HISKP
Theory Seminar
Universität Bonn

RUHR UNIVERSITÄT BOCHUM RUB

Finite volume NN system using plane wave expansion and eigenvector continuation

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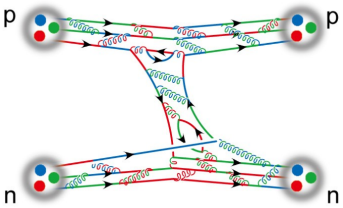
Contents

Introduction

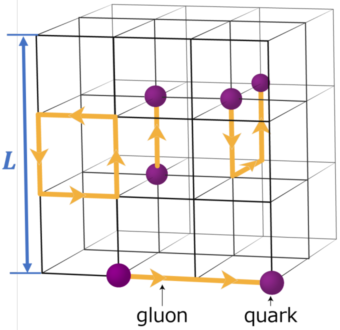
lattice QCD and finite volume energy levels

- QCD is the fundamental theory of the strong interaction

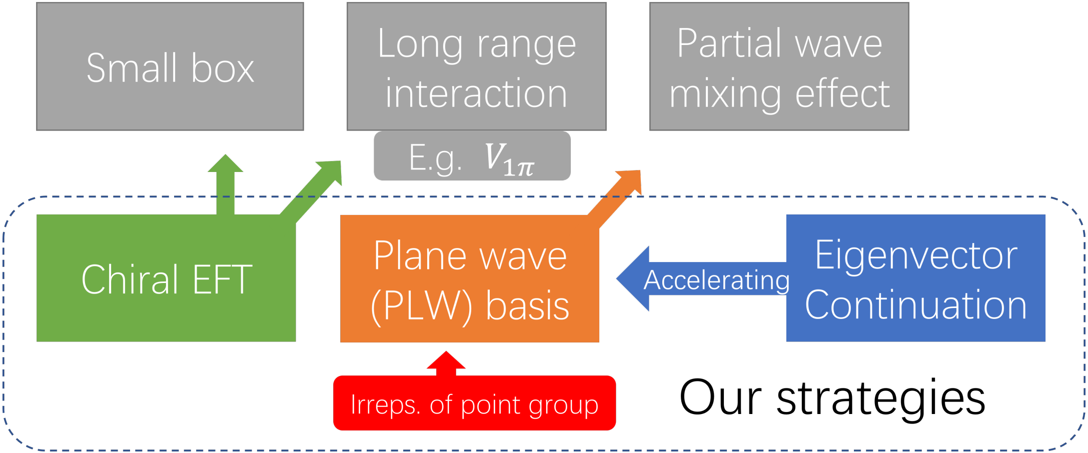
$$\mathcal{L}_{QCD} = \sum_f \bar{q}_f (i\not{D} - \mathcal{M} q_f) - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu,a} \tag{1}$$



- 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 observables 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



Beyond Lüscher's formula



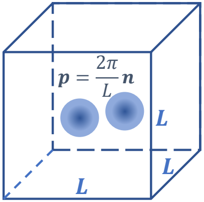
Lüscher's formula

Quantization of momentum

- boundary conditions in the cubic box

$$\psi(\mathbf{x}_1, \mathbf{x}_2) = \psi(\mathbf{x}_1 + \mathbf{n}_1 L, \mathbf{x}_2 + \mathbf{n}_2 L) \quad (2)$$

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



- $\boldsymbol{d} = (0, 0, 0)$: cubic group O_h
- The rotation symmetry is broken: $SO(3) \to O_h$

$\Rightarrow$ $\{l, m\}$ are not good quantum numbers to label states

$\Rightarrow$ The FV energy should be classified by irreducible representations (irrepss.) of O_h group

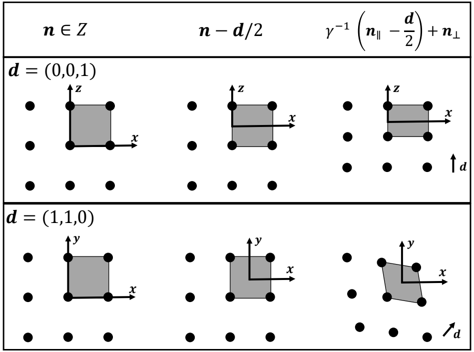
$$\{l, m\} \to \{A_1, A_2, E, T_1, T_2\}$$

$\Rightarrow$ Partial wave mixing: for $l \neq l$ and $m \neq m'$

$$\langle lm|H^{FV}|l'm'\rangle \neq 0$$

Moving system

- Moving system in the box $\boldsymbol{d} \neq 0$
  - $\Rightarrow$ For LQCD, changing box size is expensive
  - $\Rightarrow$ Calculate E^{FV} of moving two-body systems in a box
- box frame (BF) and center of mass frame (CMF)
- The mesh of momentum in CMF (Focus on $m_1 = m_2$)
  - $\Rightarrow$ $\boldsymbol{d} = (0, 0, 1)$, D_{4h} group
  - $\Rightarrow$ $\boldsymbol{d} = (1, 1, 0)$, D_{2h} group
  - $\Rightarrow$ $\boldsymbol{d} = (1, 1, 1)$, D_{3d} group
  - $\Rightarrow$ ...



Rummukainen:1995vs,Leskovec:2012gb

Lüscher's formula

- Lippmann-Schwinger equation in the finite volume

Luscher:1990ux,Polejaeva:2012ut

$$T^L(\boldsymbol{p},\boldsymbol{q};z) = V(\boldsymbol{p},\boldsymbol{q}) + \int \frac{d^3\boldsymbol{k}}{(2\pi)^3} V(\boldsymbol{p},\boldsymbol{q}) G_0^L(\boldsymbol{k};z) T(\boldsymbol{k};z)$$

$$G_0^L(\boldsymbol{k},z) = (\frac{2\pi}{L})^3 \sum_{\boldsymbol{p}\in\frac{2\pi}{L}\boldsymbol{n}} \frac{2\mu\delta^3(\boldsymbol{p}-\boldsymbol{k})}{q_0^2-\boldsymbol{p}^2} = \text{P.V.}\frac{2\mu}{q_0^2-\boldsymbol{k}^2} + G_F(\boldsymbol{k},z) = G_K(\boldsymbol{k},z) + G_F(\boldsymbol{k},z)$$

with $z = m_1 + m_2 + \frac{q_0^2}{2\mu}$.

- The "$=$" relation is valid up to the exponentially suppressed terms in L
- K matrix in the infinite volume: $K = V + VG_K K$

$$T^L = V + V(G_K + G_F)T^L = K + KG_F T^L$$

- E^{FV} corresponding to poles of T^L : interaction-independent form

$$\det[1-KG_F] = 0, \text{ or } \det[G_F - K^{-1}]=0$$

- Expanding it in partial wave basis

$$\det[G_F - K^{-1}] = 0, \Rightarrow \det[M_{l'm',lm} - \delta_{ll'}\delta_{mm'} \cot\delta_l] = 0 \tag{4}$$

$\Rightarrow$ Determinate equation of a matrix with infinite dimensions.

$\Rightarrow$ Truncate at some l_{max}

- Reduce to irreps. Γ_i of point group

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

$\Rightarrow$ Obtain the basis of the irreps. $|lm\rangle \to |\Gamma, l, \alpha\rangle$ (Projection operator technique) Bernard:2008ax

- Lüscher quantization conditions: $\det\left[M^{(\Gamma,\boldsymbol{P})}_{ln,l'n'} - \delta_{ll'}\delta_{nn'}\cot\delta_l\right] = 0$

Luscher:1990ux,Rummukainen:1995vs,Feng:2004ua,Kim:2005gf,Fu:2011xz,Polejaeva:2012ut,Leskovec:2012gb,Gockeler:2012yj,...

Lüscher's formula

- Example $\boldsymbol{d} = (0,0,1)$, $\Gamma = A_1^+$, w_{lm} depends on E but independent on V

$$\det\left[M^{(\Gamma,\boldsymbol{P})}_{ln,l'n'} - \delta_{ll'}\delta_{nn'}\cot\delta_l\right] = 0, \quad M^{(A_1^+,\boldsymbol{d})} = \begin{bmatrix} w_{00} & -\sqrt{5}w_{20} & \cdots \\ -\sqrt{5}w_{20} & w_{00} + \frac{10}{7}w_{20} + \frac{18}{7}w_{40} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \tag{5}$$

- Truncate at $l_{max} = 0$, one-to-one relation: $\delta_0(E^{FV}) \sim E^{FV}$
- Truncate at $l_{max} > 0$, no one-to-one relations
  - $\Rightarrow$ E.g $\{E_1^{FV}, E_2^{FV}\} \not\Rightarrow \{\delta_S(E_1^{FV}), \delta_S(E_2^{FV}), \delta_D^{FV}(E_1^{FV}), \delta_D^{FV}(E_2^{FV})\}$
  - $\Rightarrow$ One has to parameterize K-matrix: effect range expansion, ..., framework-dependent
  - $\Rightarrow$ root-finding algorithm
- Lüscher's formula: quantization conditions in partial wave basis
- Why not quantization conditions in plane wave basis + Hamiltonian method?

Beyond Lüscher's formula

- One possible reason to prevent us from the quantization conditions in plane wave basis:

  $\Rightarrow$ The dimensions of the matrix could be large~$\mathcal{O}(1000)$

- Hamiltonian method of Adelaide group

  Hall:2013qba,Wu:2014vma,Liu:2015ktc,Li:2021mob

$$T_l(p,q) = V_l(p,q) + \int dp' p'^2 V_l(p,p') \frac{2\mu}{k^2 - p'^2 + i\epsilon} T_l(p',q)$$

$$T_l^L(p_m,p_n) = V_l(p_m,p_n) + \left(\frac{2\pi}{L}\right)^3 \sum_i \frac{C_3(i)}{4\pi} p_i^2 V_l(p_m,p_i) \frac{2\mu}{k^2 - p_i^2} T_l^L(p_i,p_n)$$

  $C_3(n)$: No. of ways of get $a^2+b^2+c^2=n$; a,b,c are integers

  $\Rightarrow$ The dimensions of the matrix is reduced

  $\Rightarrow$ Become complicate for the moving systems

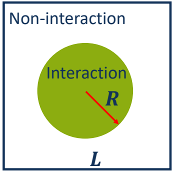
  $\Rightarrow$ Based on partial wave decomposition, hard to consider partial wave mixing effect

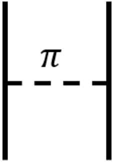
- Our strategies: plane wave expansion + eigenvector continuation

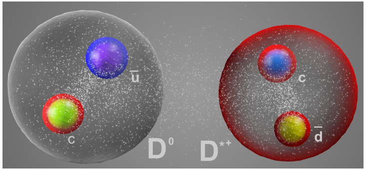
Beyond Lüscher's formula

- Lüscher's quantization condition become exact $L \gg R$, negligible $e^{-L/R}$ effect
  - $\Rightarrow$ Long range interaction could be very important: one-pion exchange
  - $\Rightarrow$ size of T_{cc} state: 7.5 ± 0.4 fm, VS LQCD simulation box e.g. $L \sim 2$ fm or 2.7 fm

    LHCb:2021auc,Padmanath:2022cvl

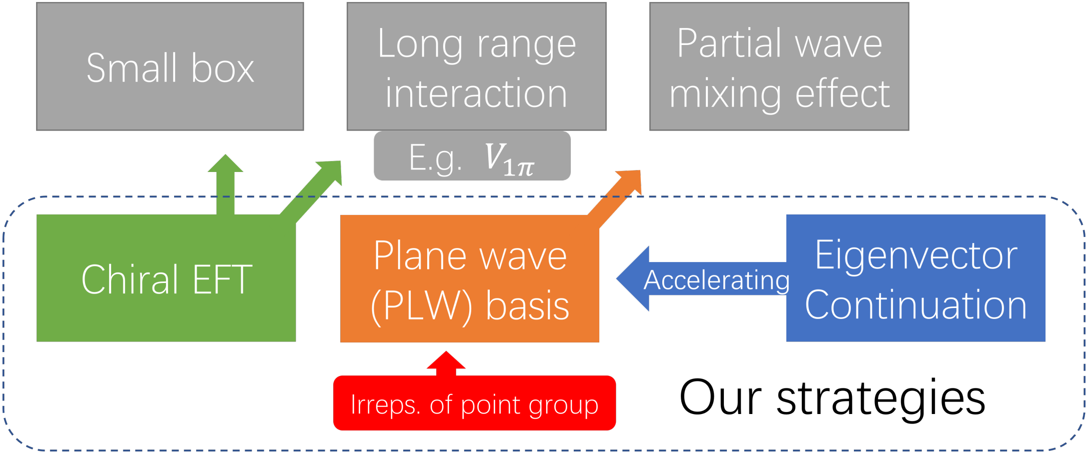






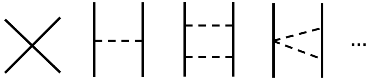
- Chiral EFT with one-pion exchange interaction

Beyond Lüscher's formula



Theoretical formalism

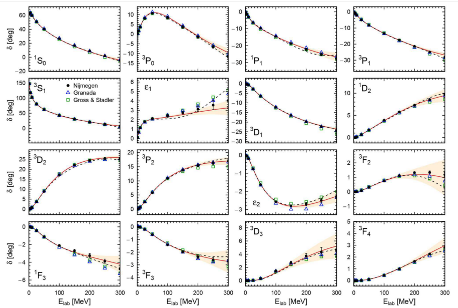
NN interaction: chiral EFT



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

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

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

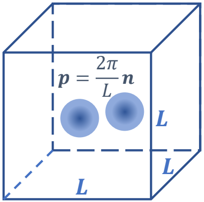


- Benefit from the known long-range interaction $V_{1\pi}$
- Low energy constants (LECs) for short-range interaction (contact interaction)
  - $\Rightarrow$ fitting lattice QCD data
  - $\Rightarrow$ $\#$ of LECs: $V^{(0)}$(+2),$V^{(2)}$(+7),$V^{(4)}$(+12); for specific irreps, the $\#$ will be small

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

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

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



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

  $\Rightarrow\ \{0,0,0\}_{1\times3}, \{0,0,a\}_{6\times3}, \{0,a,a\}_{12\times3}, \{0,a,b\}_{24\times3}...$

- 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: $\{0,0,a\}_{6\times3} = 2T_1^+ \oplus T_2^+ \oplus A_1^- \oplus E_1^- \oplus T_1^- \oplus T_2^-$
- 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

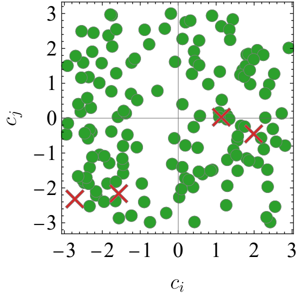
- dim of the $\mathbb{H}_\Gamma$: cubic function of L^{-1}

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

Towards a practical approach: eigenvector continuation

- Plane wave basis+Eigenvector continuation

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



- Rayleigh-Ritz variational principle:

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

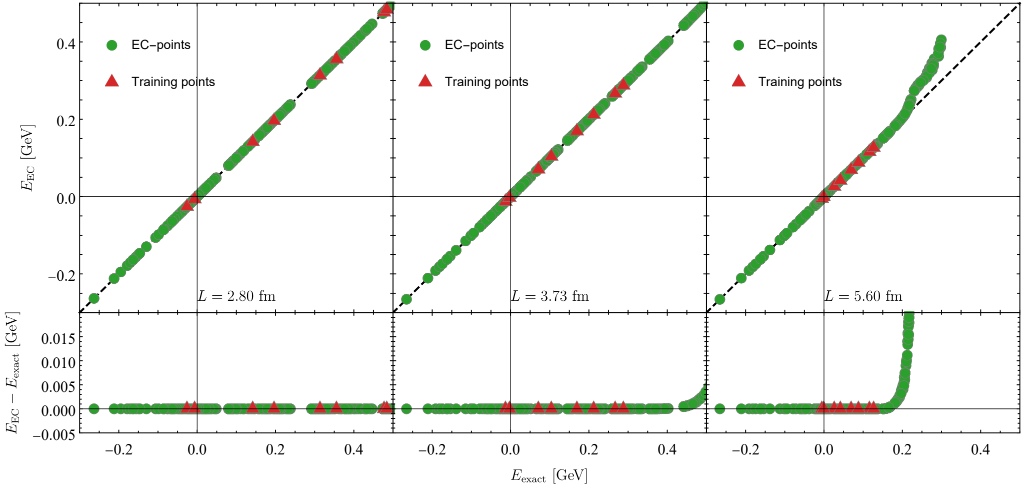
$$|\psi\rangle = a_m|\phi_m\rangle, \quad \langle\phi_m|H(c_i)|\phi_n\rangle a_n = \mathcal{E}\langle\phi_m|\phi_n\rangle a_n$$

  $\Rightarrow$ 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

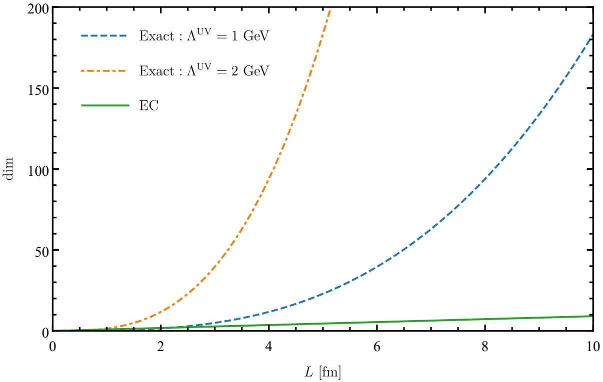
- Interaction: V_{contact} with 2 LECs $\{c_1, c_2\}$ + $V_{1\pi}$ in $L = \{2.70, 3.73, 5.60\}$ boxes
- Training points: $\{c_1^{\text{phy}}, 0\}$, $\{0, c_2^{\text{phy}}\}$; keep the first four energy levels as basis, dim=8



Eigenvector continuation

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

- dim is linear function $\frac{1}{L}$: linear VS cubic
- $\text{dim}^{EC} \sim \mathcal{O}(10)$
- 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

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

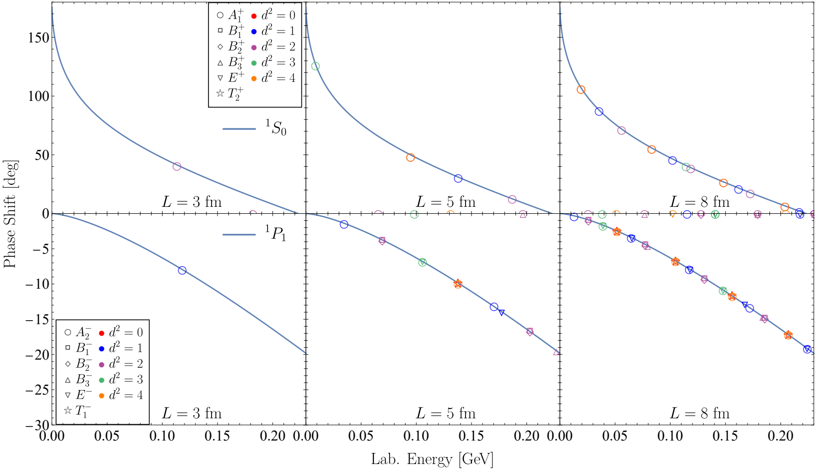
$\Rightarrow$ Easy-to-use interface: no need to know the details of χEFT

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)

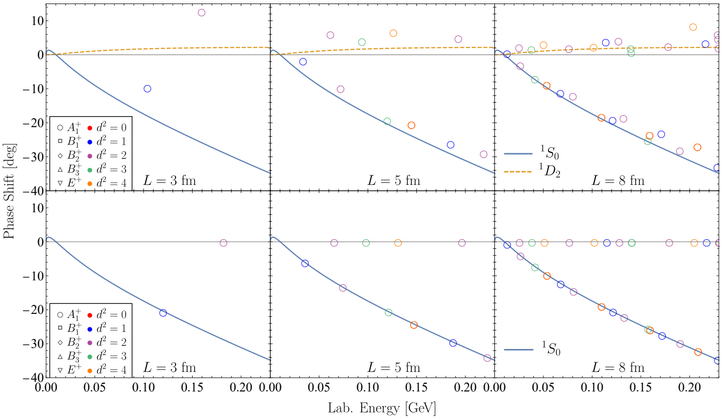
Larger L, denser E^{FV}s

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:

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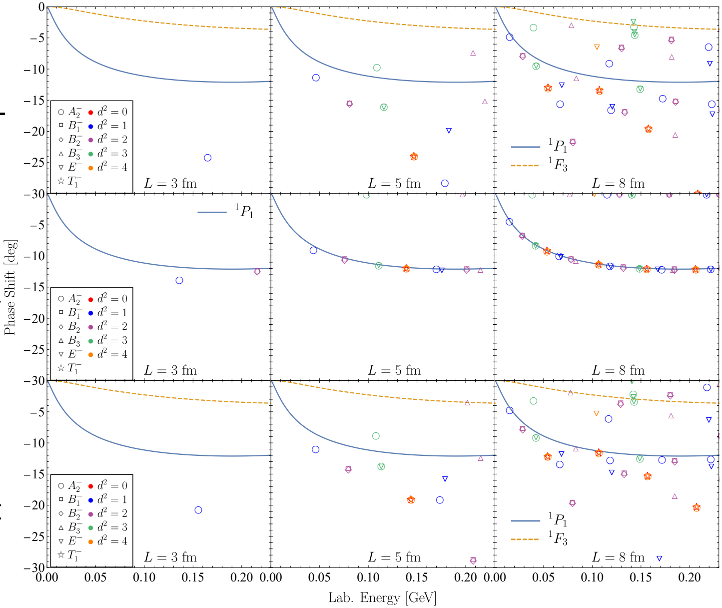
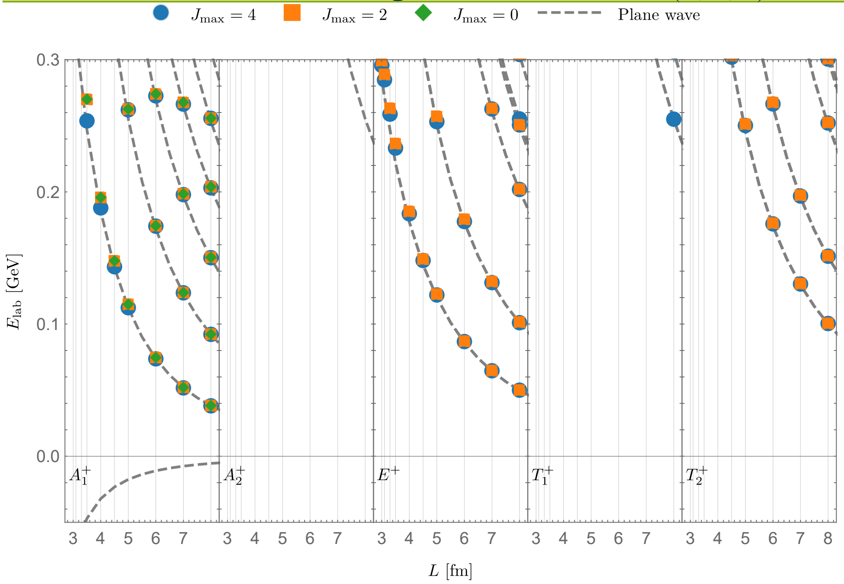


Scattering state: $S=0$, $d=(0,0,0)$, even-parity



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

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

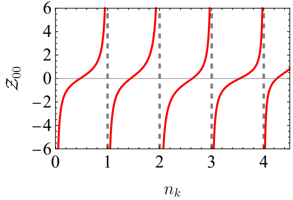
  - $\Rightarrow$ δ as input, truncated at different J_{max},
  - $\Rightarrow$ root-finding:

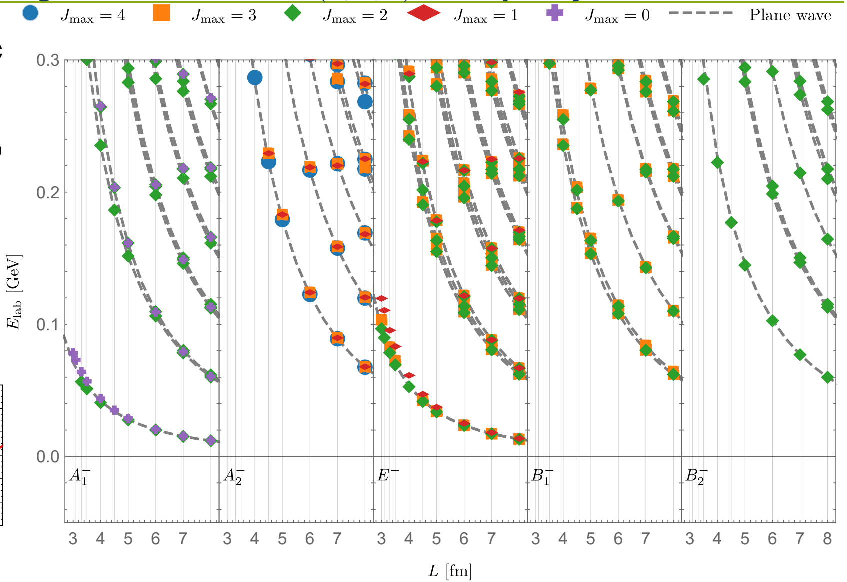
Woss:2020cmp,HSC

$L=$ {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

$$\kappa = \kappa_0 + \frac{Z^2}{L} F(L, \kappa_0) + \mathcal{O}(e^{-2\kappa L}) \tag{6}$$

  $\Rightarrow$ κ: Binding momentum, κ_0 in infinite volume

  $\Rightarrow$ For $\boldsymbol{d} = (0,0,0)$, $F(L,\kappa) = 6e^{-\kappa L} + 6\sqrt{2}e^{-\sqrt{2}\kappa L} + \frac{8}{\sqrt{3}}e^{-\sqrt{3}\kappa L}$

  $\Rightarrow$ Expand the Lüscher's formula for scattering states (analytical continuation) at the κ_0

- Leading order χEFT interaction: $V_{\text{contact}} + V_{1\pi}$

  $\Rightarrow$ $m_\pi = 138, 300, 450$ MeV, tuning the V_{contact} to permit bound states B_d =2, 10, 20 MeV

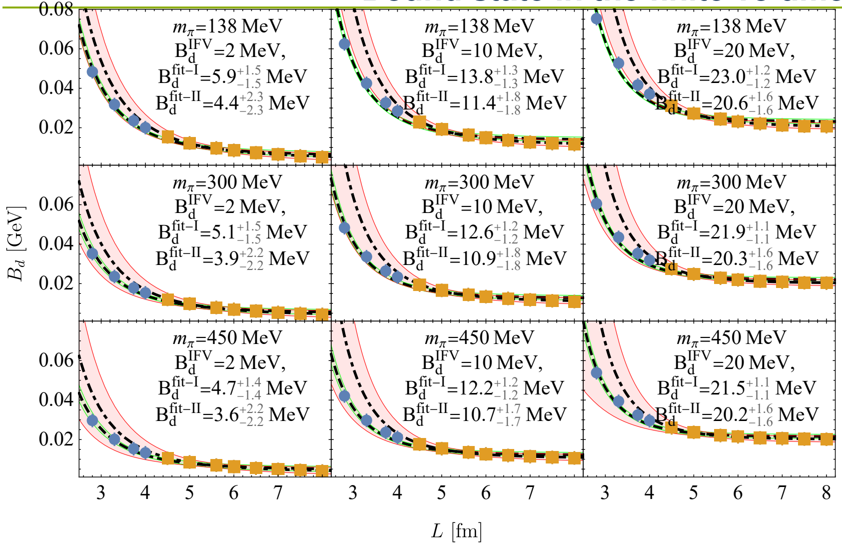
- Generate FV energy levels from PLW approach,

  $\Rightarrow$ 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

  $\Rightarrow$ 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

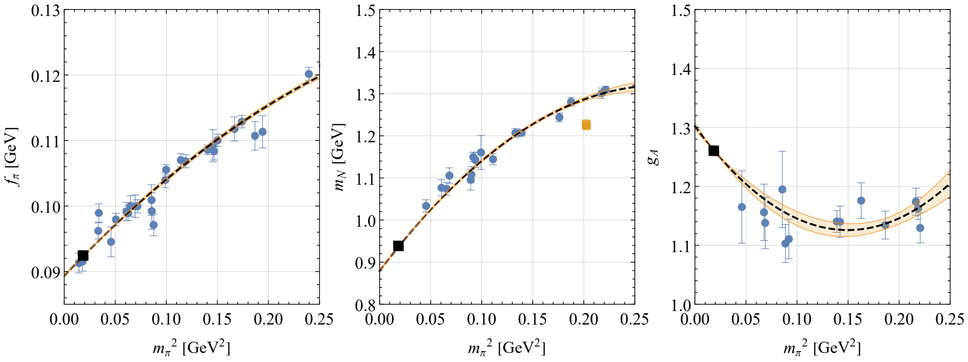
$$\kappa = \kappa_0 + \frac{Z^2}{L} F(L, \kappa_0) + \mathcal{O}(e^{-2\kappa L})$$

- 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

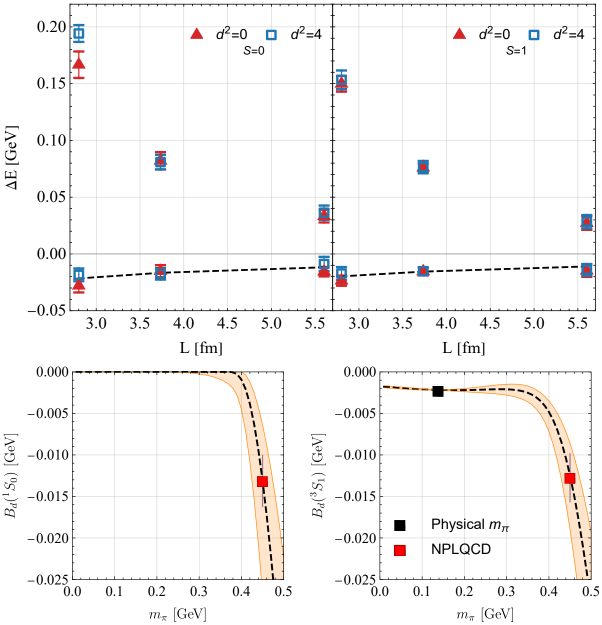
- NPLQCD data: $m_\pi = 450$ MeV — Orginos:2015aya,Illa:2020nsi
- For such a large pion mass, the validity of χEFT is questionable, a proof-of-principle
- Pion mass dependent of g_A, f_π, m_N from lattice QCD — Alexandrou:2013joa, Budapest-Marseille-Wuppertal:2013vij



Fitting results

- NPLQCD data Orginos:2015aya,Illa:2020nsi
- χEFT to NLO
- Contact terms:
  - $\Rightarrow C_i^{phy} \rightarrow C_i^{phy}[1 + a_i(1 - \frac{m^2}{m^2_{\text{phy}}})]$
  - $\Rightarrow$ 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, $\chi^2/\text{d.o.f} = 0.87$
- For S=0, $\chi^2/\text{d.o.f} = 0.92$



Summary and Outlook

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- 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_π =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!