Three-particle dynamics in a finite volume

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

arXiv:1706.07700, arXiv:1707.02176 + ongoing work

Hirschegg 2018, “Multiparticle resonances in hadrons, nuclei, and ultracold gases,”

15 January 2018

Plan

- Introduction
- Non-relativistic EFT and dimer picture
- Independence from the off-shell effects
- Symmetries of the box and the finite volume spectrum
- Role of the three-body force:
  three-particle bound state
  shift of the ground-state level
- Conclusions, outlook

Extraction of the observables on the lattice

Motivation:

$\hookrightarrow$ Decays into the three-particle final states (examples: $\eta \to 3\pi$, $\omega \to 3\pi$, Roper resonance, etc.)

$\hookrightarrow$ Nuclear physics on the lattice

Three-particle sector: continuum

- bound states
- elastic scattering, rearrangement reactions
- breakup...

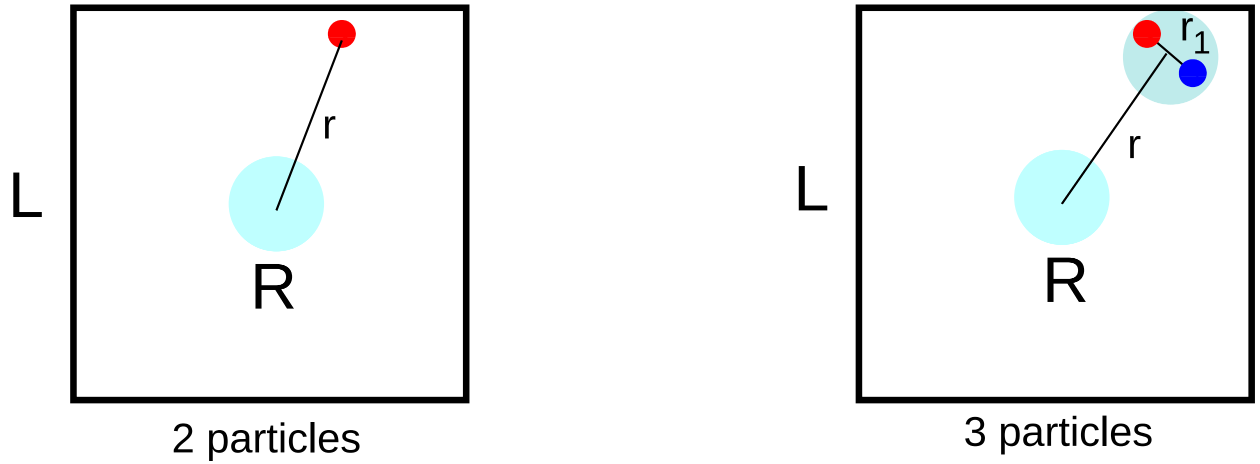
Three-particle sector: finite volume

- two-particle *and* three-particle energy levels *both below and above* the pertinent thresholds

How does one extract infinite-volume observables from lattice data?

Three particles in a finite volume: the problem

Two-particle scattering: The wave function always in the asymptotic form near the walls: no off-shell effects!



- The three-particle wave function near the box walls is not always described by the asymptotic wave function
- Is the three-particle spectrum determined solely in terms of the S-matrix?

The history

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 + analiticity

$\hookrightarrow$ The quantization condition rather complicated, not well suited for the analysis of the lattice data

$\hookrightarrow$ What is the convenient set of observables to be extracted?

The strategy

- If $R \ll L$ (large boxes $\to$ small momenta), the energy spectrum can be calculated, using non-relativistic EFT in a finite volume
- Effective couplings matched to the observables in the infinite volume *on the mass shell*

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

- Analysis of the lattice data: determine these couplings from the fit to the spectrum, calculate the S-matrix from the dynamical equations

$\hookrightarrow$ Effective couplings form a convenient set of the parameters to be determined on the lattice $\to$ contain only exponentially suppressed effects at large L.

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:

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

- Two frameworks algebraically equivalent
- 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

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

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

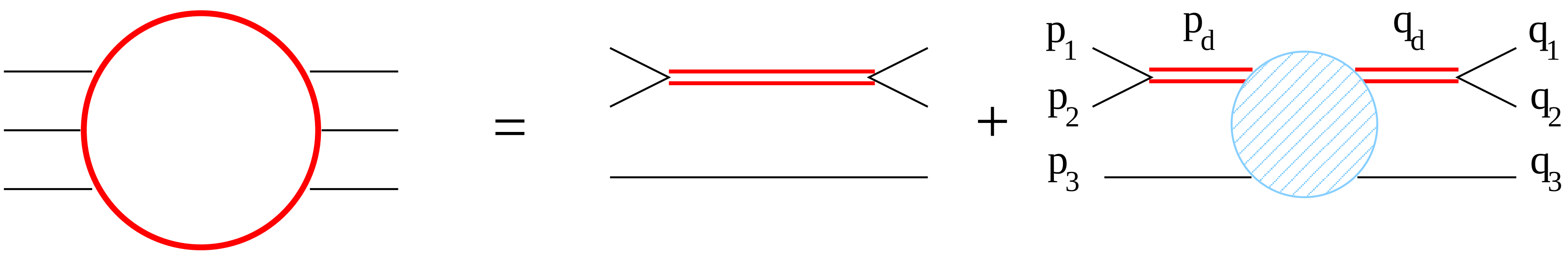
$\hookrightarrow$ The S-matrix does not depend on D_4''!

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

- 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

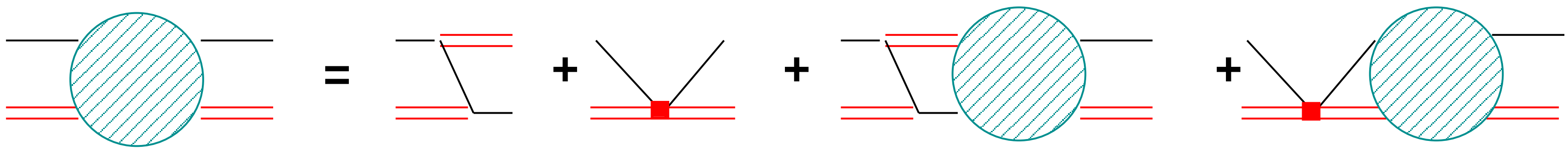
Off-shell dimers are physical:



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

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

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

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

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

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

- Poles of $\mathcal{M}_L$ $\quad\to\quad$ 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 $\quad\to\quad$ 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 $T_L^{(3)}$:

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

- Agrees with: Polejaeva and AR, Hansen and Sharpe, Briceno and Davoudi, Mai and Döring
- Differs by the choice of the cutoff on the spectator momentum $\mathbf{k}$
- The spectrum is determined only by the on-shell input!

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,

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

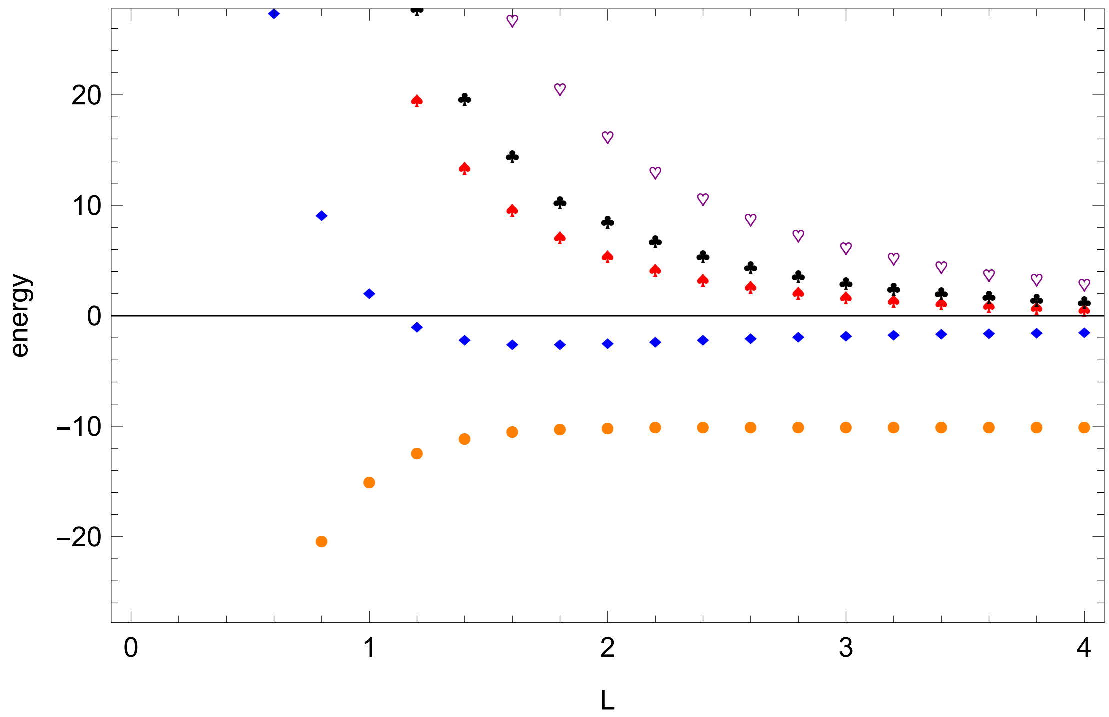
Projecting back the components:

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

The quantization condition in the new basis partially diagonalizes

See more on this in J.-Y. Pang's talk!

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



- The spectrum both below and above the three-particle threshold is given

Extraction of the three-body couplings from the lattice data

Two different scenarios:

- The three particle bound state exists
  - For a single L, the coupling H_0 (at a given cutoff Λ and scattering length a) can be fitted to the binding energy.
  - In order to determine higher-order couplings, more data points are necessary
- The three-particle bound states do not exist
  - 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
  - The leading-order shift of the ground state comes at $O(L^{-3})$. The coupling H_0 contributes at $O(L^{-6})$
  - *Consistency:* three-body couplings appear at higher orders in the perturbative expansion of the scattering amplitude

1. Energy shift of the three-particle bound state

Unitary limit $a \to \infty$: U.-G. Meißner, G. Rios and AR, PRL 114 (2015) 091602

See also M. T. Hansen and S. R. Sharpe, PRD 95 (2017) 034501

Using Poisson's formula...

$$\mathcal{M}_L(\mathbf{p},\mathbf{q};E) = Z(\mathbf{p},\mathbf{q};E) + 8\pi \int_{\mathbf{k}}^{\Lambda} Z(\mathbf{p},\mathbf{q};E)\hat{\tau}_L(\mathbf{k};E)\mathcal{M}_L(\mathbf{k},\mathbf{q};E)$$

$$\hat{\tau}_L(\mathbf{k};E) = \frac{1+\sum_{\mathbf{n}\neq\mathbf{0}} e^{iL\mathbf{n}\mathbf{k}}}{\tau^{-1}(\mathbf{k};E) + \underbrace{\Delta_L(\mathbf{k};E)}_{\text{zeta-function}}} = \tau(\mathbf{k};E) + \sum_{\mathbf{n}\neq\mathbf{0}} e^{iL\mathbf{n}\mathbf{k}}\tau(\mathbf{k};E) + \cdots$$

$$\hookrightarrow \quad \Delta E = 8\pi \int_{\mathbf{k}}^{\Lambda} \big[\Psi(\mathbf{k})\big]^2 \sum_{\mathbf{n}\neq\mathbf{0}} e^{iL\mathbf{n}\mathbf{k}}\tau(\mathbf{k};E) + \cdots$$

Normalization condition

$$-8\pi\int_{\mathbf{p}}^{\Lambda}\big[\Psi(\mathbf{p})\big]^2\frac{\partial\tau(\mathbf{p};E)}{\partial E}-(8\pi)^2\int_{\mathbf{p}}^{\Lambda}\int_{\mathbf{q}}^{\Lambda}\Psi(\mathbf{p})\tau(\mathbf{p};E)\frac{\partial Z(\mathbf{p},\mathbf{q};E)}{\partial E}\tau(\mathbf{q};E)\Psi(\mathbf{q})=1$$

Faddeev-Minlos solution: $\Lambda\to\infty$ and $H(\Lambda)=0$.

$$\Psi_0(p)=iN_0\frac{\kappa}{p}\,\sin(s_0u)\,,\qquad u=\ln\left(\frac{\sqrt{3}}{2}\,\frac{p}{\kappa}+\sqrt{\frac{3p^2}{4\kappa^2}+1}\right),\quad E=\frac{\kappa^2}{m}$$

Asymptotic normalization coefficient

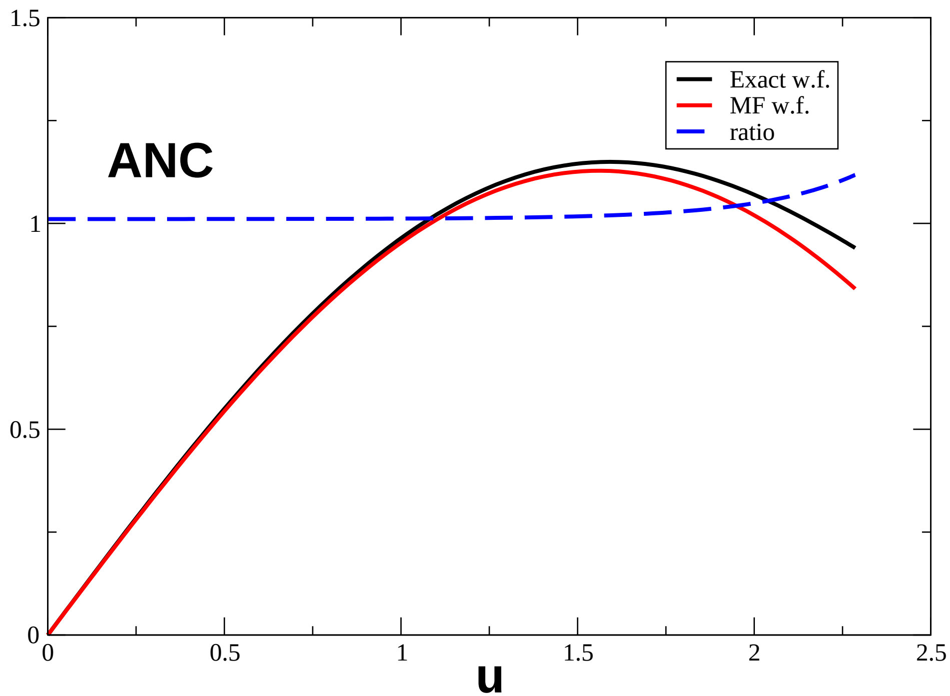
$$\mathcal{A}=\lim_{p\to 0}\Psi(p)/\Psi_0(p)$$

No derivative couplings: $\mathcal{A}=1+O(\kappa/\Lambda)$

Derivative couplings: $\mathcal{A}\neq 1$

Energy shift in the unitary limit

U.-G. Meißner, G. Rios and AR, PRL 114 (2015) 091602



$$\frac{\Delta E}{|E|} = c(\kappa L)^{-3/2}\mathcal{A}^2 \exp\left(-\frac{2\kappa L}{\sqrt{3}}\right)$$

$\mathcal{A} = 1 + O(\kappa/\Lambda)$ in the absence of derivative couplings

Going beyond unitary limit

$$\Delta E \propto \int_{\mathbf{p}}^{\Lambda} \frac{\big[\Psi(\mathbf{p})\big]^2 e^{iL\mathbf{n}\mathbf{p}}}{-a^{-1} + \sqrt{\frac{3}{4}\,\mathbf{p}^2 + \kappa^2}}\,, \qquad |\mathbf{n}| = 1$$

$\Psi(\mathbf{p})$ is only weakly singular in the low-momentum region $\to$ const.

$$\Delta E = \frac{\#}{aL}\exp\left(-\frac{2}{\sqrt{3}}\sqrt{\kappa^2 - \frac{1}{a^2}}\,L\right) + \frac{\#}{(\kappa L)^{3/2}}\exp\left(-\frac{2\kappa L}{\sqrt{3}}\right) + \cdots$$

1. Lüscher equation, bound state of a particle and a dimer
2. Three-particle bound state in the unitary limit

2. Energy shift of the three-particle ground state

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

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

- The coupling d_3 contains two-body contributions (scattering length, effective radius) as well as the three-body term
- Three-bedy 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-Lopez, A. Rusetsky and C. Urbach, in preparation

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

- 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?

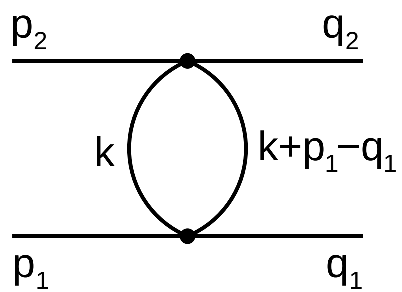
Exponentially suppressed contribitions: 2-body levels

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!

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