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Finite volume NN system using plane wave exansion and eigenvector continuation

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Based on JHEP10(2021)051 and paper in preparation

Together with Evgeny Epelbaum (RUB)

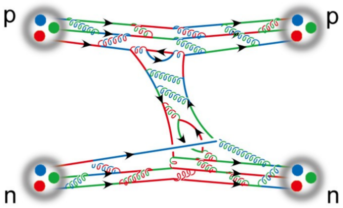
Contents

Lüscher’s formula

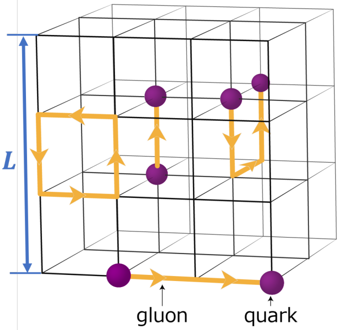
lattice QCD and finite volume energy levels

- QCD is the fundamental theory of the strong interaction

$$\mathcal{L}_{QCD} = \sum_f \bar{q}_f (i\not{D} - \mathcal{M} q_f) - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu,a} \tag{1}$$



- Extract nuclear forces from QCD? Lattice QCD!
  - ⇒ formulated on a lattice of points in space and time in a finite volume (FV)



- How to extract observable in the infinite volume from a finite volume calculation?
  - ⇒ Lüscher's formula: energy levels in FV: $E^{FV} \sim \delta^l$ Luscher:1990ux
  - ⇒ HAL QCD: Bethe–Salpeter amplitude → potential Ishii:2006ec

Two particles in a box

- Periodic boundary condition: $\psi(\mathbf{x}_1, \mathbf{x}_2) = \psi(\mathbf{x}_1 + \mathbf{n}_1 L, \mathbf{x}_2 + \mathbf{n}_2 L)$

  $\Rightarrow$ Equivalently, discrete momentum:

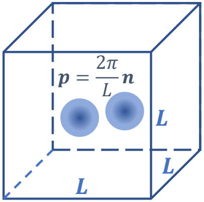
$$\boldsymbol{p}_1 + \boldsymbol{p}_2 = \boldsymbol{P}, \quad \boldsymbol{p}_1 = \frac{2\pi}{L}\boldsymbol{n}, \quad \boldsymbol{P} = \frac{2\pi}{L}\boldsymbol{d}, \qquad \boldsymbol{n}, \boldsymbol{d} \in Z^3$$

- The rotation symmetry is broken: $SO(3) \to O_h$

  $\Rightarrow$ $\{l, m\}$ is not good quantum number to label states

  Representation of the eigenstates: $\{l, m\} \to \{A_1, A_2, E, T_1, T_2\}$

  $\Rightarrow$ Partial wave mixing: $\langle lm|H^{FV}|l'm'\rangle \neq 0$ for $l \neq l$ and $m \neq m'$



- Moving system in the box $\boldsymbol{d} \neq 0$ introduce other point groups: D_{4h}, D_{2h},...

  $\Rightarrow$ For lattice QCD, changing box size is expensive

  $\Rightarrow$ To extract more information, calculate energies of moving two-body systems in a box

Lüscher's formula and beyond

- Lüscher's quantization condition:

$$\det[\delta_{ll'} \cot \delta_l(E) - M_{l,l'}(E)] = 0$$

$\Rightarrow$ Neglect partial wave mixing $E^{FV} \sim \delta_l(E^{FV})$, one-to-one relation,

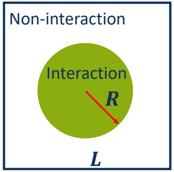
otherwise, parameterize K-matrix, root-finding algorithm

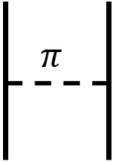
$\Rightarrow$ $L \gg R$, negligible $e^{-L/R}$ effect

LSE : $T^L = K + K G_F T^L$

$$\det[K^{-1} - G_F] = 0$$

V-dependent kinematic term

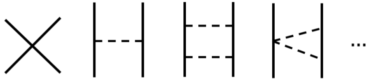




- Long-range interaction, e.g. $V_{1\pi}^{NN}$? Small box? Partial wave mixing?
- New framework: (1)Plane wave (PLW) basis+ (2) Chiral EFT+(3)Eigenvector continuation

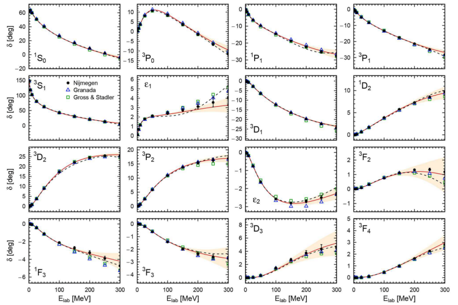
Theoretical formalism

NN interaction: chiral EFT



$$V(\vec{p}', \vec{p}) = V_{\text{contact}} + V_{1\pi} + V_{2\pi}$$

- Derived in the momentum space, E-independent
- Semilocal momentum-space regularization Reinert:2017usi



$$V_{1\pi}(\vec{p}', \vec{p}) = -\frac{g_A^2}{4F_\pi^2}\left(\frac{\vec{\sigma}_1 \cdot \vec{q}\vec{\sigma}_2 \cdot \vec{q}}{q^2 + m_\pi^2} + C(m_\pi)\vec{\sigma}_1 \cdot \vec{\sigma}_2\right) e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}$$

- Benefit from the known long-range interaction $V_{1\pi}$
- Low energy constants (LECs) for short-range interaction (contact interaction)

  $\Rightarrow$ fitting lattice QCD data

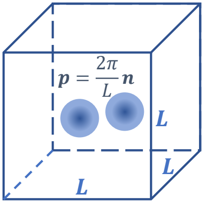
  $\Rightarrow$ $\#$ of LECs: $V^{(0)}$(+2),$V^{(2)}$(+7),$V^{(4)}$(+12); for specific irreps, the $\#$ will be small

Hamiltonian approach in Plane wave basis: $|\boldsymbol{p}_n, \boldsymbol{\eta}\rangle$

- $|\boldsymbol{p}_n, \boldsymbol{\eta}\rangle$: $\boldsymbol{p}_n$ discrete momentum, $\boldsymbol{\eta}$: polarization vector for $S=1$

$$\hat{D}(g)|\boldsymbol{p}, \boldsymbol{\eta}\rangle = |g\boldsymbol{p}, g\boldsymbol{\eta}\rangle, \hat{P}|\boldsymbol{p}, \boldsymbol{\eta}\rangle = |-\boldsymbol{p}, \boldsymbol{\eta}\rangle$$

$$\langle \boldsymbol{p}_{n'}, \boldsymbol{\eta}'^{\dagger}|\hat{D}(g)|\boldsymbol{p}_n, \boldsymbol{\eta}\rangle = \delta_{\boldsymbol{n}'\boldsymbol{n}} \left(\boldsymbol{\eta}'^{\dagger} \cdot g\boldsymbol{\eta}\right)$$



Periodic boundary condition

- $\{|\boldsymbol{p}_n, \boldsymbol{\eta}\rangle\}$ form the representation space of corresponding point group
- LSE become matrix equation $\mathbb{T} = \mathbb{V} + \mathbb{V}\mathbb{G}\mathbb{T}$
- Finite volume levels $\Rightarrow$ Eigenvalue problem

$$\det\left(\mathbb{G}^{-1} - \mathbb{V}\right) = 0 \rightarrow \det\left(\mathbb{H} - E\mathbb{I}\right) = 0,$$

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

$$\mathbb{H} \xrightarrow{\text{reduction}} \text{diag}\{\mathbb{H}_{\Gamma_i}, \mathbb{H}_{\Gamma_j}, \ldots\} \Rightarrow \quad \mathbb{H}_{\Gamma}\boldsymbol{v} = E_{\Gamma}\boldsymbol{v}$$

Hamiltonian approach in Plane wave basis: $|p_n, \eta\rangle$

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

  $\Rightarrow \{0,0,0\}_{1\times 3}, \{0,0,a\}_{6\times 3}, \{0,a,a\}_{12\times 3}, \{0,a,b\}_{24\times 3}\ldots$

- Reduce to irreducible representations (irreps): projection operator

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

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

- An example: $\{0,0,a\}_{6\times 3} = 2T_1^+ \oplus T_2^+ \oplus A_1^- \oplus E_1^- \oplus T_1^- \oplus T_2^-$
- 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 $|p_n\rangle \rightarrow$ irreps

- dim of the $\mathbb{H}_\Gamma$: cubic function of L^{-1}

$$\mathrm{dim} \sim \left(\frac{\Lambda_{\mathrm{UV}}}{2\pi/L}\right)^3 \times \frac{1}{10} \sim \mathcal{O}(1000)$$

Towards a practical approach: eigenvector continuation

- Plane wave basis+Eigenvector continuation

  Dick Furnstahl's talk

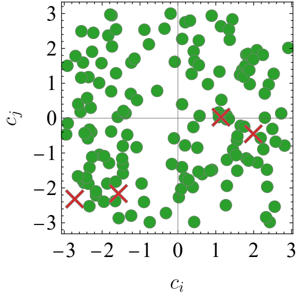
  $\Rightarrow$ Eigenvector continuation (EC) with subspace learning Frame:2017fah,Demol:2019yjt,Furnstahl:2020abp,Yapa:2022nnv

- Rayleigh-Ritz variational principle:

$$\mathcal{E}[\psi] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}, \quad E_{ground} = \mathcal{E}_{min}$$

$$|\psi\rangle = a_m|\phi_m\rangle, \quad \langle\phi_m|H(c_i)|\phi_n\rangle a_n = \mathcal{E}\langle\phi_m|\phi_n\rangle a_n$$

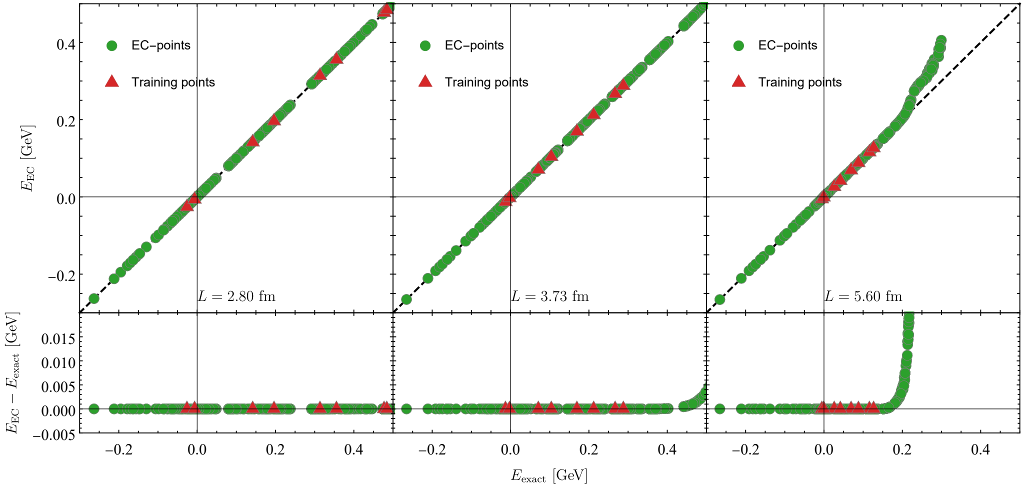
  $\Rightarrow$ choose the trial function (basis) properly



- To fit or quantify uncertainty: solve above Eqs. with different $\{c_i\}$ repeatedly
- EC basis: eigenvectors from a selection of parameter sets $\{c_i\}^1, \{c_i\}^2$, ...(training point)
- Naturalness of low energy constants (LEC) of EFT (~ 1) make the EC more reliable

Eigenvector continuation

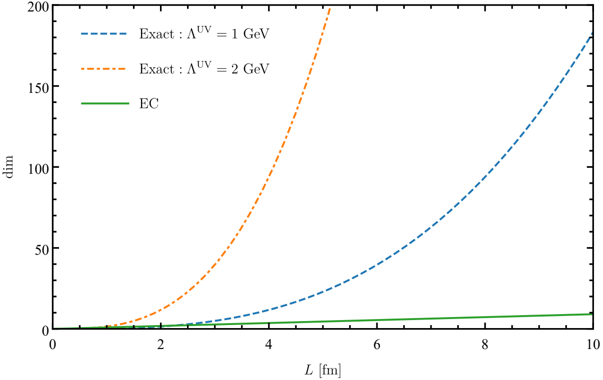
- Interaction: V_{contact} with 2 LECs $\{c_1, c_2\}$ + $V_{1\pi}$ in $L = \{2.70, 3.73, 5.60\}$ boxes
- Training points: $\{c_1^{\text{phy}}, 0\}$, $\{0, c_2^{\text{phy}}\}$; keep the first four energy levels as basis, dim=8



Eigenvector continuation

$$\dim^{EC} = \frac{2\pi p}{L} \times n_{\text{training}}$$

- dim is linear function $\frac{1}{L}$: linear VS cubic
- $\dim^{EC} \sim \mathcal{O}(10)$
- The subspace learning is the one-time cost



- After subspace learning, we can provide the $\mathbb{H}_0^{EC}$ and $\mathbb{V}_i^{EC}$ to the lattice community

$$\mathbb{H}^{EC} = \mathbb{H}_0^{EC} + c_i \mathbb{V}_i^{EC}, \quad \mathbb{H}^{EC}\boldsymbol{v} = E\boldsymbol{v}$$

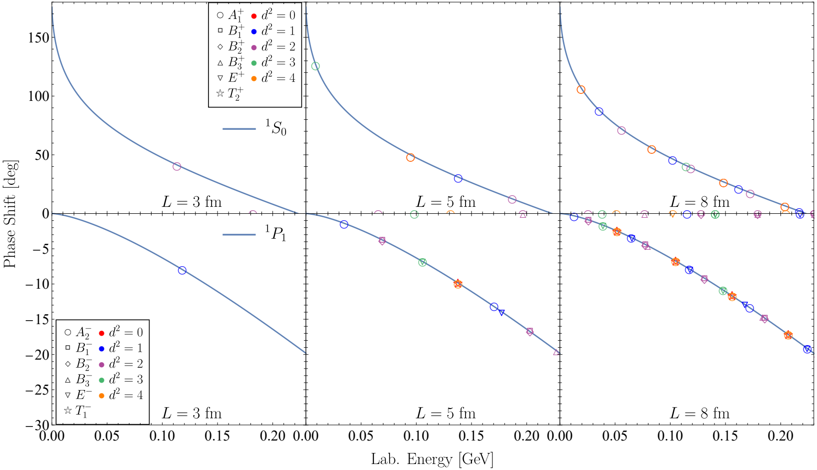
$\Rightarrow$ Easy-to-use interface: no need to know the details of χEFT

Scattering states: Lüscher’s formula VS PLW

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)

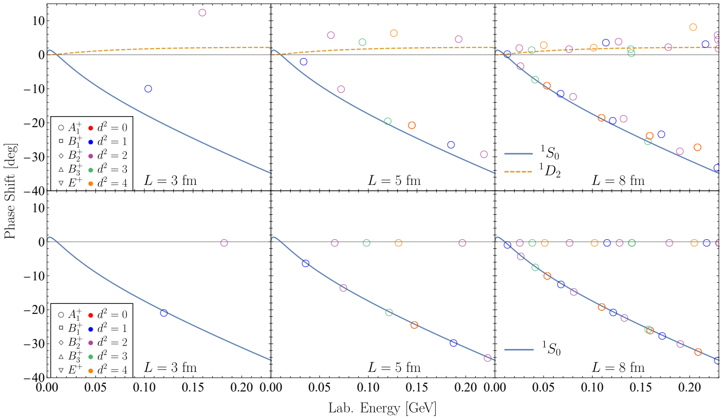
Larger L, denser E^{FV}s

Vanishing δ: D,F...waves

- The lowest PW Lüscher's formula works accurately: short range + w/o PW mixing

One-pion exchange: even-parity

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

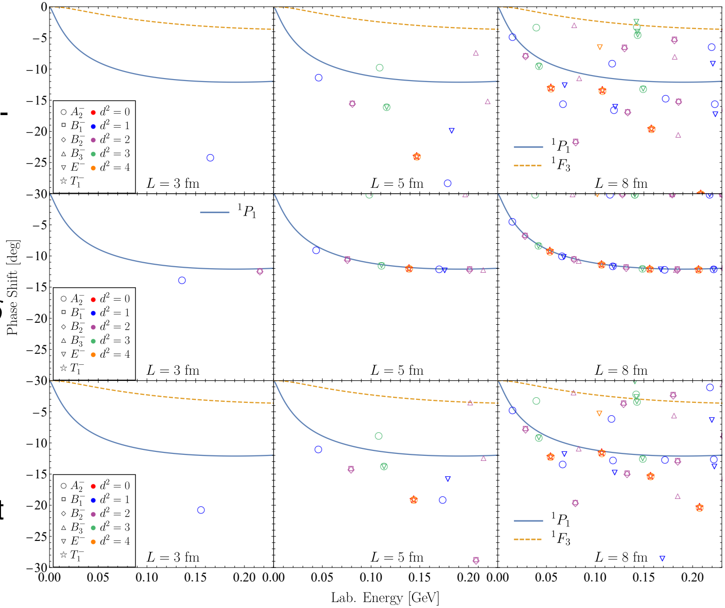


- Upper: full OPE
  - $\Rightarrow$ Large deviation for $L = 3$ fm
  - $\Rightarrow$ Good for $L \geq 5$fm
- Lower: S-wave-projected OPE
  - $\Rightarrow$ Switch off higher PW $V_{l>0}$
  - $\Rightarrow$ The deviation disappear

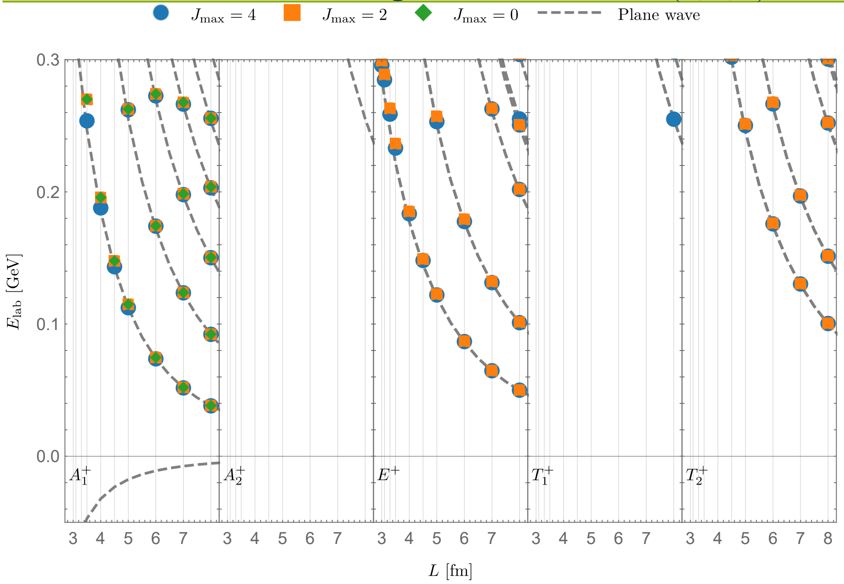
One-pion exchange: odd-parity

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

2107.04430



Scattering state: $S = 0$, $d = (0,0,0)$, even-parity



- PLW: with NNLO χEFT
- Lüscher QC:
  - $\Rightarrow$ Generate the phase shift (δ) to $J = 5$

$$\det[M^{\Gamma}_{l,l'} - K^{-1}(\delta)] = 0$$

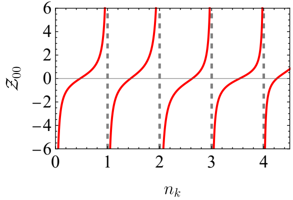
  - $\Rightarrow$ δ as input, truncated at different J_{max},
  - $\Rightarrow$ root-finding:

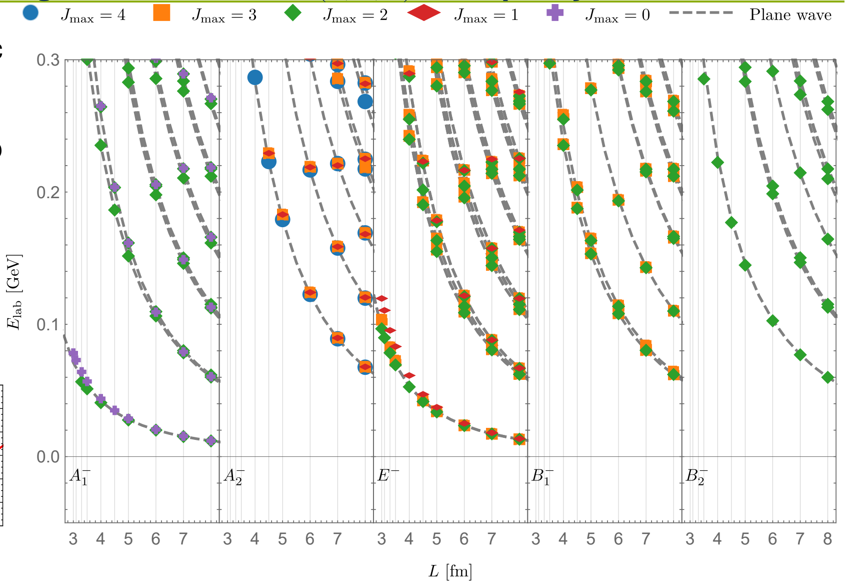
Woss:2020cmp,HSC

L ={3.0,3.1,3.3,3.5,4.0,4.5,5.0,6.0,7.0,8.0} fm

Scattering state: $S = 1$, $d = (0, 0, 1)$, odd-parity

- The PLW works: static and moving systems
- The QC converge to PLW results
- The discrepancy:
  - $\Rightarrow$ small box
  - $\Rightarrow$ low $J_{\max}$ QC





- The small differences in E^{FV} energy level could mean large difference in δ

Bound states: Lüscher’s formula VS PLW

Bound state in the finite volume

- Bound state Lüscher's formula

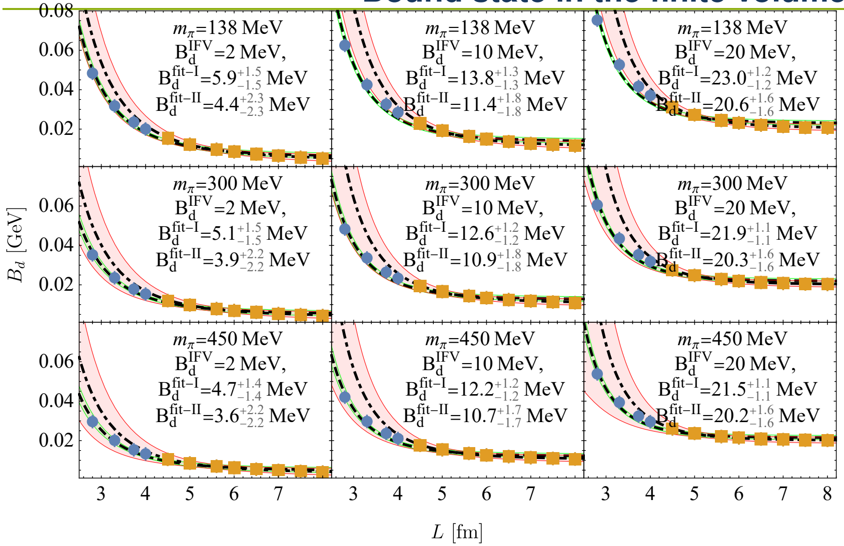
Luscher:1985dn, Koenig:2011xdn, Davoudi:2011md, Briceno:2014oea

$$\kappa = \kappa_0 + \frac{Z^2}{L} F(L, \kappa_0) + \mathcal{O}(e^{-2\kappa L}) \quad (2)$$

  - ⇒ κ: Binding momentum, κ_0 in infinite volume
  - ⇒ For $\boldsymbol{d} = (0,0,0)$, $F(L,\kappa) = 6e^{-\kappa L} + 6\sqrt{2}e^{-\sqrt{2}\kappa L} + \frac{8}{\sqrt{3}}e^{-\sqrt{3}\kappa L}$
  - ⇒ Expand the Lüscher's formula for scattering states (analytical continuation) at the κ_0

- Leading order χEFT interaction: $V_{\text{contact}} + V_{1\pi}$
  - ⇒ $m_\pi = 138, 300, 450$ MeV, tuning the V_{contact} to permit bound states $B_d =$2, 10, 20 MeV
- Generate FV energy levels from PLW approach,
  - ⇒ Box size: $2.80, 3.3, 3.73, 4.0, 4.5, 5.0, 5.60, 6.0, 6.5, 7.0, 7.5, 8.0$ fm
  - ⇒ assign constant uncertainties
- Extract the B_d^{IFV} (κ_0) by fitting energy levels with above exponential relations

Bound state in the finite volume



Fit-I: All inputs; Fit-II: only orange points

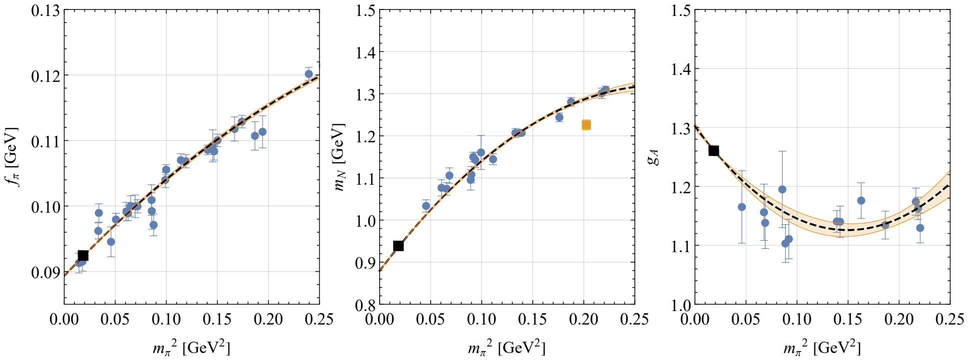
$$\kappa = \kappa_0 + \frac{Z^2}{L} F(L, \kappa_0) + \mathcal{O}(e^{-2\kappa L})$$

- The best fitting does not depend on constant uncertainties of E^{FV}
- The best fit of B_d^{fit}
  - $\Rightarrow$ biased
  - $\Rightarrow$ $B_d^{\text{fit}} > B_d^{\text{IFV}}$
  - $\Rightarrow$ Smaller m_π, larger bias
- Drop small box inputs decrease the bias
- The bias (small boxes, small m_π) is the chance of PLW method

Fitting the NPLQCD data

Pion-mass dependence

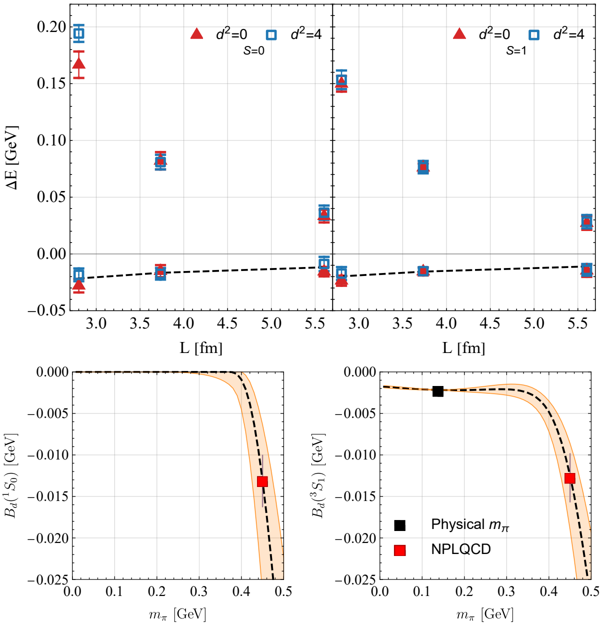
- NPLQCD data: $m_\pi = 450$ MeV — Orginos:2015aya,Illa:2020nsi
- For such a large pion mass, the validity of χEFT is questionable, a proof-of-principle
- Pion mass dependent of g_A, f_π, m_N from lattice QCD — Alexandrou:2013joa, Budapest-Marseille-Wuppertal:2013vij



Fitting results

- NPLQCD data Orginos:2015aya,Illa:2020nsi
- χEFT to NLO
- Contact terms:
  - $\Rightarrow C_i^{phy} \to C_i^{phy}[1 + a_i(1 - \frac{m^2}{m_{\text{phy}}^2})]$
  - $\Rightarrow$ reduce to physical one for $m = m_{\text{phy}}$
  - $\Rightarrow$ three a_i for $S = 1$
  - $\Rightarrow$ two a_i for $S = 0$
- Inputs: ground states

  $L = \{2.801, 3.734, 5.602\}$ fm $\otimes\ d^2 = \{0, 4\}$
- For S=1, χ^2/d.o.f $= 0.87$
- For S=0, χ^2/d.o.f $= 0.92$



Summary and Outlook

Summary and Outlook

- An alternative approach of Lüscher's formula to investigate NN in the box
  - ⇒ Plane wave expansions: include the partial wave mixing effect
  - ⇒ χEFT: benefit from the known long-range interaction $V_{1\pi}$, works well for small boxes
  - ⇒ Eigenvector continuation: accurate and fast, provides an interface
- Scattering states: high partial wave in QC is important, especially in small box
- Bound states: the exponential relations are biased in small box and small m_π
- Fitting to NPLQCD at $m_\pi =$450 MeV
- Outlook
  - ⇒ The advantages would be more obvious for physical m_π
  - ⇒ Refined analysis of pion mass dependence
  - ⇒ Used for D^*D, $D^*\bar{D}$ [T_{cc}, $X(3872)$] interaction

Thank you!

Back up

Bound states in FV...

Luscher formule

Davoudi:2011md

$$T^{-1} + iq = q\cot\delta(q) = \frac{2}{L\sqrt{\pi}}\mathcal{Z}_{00}(n_q^2) \tag{3}$$

Approx.1 Higher PW is neglected

bound states $q = i\kappa$

$$T^{-1}(\kappa) - \kappa = \frac{2}{L\sqrt{\pi}}\mathcal{Z}_{00}(-n_\kappa^2) = \frac{1}{L}F(L,\kappa) - \kappa \tag{4}$$

$$T^{-1}(\kappa) = \frac{1}{L}F(L,\kappa) \tag{5}$$

$$F(L,\kappa) = \sum_{\boldsymbol{m}\neq\boldsymbol{0}} \frac{1}{|\boldsymbol{m}|} e^{-\mathrm{i}2\pi\boldsymbol{m}\cdot\boldsymbol{d}} e^{-|\boldsymbol{m}|\kappa L}, \quad F \sim e^{-\kappa L} \tag{6}$$

Lüscher's formula

- Lippmann-Schwinger equation in FV: $T^L = K + KG_F T^L$ Luscher:1990ux,Polejaeva:2012ut

$$G_0^L(\boldsymbol{k}, z) = (\frac{2\pi}{L})^3 \sum_{\boldsymbol{p}} \frac{2\mu\delta^3(\boldsymbol{p}-\boldsymbol{k})}{\boldsymbol{p}^2 - q_0^2}, \quad G_F = G_0^L - G_K(\boldsymbol{k}, z) \tag{7}$$

- Partial wave expansion: l is not a good quantum number

$$\langle \boldsymbol{p}|T^L|\boldsymbol{q}\rangle = 4\pi \sum_{l'm'lm} Y_{l'm'}(\hat{\boldsymbol{p}}) T^L_{l'm',lm}(p,q,z) Y^*_{lm}(\hat{\boldsymbol{q}})$$

$$\langle \boldsymbol{p}|K|\boldsymbol{q}\rangle = 4\pi \sum_{lm} Y_{lm}(\hat{\boldsymbol{p}}) K_l(p,q,z) Y^*_{lm}(\hat{\boldsymbol{q}}), \quad \tan\delta_l(q_0) = \frac{\mu p}{2\pi} K_l(q_0, q_0; z)$$

- E^{FV} corresponding to poles of $T^L \Leftarrow \det[1 - KG_F] = 0$, interaction-independent

$$\det[F_{l'm',lm}] = 0 \Rightarrow \begin{vmatrix} F_{\Gamma_1} & & \\ & F_{\Gamma_2} & \\ & & \ddots \end{vmatrix} = 0, \quad \det[F_{\Gamma_i}] = 0 \tag{8}$$

- Truncate at some l, reduced to irreps. of cubic group (Projection operator technique)

Bound states in FV

$$T^{-1}(\kappa) = \frac{1}{L} F(L, \kappa) \tag{9}$$

$$T^{-1}(\kappa_0) = 0, \quad \kappa = \kappa_0 + \kappa_1 + \kappa_2 + .. \tag{10}$$

$$T^{-1}(\kappa) = 0 + T^{-1'}(\kappa_0)(\kappa_1 + \kappa_2) + ... = \frac{1}{L} F(L, \kappa_0) + \frac{1}{L} F'(L, \kappa_0)(\kappa_1) + ... \tag{11}$$

Approx 2. Ignoring Left-hand cut

$$\frac{1}{L} F(L, \kappa_0) = T'^{-1}(\kappa_0)\kappa_1, \quad \kappa_1 \sim e^{-\kappa L} \tag{12}$$

$$\kappa = \kappa_0 + \frac{Z^2}{L} F(L, \kappa_0) + \mathcal{O}(e^{-2\kappa L}) \tag{13}$$

Approx 3. The perturbation: precise up to $\mathcal{O}(e^{-2\kappa L})$

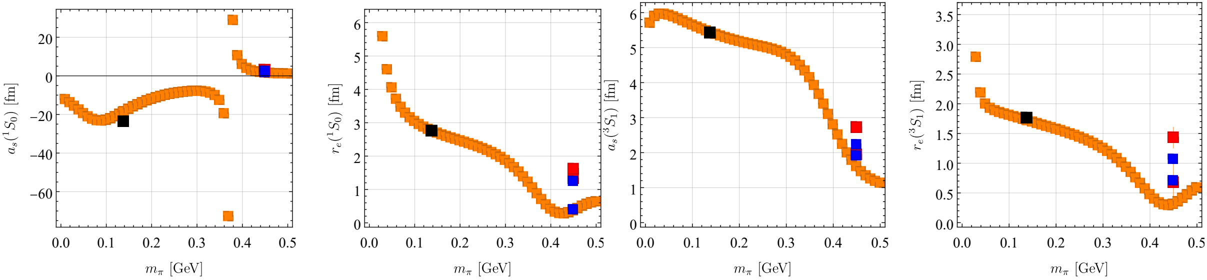
Bound states in FV

$$\kappa = \kappa_0 + \frac{Z^2}{L} F(L, \kappa_0) + \mathcal{O}(e^{-2\kappa L}) \tag{14}$$

$$\begin{aligned}
\boldsymbol{d} = (0,0,0) : & F(L,\kappa) = 6e^{-\kappa L} + 6\sqrt{2}e^{-\sqrt{2}\kappa L} + \frac{8}{\sqrt{3}}e^{-\sqrt{3}\kappa L}, \\
\boldsymbol{d} = (0,0,1) : & F(L,\kappa) = 2e^{-\kappa L} - 2\sqrt{2}e^{-\sqrt{2}\kappa L} - \frac{8e^{-\sqrt{3}\kappa L}}{\sqrt{3}}
\end{aligned} \tag{15}$$

Approx 4. Truncation of the $F(L, \kappa)$

effective range parameter



Non-interacting systems

- Two particles on-shell, Lorentz boost to CMF

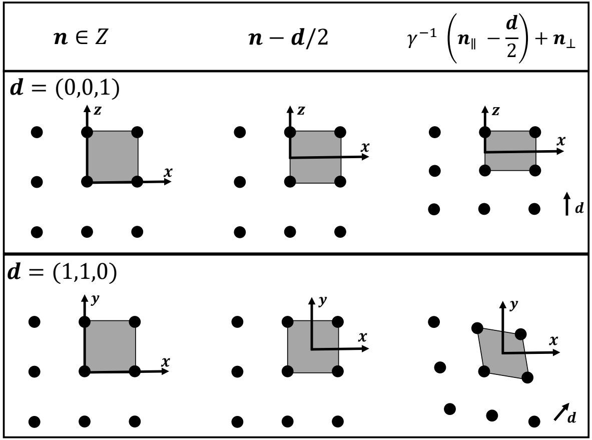
Rummukainen:1995vs,Leskovec:2012gb

$$\boldsymbol{p}_1^* = \gamma^{-1}\left(\boldsymbol{p}_{1\parallel} - \frac{1}{2}A\boldsymbol{P}\right) + \boldsymbol{p}_{1\perp}, \quad A \equiv 1 + \frac{m_1^2 - m_2^2}{E^{*2}}, \quad \gamma = \frac{\sqrt{E^{*2} + P^2}}{E^*} \tag{16}$$

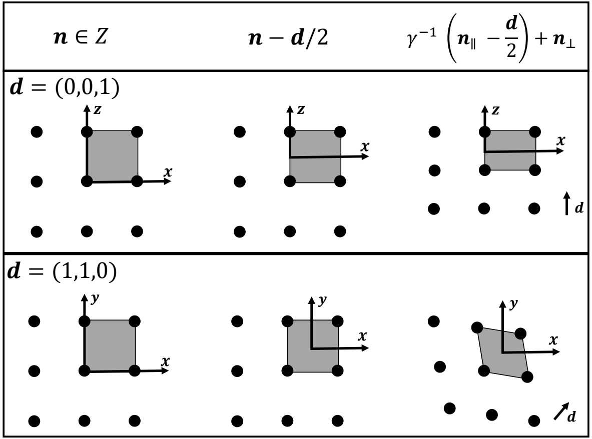
- If $m_1 \neq m_2$, no space inversion symmetry

Ziwen Fu, Phys.Rev.D85,014506; Leskovec:2012gb

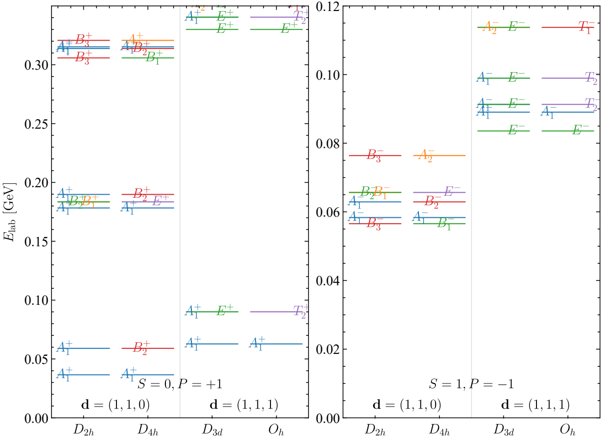
- Focus on $m_1 = m_2$ with parity
- $\boldsymbol{d} = (0, 0, 1)$, D_{4h} group
- $\boldsymbol{d} = (1, 1, 0)$, D_{2h} group
- $\boldsymbol{d} = (1, 1, 1)$, D_{3d} group
- For non-relativistic system $\gamma = 1$



Irreps

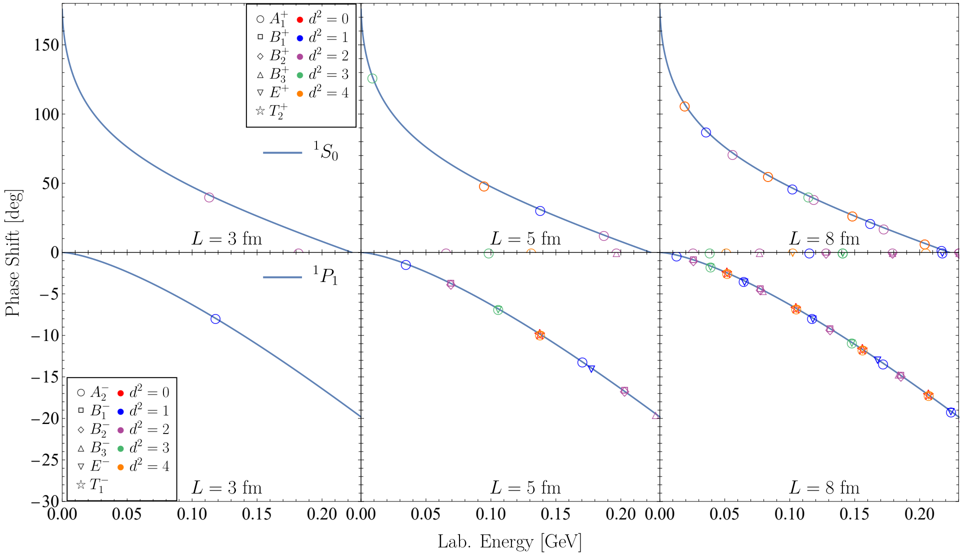


n ∈ Z
n − d/2
γ⁻¹ (n∥ − d/2) + n⊥
d = (0,0,1)
d = (1,1,0)
z
x
y
d

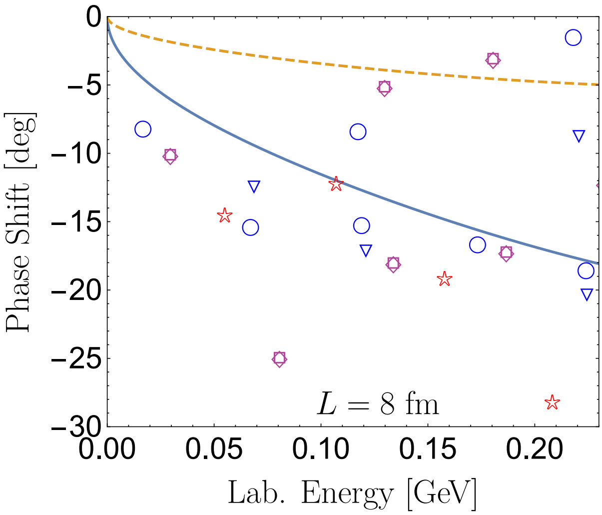


E_lab [GeV]
S = 0, P = +1
S = 1, P = −1
d = (1, 1, 0)
d = (1, 1, 1)
D_2h
D_4h
D_3d
O_h

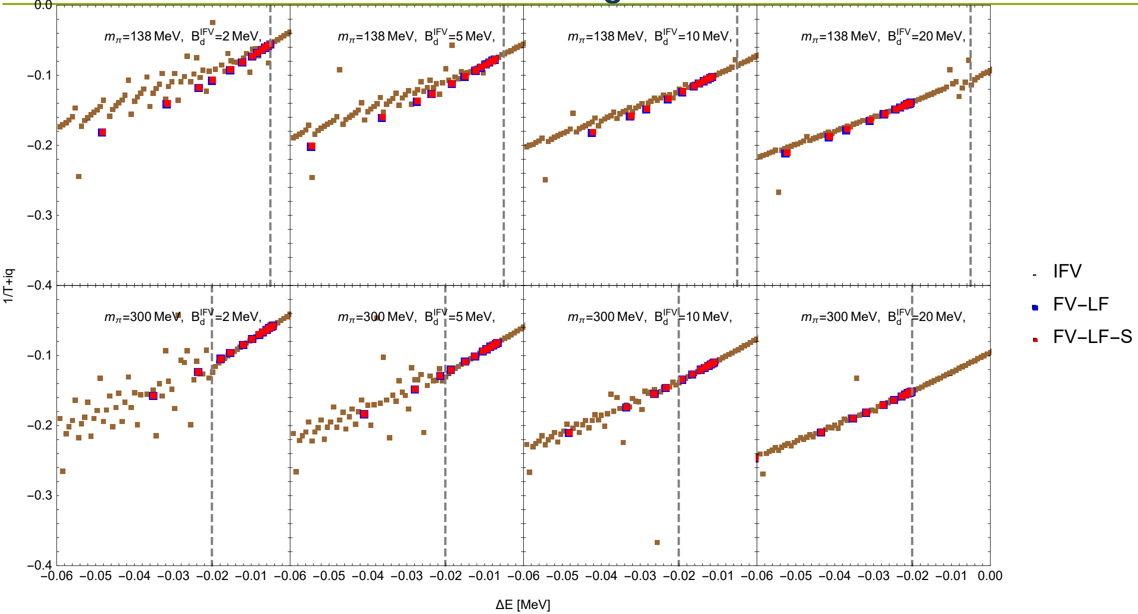
Partial-wave-contact



Partial-wave-P-wave



Partial-wave mixing for bound states



Partial-wave mixing for bound states