Finite Volume Spectrum of the 3-body System

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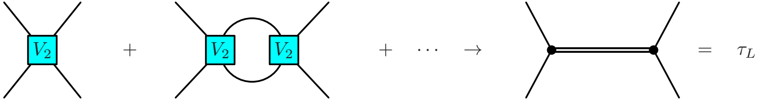
Multiparticle resonances in hadrons, nuclei, and ultracold gases

1. Formalism
   - Quantization condition
   - Projection onto the irreps of the octahedral group
2. 3-body Spectrum in a Finite Volume
   - Solution of quantization condition
   - Identification of the spectrum in a finite volume
3. Conclusions

Particle-dimer formalism

(H.-W. Hammer, J.-Y. Pang and A. Rusetsky, arXiv: 1706.07700, arXiv: 1707.02176)

- A dimer:



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

- Particle-dimer scattering:

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

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

- See more in Akaki Rusetsky's and Michael Döring's talk

Quantization Condition

Poles in the 3-particle amplitude $\rightarrow$ energy spectrum

$$\det\left(\tau_L^{-1}(\mathbf{q};E)\delta_{\mathbf{pq}} - \frac{8\pi}{L^3}Z(\mathbf{p},\mathbf{q};E)\right) = 0$$

Assumptions:

- Kinematics

  3 identical scalar particles & Non-relativistic kinematics.

  Non-identical particles, relativistic kinematics will be included later.

- Dynamics

  S-wave 2-body interaction & Non-derivative 3-body interaction.
  Higher partial waves, derivative couplings will be included later.

Breakdown of the Partial Wave Expansion (PWE)

- Breakdown of PWE in a finite volume

  Rotational symmetry broken.

  Expansion in the Legendre polynomials does not converge for singular potentials, *e.g.*, $Z(\mathbf{p},\mathbf{q};E)=\frac{1}{\mathbf{p}^2+\mathbf{q}^2+\mathbf{pq}-mE}+\frac{H_0(\Lambda)}{\Lambda^2}$ is singular above the break-up threshold.

  (M. Döring and M. Mai, arXiv:1709.08222)

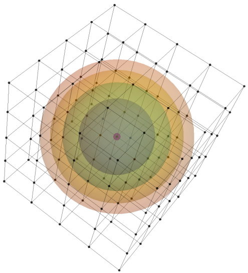
- Octahedral group O_h on the lattice

  24 rotations R_a, $(a=1,\cdots,24)$.

  Inversion of all 3 axis, I.

  48 elements, $R_a, R_a I$ in the group O_h.

Discrete Momenta



- Discrete momenta $\mathbf{p} = 2\pi\mathbf{n}/L, \quad (\mathbf{n} \in \mathbb{Z}^3)$.
  Further, we measure momenta in unit $\frac{2\pi}{L}$.

- Integral over continuous momenta vs. Sum over discrete momenta

Infinite volume, $\int d^3p f(\mathbf{p}) = \underbrace{\int p^2 dp}_{\text{different surfaces}} \underbrace{\int d\Omega_p}_{\text{solid angle inside the surface}} f(p, \Omega_p)$.

Finite volume: $\sum_{\mathbf{p}} f(\mathbf{p}) = \underbrace{\sum_s}_{\text{different shells}} \underbrace{\sum_{\hat{p}}}_{\text{orientations inside shell } s} f(s, \hat{p})$.

Shells

Shell is a set of momenta with the same $|\mathbf{p}|$, which can be obtained from reference momentum $\mathbf{p}_0$, $\mathbf{p} = g\mathbf{p}_0, \quad g \in O_h$.

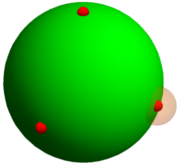
- Shell 0 $(0,0,0)$
  1 orientation. $\mathbf{p}_0(0) = (0,0,0)$. 48 Symmetry trans. on $\mathbf{p}_0$: $g\mathbf{p}_0 = \mathbf{p}_0$.

- Shell 1
  $(1,0,0),(0,1,0),(0,0,1),(-1,0,0),\cdots$

  6 orientations.

  Reference momentum $\mathbf{p}_0(1) = (1,0,0)$.

  $g\mathbf{p}_0(1)$ generates shell 1.
  Each momentum produced $48/6 = 8$ times.



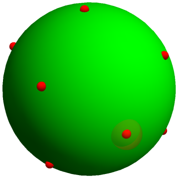
- **Shell 2**

  $(1,1,0),(1,0,1),(0,1,1),(1,-1,0),\cdots$

  12 orientations.

  Reference momentum $\mathbf{p}_0(2) = (1,1,0)$.

  $g\mathbf{p}_0(2)$ generates shell 2.
  Each momentum produced $48/12 = 4$ times.



- **Shell s**

  Continue increasing the length of momentum.

  ϑ_s orientations, $g\mathbf{p}_0(s)$ generates shell s. Each momentum produced G/ϑ_s times.

  Reference momentum $\mathbf{p}_0(s)$ is chosen arbitrarily. Nothing depends on this choice.

- Degenerate shells, *e.g.*, shell 8 and 9

  $(3,0,0),(0,3,0),(0,0,3),\cdots.$

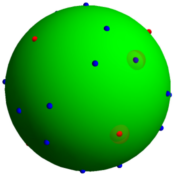
  Reference momentum $\mathbf{p}_0(8)=(3,0,0)$.

  $(2,2,1),(2,1,2),(1,2,2),\cdots.$

  Reference momentum $\mathbf{p}_0(9)=(2,2,1)$.

  Radius of the shells 8 and 9 are both 3.

  They are different shells.
  $g\mathbf{p}_0(8)$ and $g\mathbf{p}_0(9)$ generate shells 8 and 9 separately.



- Sum over shells All momenta in a given shell are produced from reference momentum.

$$\sum_{\mathbf{p}} f(\mathbf{p}) = \underbrace{\sum_s}_{\text{different shells}} \underbrace{\frac{\vartheta_s}{G}\sum_g}_{\text{orientations inside shell } s} f(g\mathbf{p}_0(s)).$$

Expansion by Matrices of Irreps.

- Analogous to PWE
  $f(\mathbf{p}) = f(p, \Omega_p) = \sqrt{4\pi}\sum_{\ell m} f_{\ell m}(p) Y_{\ell m}(\Omega_p)$. Spherical harmonics.
  $f(\mathbf{p}) = f(g\mathbf{p}_0(s)) = \sum_{\Gamma, ij} f_{ij}^{(\Gamma)}(s) T_{ij}^{(\Gamma)}(g)$. Matrices of irreps

- Matrices of irreps (V. Bernard, *et.al.*, arXiv:0806.4495)
  48 group elements, g represented in 10 irreps. $\Gamma = A_1^{\pm}, A_2^{\pm}, E^{\pm}, T_1^{\pm}, T_2^{\pm}$, $T^{(\Gamma)}(g)$.
  1. 1 dimensional A_1, A_2 : $T^{(A_1^{\pm}, A_2^{\pm})}(g) = \pm 1$;
  2. 2 dimensional E: $T^{(E^{\pm})}(g)$ are 2×2;
  3. 3 dimensional T_1, T_2: $T^{(T_1^{\pm}, T_2^{\pm})}(g)$ are 3×3.

- Orthogonality and closure relation Expansion is complete.
  $\sum_g T_{ij}^{(\Gamma)*}(g) T_{i'j'}^{(\Gamma')}(g) = \delta_{\Gamma\Gamma'} \delta_{ii'} \delta_{jj'} \frac{G}{s_\Gamma}$ and $\sum_{\Gamma, ij} \frac{s_\Gamma}{G} T_{ij}^{(\Gamma)}(g) T_{ij}^{(\Gamma)*}(g') = \delta_{gg'}$.

Reduction of the Quantization Condition

Homogeneous STM equation in a finite volume, $\mathscr{F}(\mathbf{p}) = \frac{8\pi}{L^3}\sum_{\mathbf{q}}^{\Lambda} Z(\mathbf{p},\mathbf{q};E)\tau_L(\mathbf{q};E)\mathscr{F}(\mathbf{q})$.

- Expansion of $\mathscr{F}(\mathbf{p})$
  $\mathscr{F}(\mathbf{p}) = \mathscr{F}(g\mathbf{p}_0(s)) = \sum_{\Gamma,ij}\mathscr{F}_{ij}^{(\Gamma)}(s)T_{ij}^{(\Gamma)}(g)$ & $\mathscr{F}_{ij}^{(\Gamma)}(s) = \frac{s_\Gamma}{G}\sum_g T_{ij}^{(\Gamma)*}(g)\mathscr{F}(g\mathbf{p}_0(s))$.

- Propagator τ_L $\tau_L(\mathbf{q};E) = \tau(g\mathbf{q};E)$.
  $\tau_L(\mathbf{q};E) = \tau_L(g\mathbf{q}_0(r);E) = \tau_L(r;E)$.

- Expansion of Z $Z(\mathbf{p},\mathbf{q};E) = Z(g\mathbf{p},g\mathbf{q};E)$.
  $Z(\mathbf{p},\mathbf{q};E) = Z(g\mathbf{p}_0(s),g'\mathbf{q}_0(r);E) = \sum_{\Gamma,ij,n}\frac{s_\Gamma}{G}T_{ij}^{(\Gamma)}(g)Z_{jn}^{(\Gamma)}(s,r;E)T_{in}^{(\Gamma)*}(g')$.
  $Z_{jn}^{(\Gamma)}(s,r;E) = \sum_g Z(\mathbf{p}_0(s),g\mathbf{q}_0(r);E)T_{jn}^{(\Gamma)}(g)$.

$\mathscr{F}_{ij}^{(\Gamma)}(s) = \frac{8\pi}{L^3}\sum_r\frac{\vartheta_r}{G}\sum_n Z_{jn}^{(\Gamma)}(s,r;E)\tau_L(r;E)\mathscr{F}_{in}^{(\Gamma)}(r) \to$

$$\boxed{\det\left(\tau^{-1}(r;E)\frac{G}{\vartheta_r}\delta_{sr}\delta_{jn} - \frac{8\pi}{L^3}Z_{jn}^{(\Gamma)}(s,r;E)\right) = 0}$$

Solution in the Infinite Volume

- Fragmentation threshold

  Particle-dimer threshold $mE_{\text{Frag}} = -1\ \text{MeV}^2$.

  Ground state of a particle and a dimer.

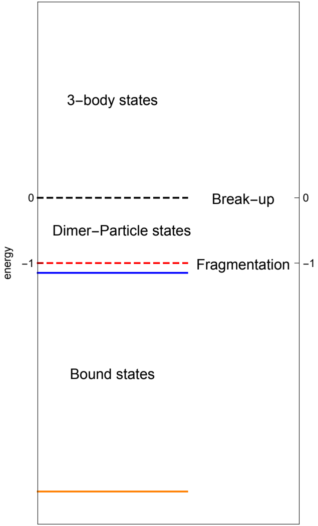
- Break-up threshold

  3-body threshold $mE_{\text{Break}} = 0\ \text{MeV}^2$.

  Ground state of 3 particles.

- Bound States

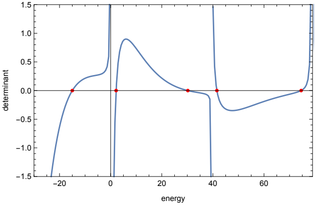
  $mE_1 = -10\ \text{MeV}^2$.
  $mE_0 = -1.016\ \text{MeV}^2$.

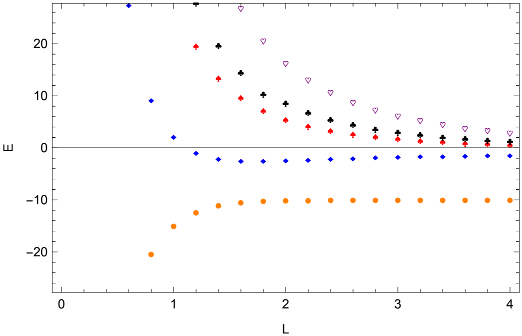


Solution of the Quantization Condition in A_1^+-Irrep

- Determinant in A_1^+-Irrep
$$\det\left(\tau(r)^{-1}\frac{G}{\vartheta_r}\delta_{sr} - \frac{8\pi}{L^3}Z^{(A_1^+)}(s,r)\right) = 0$$

1. Projection
2. Determinant and zero points



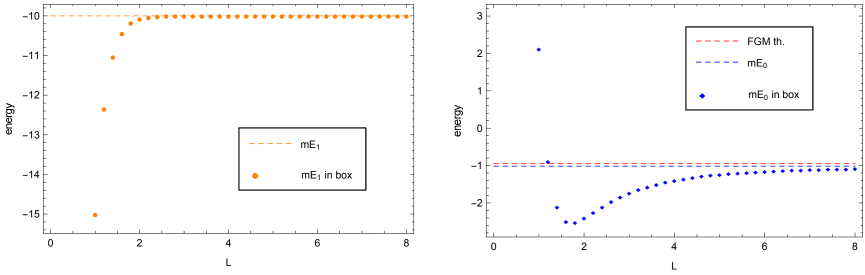


- Spectra in a box

  5 energy levels near th. in a box.

  2 bound states and 3 scattering states.

Bound States in a Box



- Infinite volume limit $mE_1(L) \to -10$ & $mE_0(L) \to -1.016$.

- Exponentially suppressed correction.

  3-body bound state $a \to \infty$, $\Delta E_1 \propto \frac{1}{L^{3/2}} \exp\left(-\frac{2}{\sqrt{3}}\kappa L\right)$.

  (U. Meißner, G. Rios and A. Rusetsky, PRL 114(9) (2015), 091602)

  Particle-dimer bound state $\kappa^2 - a^{-2} \ll \kappa^2$, $\Delta E_0 \propto \frac{1}{L} \exp\left(-\frac{2}{\sqrt{3}}\sqrt{\kappa^2 - a^{-2}}L\right)$.

  (M. Lüscher, NPB 354 (1991) 531)

- Theoretical Calculation

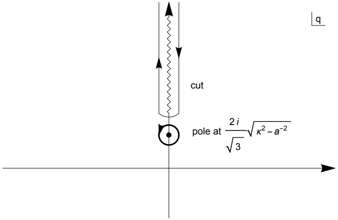
$$\mathcal{M}_L(\mathbf{p},\mathbf{k};E) = \mathcal{M}(\mathbf{p},\mathbf{k};E) + 8\pi \int^{\Lambda} \frac{d^3q}{(2\pi)^3} \mathcal{M}(\mathbf{p},\mathbf{q};E)\delta\tau_L(\mathbf{q};E)\mathcal{M}_L(\mathbf{q},\mathbf{k};E),$$

where $\delta\tau_L = \sum_{\mathbf{n}\neq 0} e^{i\mathbf{nq}L}\tau(\mathbf{q};E) + O(\frac{1}{L})$.

$$\Delta E = 8\pi \int \frac{d^3q}{(2\pi)^3} \phi^\dagger(\mathbf{q}) \sum_{\mathbf{n}\neq 0} e^{i\mathbf{nq}L}\tau(\mathbf{q})\phi(\mathbf{q}) + \cdots.$$

Contour integral on the complex plane.

1. Regular w.f. $\phi(\mathbf{q}) \sim$ const.
2. Cut and pole of $\tau(\mathbf{q};E) = \frac{1}{-a^{-1}+\sqrt{\frac{3}{4}\mathbf{q}^2 - mE - i\varepsilon}}$



$$\boxed{\Delta E = \frac{\kappa^2}{m}\left[\frac{1}{(\kappa L)^{3/2}} C \exp\left(-\frac{2}{\sqrt{3}}\kappa L\right) + \frac{1}{\sqrt{(\kappa a)^2 - 1}}\frac{1}{(\kappa L)} C' \exp\left(-\frac{2}{\sqrt{3}}\sqrt{\kappa^2 - a^{-2}}L\right)\right]}$$

$$\boxed{\Delta E = \frac{\kappa^2}{m}\left[\frac{1}{(\kappa L)^{3/2}} C \exp\left(-\frac{2}{\sqrt{3}}\kappa L\right) + \frac{1}{\sqrt{(\kappa a)^2-1}}\frac{1}{(\kappa L)} C' \exp\left(-\frac{2}{\sqrt{3}}\sqrt{\kappa^2 - a^{-2}} L\right)\right]}$$

- 2 types of contributions

  3-body contribution: $\frac{1}{(\kappa L)^{3/2}} \exp\left(-\frac{2}{\sqrt{3}}\kappa L\right)$

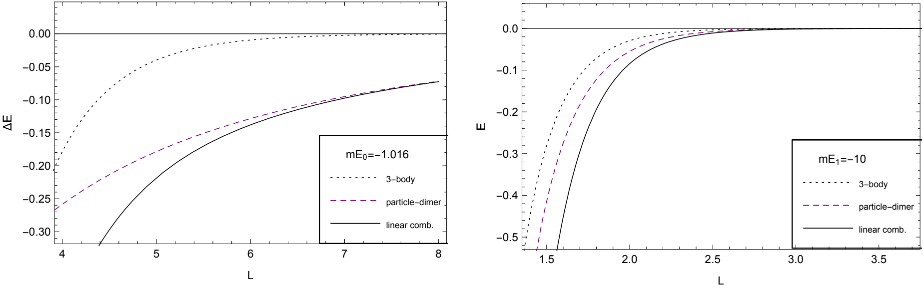
  Particle-dimer contribution: $\frac{1}{\sqrt{(\kappa a)^2-1}}\frac{1}{(\kappa L)} \exp\left(-\frac{2}{\sqrt{3}}\sqrt{\kappa^2 - a^{-2}} L\right)$

  1. Suppressed as $\kappa^2 \gg a^{-2}$
  2. Dominating as $\kappa^2 - a^{-2} \ll \kappa^2$

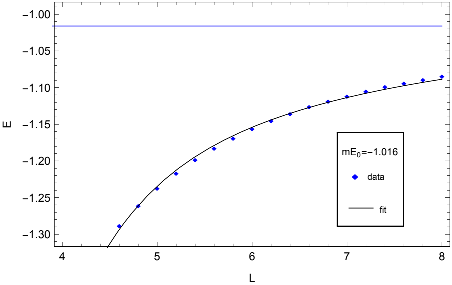
- $C$and C' The two coefficients are related to infinite volume wave function $\phi(\mathbf{q})$.

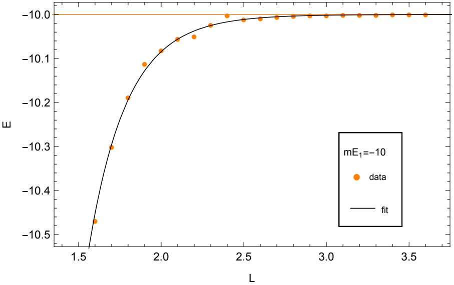
- **Identification**

  Energy shift of bound state $mE_0 = -1.016$ is dominated by particle-dimer contribution. In case of $mE_1 = -10$, both contributions are comparable in magnitude.

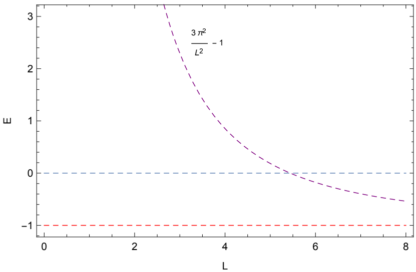


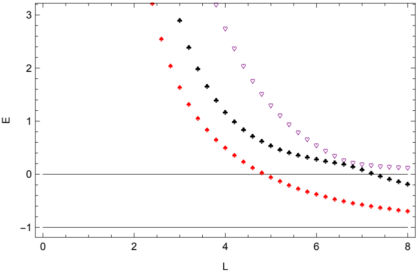
- Identification
  1. We identify the state with $mE_0 = -1.016$ as predominately particle-dimer state.
  2. A state with $mE_1 = -10$ is mixture.





Scattering States above threshold





- Free 3-body state & Free particle-dimer state

  Free 3-body state: $mE = \frac{\mathbf{p}^2}{2} + \frac{\mathbf{q}^2}{2} + \frac{(-\mathbf{p}-\mathbf{q})^2}{2}$

  Grd. st. $\mathbf{p} = \mathbf{q} = \frac{2\pi}{L}(0,0,0) \to mE = 0$

  Free particle-dimer state: $mE = \left(\frac{\mathbf{p}^2}{4} - \frac{1}{a^2}\right) + \frac{(-\mathbf{p})^2}{2}$

  Grd. st. $\mathbf{p} = \frac{2\pi}{L}(0,0,0) \to mE = -1$

  1st excited st. $\mathbf{p} = \frac{2\pi}{L}(0,0,1)$ or $(0,1,0)\cdots \to mE = \frac{3\pi^2}{L^2} - 1$

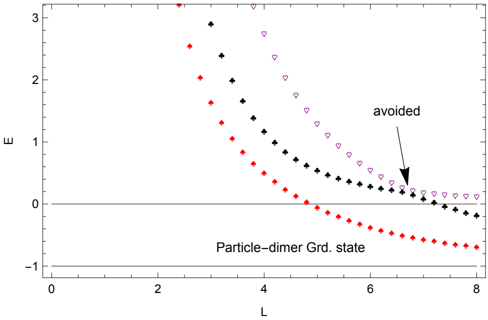
- Identify particle-dimer ground state

  The lowest-lying energy level above threshold tends to particle-dimer threshold individually.

- Avoided

  The second and third energy levels exhibit avoided level crossing.

  How to identify them?

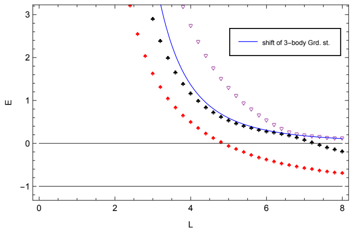


- Shift of 3-body ground state

  Theoretical calculations:

  $$mE(L) = \frac{12\pi a}{L^3} - \frac{12a^2}{L^4}\mathscr{I} + \frac{12a^3}{\pi L^5}\left(\mathscr{I}^2 + \mathscr{J}\right) + o\left(\frac{1}{L^5}\right).$$

  (S. Beane *et.al.*, arXiv:0707.1670, S. Sharpe, arXiv:1707.04279)



- Identification of 3-body Ground State and Particle-dimer 1st Excited State

  Before avoided level crossing, the 2nd level is a 3-body state and the 3rd level is a particle-dimer state

  After avoided level crossing, they exchange their roles.

  Finally, the 3-body state tends to the 3-body threshold $mE = 0$ and particle-dimer state to the particle-dimer threshold $mE = -1$.

- In a finite volume, the quantization condition is projected onto the different irreps of the octahedral group.
- The spectra of A_1^+-irrep are calculated. The individual energy levels are identified in terms of bound states, as well as particle-dimer and 3-particle scattering states.

- Outlook
  - Derive the perturbative shift for the particle-dimer states. Use this result for the identification of the corresponding energy levels.
  - Use the method to predict the outcome of lattice simulation in the realistic systems.

Thank you for your attention!