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Two-particle scattering in the finite volume using plane wave basis

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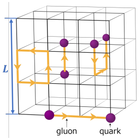
Together with Evgeny Epelbaum (RUB)

Contents

Lüscher's formula and beyond

- LQCD: formulated on a lattice of points in spacetime in a finite volume (FV)
- LQCD results: energy levels in FV
- Lüscher's formula:$\det\left[M^{(\Gamma,\boldsymbol{P})}_{ln,l'n'}(E)-\delta_{ll'}\delta_{nn'}\cot\delta_l\right]=0$ Luscher:1990ux

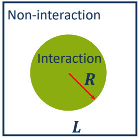


$\Rightarrow$ Derivation: LSE in FV + Partial wave expansion Luscher:1990ux,Polejaeva:2012ut

- **Model-independent, One-to-one:** $E^{FV}\sim\delta^l$

$\Rightarrow$ $L\gg R$, neglect $e^{-L/R}$ effect; Caveat: E.g. 1-π exchange Sato:2007ms,Jansen:2015lha

$\Rightarrow$ No partial wave (PW) mixture; Caveat:rotational symmetry in FV Luscher:1990ux



- To improve:

$\Rightarrow$ Parameterize T-matrix within theoretical frameworks, e.g. effective range expansion

$\Rightarrow$ Alternative approaches: HAL QCD, UChPT in FV, Hamiltonian EFT... Ishii:2006ec,Doring:2011vk,Wu:2014vma,...

- Our approach

$\Rightarrow$ Plane wave expansion $|\frac{2\pi}{L}\boldsymbol{n}\rangle$→LSE to get quantization conditions Lee:2020fbo

$\Rightarrow$ Long range interaction: effective field theory (long-range:known, short-range:$\leftarrow$ LQCD)

Theoretical formalism

Lippmann-Schwinger equation in FV

- LSE become matrix equation $\mathbb{T} = \mathbb{V} + \mathbb{V}\mathbb{G}\mathbb{T}$

$$\mathbb{T}_{\boldsymbol{n}',\boldsymbol{n}} = T\left(\frac{2\pi}{L}\boldsymbol{n}', \frac{2\pi}{L}\boldsymbol{n}; E\right), \quad \mathbb{G}_{\boldsymbol{n},\boldsymbol{n}'} = \frac{1}{L^3}\frac{1}{E - \frac{q_{\boldsymbol{n}}^2}{m_N}}\delta_{\boldsymbol{n}',\boldsymbol{n}}, \quad \text{truncation at } n^2 < n_{max}^2$$

- If the potential is energy-independent $\Rightarrow$ Eigenvalue problem

$$\det\left(\mathbb{G}^{-1} - \mathbb{V}\right) = 0 \to \det\left(\mathbb{H} - E\mathbb{I}\right) = 0, \quad \text{with} \quad \mathbb{H}_{\boldsymbol{m},\boldsymbol{n}} = \frac{1}{L^3}\mathbb{V}_{\boldsymbol{m},\boldsymbol{n}} + \frac{q_{\boldsymbol{n}}^2}{m_N}\delta_{\boldsymbol{m},\boldsymbol{n}}$$

- Reduce the $\mathbb{H}$ according to irreducible representations (irreps) of the point group

$$\mathbb{H} \xrightarrow{\text{reduction}} \underbrace{\begin{pmatrix} \mathbb{H}_{\Gamma_i} & & \\ & \mathbb{H}_{\Gamma_j} & \\ & & \ddots \end{pmatrix}}_{\text{block-diagnal}}, \quad \det\left(\mathbb{H}_\Gamma - E_\Gamma \mathbb{I}\right) = 0$$

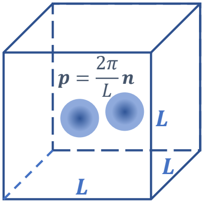
- If the potential is E-dependent, $\det[\mathbb{M}_\Gamma(E)] = 0$, root-finding algorithm

Representation space spanned by $|p_n\rangle$

- The representation of cubic group (O_h)

$$\{n_1,n_2,n_3\} \equiv \{|n_1,n_2,n_3\rangle \text{ + perm. } n_1,n_2,n_3 \text{ + change signs}\}$$

$$\langle \boldsymbol{n}'|\hat{D}(g)|\boldsymbol{n}\rangle = \delta_{\boldsymbol{n}',g\boldsymbol{n}}$$



- Seven patterns of representation space $\{n_1,n_2,n_3\}_{dim}$

$$\Rightarrow \{0,0,0\}_1, \{0,0,a\}_6, \{0,a,a\}_{12}, \{0,a,b\}_{24}, \{a,a,a\}_8, \{a,a,b\}_{24}, \{a,b,c\}_{48}$$

- Reduce to irreducible representations (irreps): projection operator

e.g. textbook by M.Dresselhaus et.al

$$\hat{P}^{\Gamma_a}_{\alpha\beta} \equiv \sum_{g_i\in G} \frac{N(\Gamma_a)}{n_G} R^{\Gamma_a}_{\alpha\beta}(g_i)^* \hat{D}(g_i), \qquad \hat{P}^{\Gamma_a}_{\alpha\alpha'}|\psi\rangle = a^{\Gamma_a}_{\alpha'}|\Gamma_a,\alpha\rangle.$$

- An example: $\{0,0,a\}_6 = A_1^+ \oplus E^+ \oplus T_1^-$

- For moving systems, elongated boxes, particles with arbitrary spin...

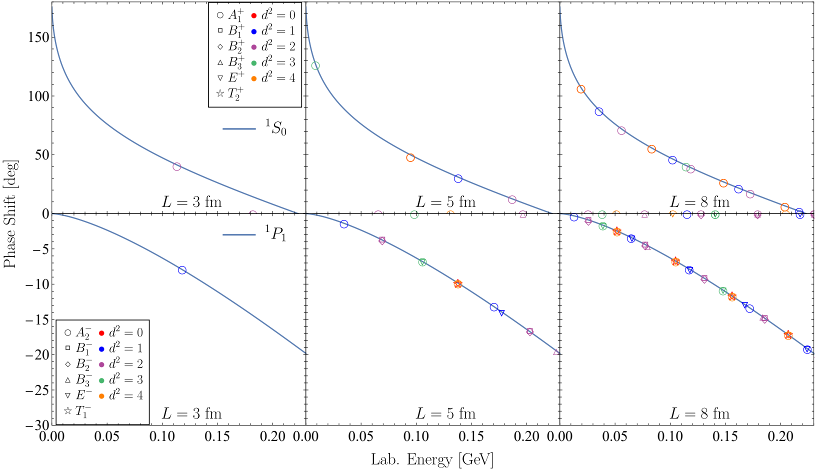
Symmetric group (character table) $\xrightarrow{\hat{P}^{\Gamma}}$ unitary irrep matrices $\xrightarrow{\hat{P}^{\Gamma}_{\alpha\beta}}$ rep space $\vert p_n\rangle \rightarrow$ irreps

Application I: spin-singlet NN scattering

Benchmark: contact interaction

- Interaction: spin singlet, ONLY contribute to S- and P-wave

$$V^{(0)}_{\text{cont}}(\boldsymbol{p},\boldsymbol{p}') = C_S, \quad V^{(2)}_{\text{cont}}(\boldsymbol{p},\boldsymbol{p}') = C_1\boldsymbol{q}^2 + C_2\boldsymbol{k}^2$$



$L = 3, 5, 8$ fm

Solid line: δ^l in IFV

Markers: E^{FV} - δ^{LF}

l_{min} Lüscher formula (LF)

Larger L, denser E^{FV}s

Vanishing δ: D,F...waves

- The single-channel Lüscher formula works accurately: short range + w/o PW mixing

ChEFT nuclear forces to NNLO

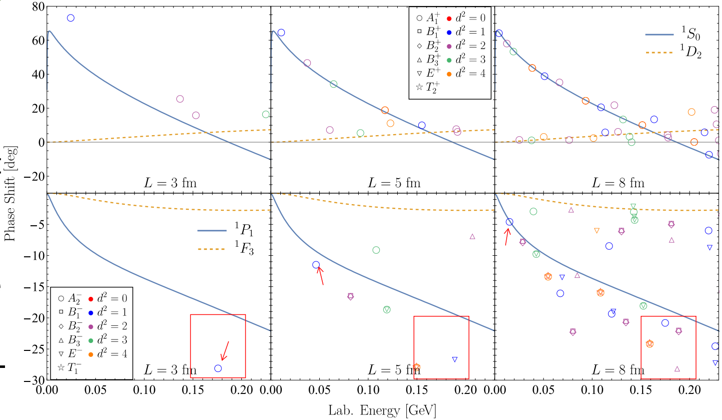
- LF: even parity
  - $\Rightarrow$ Large deviation for $L = 3$ fm
  - $\Rightarrow$ Good for $L \geq 5$ fm

Sato:2007ms

- LF: odd parity
  - $\Rightarrow$ Near-thresh.: $\delta \to$ exact ones
  - $\Rightarrow$ Deviation$\uparrow$ with $E\uparrow$
  - $\Rightarrow$ $L\uparrow$ cannot improve the LF results at higher E
  - $\Rightarrow$ Large deviation for $L = 8$ fm
  - $\Rightarrow$ $L\uparrow$ improves the LF results for single state
  - $\Rightarrow$ The reason of deviation? PW mixing??

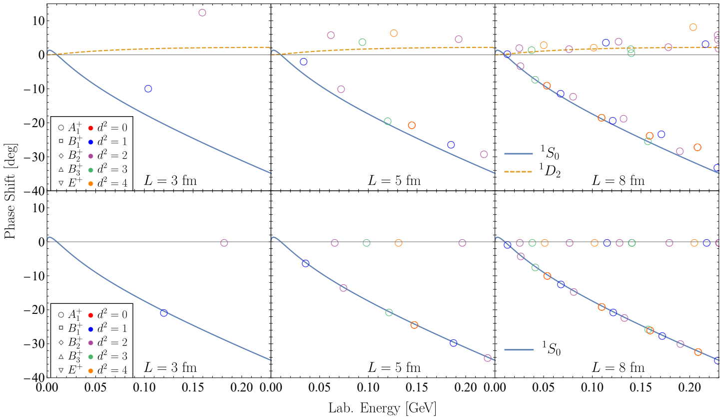
Interaction Epelbaum:2003xx

$$V = V^{(0)}_{\text{cont}} + V^{(0)}_{1\pi} + V^{(2)}_{\text{cont}} + V^{(2)}_{2\pi} + V^{(2)}_{1\pi} + V^{(3)}_{2\pi}$$



One-pion exchange: even-parity

$$V(\boldsymbol{p},\boldsymbol{p}') = \sum_l \frac{2l+1}{4\pi} V_l(p,p') P_l(z), \quad V_{\text{S-wave}}(\boldsymbol{p},\boldsymbol{p}') = (4\pi)^{-1} V_0(p,p') P_0(z)$$



- Upper: full OPE
  - ⇒ Deviations are qualitatively similar to NNLO results
  - ⇒ Large deviation for $L = 3$ fm
  - ⇒ Good for $L \geq 5$fm
- Lower: S-wave-projected OPE
  - ⇒ Switch off higher PW $V_{l>0}$
  - ⇒ The deviation disappear

One-pion exchange: odd-parity

- The upper:full OPE
  - ⇒ Deviations are qualitatively similar to NNLO results
  - ⇒ Deviations are large regardless of L
- The middle: P-wave OPE
  - ⇒ Switch off higher PW $V_{l>1}$
  - ⇒ LF reproduces the P-wave δ accurately
- The lower: P-wave + F-wave OPE
  - ⇒ Mixing effect from F-wave
  - ⇒ Sensitive to the 2ed lowest PW:

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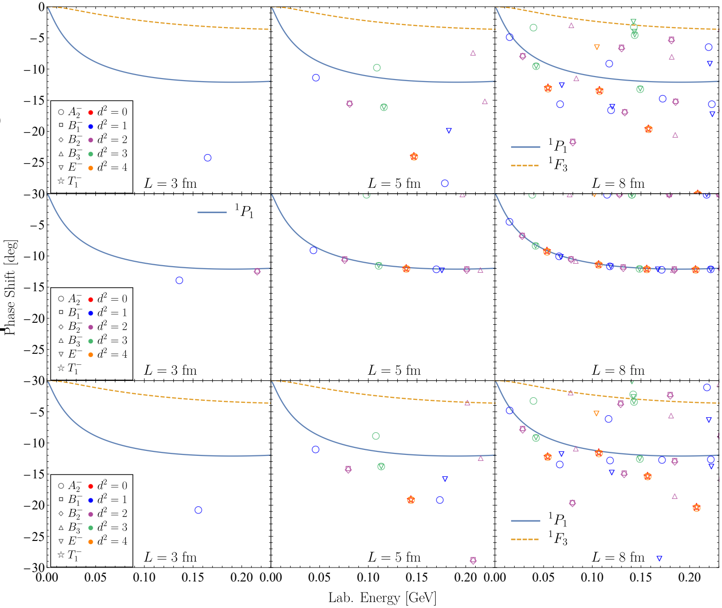
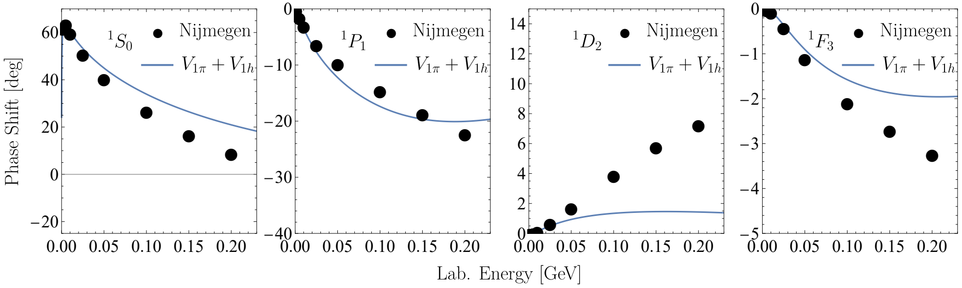


EFT-inspired fitting: toy model

- Long-range (OPE) interaction ⇒one-to-one LF fails due to PW mixing
- Known OPE⇒ EFT-inspired approach to fitting E^{FV}
- Mimic LQCD data: Toy model to generate FV energies, m_h=0.5 GeV

$$V_{\text{toy}} = V_{1\pi} + V_{1h} = -\left(\frac{g_A}{2F_\pi}\right)^2 \frac{M_\pi^2}{\boldsymbol{q}^2+M_\pi^2}\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 + \left(c_{h1} + c_{h2}\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\right)\frac{1}{\boldsymbol{q}^2+m_h^2}$$



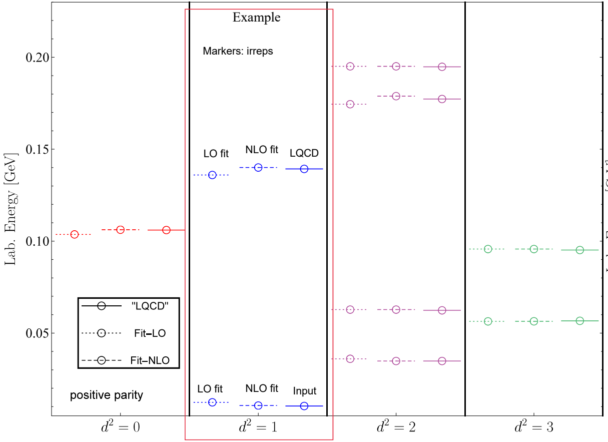
- Fit the FV energy levels with $V_{\text{EFT}} = V^{(0)}_{\text{OPE}} + V^{(0)}_{\text{cont}} + V^{(2)}_{\text{cont}} + V^{(4)}_{\text{cont}} + \ldots$

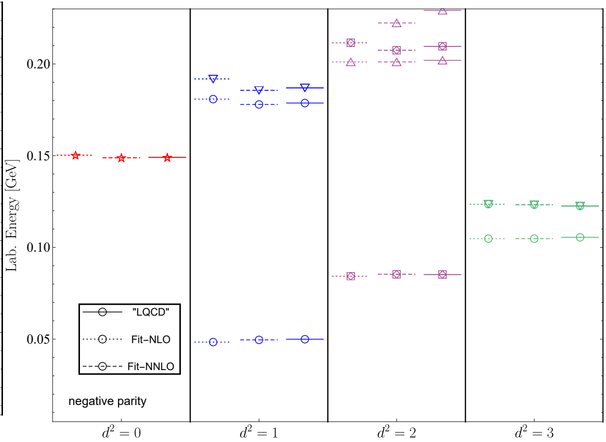
EFT-inspired fitting: results

- Fitting: Determinant residual method

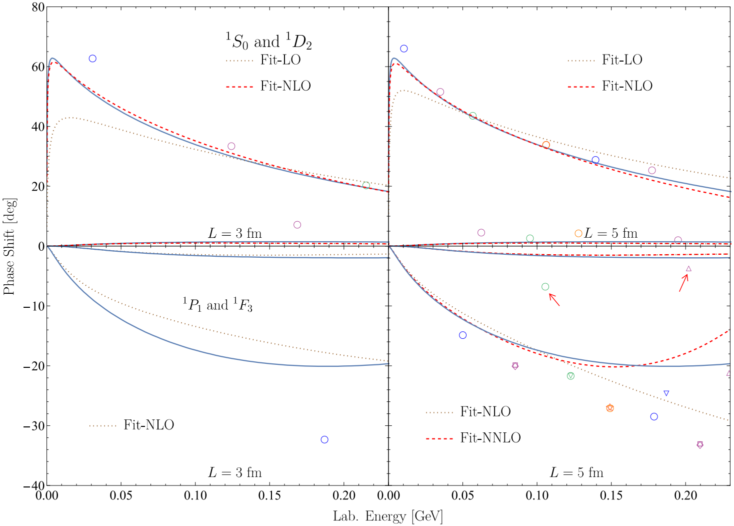
Morningstar:2017spu

- The ground state for each irrep is input
- Good agreement and improved with orders





EFT-inspired fitting VS Lüscher formula



- Improved with orders
  - ⇒ 1-para.: rough
  - ⇒ 2-para: improved
- Uncover "underlying" theory
- Good fit for small box
  - ⇒ e.g. S-wave, $L = 3$ fm
- Higher PW dominant energy will NOT fail the fit

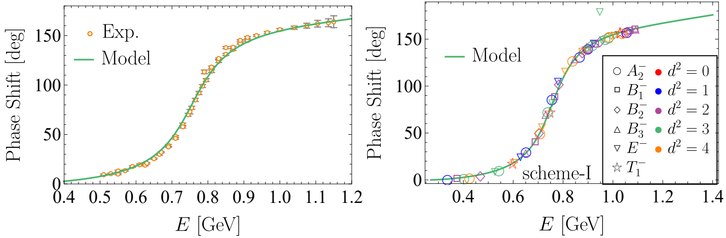
Application II: ρ-channel $\pi\pi$ scattering

$\pi\pi$ finite volume energy levels

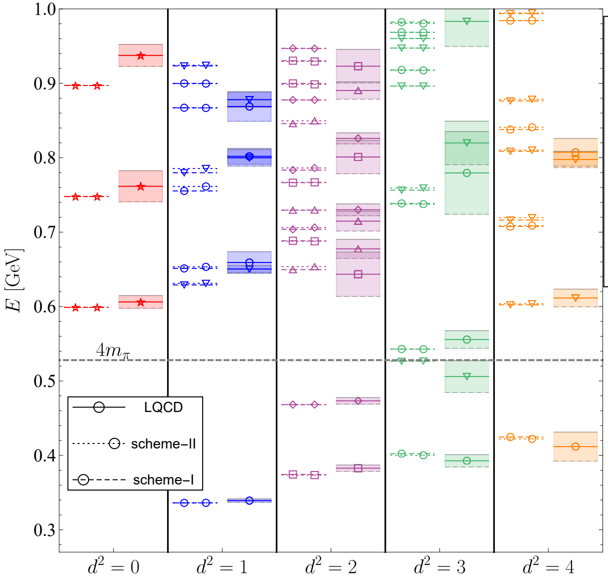
- Reduced Bethe-Salpeter equation
- Phenomenological model:3 para. (f, G_V and M_0) depict the δ in infinite volume Chen:2012rp

$$V(\boldsymbol{p}, \boldsymbol{p}'; E) = -\frac{2\boldsymbol{p}\cdot\boldsymbol{p}'}{f^2}\left(1 + \frac{2G_V^2}{f^2}\frac{E^2}{M_0^2 - E^2}\right) \quad \text{only P-wave}$$

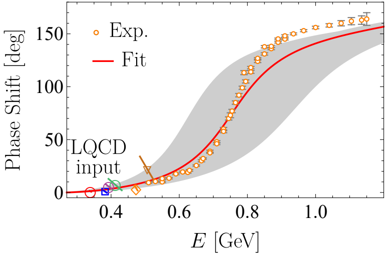
- Plane wave expansion of BSE in FV ($L = 4.3872$ fm)
- Energy-dependent potential⇒ root-finding algorithm⇒energy level
- Lüscher formula works well (short range interaction without PW mixing)



Compare with and fit the lattice QCD results



- Lattice QCD results from ETMC Fischer:2020fvl
  $\Rightarrow L = 4.3872,\ m_\pi = 132$ MeV
- Compare our E^{FV} with LQCD results
- Fit the E^{LQCD} below $4m_\pi$
- Agree with Exp. results well
- Large uncertainty due to simple model



Summary

Summary

- A proof-of-principle of an alternative method of Lüscher's formula
- LSE or BSE in plane wave expansion+projection operator technique reduction to irreps

  $\Rightarrow$ Including partial wave mixing effect naturally, avoid complications of PW expansion

  $\Rightarrow$ Rest and moving two-particle systems
- Non-relativistic example: spin-singlet NN

  $\Rightarrow$ S-wave dominant states: LF works well for $L \gtrsim 5$ fm

  $\Rightarrow$ P-wave dominant states: OPE$\rightarrow$large PW mixing effect regardless the box size

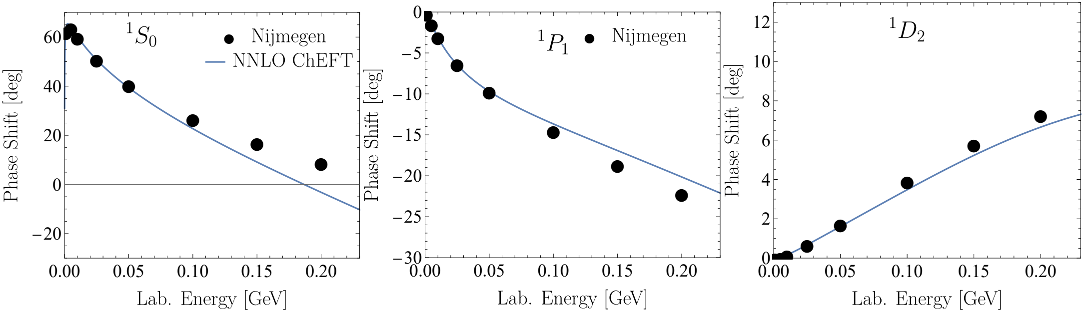
  $\Rightarrow$ EFT-based approach in the plane wave basis: $V_{1\pi} + V_{1h} \underset{\text{data}}{\overset{\text{fit}}{\leftrightarrows}} V_{1\pi} + V^{(0)}_{\text{cont}} + V^{(2)}_{\text{cont}} \cdots$

  $\Rightarrow$ Advantages: 1) **insensitive to PW mixing artifact**; 2) **small box (long-range interaction)**
- Relativistic example: ρ-channel $\pi\pi$: compare and fit with LQCD results from ETM
- On-going: SMS NN force, $S = 1$, LF with PW mixng VS plane wave +EFT, Real LQCD NN data

Thanks for your attention!

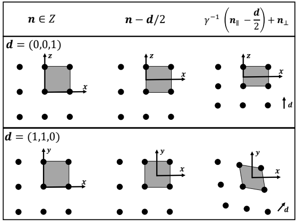
Backup

NNLO ChEFT nuclear forces



Projection operator technique

- Identify the symmetric group and its elements and character table



- Construct the unitary irrep matrices with character projection operation

$$\hat{P}^{\Gamma_a} \equiv \sum_{\alpha} \hat{P}^{\Gamma_a}_{\alpha\alpha} = \sum_{g_i \in G} \frac{N(\Gamma_a)}{n_G} \chi^{\Gamma_a}(g_i) \hat{D}(g_i), \quad \hat{P}^{\Gamma_a}|\psi\rangle = \sum_{\alpha} a^{\Gamma_a}_{\alpha} |\Gamma_a, \alpha\rangle$$

- Reduce the representation to the direct sum of irreps.

$$\hat{P}^{\Gamma_a}_{\alpha\beta} \equiv \sum_{g_i \in G} \frac{N(\Gamma_a)}{n_G} R^{\Gamma_a}_{\alpha\beta}(g_i)^* \hat{D}(g_i), \quad \hat{P}^{\Gamma_a}_{\alpha\alpha'}|\psi\rangle = a^{\Gamma_a}_{\alpha'} |\Gamma_a, \alpha\rangle.$$

Moving system

$$\boldsymbol{p}^* = \boldsymbol{n}^* \frac{2\pi}{L}, \quad \boldsymbol{n}^* \in P_d$$
$$P_d = \{\gamma^{-1}(\boldsymbol{n}_\parallel - \frac{1}{2}\boldsymbol{d}) + \boldsymbol{n}_\perp\}, \quad \boldsymbol{n} \in Z^3$$

For $\boldsymbol{d} = (a, a, a)$: at most seven patterns

$$\{n_1, n_2, n_3\} = \{|n_1, n_2, n_3\rangle \text{ with permutations of } n_1, n_2, n_3 \text{ and changing signs}\}$$

For $\boldsymbol{d} = (0, 0, a)$ and $\boldsymbol{d} = (a, a, 0)$: at most eight pattern

$$\{n_1, n_2; n_3\} = \{|n_1, n_2, n_3\rangle \text{ with permutations of } n_1 \text{and } n_2 \text{ and changing signs}\}.$$

Hamiltonian EFT of Adelaide group

Hamiltonian EFT:	PW LSE	$\to$	discretize $\lvert\boldsymbol{p}\rvert = \frac{2\pi}{L}n$			Hall:2013qba,Wu:2014vma,Liu:2015ktc
Our work:	3D LSE	$\to$	discretize $\boldsymbol{p} = \frac{2\pi}{L}\boldsymbol{n}$	$\to$	Reduce to irrep. Γ	

$$V(\boldsymbol{p},\boldsymbol{p}') = \sum_l \frac{2l+1}{4\pi} V_l(p,p') P_l(z)$$

$$T(\boldsymbol{p},\boldsymbol{p}') = V(\boldsymbol{p},\boldsymbol{p}') + \int \frac{d^3\boldsymbol{q}}{(2\pi)^3} V(\boldsymbol{p},\boldsymbol{q}) G(q) T(\boldsymbol{q},\boldsymbol{p}')$$

$$T^l(p,p') = V^l(p,p') + \int \frac{q^2 dq}{(2\pi)^3} V^l(p,q) G(q) T^l(q,p')$$

- For S-wave: $V_0(p,p') \neq 0$ and $V_l(p,p') = 0$ for $l > 0$; two approaches are the same
- For the higher PW, e.g.: $V(\boldsymbol{p},\boldsymbol{p}') = \frac{3}{4\pi} V_1(p,p') P_1(z)$

$\Rightarrow$ The Adelaide group in fact assume a

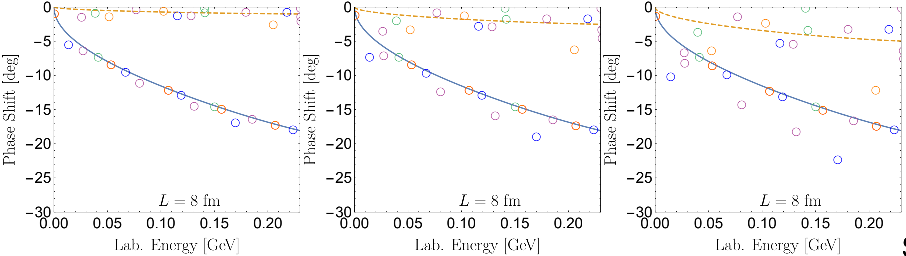
$$V(\boldsymbol{p},\boldsymbol{p}') = \frac{1}{4\pi}\tilde{V}_0(p,p') = \frac{1}{4\pi}V_1(p,p')$$

convergence of partial wave expansion

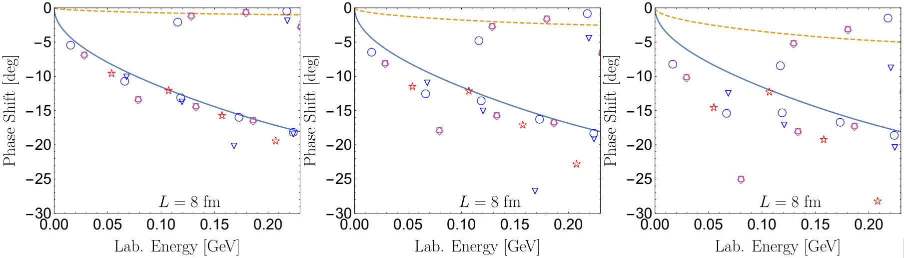
- Near-threshold behavior: $\delta_l \sim p_{\text{on}}^{2l}$
- Only valid below the t-channel singularity: $E_{\text{lab}} \sim \frac{2M_\pi^2}{m_N} \sim 10$ MeV
- For higher energy, the convergence of partial wave expansion become slow
- E.g. To calculate differential cross section at $E_{\text{lab}} = 300$ MeV to 1% accuracy, $j_{max} = 16$ is needed

PW mixing

$$V(p,p',z) = \sum_l \frac{l+1}{4\pi} V_l P_l(z), \quad V_{l=0} = V_{l=1} = C_1, \quad V_{l=2} = V_{l=3} = C_2, \quad C_2 = 10c_2, 15c_2, 50c_2$$

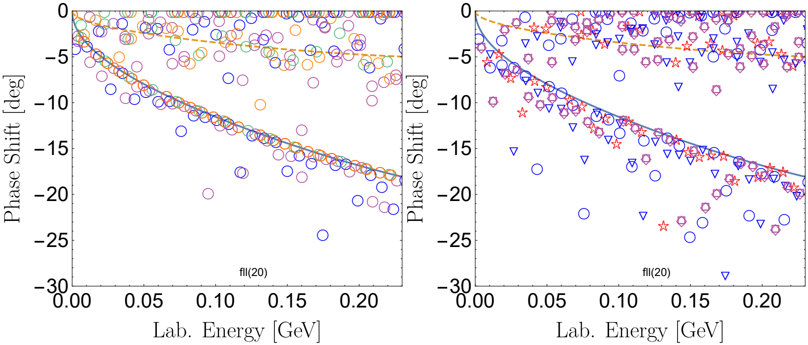


S-D mixing



P-F mixing

PW mixing: $L = 20$ fm



Root-finding and determinate residual method

$$\det[\mathbb{M}_\Gamma(E)] = 0$$

$$\Omega_\Gamma(E;\mu) \equiv \prod \frac{\lambda_{\Gamma,i}(E)}{\sqrt{\lambda_{\Gamma,i}(E)^2 + \mu^2}}, \qquad \det\left[\mathbb{M}_\Gamma(E)\right] = \prod_i \lambda_{\Gamma,i}(E)$$

- root-finding: $\Omega_\Gamma(E;\mu) = 0$
- determinate residual method

$$\chi^2 = \sum_{\Gamma,i} \frac{\Omega_\Gamma(E_{\Gamma,i})^2}{\sigma[\Omega_\Gamma(E_{\Gamma,i})]^2},$$

Computational cost- an estimation

- For NN: $n^2 \leq 100$, dim $\approx \frac{4}{3}\pi n^3 \approx 4000$, $\mathrm{dim}_\Gamma \approx 4000/12$
- For $\pi\pi$: $n^2 \leq 50$, dim $\approx \frac{4}{3}\pi n^3 \approx 1500, \mathrm{dim}_\Gamma \approx 1500/12$
- Accelerating the calculation: eigenvector continuation??

Frame:2017fah

Fitting details

- Fit the FV energies with $V_{\text{EFT}} = V^{(0)}_{\text{OPE}} + V^{(0)}_{\text{cont}} + V^{(2)}_{\text{cont}} + V^{(4)}_{\text{cont}} + \ldots$

$$V^{(0)}_{\text{cont}} = \frac{1}{4\pi}\tilde{C}_{^1S_0}, \quad V^{(2)}_{\text{cont}} = \frac{1}{4\pi}C_{^1S_0}(p^2 + p'^2)$$

$$V^{(2)}_{\text{cont}}(p, p', z) = \frac{3}{4\pi}C_{^1P_1}pp'z, \quad V^{(4)}_{\text{cont}}(p, p', z) = \frac{3}{4\pi}D_{^1P_1}pp'(p^2 + p'^2)z$$