O_h} (T_{ij}^{(\Gamma)}(g))^* f(g\mathbf{p}_0)\,, \qquad G = \text{dim}(O_h) = 48$$

The quantization condition in the new basis partially diagonalizes

An alternative method of expansion: see Maxim Mai's talk

The expansion of the kernel

The kernel is invariant under O_h: $Z(g\mathbf{p},g\mathbf{q})=Z(\mathbf{p},\mathbf{q})$

$$
\begin{aligned}
Z_{nm}^{(\Gamma\Gamma',ij)}(r,s) &= \sum_{g,g'\in O_h}(T_{in}^{(\Gamma)}(g'))^*Z(g'\mathbf{p}_0(r),g\mathbf{k}_0(s))T_{jm}^{(\Gamma')}(g) \\
&= \sum_{g,g'\in O_h}(T_{in}^{(\Gamma)}(g'))^*Z(\underbrace{g^{-1}g'}_{=g''}\mathbf{p}_0(r),\mathbf{k}_0(s))T_{jm}^{(\Gamma')}(g) \\
&= \sum_{g,g''\in O_h}\sum_k(T_{ik}^{(\Gamma)}(g))^*(T_{kn}^{(\Gamma)}(g''))^*Z(g''\mathbf{p}_0(r),\mathbf{k}_0(s))T_{jm}^{(\Gamma')}(g) \\
&= \sum_{g''\in O_h}\sum_k\frac{G}{s_\Gamma}\,\delta_{\Gamma\Gamma'}\delta_{ij}\delta_{km}(T_{kn}^{(\Gamma)}(g''))^*Z(g''\mathbf{p}_0(r),\mathbf{k}_0(s)) \\
&= \frac{G}{s_\Gamma}\,\delta_{\Gamma\Gamma'}\delta_{ij}\sum_{g\in O_h}(T_{mn}^{(\Gamma)}(g))^*Z(g\mathbf{p}_0(r),\mathbf{k}_0(s)) \\
&= \frac{G}{s_\Gamma}\,\delta_{\Gamma\Gamma'}\delta_{ij}Z_{nm}^{(\Gamma)}(r,s)
\end{aligned}
$$

Reduction of the equation

The equation determining the energy spectrum:

$$f(\mathbf{p}) = \frac{8\pi}{L^3} \sum_s \sum_{g\in O_h} \frac{\vartheta(s)}{G} Z(\mathbf{p}, g\mathbf{k}_0(s))\tau(s) f(g\mathbf{k}_0(s))$$

$\vartheta(s)$: the multiplicity of the shell s

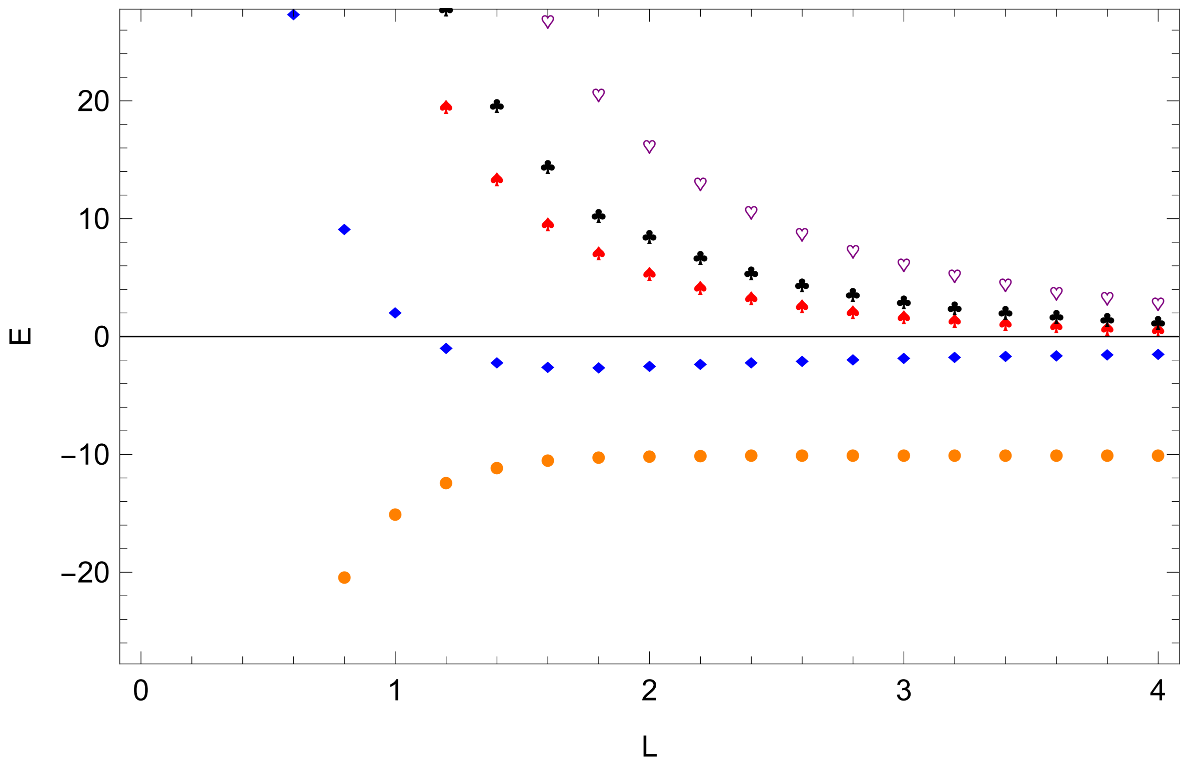
Projecting the equation on a given irrep Γ:

$$f_i^{(\Gamma)}(r) = \frac{8\pi}{L^3} \sum_s \frac{\vartheta(s)\tau(s)}{G} \sum_j Z_{ij}^{(\Gamma)}(r,s) f_j^{(\Gamma)}(s)\,.$$

The quantization condition partially diagonalizes

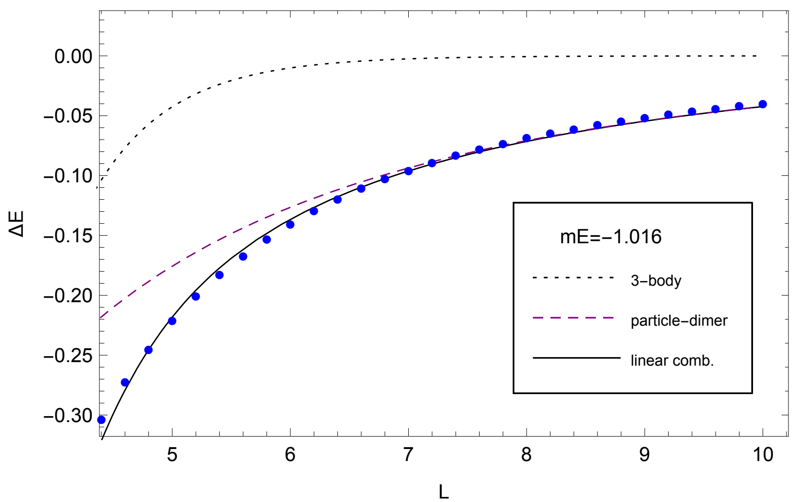
$$\det\left(\tau(s)^{-1}\vartheta(s)^{-1}\delta_{rs}\delta_{ij} - \frac{8\pi}{L^3}\frac{1}{G} Z_{ij}^{(\Gamma)}(r,s)\right) = 0\,.$$

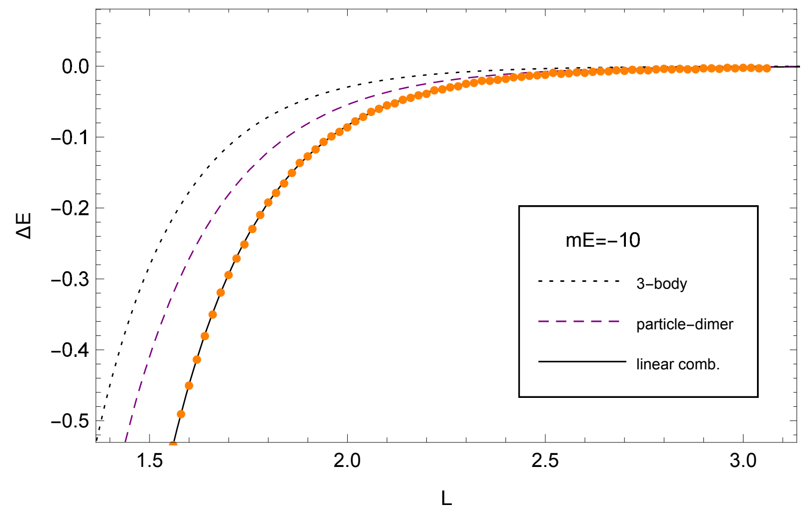
The finite-volume spectrum in the A_1 irrep, CM frame



- $m = a = 1,\ \Lambda = 225,\ H_0(\Lambda) = 0.192$
- The spectrum both below and above the three-particle threshold

Bound-state spectrum: $E = -1.016$ and $E = -10$



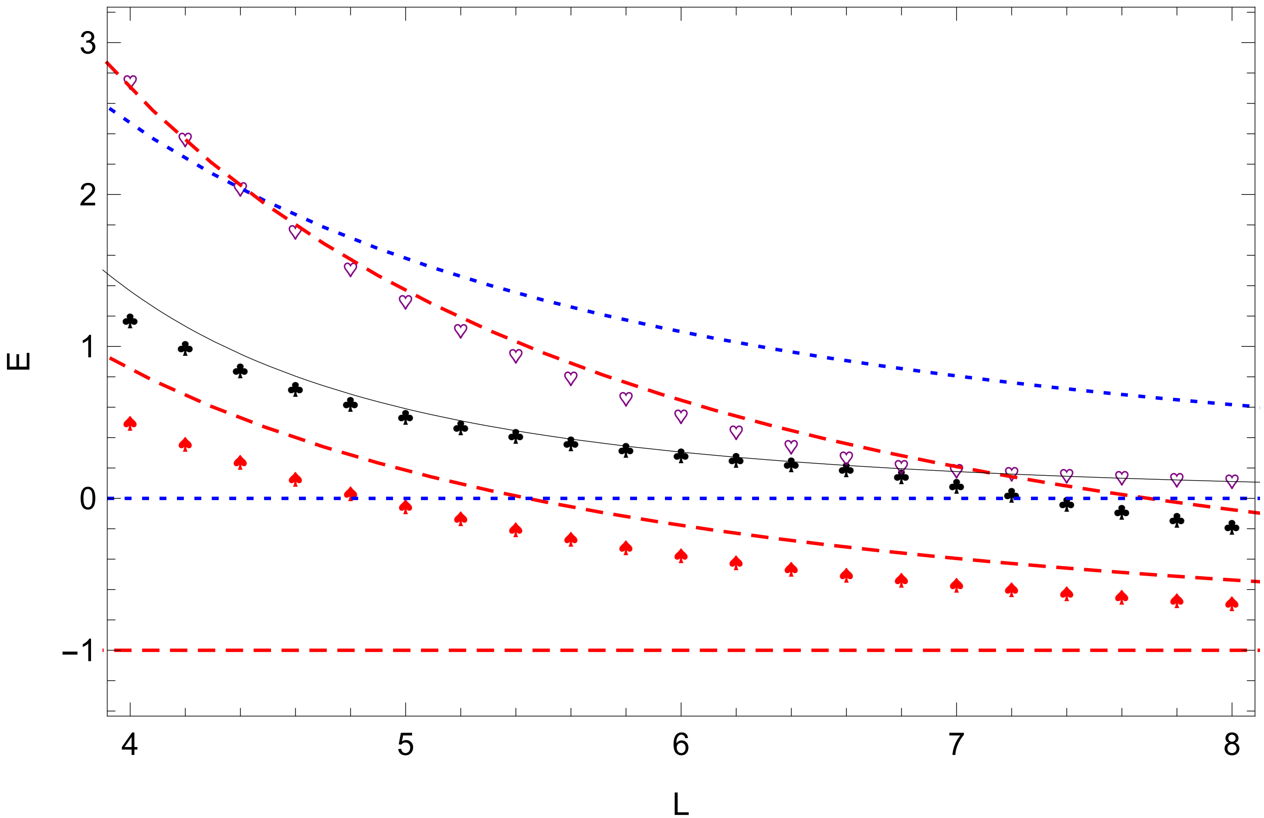


Three-particle: $\dfrac{C}{L^{3/2}}\,\exp\left(-\dfrac{2}{\sqrt{3}}\,\kappa L\right)$

Particle-dimer: $\dfrac{C'}{L}\,\exp\left(-\dfrac{2}{\sqrt{3}}\,\sqrt{\kappa^2 - a^{-2}}L\right)$

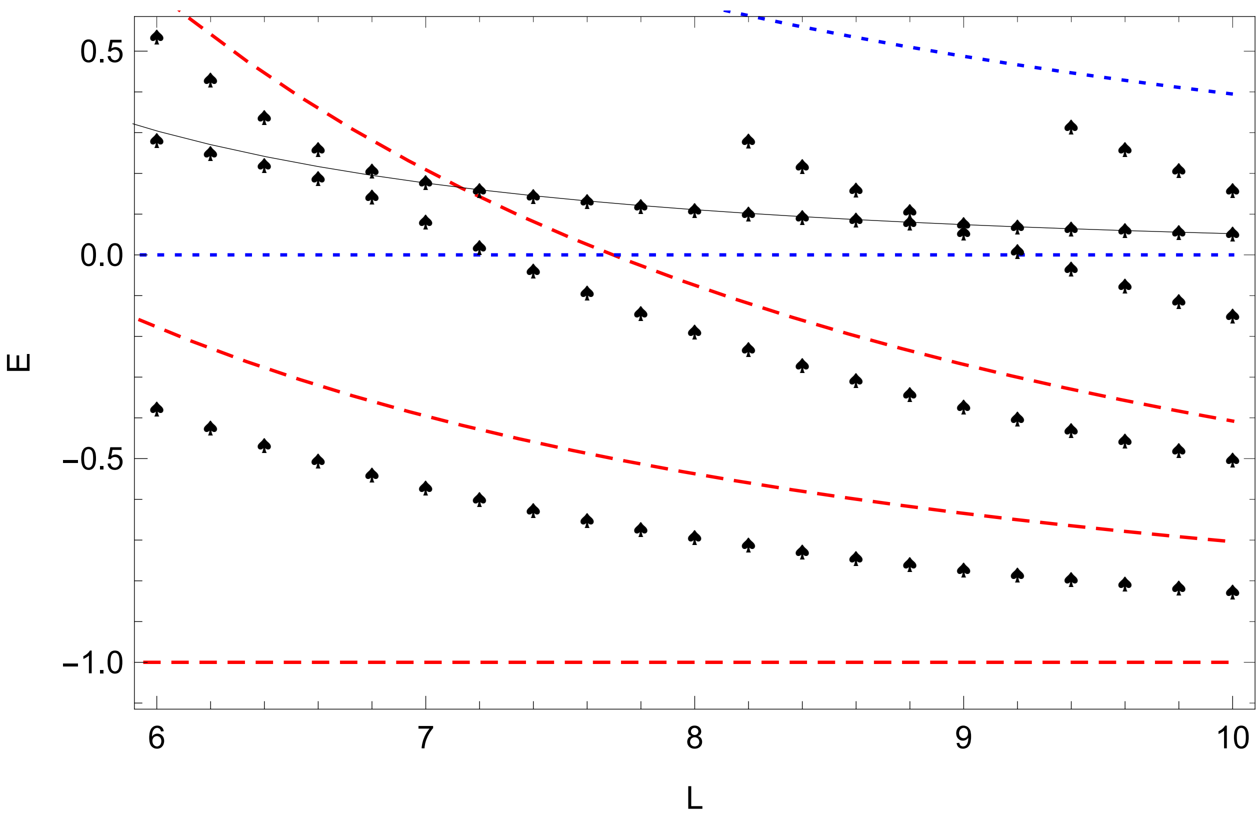
. . . or, a linear combination thereof

Scattering states



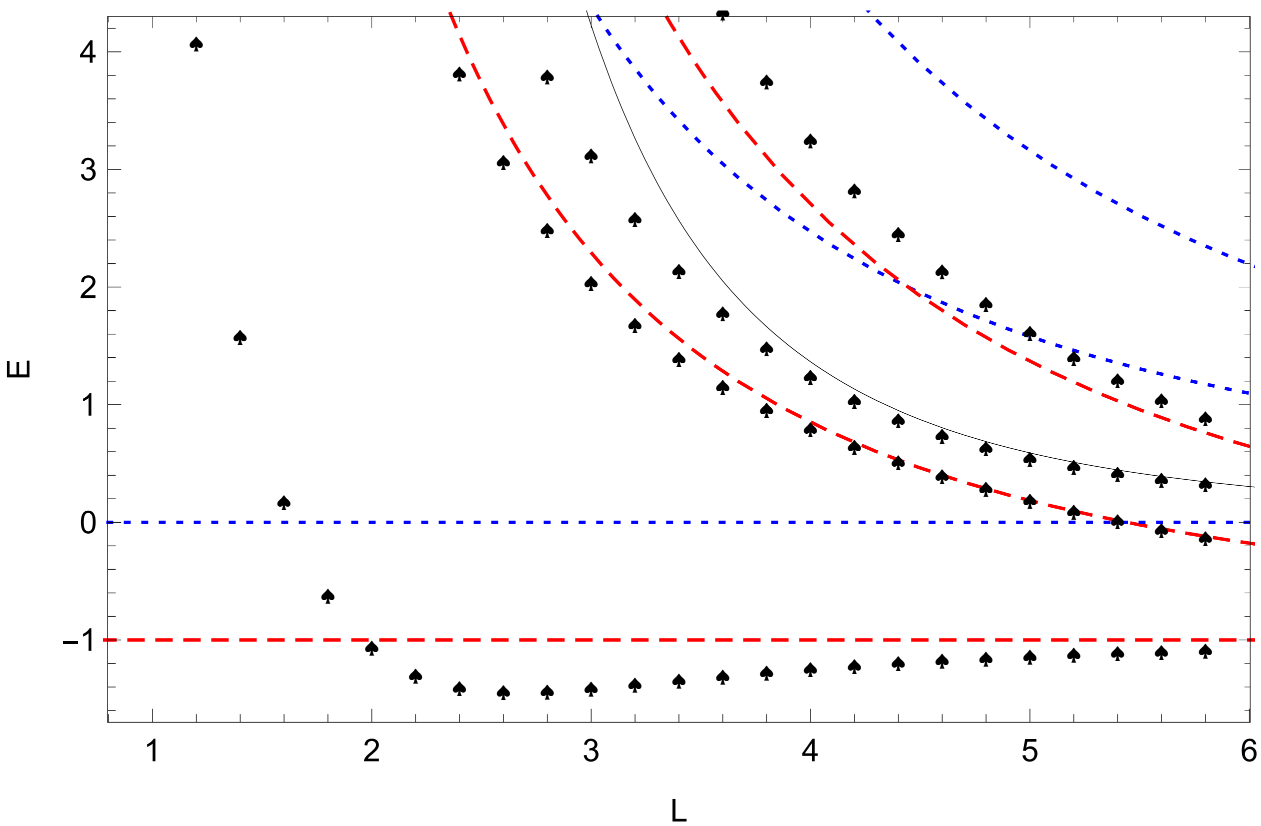
$$\Delta E = \frac{12\pi a}{L^3} - \frac{12a^2}{L^4}\mathcal{I} + \frac{12a^3}{\pi L^5}(\mathcal{I}^2 + \mathcal{J}) + O(L^{-6})\,, \quad \mathcal{I} \simeq -8.914,\ \mathcal{J} \simeq 16.532$$

Avoided level crossing



- Avoided level crossing between 3-particle and particle-dimer states
- Where is the (displaced) particle-dimer threshold?

Pushing up the energy level by a shallow bound state



- Change the parameters: the shallow bound state disappears
- Displaced threshold can be easily identified!

Extraction of the three-body couplings from the lattice data

The energy level displacements can be treated in perturbation theory, are known up to and including $O(L^{-7})$:

S.R. Beane, W. Detmold and M.J Savage, PRD 76 (2007) 074507; W. Detmold and M.J. Savage, PRD 77 (2008) 057502; S.R. Sharpe, PRD 96(2017) 054515 . . .

$$\Delta E_2 = \frac{4\pi\alpha}{mL^3}\left(1 + \frac{c_1}{L} + \frac{c_2}{L^2} + \frac{c_3}{L^3}\right) + O(L^{-7})$$

$$\Delta E_3 = \frac{12\pi a}{mL^3}\left(1 + \frac{d_1}{L} + \frac{d_2}{L^2} + \frac{\bar{d}_3}{L^3}\ln L + \frac{d_3}{L^3}\right) + O(L^{-7})$$

- The coupling d_3 contains two-body contributions (scattering length, effective radius) as well as the three-body term
- Three-body contributions can be separated, if the many-body states (4,5,. . . particles) are included
- Multipion systems in lattice QCD has been considered
  S.R. Beane, W. Detmold, T.C. Luu, K. Orginos, M.J. Savage and A. Torok, PRL 100 (2008) 082004

Energy shift in the φ^4 theory

F. Romero-López, A. Rusetsky and C. Urbach, in preparation

$$S = \sum_x \left(-\kappa \sum_\mu (\varphi_x^* \varphi_{x+\mu} + c.c.) - \lambda(|\varphi_x|^2 - 1)^2 + |\varphi_x|^2 \right)$$

- The calculations are performed for different values of L
- For our choice of parameters λ and κ: perturbative, the phase shift does nor exceed few degrees
- Single particle mass: perfectly fits the one-loop expression:

$$M(L) - M = \text{const}\,\frac{K_1(ML)}{(ML)^{1/2}} \sim \text{const}\,\frac{\exp(-ML)}{(ML)^{3/2}}$$

- Extracting H_0 at small L: does one have control over exponentially suppressed contributions?

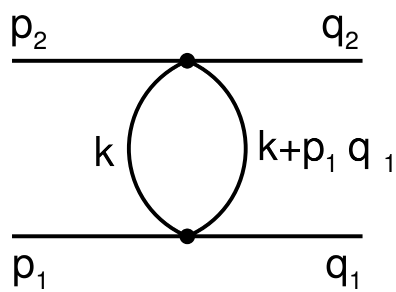
Exponentially suppressed contribitions: 2-body levels

Using quasi-potential reduction of the Bethe-Salpeter equation. . .

$$E_2 - 2M(L) = \frac{1}{L^3}\, T_L(\mathbf{0},\mathbf{0},E_2)$$

$$T_L = \bar{T}_L + \bar{T}_L(g'_L - g_\infty)T_L\,, \qquad \bar{T}_L = V_L + V_L g_\infty \bar{T}_L$$

Leading exponentially suppressed term:



$$V_L - V_\infty \sim \frac{\exp(-ML)}{(ML)^{1/2}} \quad \hookrightarrow \quad E_2 - 2M(L)\Big|_{\text{exp}} \sim \frac{\exp(-ML)}{(ML)^{7/2}} + \cdots$$

$\hookrightarrow$ The difference $E_2 - 2M(L)$ already captures the leading exponentially suppressed contribution. The correction coming from the potential is suppressed by an additional factor L^{-2}

Preliminary results of simulations

- The single-particle mass $M(L)$, as well as two- and three-particle levels E_2 and E_3 have been measured for different values of L from $L=4$ until $L=24$.
- The two-body scattering lenght a and the effective radius r have been extracted
- The three-body force has been extracted: definitely different from zero!

Fernando Romero-López can tell more during his short talk . . .

Conclusions

- An EFT formalism in a finite volume is proposed to analyze the data in the three-particle sector
- The low-energy couplings $H_0, H_2, \ldots$ are fitted to the spectrum; S-matrix is obtained through the solution of equations
- A systematic approach: allows the inclusion of higher partial waves, derivative couplings, two $\to$ three transitions, relativistic kinematics,$\ldots$
- Equivalent to other known approaches, much easier to use!
- Reduction of the quantization condition is possible, according to the octahedral symmetry
- Extraction of the three-body couplings both in non-perturbative and perturbative regimes is discussed, backed by the lattice results in the φ^4 theory

Outlook

- Three-particle Lellouch-Lüscher formula
- Three-nucleon interactions: inclusion of the long-range forces
- Inclusion of relativistic effects, higher partial waves, spin, partial wave mixing, etc
- Full group-theoretical analysis of the three-particle equation in the rectangular box including moving frames and the higher partial waves
- Derivation of the shift of the three-particle and *particle-dimer* ground-state levels from the quantization condition