The 39th International Symposium on Lattice Field theory (Lattice 2022)
Bonn, Germany, from August 8 to August 13

RUHR UNIVERSITÄT BOCHUM RUB

Finite volume NN system using plane wave exansion and eigenvector continuation

Lu Meng (孟 璐)

Ruhr-Universität Bochum

11 August, 2022

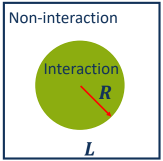
Based on papaer in preparation

Together with Evgeny Epelbaum (RUB)

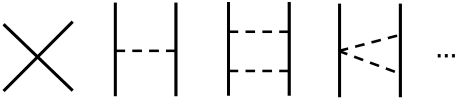
Contents

Lüscher's formula and beyond

- Lüscher's formula (LF) Luscher:1990ux
  - $\Rightarrow$ To include partial wave (PW) mixture effect: $\det[M^{\Gamma}_{l,l'} - K^{-1}] = 0$, ~~one-to-one~~, parameterize T-matrix, root-finding algorithm
  - $\Rightarrow$ $L \gg R$, negligible $e^{-L/R}$ effect



- Long-range interaction: e.g. 1-π exchange for NN and $\bar{D}^* D/\bar{D}D^*[X(3872)]$ Sato:2007ms,Jansen:2015lha
  - $\Rightarrow$ Non-relativistic approx. is good for NN force (No cross symmetry, no t-cut) Raposo's talk
- (1)Plane wave (PLW) expansion +(2) Chiral effective field theory (EFT): Meng:2021uhz
  - $\Rightarrow$ Including partial mixing conveniently, works well for small box and long-rang interaction
- Make the approach practical
  - $\Rightarrow$ (3)Eigenvector continuation
  - $\Rightarrow$ Compare it with Lüscher's formula
  - $\Rightarrow$ Fit NPLQCD results at $m_\pi = 0.45$ GeV

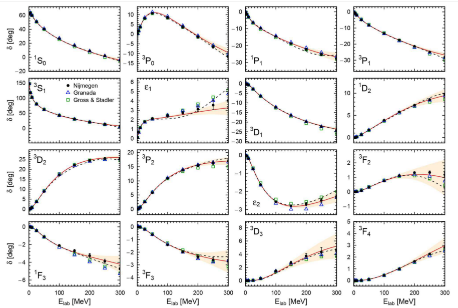


Theoretical formalism

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 potential
- Semilocal momentum-space regularization Reinert:2017usi

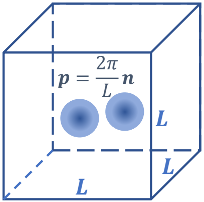


$$V_{1\pi}(\vec{p}', \vec{p}) = -\frac{g_A^2}{4F_\pi^2}\left(\frac{\vec{\sigma}_1 \cdot \vec{q}\vec{\sigma}_2 \cdot \vec{q}}{q^2 + m_\pi^2} + C(m_\pi)\vec{\sigma}_1 \cdot \vec{\sigma}_2\right) e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}$$

- Benefit from the known long-range interaction one-pion-exhcange (OPE)
- Low energy constants (LECs) for short-range interaction (contact interaction)

  $\Rightarrow$ fitting lattice QCD data

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 $S = 1$

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

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

- $\{|\boldsymbol{p}_n, \boldsymbol{\eta}\rangle\}$ form the representation space of corresponding point group
- Finite volume energy levels: eigenvector problem

$$\det\left(\mathbb{H} - E\mathbb{I}\right) = 0 \quad \text{or} \quad \mathbb{H}\boldsymbol{v} = E\boldsymbol{v} \qquad (1)$$

- Lüscher formula is the quantization condition (QC) in partial wave basis

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

- We now get the QC in plane wave (PLW) expansion

  $\Rightarrow$ eigenvector problem is easier to be solved than a general root-finding problem

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

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

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

- Reduce to irreducible representations (irreps): projection operator

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

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

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

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

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

$$\dim \sim \left(\frac{\Lambda_{\text{UV}}}{2\pi/L}\right)^3 \times \frac{1}{12} \sim \mathcal{O}(1000)$$

Towards a practical approach: eigenvector continuation

- Plane wave basis+Eigenvector continuation   W.Detmold'S talk: Gaussian basis+ impoved stochastic variational method

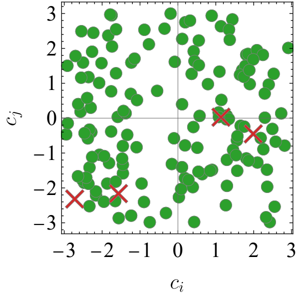
  $\Rightarrow$ Eigenvector continuation (EC) with subspace learning Frame:2017fah,Demol:2019yjt,Furnstahl:2020abp,Yapa:2022nnv

- Rayleigh-Ritz variational principle:

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

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

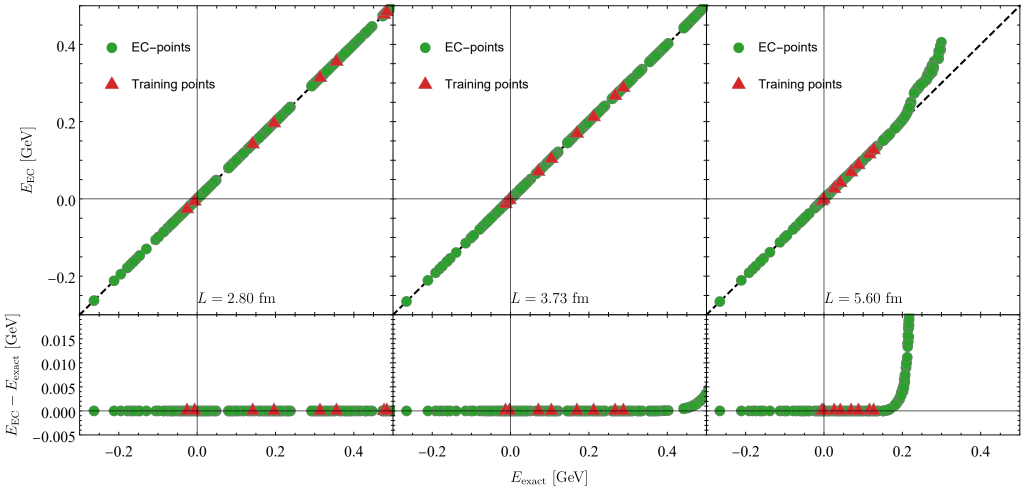
  $\Rightarrow$ Generalized to excited state



- To fit or quantify uncertainty: solve above Eqs. with different $\{c_i\}$ repeatly
- 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

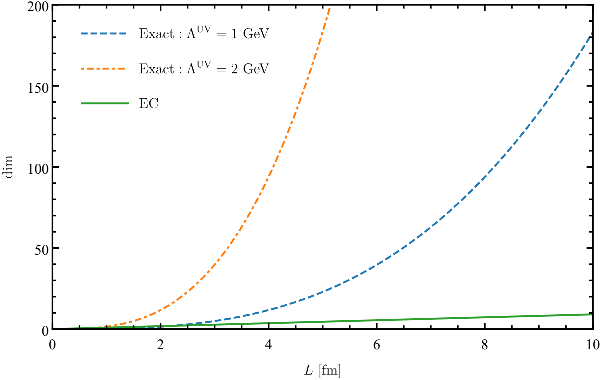
- Interaction: V_{contact} with 2 LECs $\{c_1, c_2\}$ + $V_{1\pi}$ in $L = \{2.70, 3.73, 5.60\}$ boxes
- Training points: $\{c_1^{\text{phy}}, 0\}$, $\{0, c_2^{\text{phy}}\}$; keep the first four energy levels as basis, dim=8



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



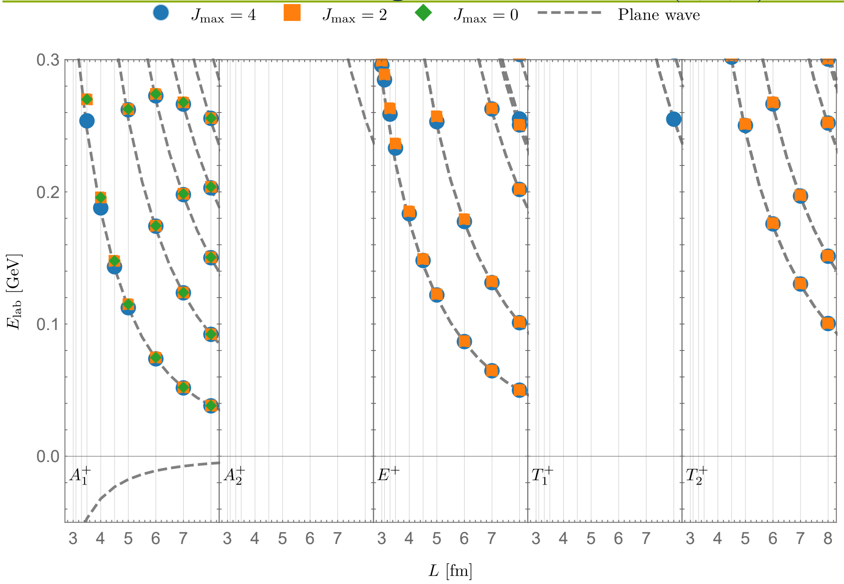
- After subspace learning, we can provide the $\mathbb{H}_0^{EC}$ and $\mathbb{V}_i^{EC}$ to the lattice community

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

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

Scattering states: Lüscher formula VS PLW

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



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

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

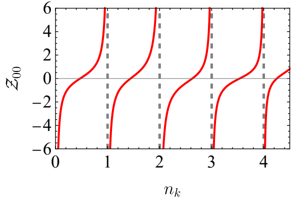
  - $\Rightarrow$ δ as input, truncated at different J_{max},
  - $\Rightarrow$ root-finding:

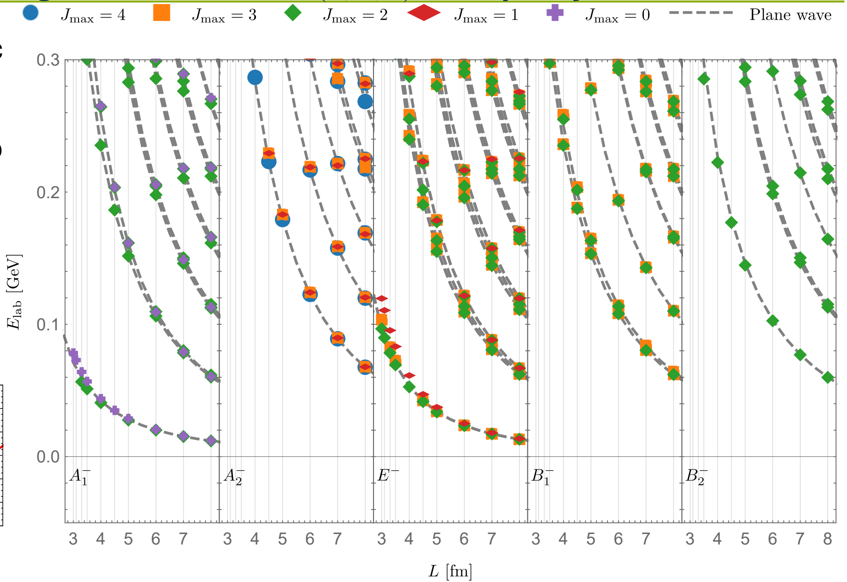
Woss:2020cmp,HSC

$L=$ {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 be large difference δ

Bound states: Lüscher formula VS PLW

Bound state in the finite volume

- Bound state Lüscher 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 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

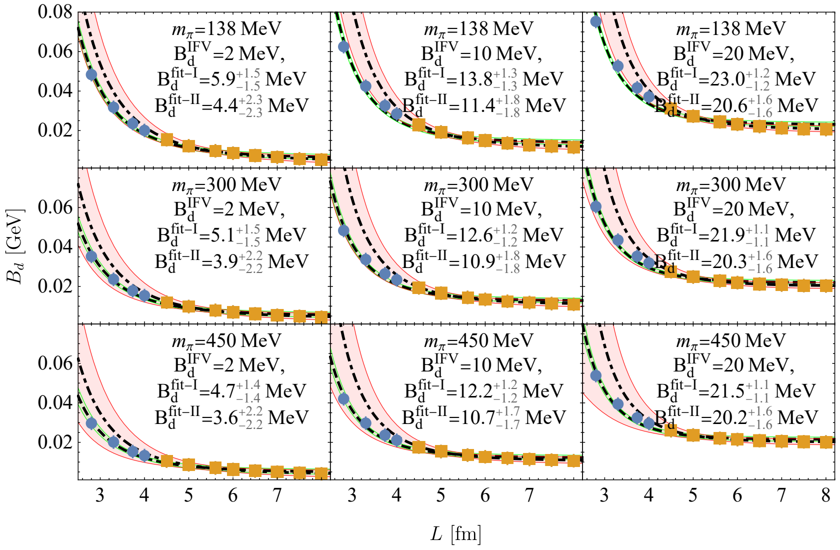
- Generate FV energy levels from PLW approach,

  ⇒ 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



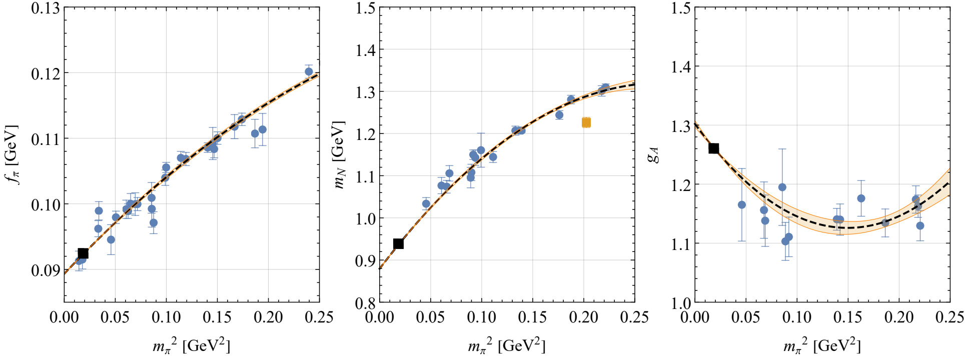
Fit-I: All inputs; Fit-II: only orange points

- 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) is the chance of PLW method

Fitting the NPLQCD data

Pion-mass dependence

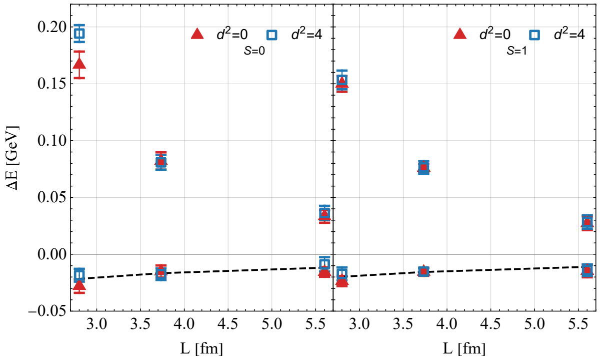
- NPLQCD data: $m_\pi = 450$ MeV Orginos:2015aya,Illa:2020nsi
- For such a large pion mass, the validity of χEFT is questionable, a proof-of-principle
- Pion mass dependent of g_A, f_π, m_N from lattice QCD Alexandrou:2013joa, Budapest-Marseille-Wuppertal:2013vij

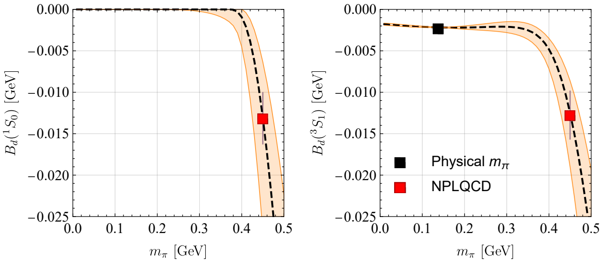


Fitting results

- NPLQCD data Orginos:2015aya,Illa:2020nsi
- χEFT to NLO
- Contact terms:
  - $\Rightarrow C_i^{phy} \to C_i^{phy}(1 - a_i \frac{m^2}{m^2_{\text{phy}}})$
  - $\Rightarrow$ 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

Summary and Outlook

- A alternative approach of Luscher 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 box
  - ⇒ Eigenvector continuation: accurate and fast, provide a interface
- Scattering states: high partial wave in QC is important, especially in small box
- Bound states: the exponential relations is 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 (T_{cc}) and $D^*\bar{D}$ [$X(3872)$]interaction ... Related talks: S.Prelovsek;S.Aoki...

Thanks!

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 $q = i\kappa$

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

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

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

Bound states in FV

$$T^{-1}(\kappa) = \frac{1}{L} F(L, \kappa) \tag{7}$$

$$T^{-1}(\kappa_0) = 0, \quad \kappa = \kappa_0 + \kappa_1 + \kappa_2 + .. \tag{8}$$

$$T^{-1}(\kappa) = 0 + T^{-1'}(\kappa_0)(\kappa_1 + \kappa_2) + ... = \frac{1}{L} F(L, \kappa_0) + \frac{1}{L} F'(L, \kappa_0)(\kappa_1) + ... \tag{9}$$

Approx 2. Ignoring Left-hand cut

$$\frac{1}{L} F(L, \kappa_0) = T'^{-1}(\kappa_0)\kappa_1, \quad \kappa_1 \sim e^{-\kappa L} \tag{10}$$

$$\kappa = \kappa_0 + \frac{Z^2}{L} F(L, \kappa_0) + \mathcal{O}(e^{-2\kappa L}) \tag{11}$$

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

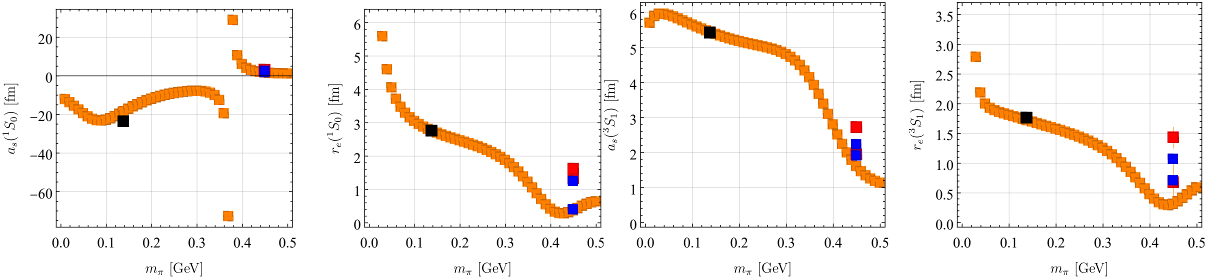
Bound states in FV

$$\kappa = \kappa_0 + \frac{Z^2}{L} F(L, \kappa_0) + \mathcal{O}(e^{-2\kappa L}) \tag{12}$$

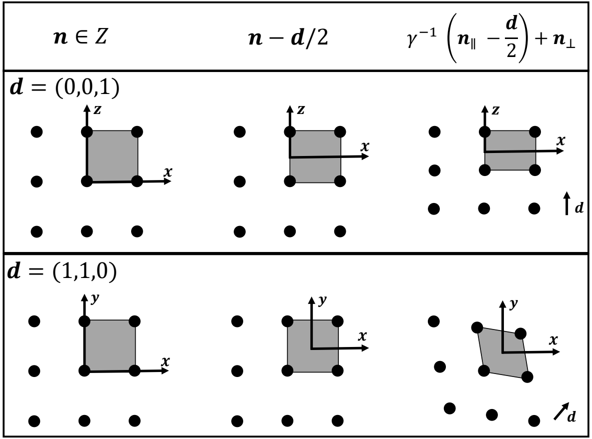
$$\begin{aligned} \boldsymbol{d} = (0,0,0) :& F(L,\kappa) = 6e^{-\kappa L} + 6\sqrt{2}e^{-\sqrt{2}\kappa L} + \frac{8}{\sqrt{3}} e^{-\sqrt{3}\kappa L}, \\ \boldsymbol{d} = (0,0,1) :& F(L,\kappa) = 2e^{-\kappa L} - 2\sqrt{2}e^{-\sqrt{2}\kappa L} - \frac{8e^{-\sqrt{3}\kappa L}}{\sqrt{3}} \end{aligned} \tag{13}$$

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

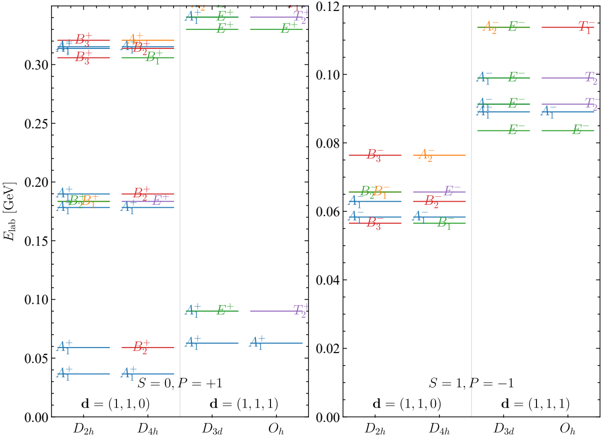
effective range parameter



Irreps

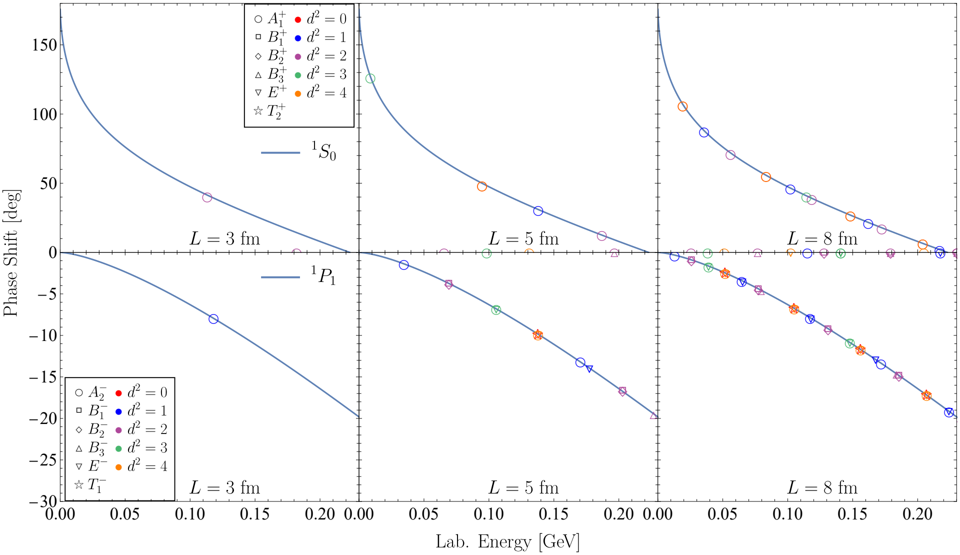


$\boldsymbol{n} \in Z$
$\boldsymbol{n} - \boldsymbol{d}/2$
$\gamma^{-1}\left(\boldsymbol{n}_\parallel - \frac{\boldsymbol{d}}{2}\right) + \boldsymbol{n}_\perp$
$\boldsymbol{d} = (0,0,1)$
$\boldsymbol{d} = (1,1,0)$

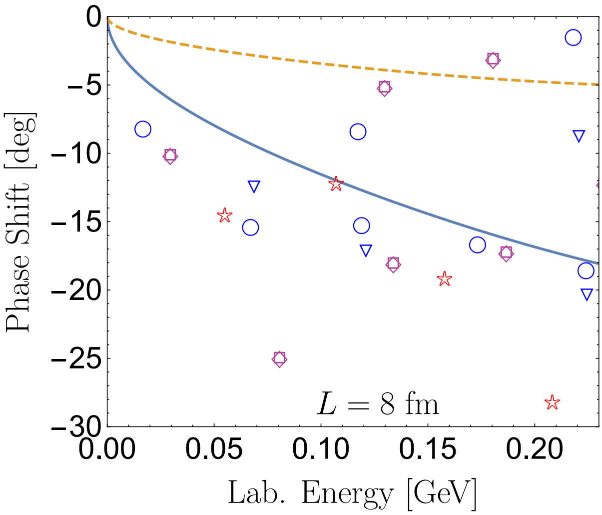


E_{lab} [GeV]
$S = 0, P = +1$
$S = 1, P = -1$
$\mathbf{d} = (1,1,0)$
$\mathbf{d} = (1,1,1)$
D_{2h}
D_{4h}
D_{3d}
O_h

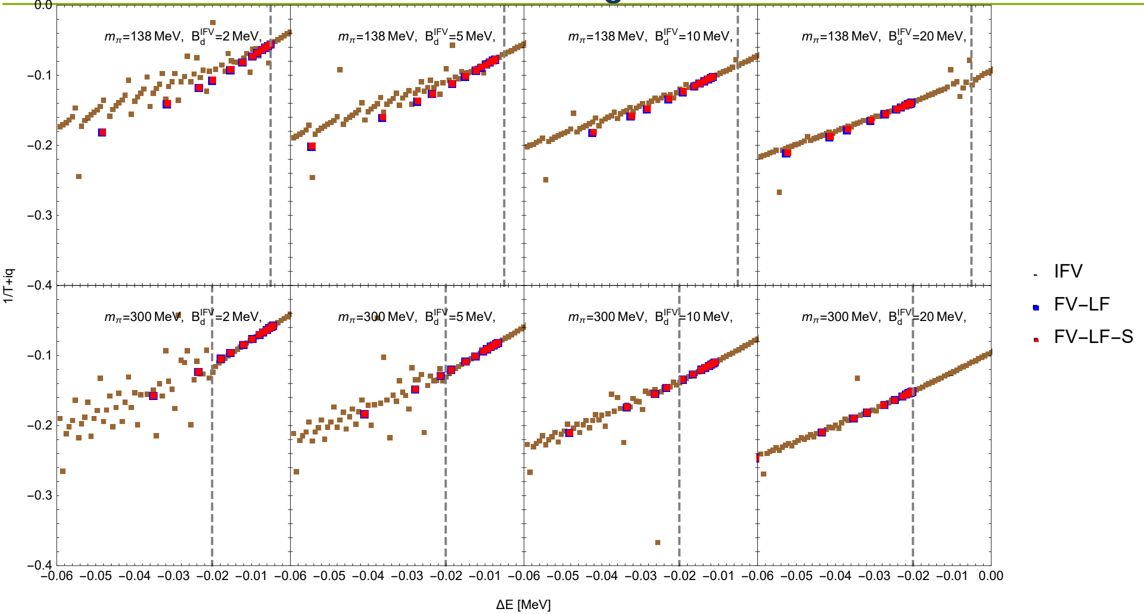
Partial-wave-contact



Partial-wave-P-wave



Partial-wave mixing for bound states



Partial-wave mixing for bound states