

Finite volume NN system using plane wave exansion and eigenvector continuation

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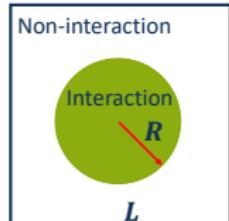
Lüscher's formula and beyond

- Lüscher's formula (LF)

Luscher:1990ux

⇒ To include partial wave (PW) mixture effect: $\det[M_{l,l'}^{\Gamma} - K^{-1}] = 0$,
~~one-to-one~~, parameterize T -matrix, root-finding algorithm

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



- Long-range interaction: e.g. $1-\pi$ exchange for NN and $\bar{D}^* D / \bar{D} D^* [X(3872)]$ Sato:2007ms,Jansen:2015lha

⇒ 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

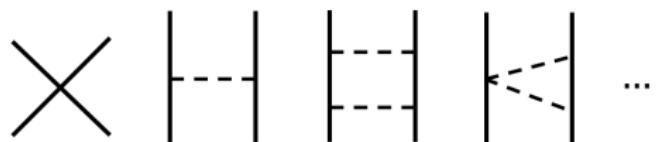
⇒ Including partial mixing naturally, works well for small box and long-range interaction

- Make the approach practical

⇒ (3)Eigenvector continuation

⇒ Compare it with Lüscher's formula

⇒ Fit NPLQCD results at $m_\pi = 0.45$ GeV



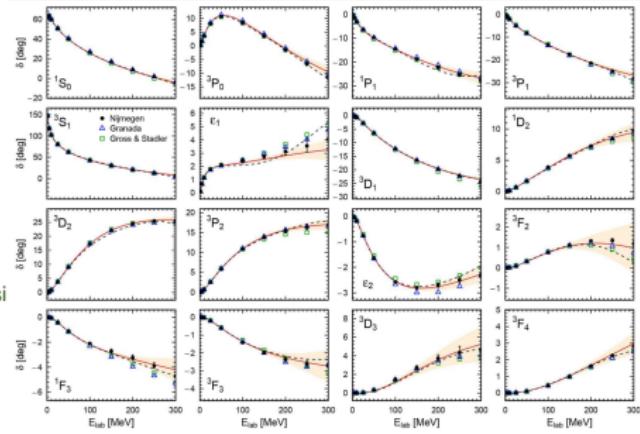
Theoretical formalism

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

- Derived in the momentum space
- E -independent potential
- Semilocal momentum-space regularization

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

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

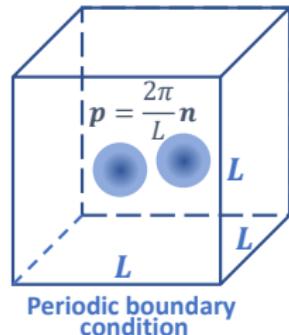


Hamiltonian approach in Plane wave basis: $|p_n, \eta\rangle$

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

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

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



- $\{|p_n, \eta\rangle\}$ form the representation space of corresponding point group
- Finite volume energy levels: eigenvalue problem

$$\det(\mathbb{H} - E\mathbb{I}) = 0 \quad \text{or} \quad \mathbb{H}\mathbf{v} = E\mathbf{v} \quad (1)$$

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

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

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

⇒ eigenvalue problem is easier to be solved than a general root-finding problem

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

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

- Reduce to irreducible representations (irreps): projection operator

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

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

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

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

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

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

Towards a practical approach: eigenvector continuation

- Plane wave basis+Eigenvector continuation

W.Detmold'S talk: Gaussian basis+ improved stochastic variational method

⇒ Eigenvector continuation (EC) with subspace learning

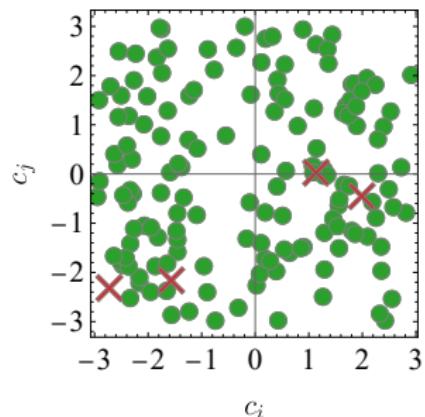
Frame:2017fah,Demol:2019yjt,Furnstahl:2020abp,Yapa:2022nnv

- Rayleigh-Ritz variational principle:

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

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

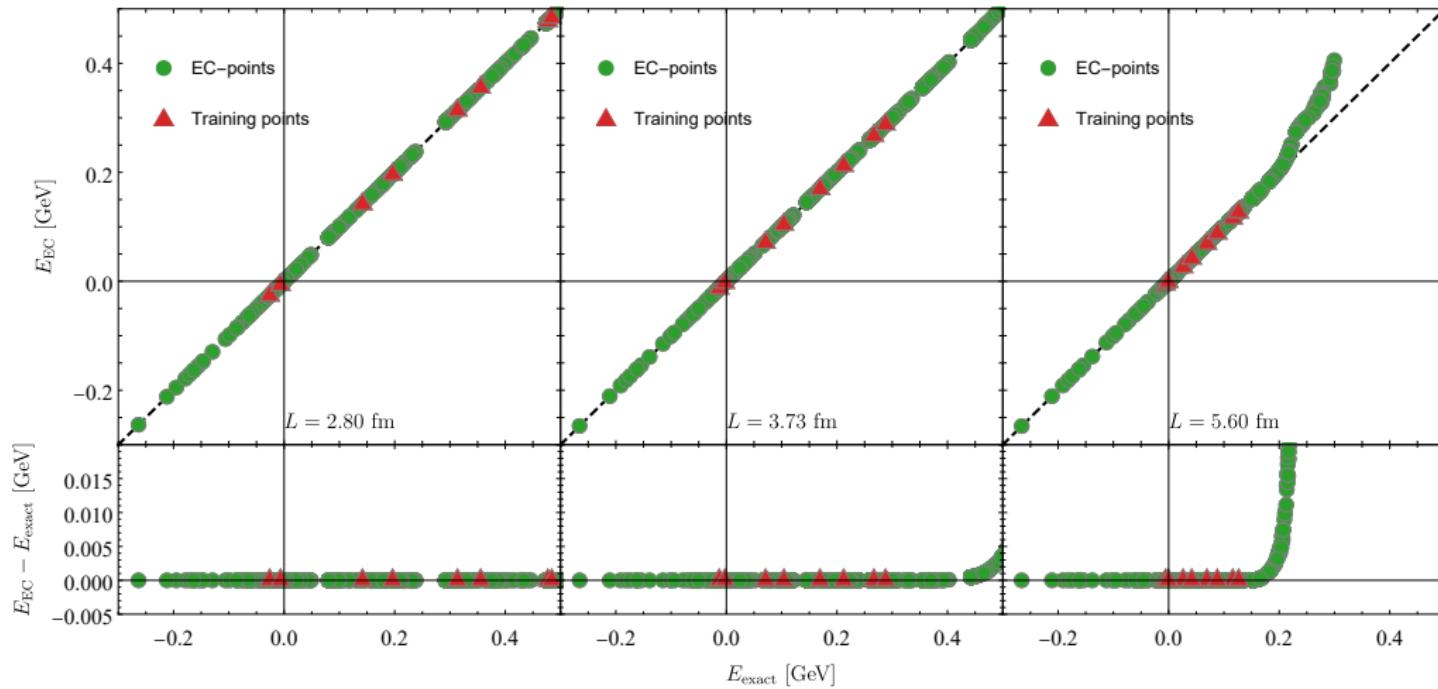
⇒ choose the trial function (basis) properly



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

Eigenvector continuation

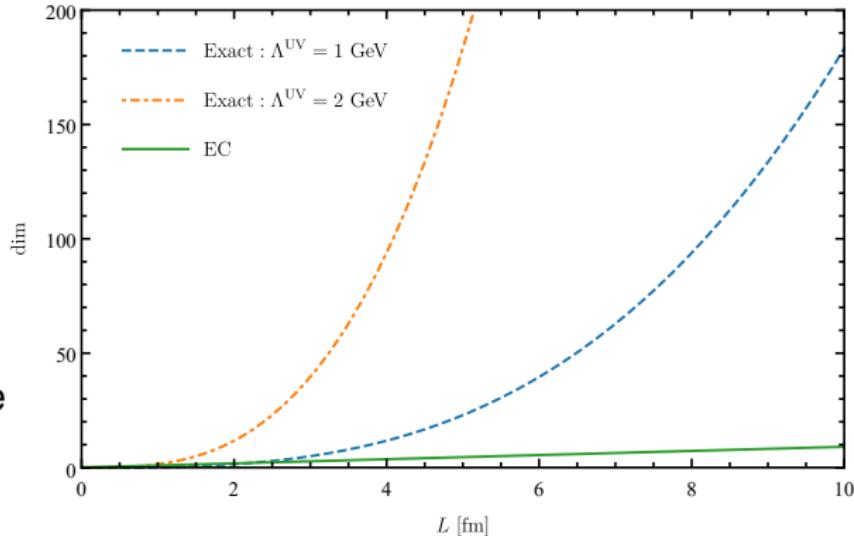
- Interaction: V_{contact} with 2 LECs $\{c_1, c_2\}$ + $V_{1\pi}$ in $L = \{2.70, 3.73, 5.60\}$ boxes
- Training points: $\{c_1^{\text{phy}}, 0\}, \{0, c_2^{\text{phy}}\}$; keep the first four energy levels as basis, dim=8



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



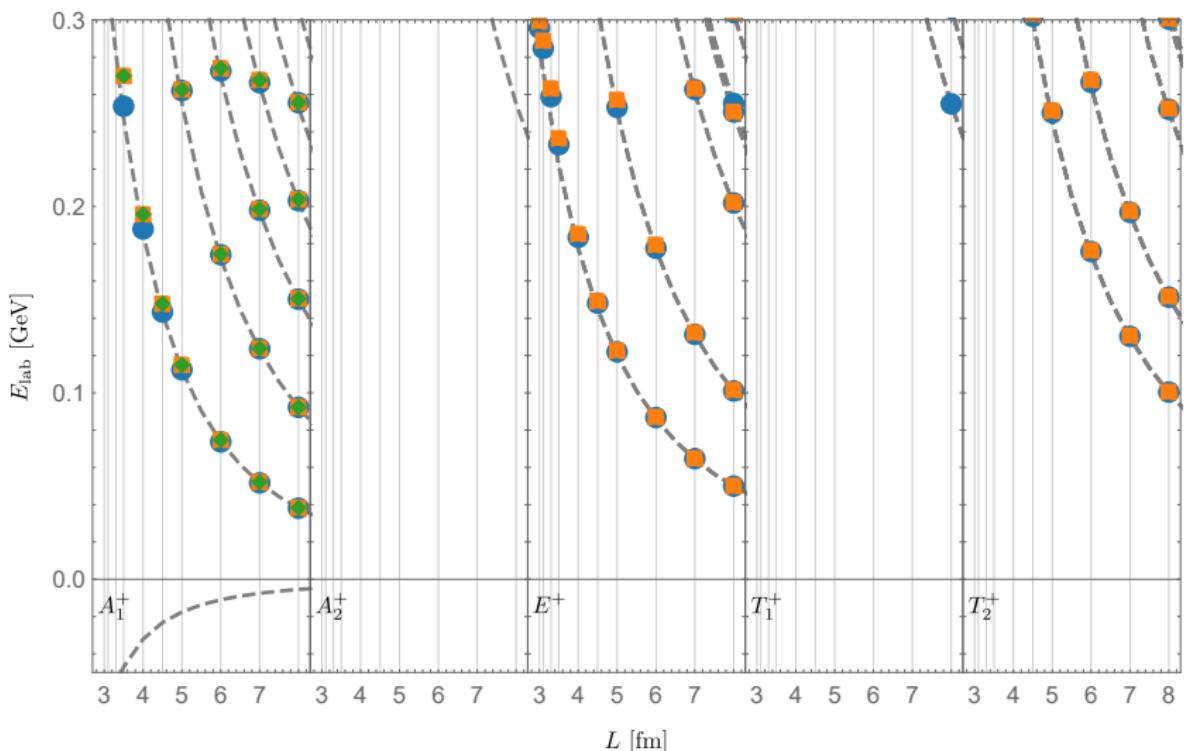
$$\mathbb{H}^{EC} = \mathbb{H}_0^{EC} + c_i \mathbb{V}_i^{EC}, \quad \mathbb{H}^{EC} \mathbf{v} = E \mathbf{v}$$

⇒ Easy-to-use interface: no need to know the details of χ EFT

Scattering states: Lüscher's formula VS PLW

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

● $J_{\max} = 4$ ● $J_{\max} = 2$ ● $J_{\max} = 0$ ----- Plane wave



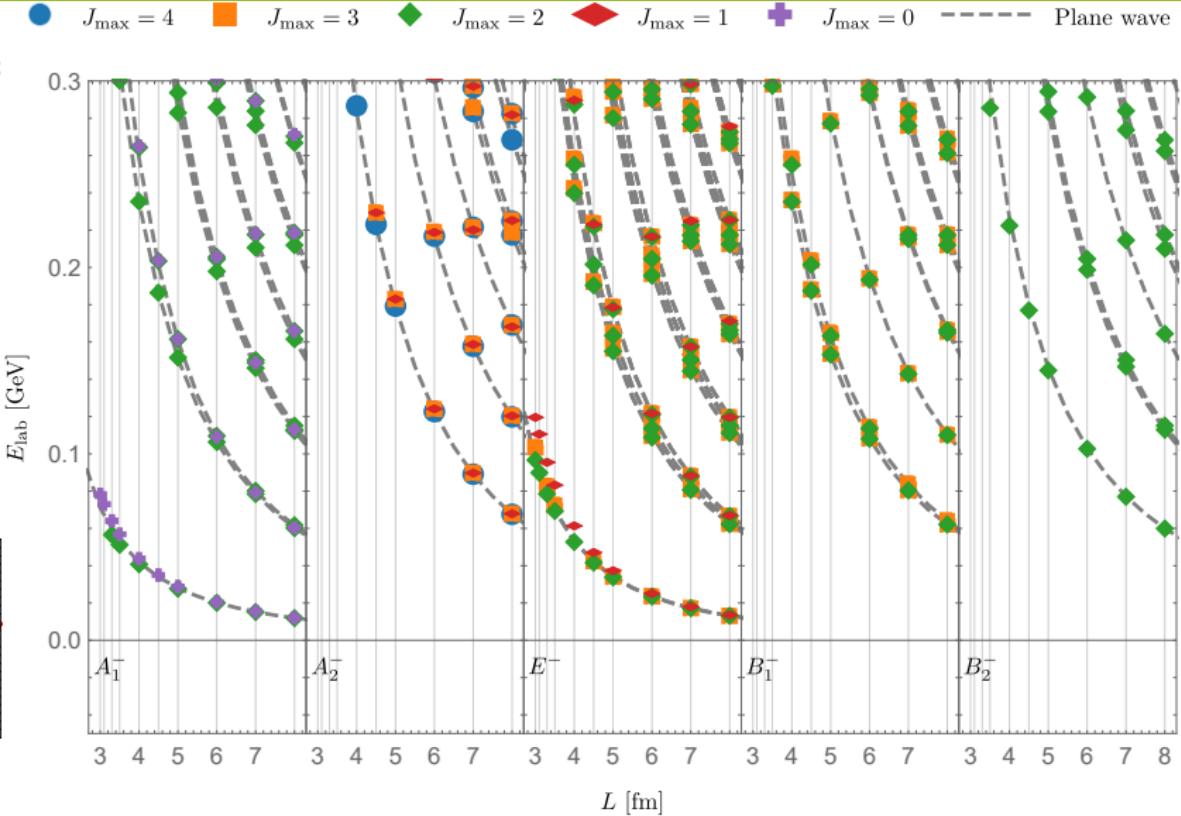
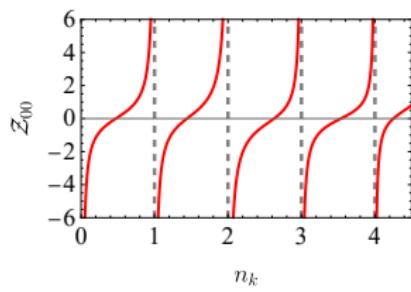
$$L = \{3.0, 3.1, 3.3, 3.5, 4.0, 4.5, 5.0, 6.0, 7.0, 8.0\} \text{ fm}$$

- PLW: with NNLO χ EFT
- Lüscher QC:
 - ⇒ Generate the phase shift (δ) to $J = 5$
 - $\det[M_{l,l'}^{\Gamma} - K^{-1}(\delta)] = 0$
 - ⇒ δ as input, truncated at different J_{\max} ,
 - ⇒ root-finding:

Woss:2020cmp,HSC

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:
 - ⇒ small box
 - ⇒ low J_{\max} QC



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

Bound states: Lüscher formula VS PLW

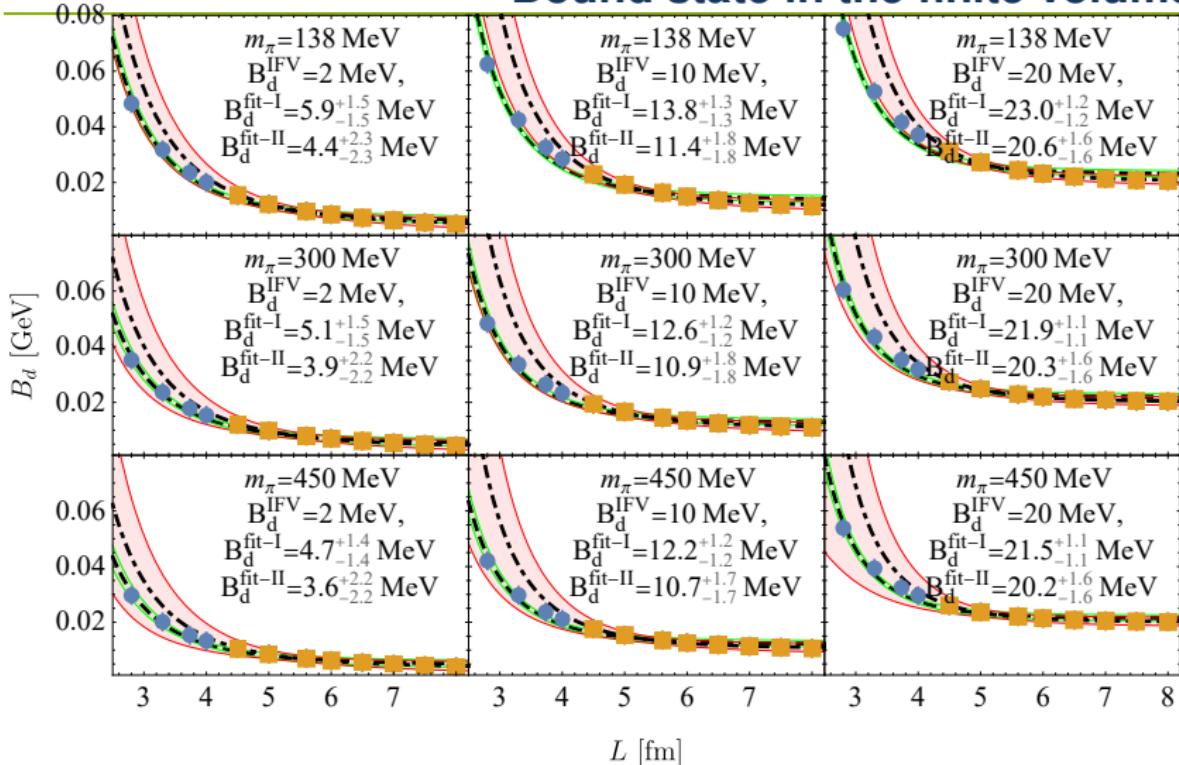
- Bound state Lüscher's formula

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 $d = (0, 0, 0)$, $F(L, \kappa) = 6e^{-\kappa L} + 6\sqrt{2}e^{-\sqrt{2}\kappa L} + \frac{8}{\sqrt{3}}e^{-\sqrt{3}\kappa L}$
- ⇒ Expand the Lüscher's formula for scattering states (analytical continuation) at the κ_0
- Leading order χ EFT 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



- 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

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

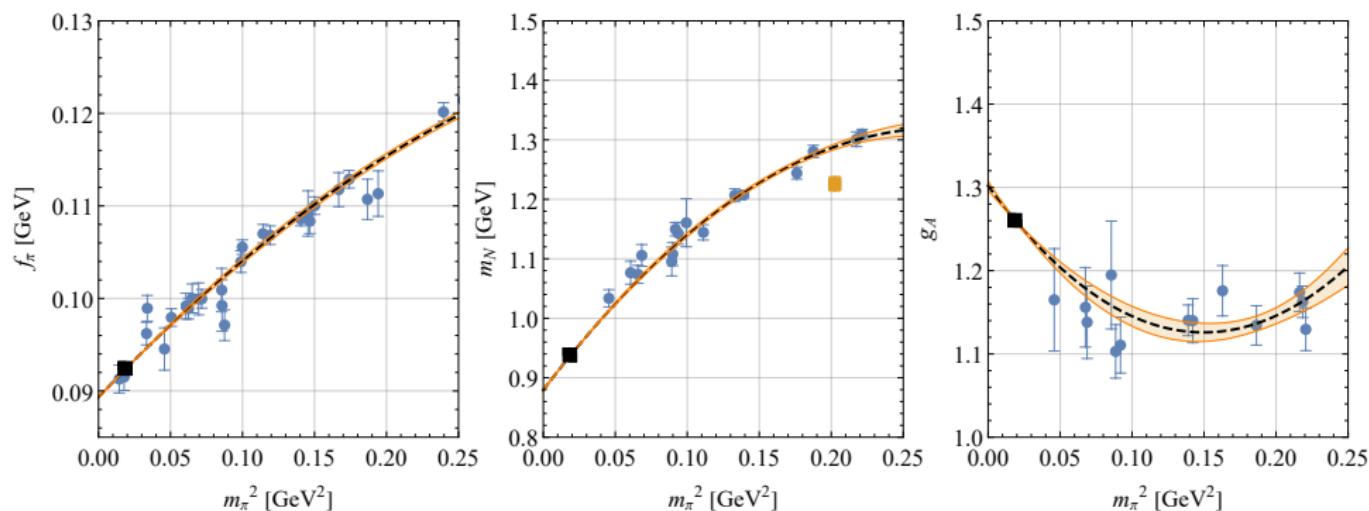
Fitting the NPLQCD data

Pion-mass dependence

- NPLQCD data: $m_\pi = 450$ MeV
- For such a large pion mass, the validity of χ EFT is questionable, a proof-of-principle
- Pion mass dependent of g_A , f_π , m_N from lattice QCD

Orginos:2015aya, Illa:2020nsi

Alexandrou:2013joa, Budapest-Marseille-Wuppertal:2013vij



Fitting results

- NPLQCD data

Orginos:2015aya, Illa:2020nsi

- χ EFT to NLO

- Contact terms:

$$\Rightarrow C_i^{phy} \rightarrow C_i^{phy} [1 + a_i (1 - \frac{m^2}{m_{phy}^2})]$$

\Rightarrow reduce to physical one for $m = m_{phy}$

\Rightarrow three a_i for $S = 1$

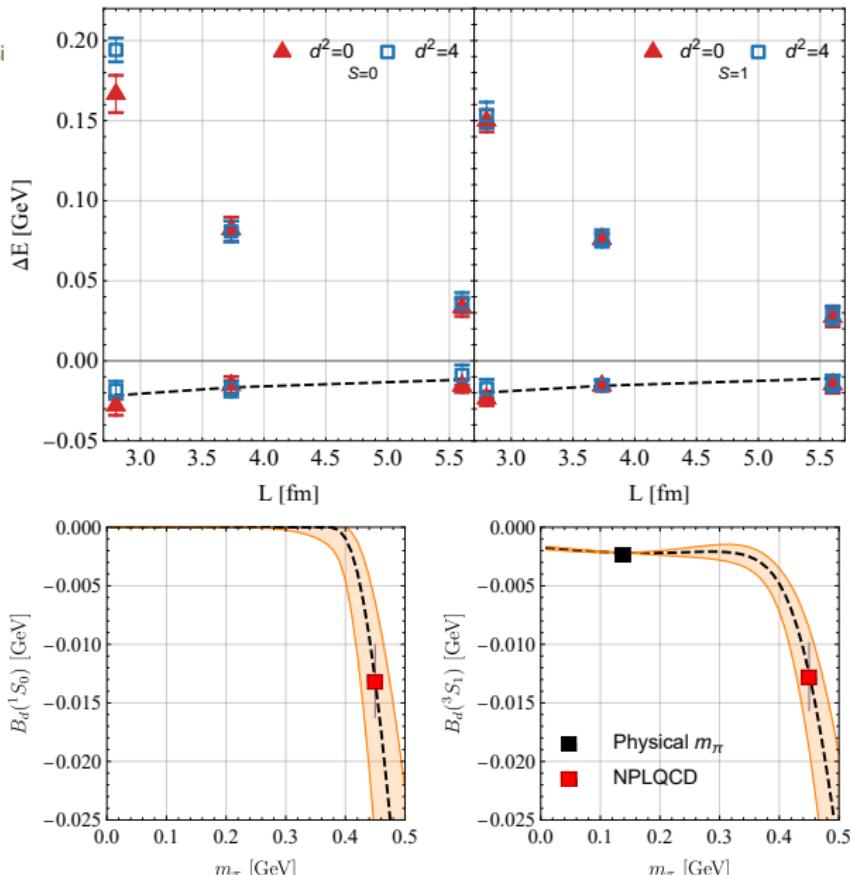
\Rightarrow two a_i for $S = 0$

- Inputs: ground states

$$L = \{2.801, 3.734, 5.602\} \text{ fm} \otimes d^2 = \{0, 4\}$$

- 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

- An alternative approach of Lüscher's formula to investigate NN in the box
 - ⇒ Plane wave expansions: include the partial wave mixing effect
 - ⇒ χ EFT: 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

Related talks: S.Prelovsek;S.Aoki...

Thanks!

Back up

Luscher formule

Davoudi:2011md

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

Approx.1 Higher PW is neglected

bound states $q = i\kappa$

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

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

$$F(L, \kappa) = \sum_{\mathbf{m} \neq 0} \frac{1}{|\mathbf{m}|} e^{-i2\pi \mathbf{m} \cdot \mathbf{d}} e^{-|\mathbf{m}|\kappa L}, \quad F \sim e^{-\kappa L} \quad (6)$$

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

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

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

Approx 2. Ignoring Left-hand cut

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

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

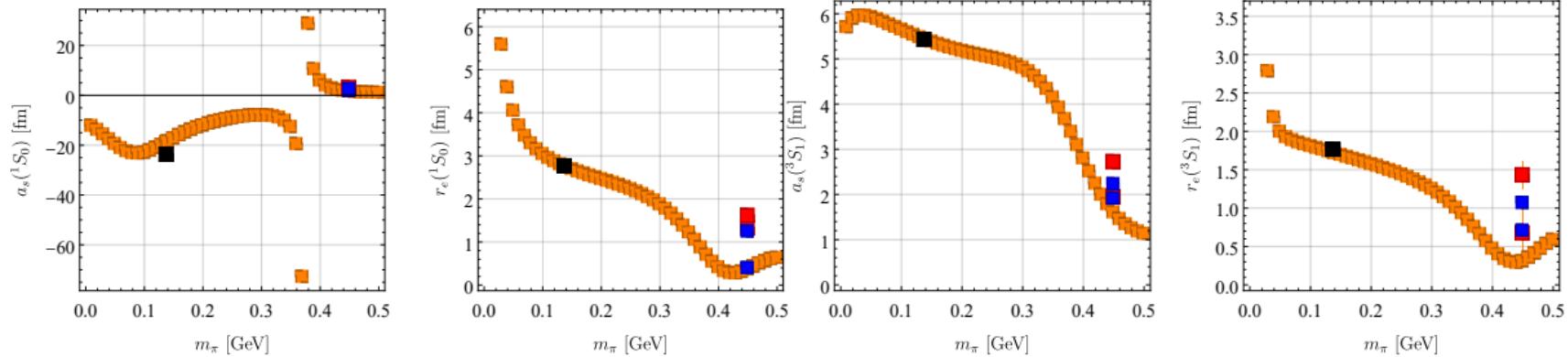
Approx 3. The perturbation: precise up to $\mathcal{O}(e^{-2\kappa L})$

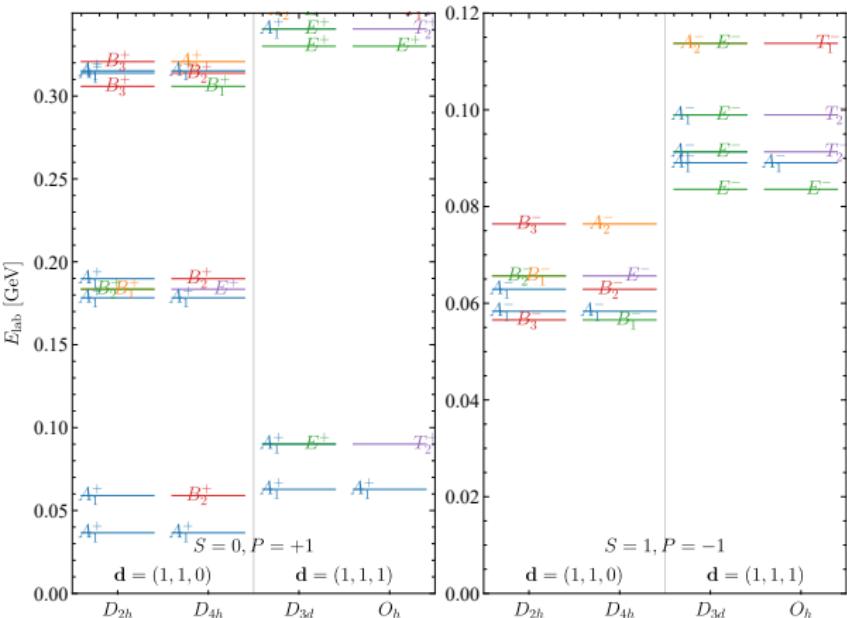
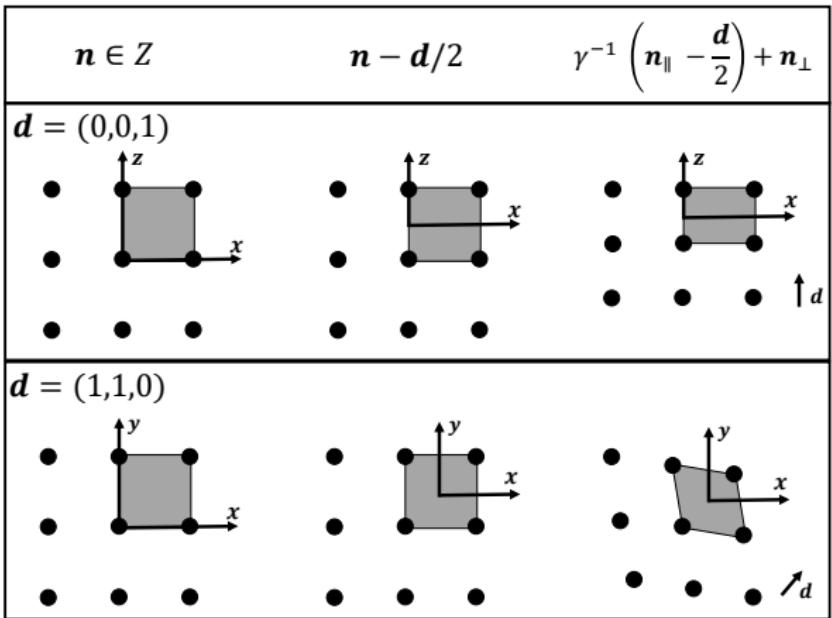
$$\kappa = \kappa_0 + \frac{Z^2}{L} F(L, \kappa_0) + \mathcal{O}(e^{-2\kappa L}) \quad (12)$$

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

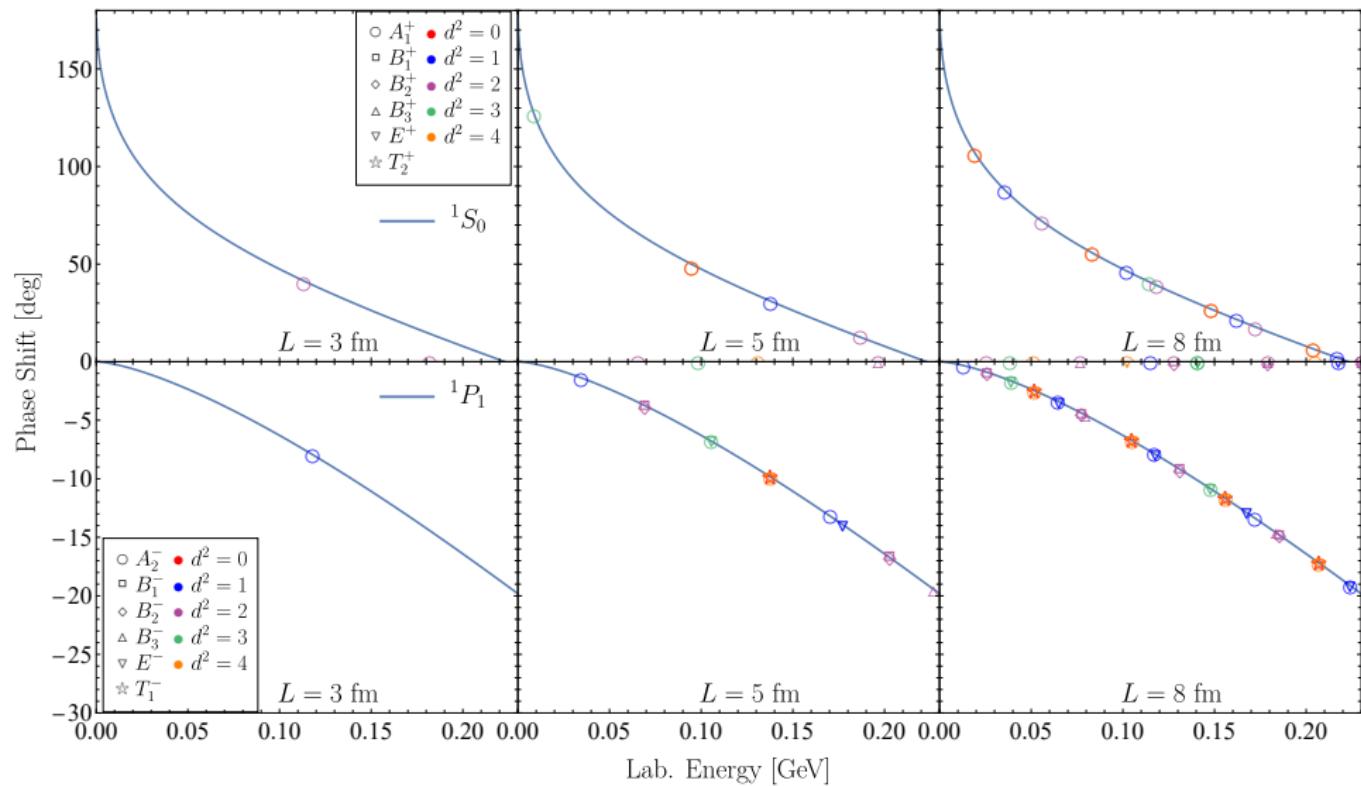
Approx 4. Truncation of the $F(L, \kappa)$

effective range parameter

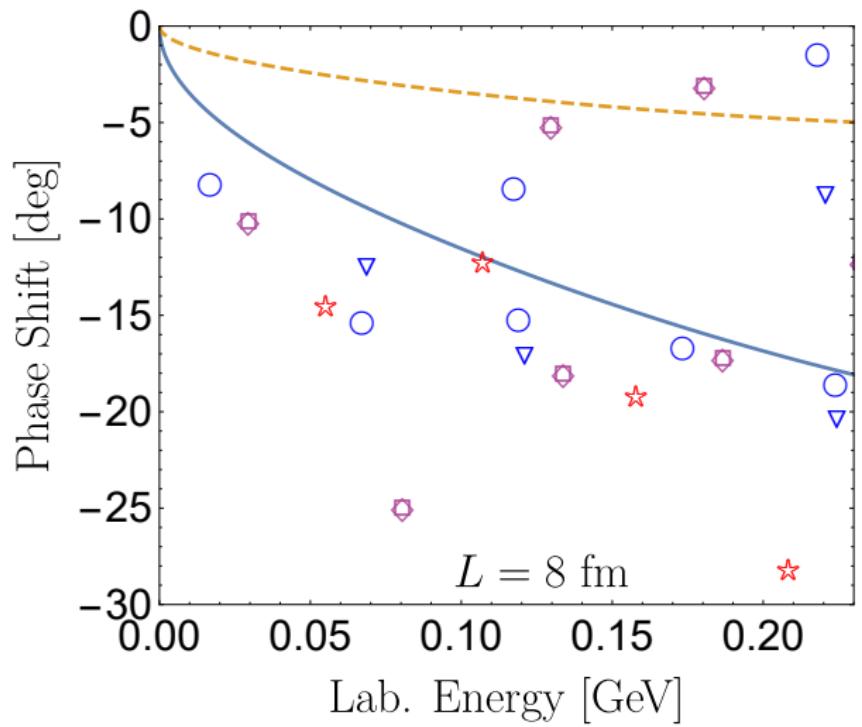




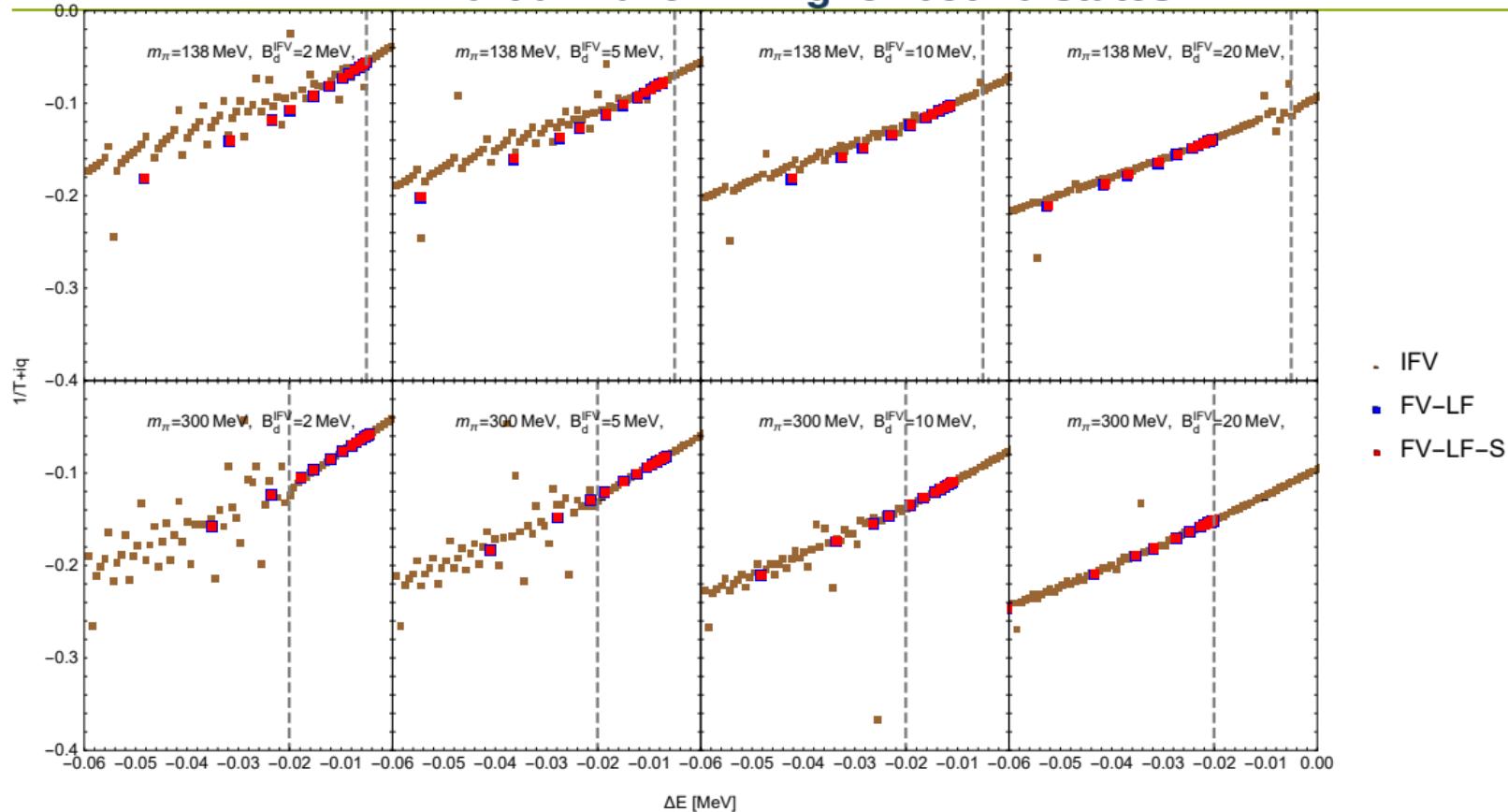
Partial-wave-contact



Partial-wave-P-wave



Partial-wave mixing for bound states



Partial-wave mixing for bound states

