RUHR UNIVERSITÄT BOCHUM RUB

# Solving the left-hand cut problem in lattice QCD: $T_{cc}$ (3875) in Hamiltonian approach


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Base on JHEP10(2021)051, PoS LATTICE2022 (2023) 201 and paper in preparation

Together with E. Epelbaum, V. Baru, A. Filin, A.M. Gasparyan, J. Gegelia

# Contents

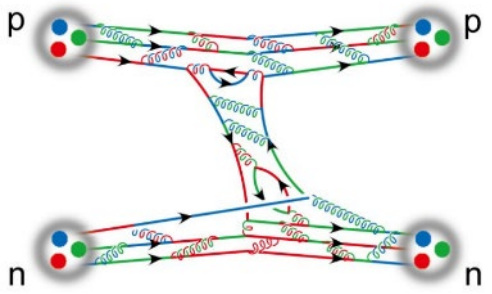
- Lüscher's formula
- Our formalism
- Preliminary results: $T_{cc}(3875)^+$ state
- Summary and outlook

# Lüscher's formula

# Lattice QCD and finite volume energy levels

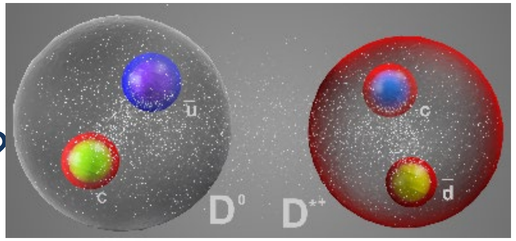
- QCD is the fundamental theory of the strong interaction

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



Nuclear force

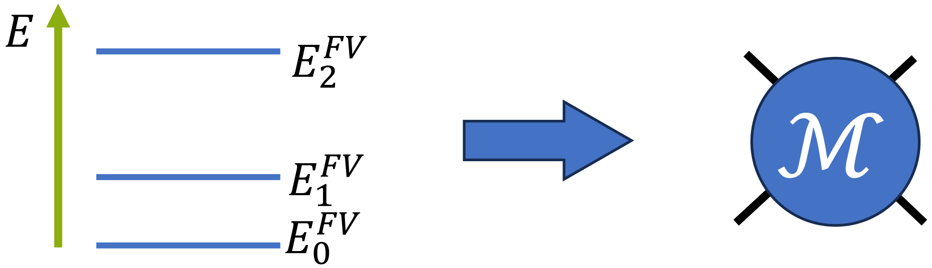
- Extract hadron-hadron interactions from QCD? Lattice QCD
  - ▶ formulated on a lattice of points in space and time in a finite volume (FV)



Hadronic molecules

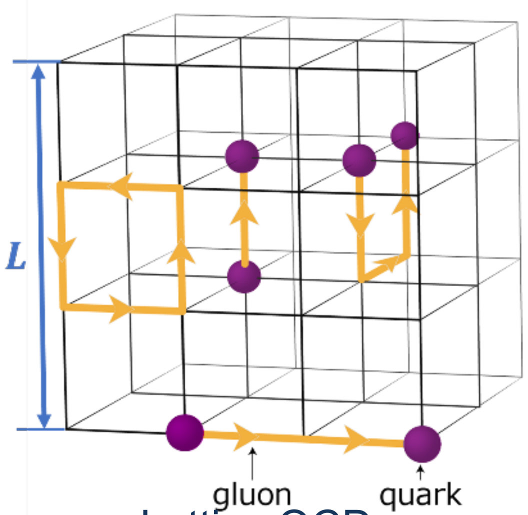
- How to extract observables in the infinite volume (IFV) from a FV calculation?
  - ▶ Energy level method: Lüscher's formula, $E^{FV} \sim \delta_l(E^{FV})$

Luscher:1990ux




  - ▶ Potential (or HAL QCD) method: Bethe–Salpeter amplitude → potential

Ishii:2006ec



Lattice QCD

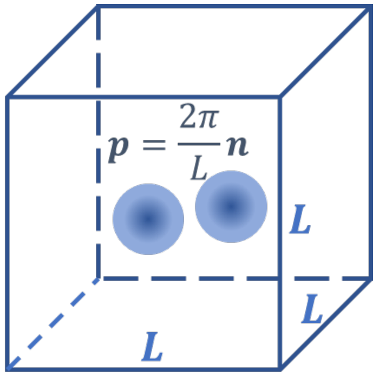
# Quantization of momentum

- Boundary conditions in the cubic box

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

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

  - ▶ 2-body rest systems: $\boldsymbol{d} = (0,0,0)$




- The rotation symmetry is broken: $SO(3) \to O_h$
  - ▶ $\{l, m\}$ are not good quantum numbers to label states
  - ▶ Partial wave mixing, for $l \neq l'$ and $m \neq m'$ ,

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

  - ▶ The FV energy should be classified by irreducible representations (irreps.) of $O_h$

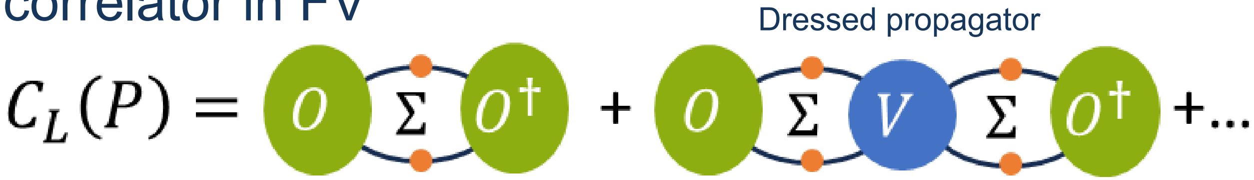
$$\{l, m\} \to \{A_1, A_2, E, T_1, T_2\}$$

- Moving system in the box $\boldsymbol{P} = \frac{2\pi}{L}\boldsymbol{d} \neq 0$
  - ▶ Other point groups, $D_{4h}$, $D_{2h}$ …
  - ▶ If $m_1 \neq m_2$, space inversion invariance is broken; states with different parities could mix

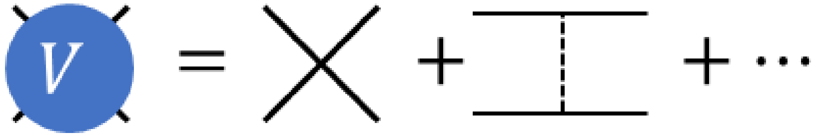
# Lüscher's formula

Luscher:1990ux, Kim:2005gf, Polejaeva:2012ut

- Two-body correlator in FV




▶ V is the Bethe-Salpeter kernel




▶ To calculate FV loops


FV loop IFV loop

$$\left[\frac{1}{L^3}\sum_{\boldsymbol{k}} - \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\right] f(k) = \begin{cases} \mathcal{O}(e^{-mL}) & \text{smooth } f(k) \\ \text{power of } L & \text{otherwise} \end{cases}$$

Only the singularities are important

▶ Only consider the two-body cut: Bethe-Salpeter kernel on-shell

$$C_L(P) = C_\infty(P) + iA\,\frac{1}{G_F^{-1}(E,L) - K(P)}\,A^\dagger$$

kinematic term K matrix in the IFV

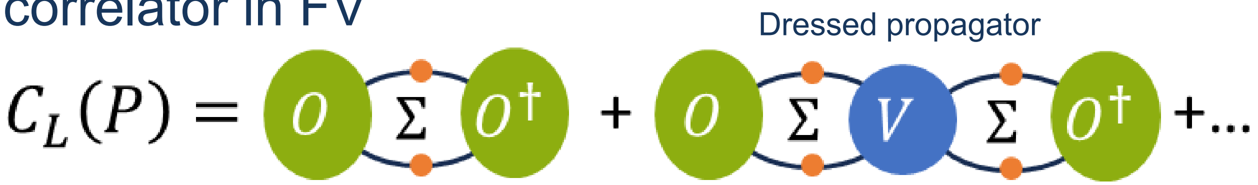
▶ Poles of $C_L$ is the FV energy levels

▶ Lüscher's formula: det $[G_F^{-1} - K] = 0$ AKA Quantization conditions (QCs)

# Lüscher's formula

Luscher:1990ux, Kim:2005gf, Polejaeva:2012ut

- Two-body correlator in FV

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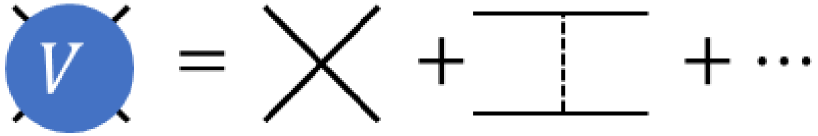


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If the left-hand cut is important?

$$C_L(P) = C_\infty(P) + iA \frac{1}{G_F^{-1}(E,L) - K(P)} A^\dagger$$

kinematic term

K matrix in the IFV

See Modified QCs Raposo:2023nex

▶ Poles of $C_L$ is the FV energy levels

▶ Lüscher's formula: $\det\left[G_F^{-1} - K\right] = 0$ AKA Quantization conditions (QCs)

# Lüscher's formula: partial wave mixing effect

- Expanding it in partial wave basis

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

  - ▶ Determinate equation of a matrix with infinite dimensions.
  - ▶ Truncate at some $l_{\max}$
- Reduce to irreps. $\Gamma_i$ of point group:: $\det\left[M^{(\Gamma,\boldsymbol{P})}_{ln,l'n'} - \delta_{ll'}\delta_{nn'}\cot\delta_l\right] = 0$
- Example $\boldsymbol{d} = (0,0,1)$, $\Gamma = A_1^+$, $w_{lm}$ depends on $E$ but independent on $V$

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

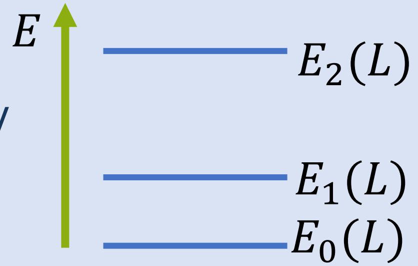
Bernard:2008ax

- 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 relation
  - ▶ E.g. $\{E_1^{FV}, E_2^{FV}\} \nRightarrow \{\delta_S(E_1^{FV}), \delta_S(E_2^{FV}), \delta_D(E_1^{FV}), \delta_D(E_2^{FV})\}$
  - ▶ One has to parameterize the K-matrix: e.g. effective range expansions (ERE)

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

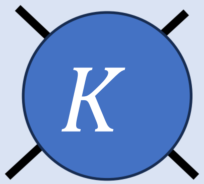
# Left-hand cuts

- Requirements of Lüscher's formula




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

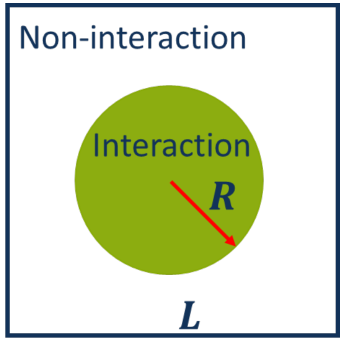
① $e^{-mL}$ effect can be neglected
② No singularity in $V$
③ Considering the PW mixing effect




IFV K-matrix

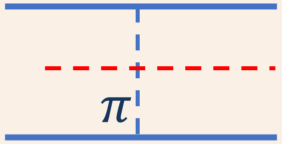
④ERE works

$k\cot\delta(k) = \frac{1}{a} + \frac{1}{2} r k^2 + \cdots$




Requirement: $\frac{L}{2} \gg R$

Typically: $m_\pi L > 3$




Left-hand cut

$$V(p,p') \sim \int_{-1}^{1} dz \frac{1}{p^2 + p'^2 - 2pp'z + m^2 + i\epsilon}$$
$$= \frac{1}{2pp'} \log\left(\frac{m^2 + (p+p')^2}{m^2 + (p-p')^2}\right)$$

on-shell: $p = p' = k$, $2\mu k^2 = E$

Branch point: $k^2 = -\frac{m^2}{4}$

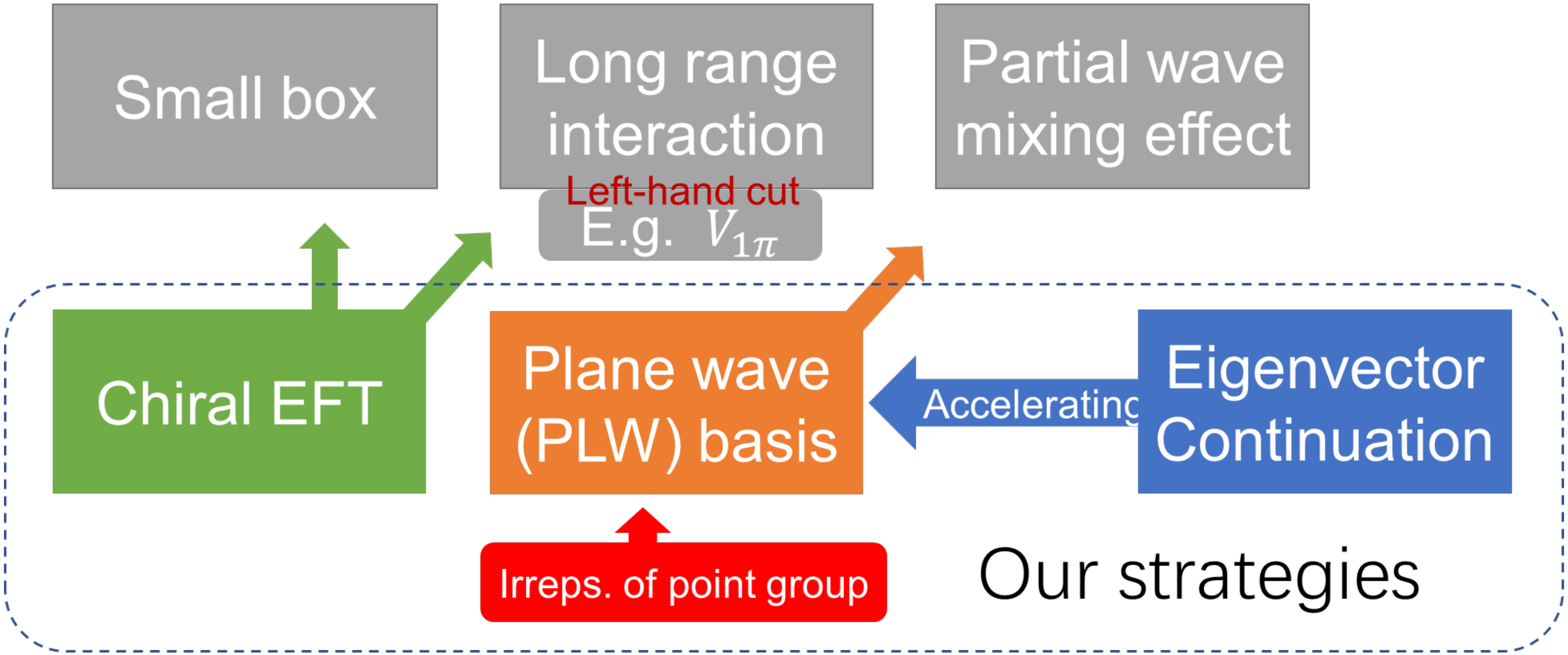
FV: LHC breaks the Lüscher's QCs ②

IFV: LHC invalidates the ERE ④

- NN system  Baru:2015ira, Baru:2016evv
- Modified ERE
- $DD^*$ systesm  Du:2023hlu

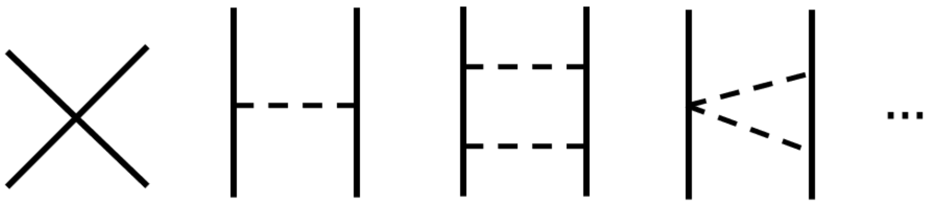
- Satisfying the four requirements are challenging for one-pion-exchange interactions

# Our formalism



# Chiral EFT

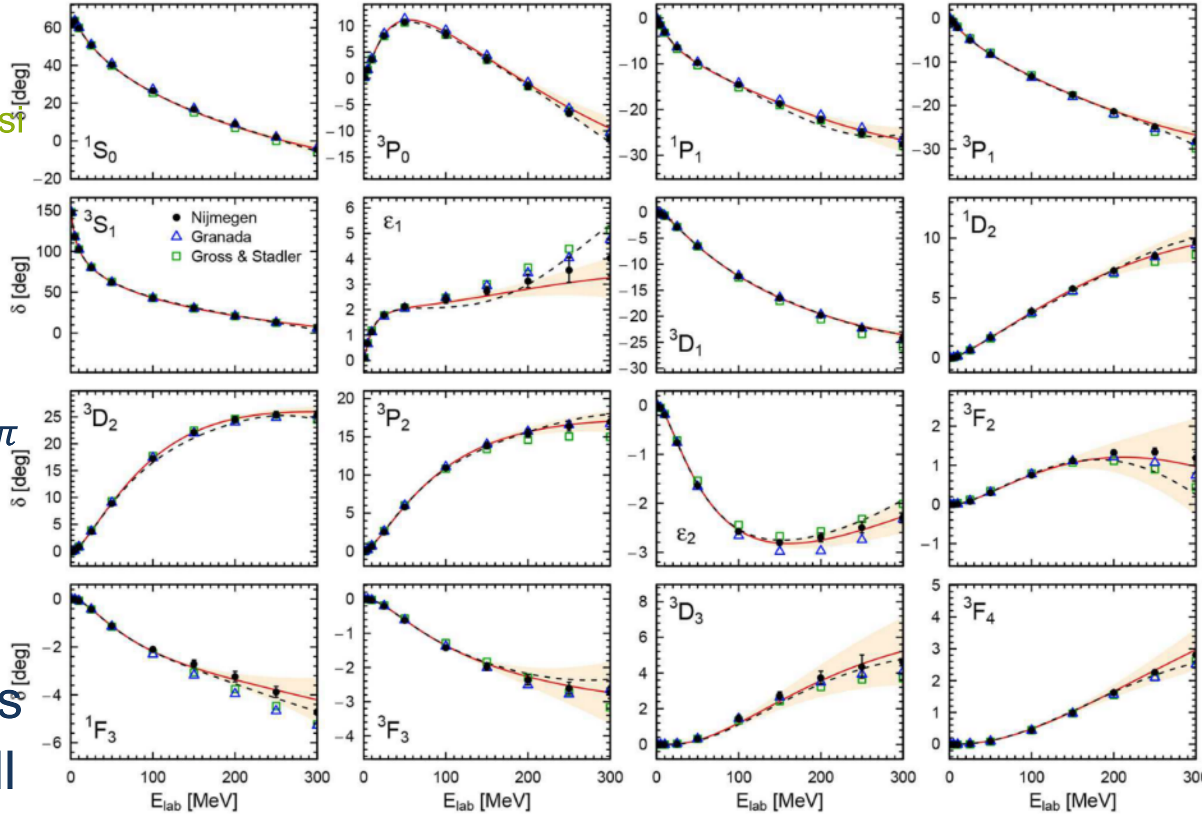
$$V(\vec{p}', \vec{p}) = V_{\text{contact}} + V_{1\pi} + V_{2\pi}$$



- 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)
  - ► fitting lattice QCD data
  - ► Decompose contact terms according to irreps
  - ► For specific irreps, the # of contact terms will be small

# Our formalism: plane wave basis expansion

- $|\boldsymbol{p}_n, \boldsymbol{\eta}\rangle$: $\boldsymbol{p}_n$ 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
- For non-relativistic systems, Lippmann-Schwinger equation (LSE)
  - ▶ matrix equation $\mathbb{T} = \mathbb{V} + \mathbb{V}\mathbb{G}\mathbb{T}$
  - ▶ Finite volume levels ⇒ 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

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

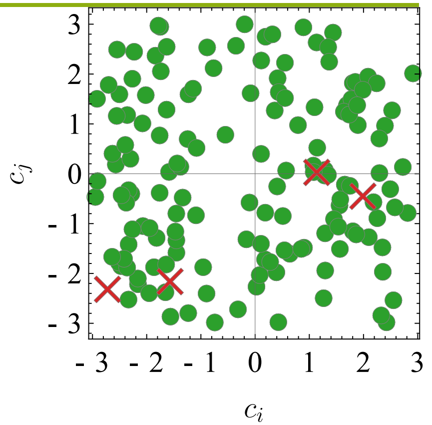
- For moving systems, elongated boxes, particles with arbitrary spin...
- dim of the $\mathbb{H}_\Gamma$: cubic function

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

# Towards a practical approach: eigenvector continuation

- Plane wave basis+Eigenvector continuation
  - ▶ Eigenvector continuation (EC) with subspace learning

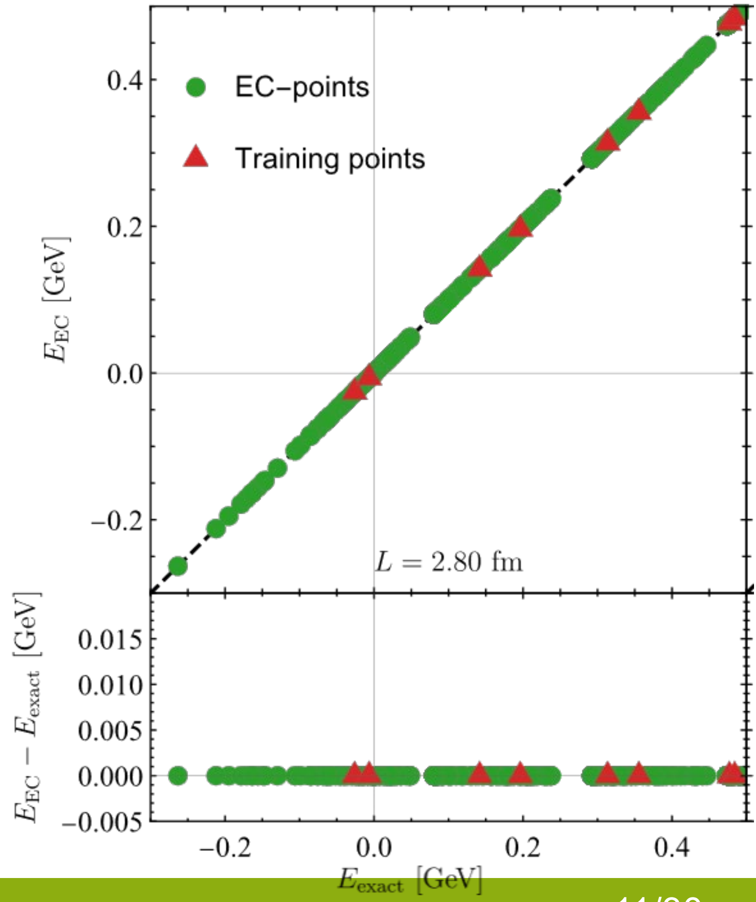
Frame:2017fah,Demol:2019yjt,
Furnstahl:2020abp,Yapa:2022nnv




- To fit or quantify uncertainty: solve eigenvalue problem with different $\{c_i\}$ repeatedly
- EC basis: eigenvectors from a selection of parameter sets $\{c_i\}_1$, $\{c_i\}_2$ ,... (training point)
- Naturalness of LECs in EFT ( ~ 1 ) makes the EC more reliable
- dim is linear function

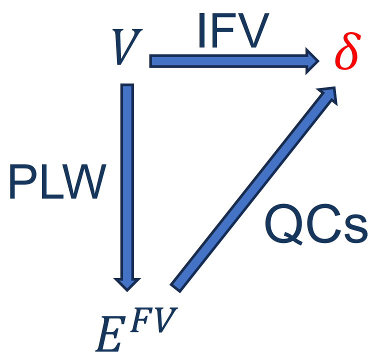
$$\dim^{EC} = \frac{p}{2\pi/L} \times n_{\text{training}} \sim \mathcal{O}(10)$$

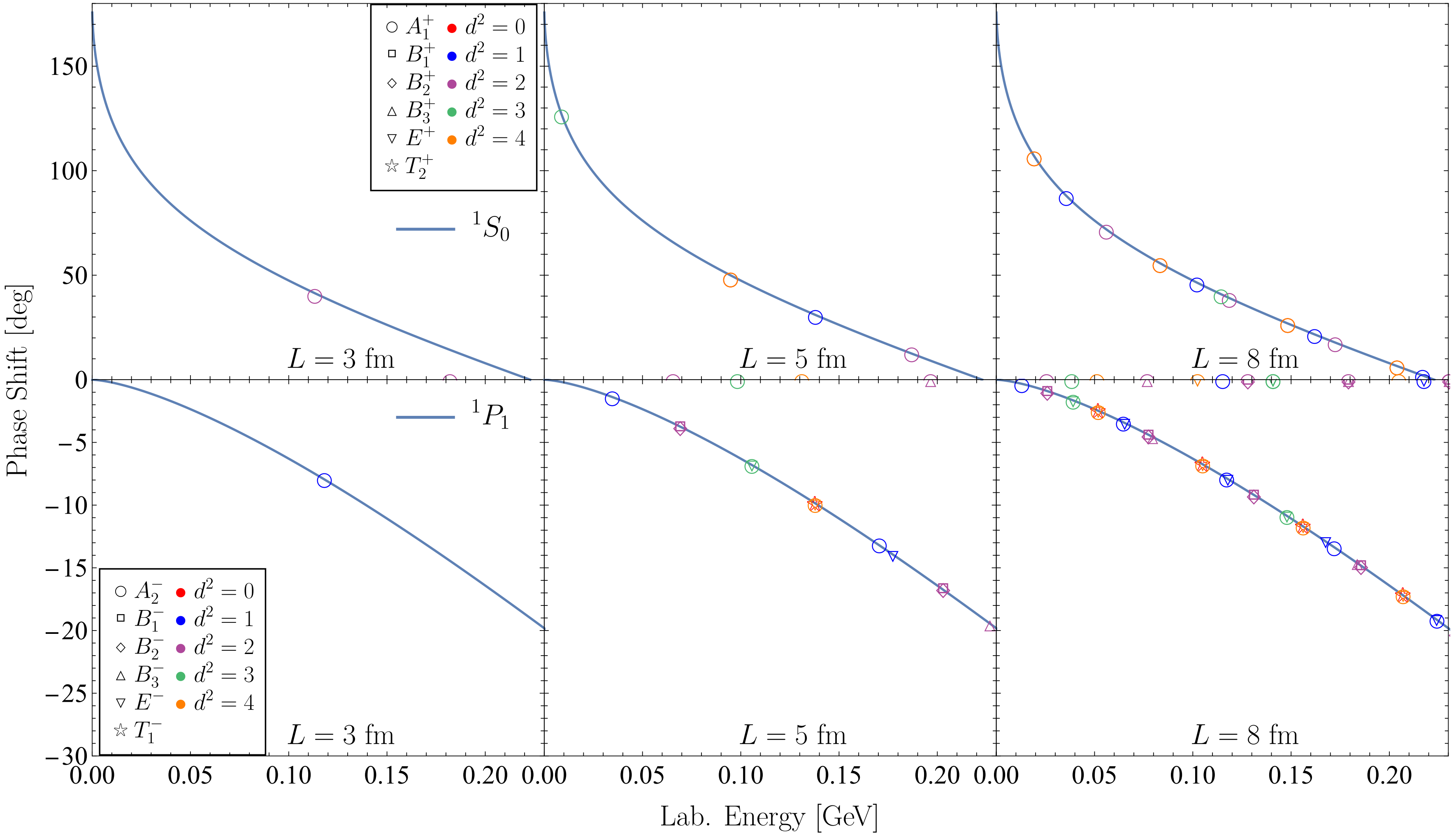
- The subspace learning is the one-time cost
- Make the calculation fast and accurate



# Benchmark: contact interaction

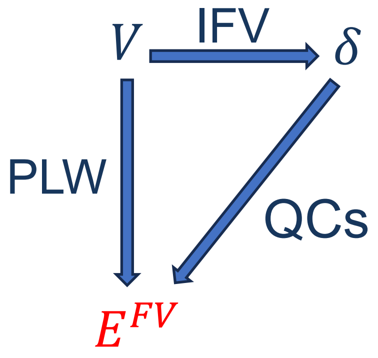
- Contact interaction: $V(\boldsymbol{p},\boldsymbol{p}') = C_S + C_1\boldsymbol{q}^2 + C_2\boldsymbol{k}^2$
- Only contribute to S-wave and P-wave



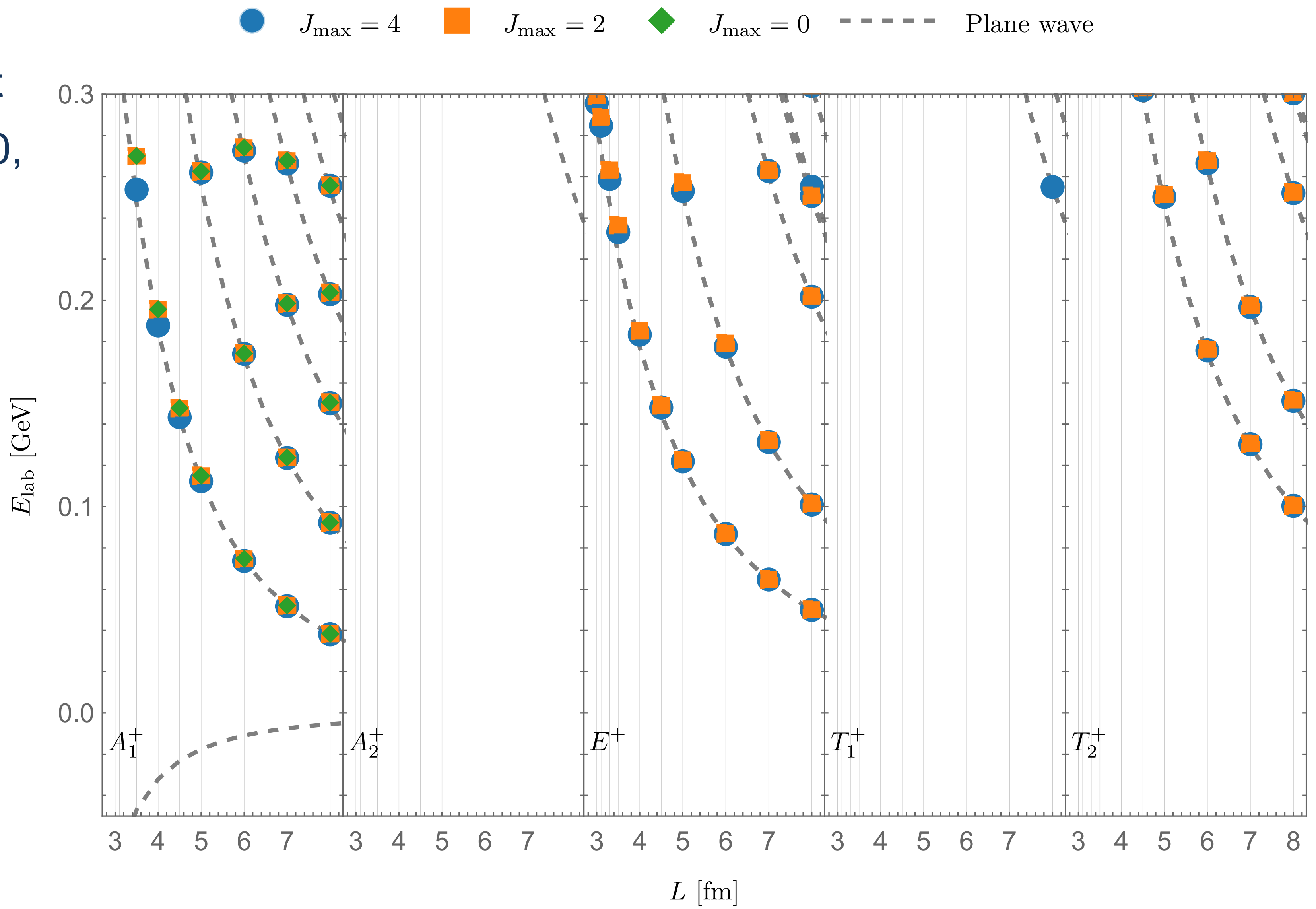



# Benchmark: chiral EFT

- ChEFT nuclear force: NNLO
- S=0, $d = (0,0,0)$, even parity
- QCs with partial mixing effect
- L={ 3.0,3.1,3.3,3.5,4.0,4.5,5.0, 6.0,7.0,8.0} fm

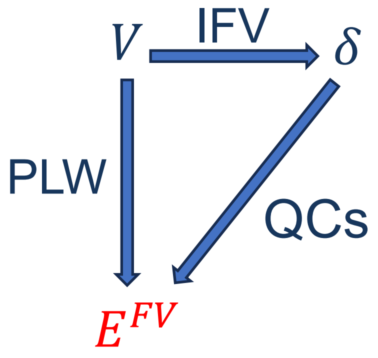


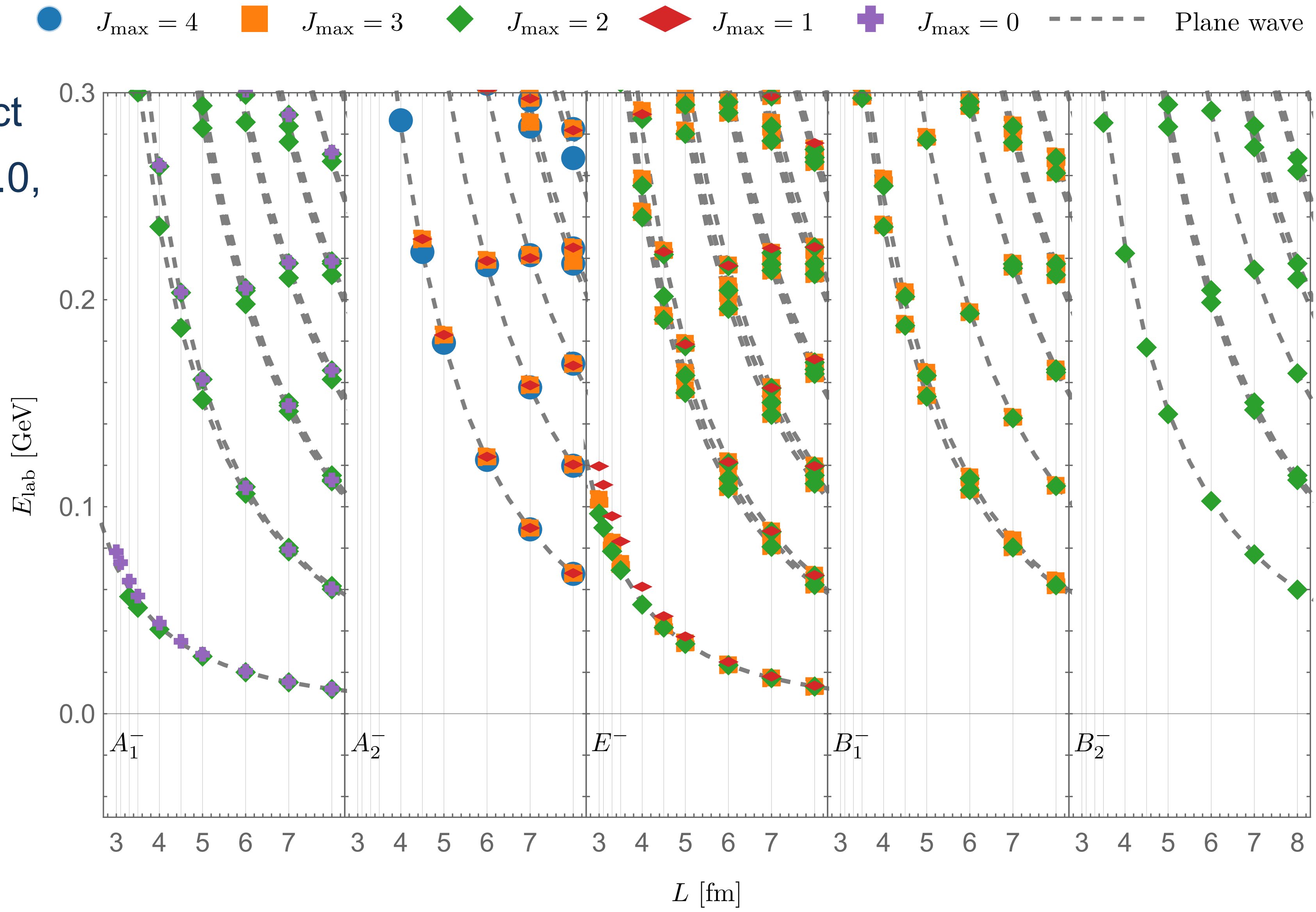

- The discrepancy
  - ▶ Small box
  - ▶ Small $J_{max}$ truncation



# Benchmark: chiral EFT

- ChEFT nuclear force: NNLO
- S=1, $d$=(0,0,1), odd parity
- QCs with partial mixing effect
- L={ 3.0,3.1,3.3,3.5,4.0,4.5,5.0, 6.0,7.0,8.0} fm

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# $T_{cc}(3875)^+$ state

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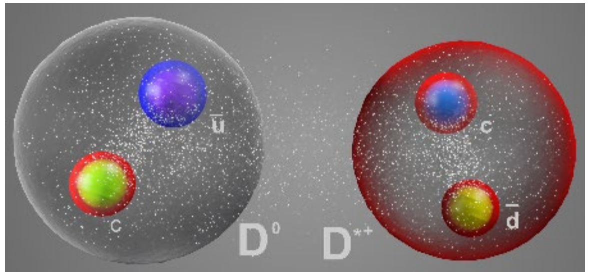
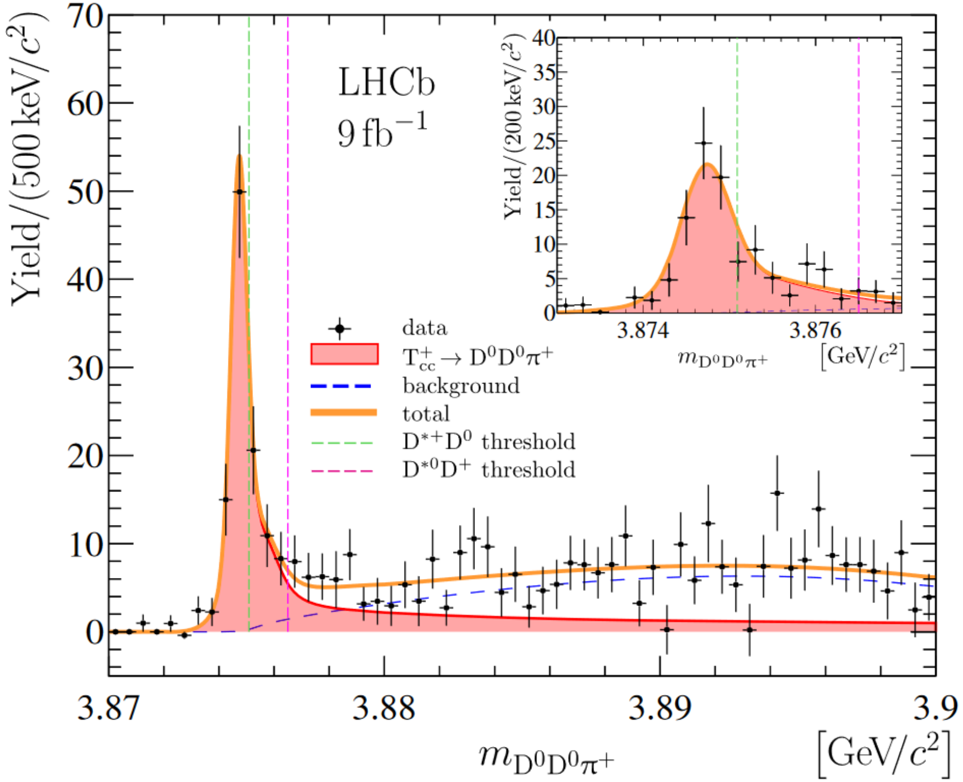
- $T_{cc}(3875)^+$ was observed in 3-body final states: $D^0D^0\pi^+$

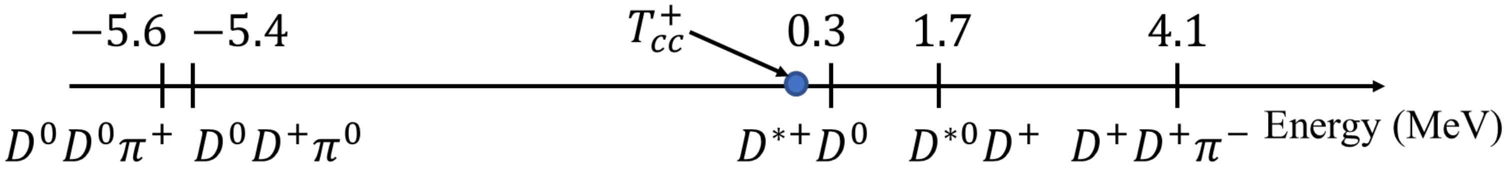
LHCb Collaboration

- Very close to $D^0D^{*+}$ thresholds: $\delta m_U \approx -360$keV, $\Gamma \approx 48$ keV
- Exotic hadrons: minimal quark content: $cc\bar{u}\bar{d}$
- Good candidates of $D^0D^{*+}$ molecule




- 3-body dynamics could be important




LHCb:2021vvq, LHCb:2021auc, Du:2021zzh, Meng:2021jnw

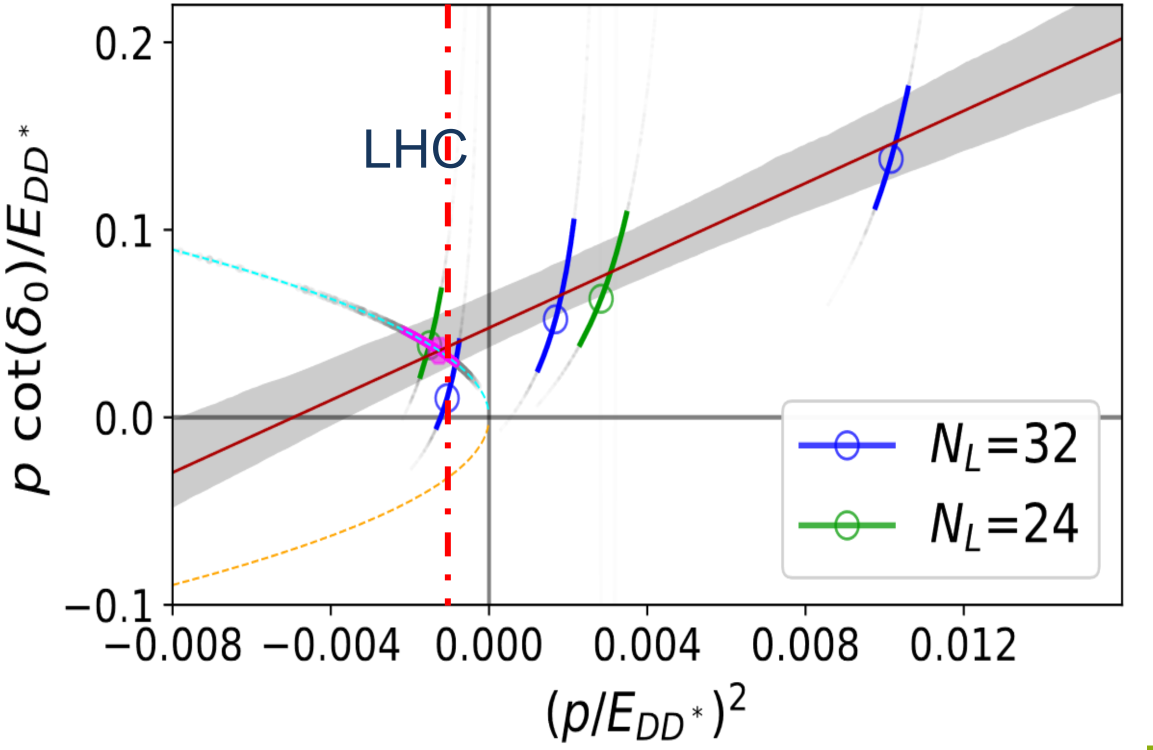
# $T_{cc}$ lattice QCD simulations

Padmanath:2022cvl

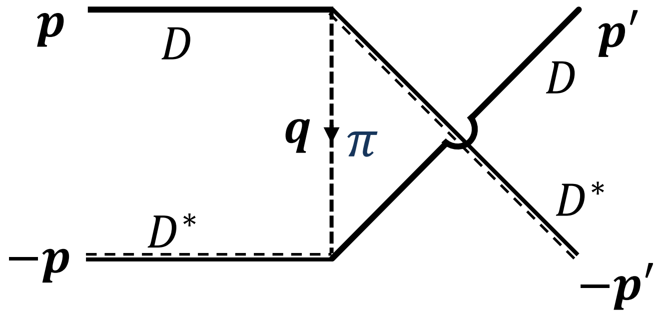
- LQCD: $m_\pi \approx$ 280 MeV, $m_D \approx 1927$ MeV, $m_{D^*} \approx 2049$ MeV, $L \approx 2.07, 2.76$ fm, $a \approx 0.086$fm
- Some quick estimations

① $e^{-mL}$ effect can be neglected
② No singularity in $V$
③ Considering the PW mixing effect

④ERE works in IFV   Du:2023hlu




RHC3




$$\frac{1}{q^2 - m_\pi^2 + i\epsilon} = \frac{-1}{\boldsymbol{q}^2 + m_\pi^2 - q_0^2 - i\epsilon} = \frac{-1}{\boldsymbol{q}^2 + m_{\text{eff}}^2 - i\epsilon}$$

Other lattice results: Cheung:2017tnt, Junnarkar:2018twb, Chen:2022vpo, Lyu:2023xro

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- Some quick estimations
  - ▶ $m_{\text{eff}}^2 = m_\pi^2 - (m_{D^*} - m_D)^2 > 0$, $m_{\text{eff}} \approx 252$ MeV
  - ▶ $m_{\text{eff}} L = 2.6, 3.5$

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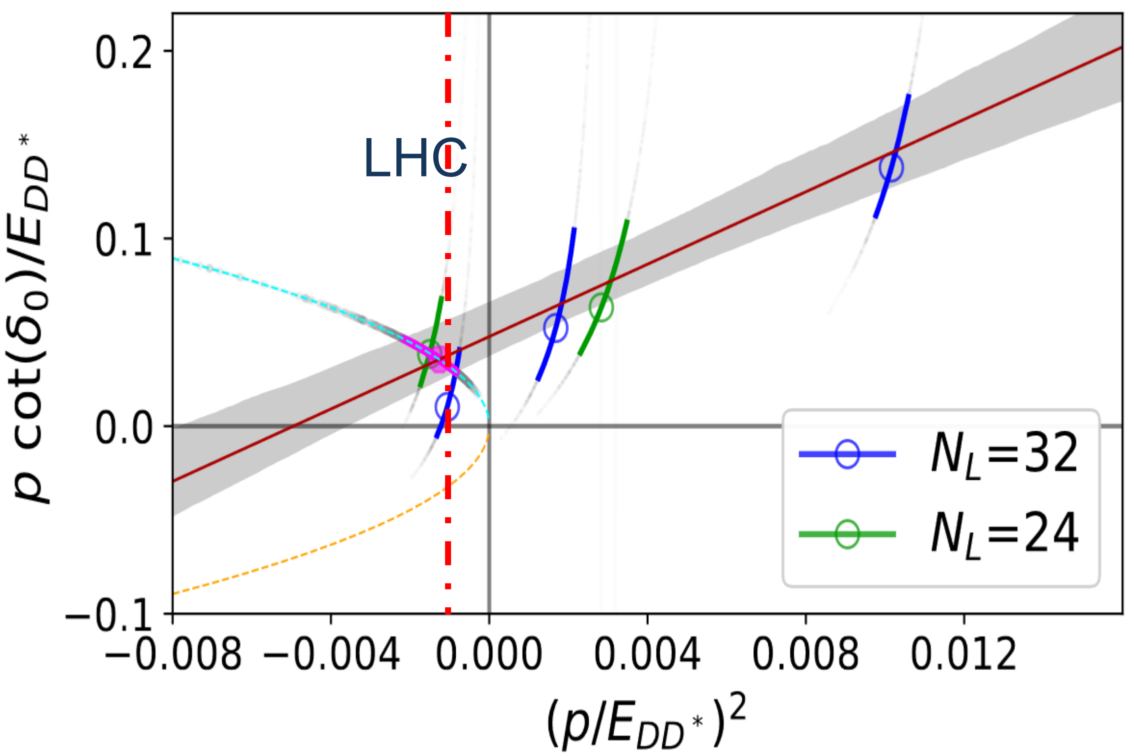


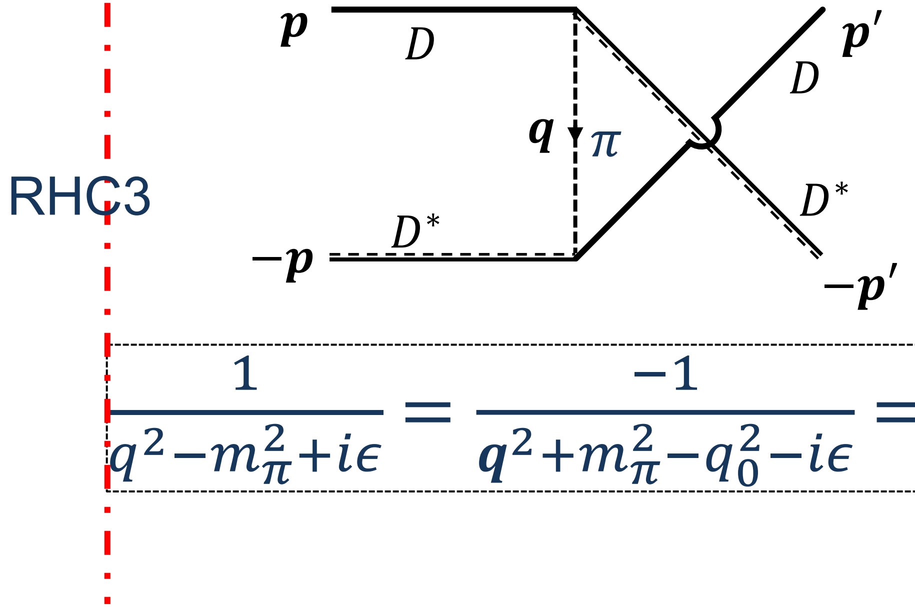


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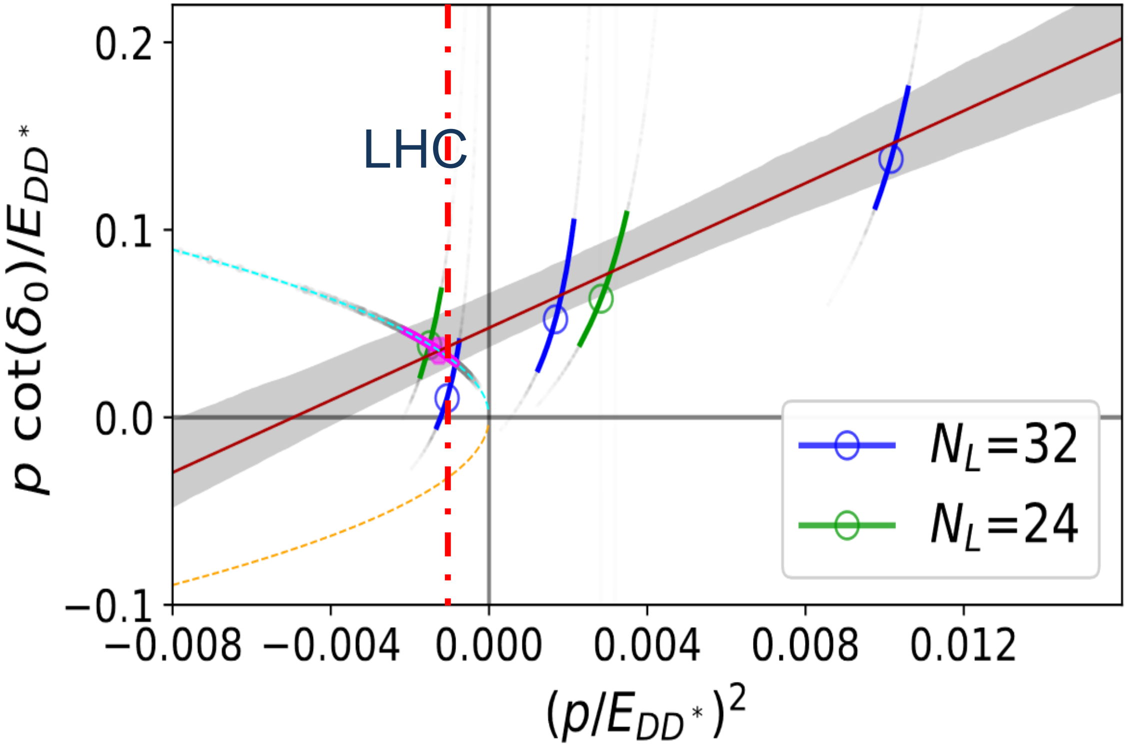
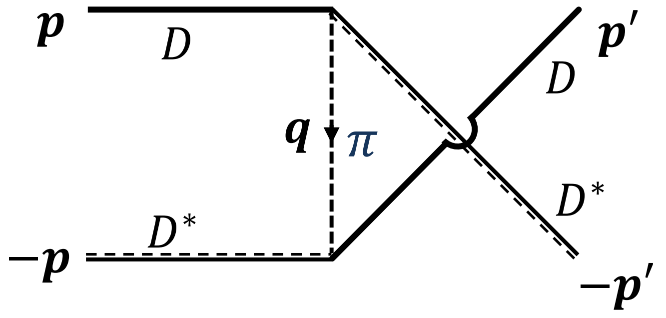



RHC3




$$\frac{1}{q^2 - m_\pi^2 + i\epsilon} = \frac{-1}{\boldsymbol{q}^2 + m_\pi^2 - q_0^2 - i\epsilon} = \frac{-1}{\boldsymbol{q}^2 + m_{\rm eff}^2 - i\epsilon}$$

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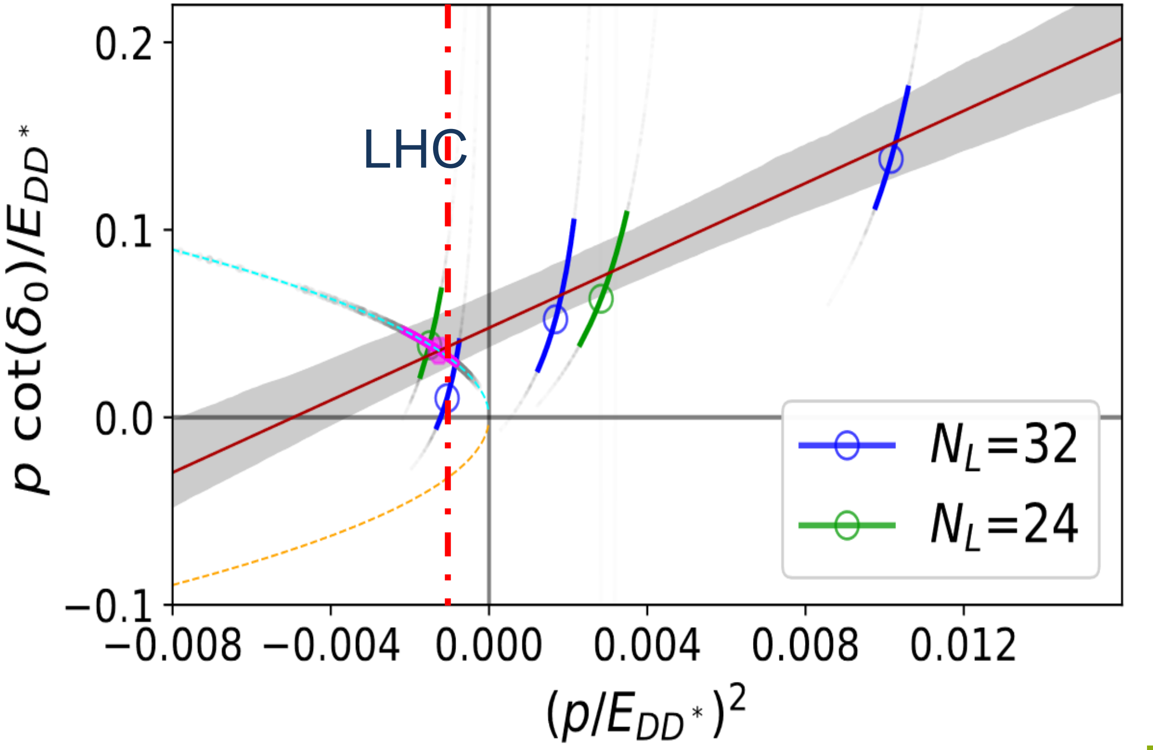
# $T_{cc}$ lattice QCD simulations

Padmanath:2022cvl

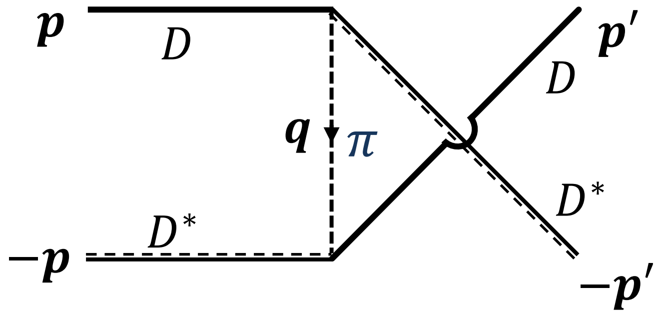
- LQCD: $m_\pi \approx$ 280 MeV, $m_D \approx 1927$ MeV, $m_{D^*} \approx 2049$ MeV, $L \approx 2.07, 2.76$ fm, $a \approx 0.086$fm
- Some quick estimations
  - ▶ $m_{\text{eff}}^2 = m_\pi^2 - (m_{D^*} - m_D)^2 > 0$, $m_{\text{eff}} \approx 252$ MeV
  - ▶ $m_{\text{eff}} L = 2.6, 3.5$
  - ▶ $p_{\text{lhc}}^2 \approx -\left(\frac{m_{\text{eff}}}{2}\right)^2 = -(126\text{ MeV})^2$

① $e^{-mL}$ effect can be neglected
② No singularity in $V$
③ Considering the PW mixing effect

④ERE works in IFV  Du:2023hlu




RHC3




$$\frac{1}{q^2 - m_\pi^2 + i\epsilon} = \frac{-1}{\boldsymbol{q}^2 + m_\pi^2 - q_0^2 - i\epsilon} = \frac{-1}{\boldsymbol{q}^2 + m_{\text{eff}}^2 - i\epsilon}$$

Other lattice results: Cheung:2017tnt, Junnarkar:2018twb, Chen:2022vpo, Lyu:2023xro

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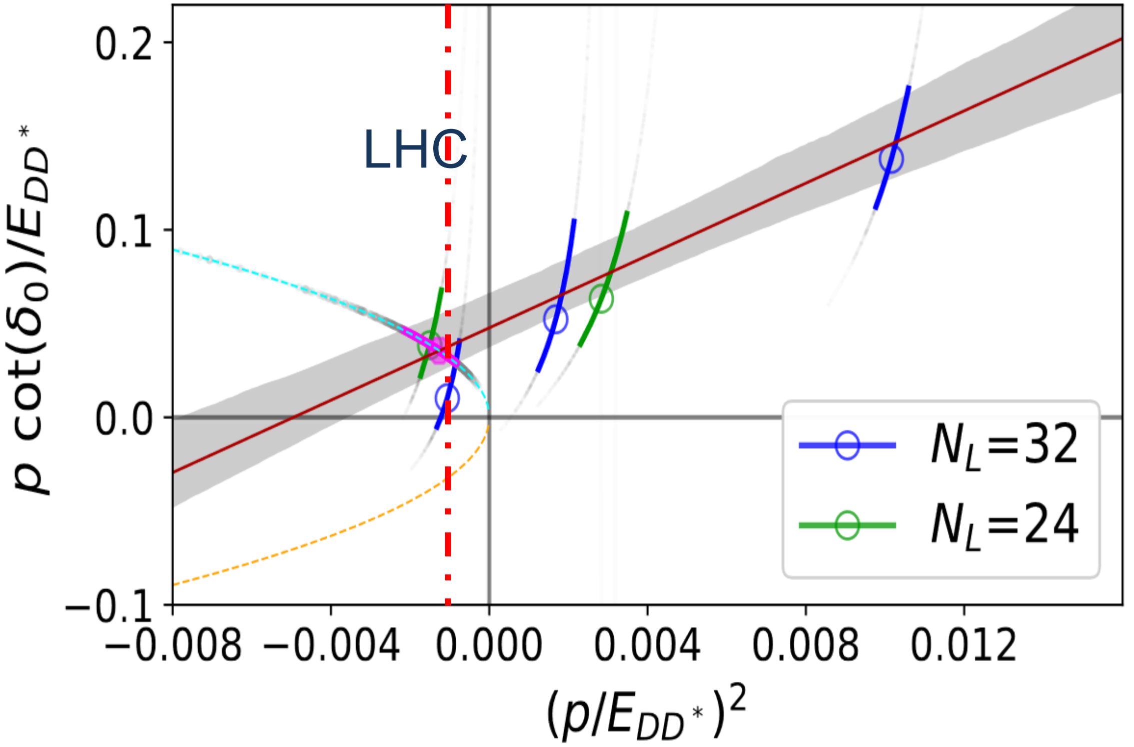


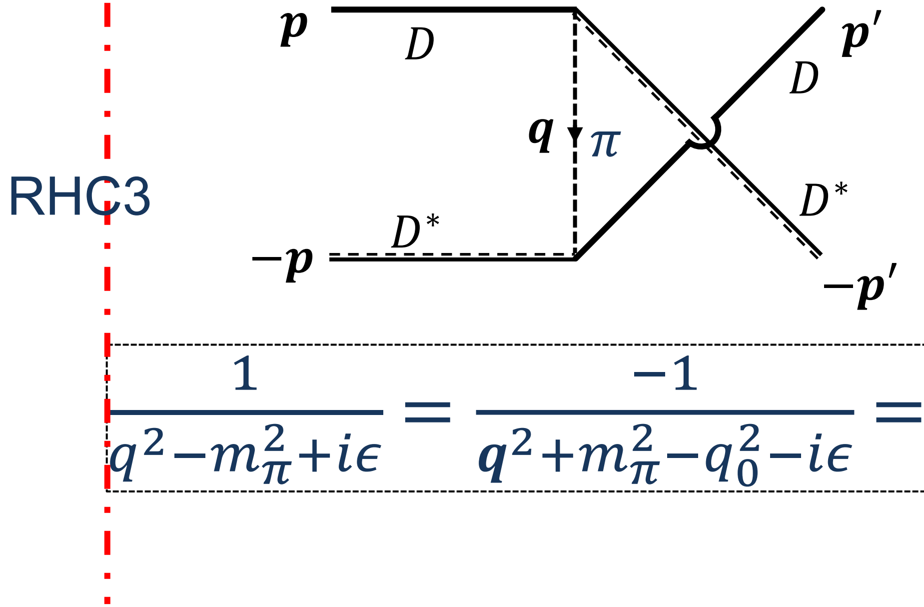


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  - ▶ $p_{\text{rhc3}}^2 \approx 2\mu_{DD^*}(2m_D + m_\pi - m_D - m_{D^*}) \approx (560\ \text{MeV})^2$

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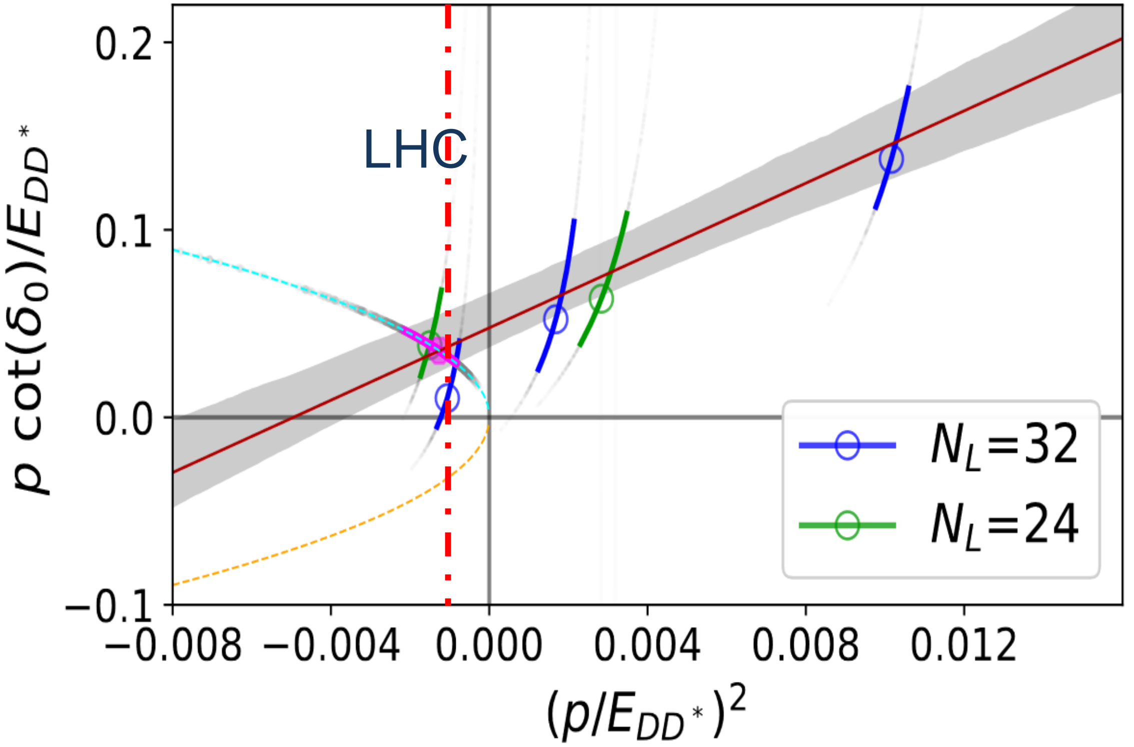


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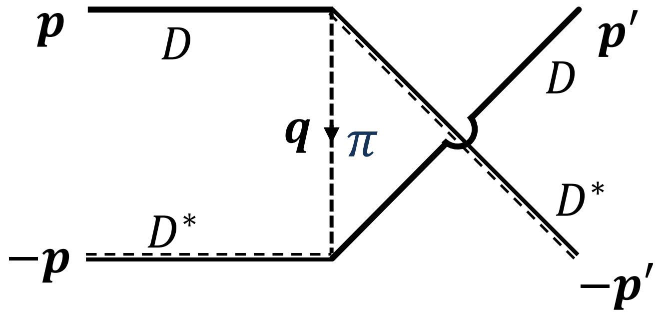


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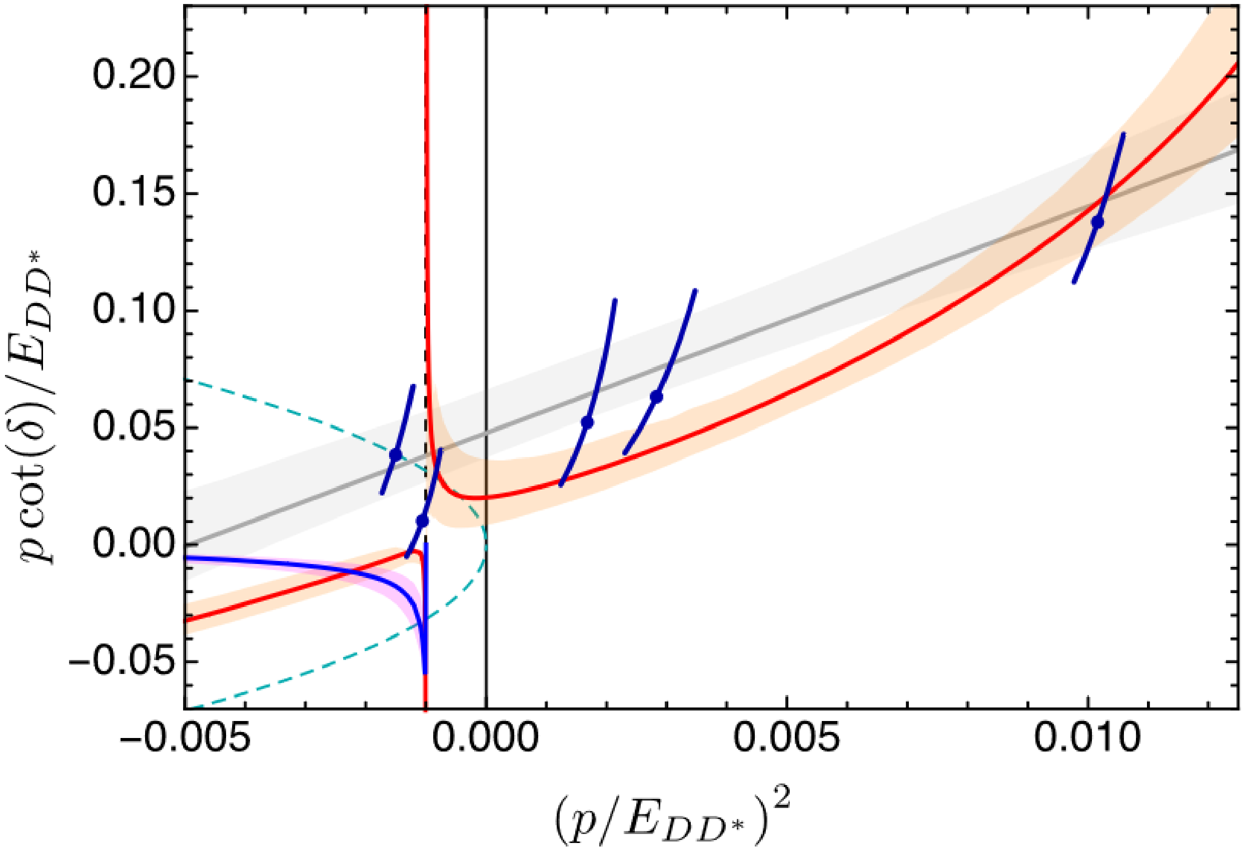
Other lattice results: Cheung:2017tnt, Junnarkar:2018twb, Chen:2022vpo, Lyu:2023xro

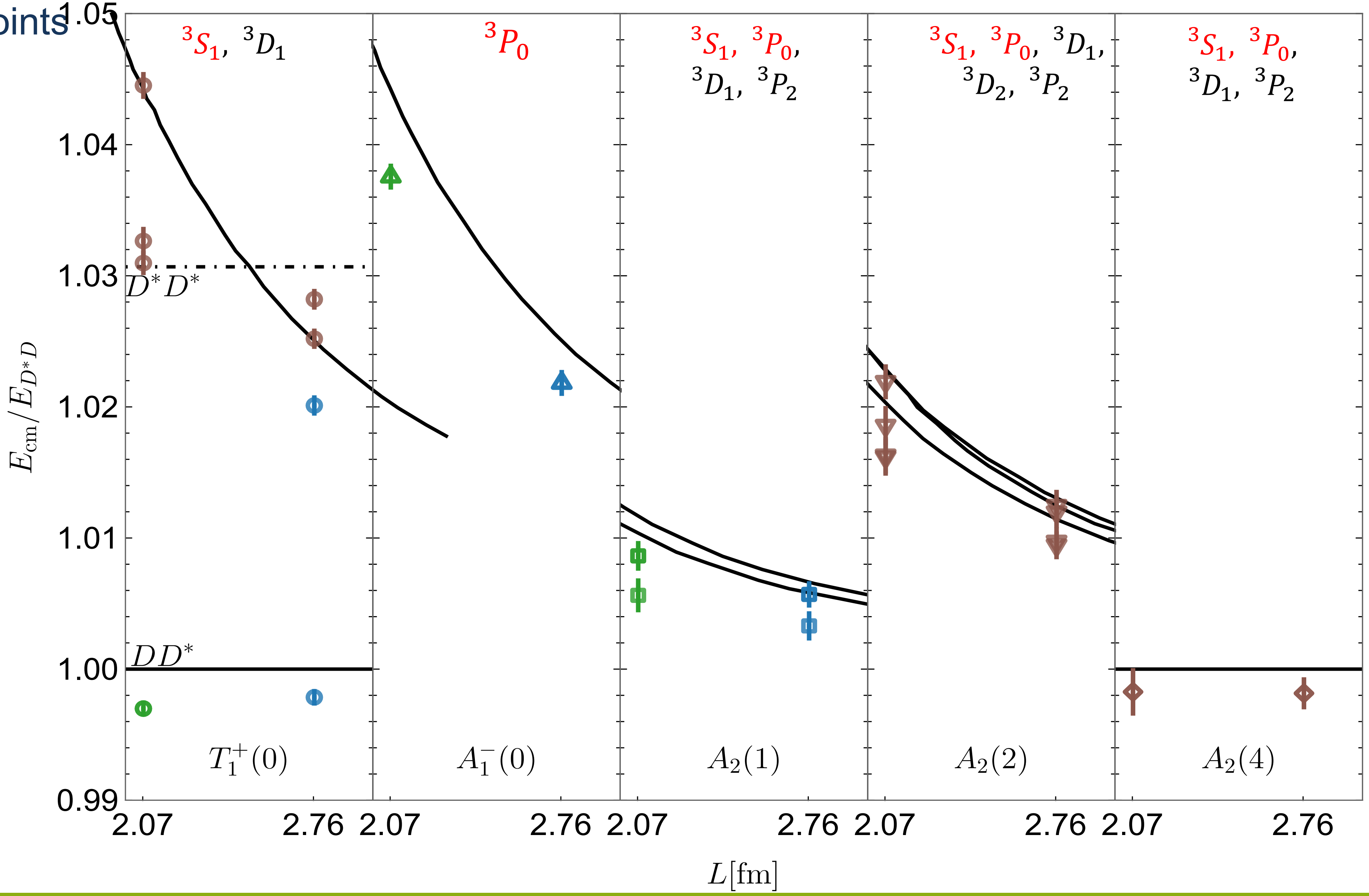
# ERE fails in IFV

- Using a Lippmann-Schwinger equation formalism, with $V = V_{OPE} + V_{\text{ctc}}^{LO} + V_{\text{ctc}}^{NLO}$ Du:2023hlu
- Conclusions: "The effective-range expansion is valid only in the very limited energy range up to the cut and as such is of little use to reliably extract the poles."
- Singular behaviors at the branch point of LHC
- Below the branch point of the LHC, $p\cot\delta$ become complex



# Lattice FV energy levels

- Green and blue points as input
- 9 inputs in total



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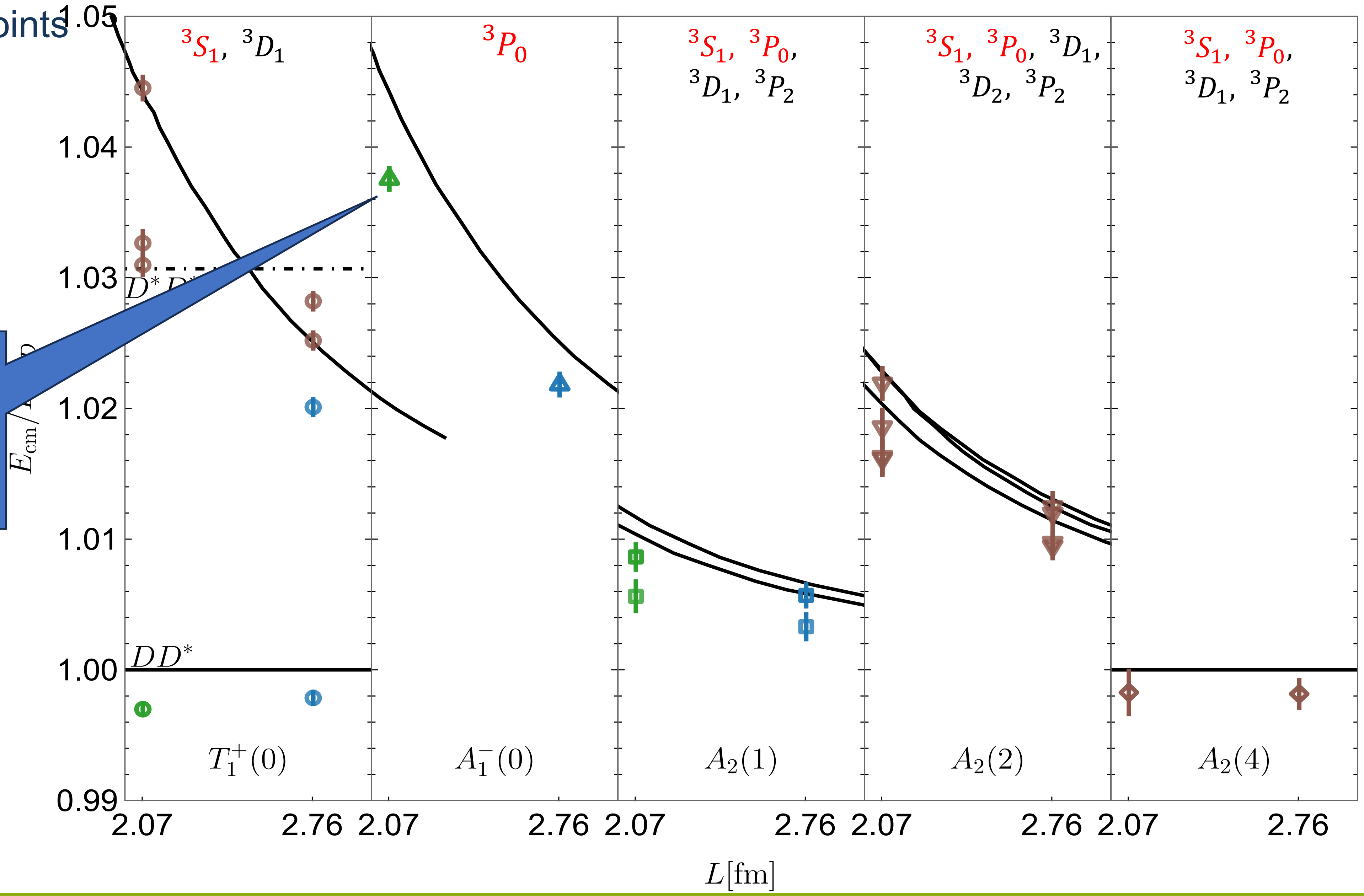


Highest input:
- relativistic effect
- large cutoff $\Lambda \geq 0.7$

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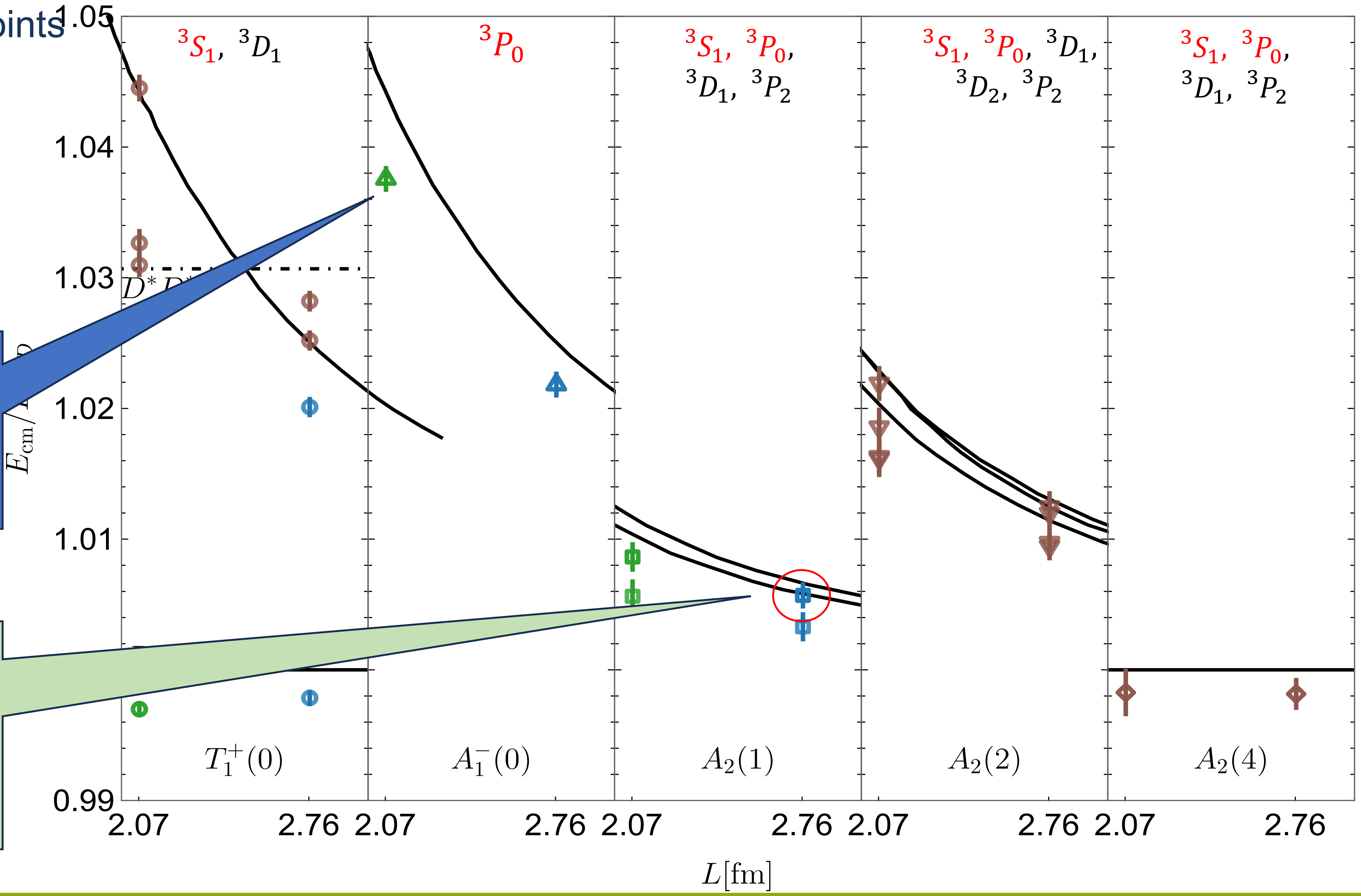



Highest input:
- relativistic effect
- large cutoff $\Lambda \geq 0.7$

Overlap with noninteracting energy levels: $\cot 0 = \infty$;

Singular in $p \cot \delta$ figures

# Relativistic formalism

- The energy levels of $A_1^-(0)$ is high, relativistic formalism

$$T(\boldsymbol{p},\boldsymbol{p}') = V(\boldsymbol{p},\boldsymbol{p}') + \int \frac{d^3\boldsymbol{q}}{(2\pi)^3} V(\boldsymbol{p},\boldsymbol{q}) \frac{1}{2w_1 w_2} \frac{(w_1+w_2)}{P_0^2-(w_1+w_2)^2+i\epsilon} T(\boldsymbol{q},\boldsymbol{p}')$$

$$w_i = \sqrt{m_i^2+\boldsymbol{q}^2}$$

$$G = i\int \frac{d^4q}{(2\pi)^4} \frac{1}{(P-q)^2-m_1^2+i\epsilon} \frac{1}{q^2-m_2^2+i\epsilon}$$

- Replace integral into summation to get $\mathbb{T}=\mathbb{V}+\mathcal{J}\mathbb{V}.\mathbb{G}.\mathbb{T}$

$$\int \frac{d^3\boldsymbol{q}}{(2\pi)^3} \to \mathcal{J}\int \frac{d^3\boldsymbol{q}_{box}}{(2\pi)^3} \to \mathcal{J}\sum_{\boldsymbol{n}} \frac{1}{L^3}$$

$\mathcal{J}$: is the Jacobian determinant of the Lorentz boost

Li:2021mob

- Get the poles

$$\det(\mathbb{H}-\lambda\mathbb{I}) = 0 \to \mathbb{H}\boldsymbol{v} = \lambda\boldsymbol{v},$$

# Interaction: ChEFT

- Contact terms to NLO

| $\mathcal{O}_1$ | $\mathcal{O}_2$ | $\mathcal{O}_3$ | $\mathcal{O}_4$ | $\mathcal{O}_5$ | $\mathcal{O}_6$ |
|---|---|---|---|---|---|
| $\boldsymbol{\epsilon}'^{\dagger}\cdot\boldsymbol{\epsilon}$ | $\boldsymbol{q}^2\boldsymbol{\epsilon}'^{\dagger}\cdot\boldsymbol{\epsilon}$ | $4\boldsymbol{k}^2\boldsymbol{\epsilon}'^{\dagger}\cdot\boldsymbol{\epsilon}$ | $4\boldsymbol{k}\cdot\boldsymbol{\epsilon}'^{\dagger}\boldsymbol{k}\cdot\boldsymbol{\epsilon}$ | $\boldsymbol{q}\cdot\boldsymbol{\epsilon}'^{\dagger}\boldsymbol{q}\cdot\boldsymbol{\epsilon}$ | $(\boldsymbol{\epsilon}'^{\dagger}\times\boldsymbol{\epsilon})\cdot(\boldsymbol{q}\times 2\boldsymbol{k})$ |

$$\boldsymbol{q}=\boldsymbol{p}'-\boldsymbol{p},\quad \boldsymbol{k}=\frac{\boldsymbol{p}'+\boldsymbol{p}}{2}$$

$$\mathcal{O}^1_{^3S_1}=\mathcal{O}_1$$

$$\mathcal{O}^2_{^3S_1}=\mathcal{O}_2+\mathcal{O}_3$$

$$\mathcal{O}_{^3S_1-^3D_1}=-\mathcal{O}_2-\mathcal{O}_3+3\mathcal{O}_4+3\mathcal{O}_5$$

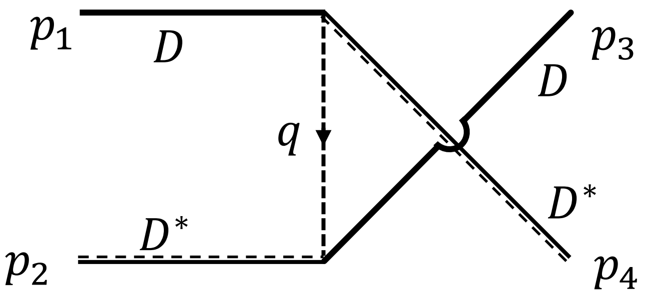
$$\mathcal{O}_{^3P_0}=-(\mathcal{O}_4-\mathcal{O}_5)+\mathcal{O}_6$$

$$\mathcal{O}_{^3P_1}=-\tfrac{3}{2}(\mathcal{O}_2-\mathcal{O}_3)+\tfrac{3}{2}(\mathcal{O}_4-\mathcal{O}_5)+\tfrac{3}{2}\mathcal{O}_6$$

$$\mathcal{O}_{^3P_2}=-\tfrac{3}{2}(\mathcal{O}_2-\mathcal{O}_3)-\tfrac{1}{2}(\mathcal{O}_4-\mathcal{O}_5)-\tfrac{5}{2}\mathcal{O}_6$$

- In present calculation: LO and NLO $^3S_1$ contact terms, NLO $^3P_0$
- Separable regulator: $e^{-\frac{p^n+p'^n}{\Lambda^n}}$, $n=2,4,6$

# One-pion-exchange interaction




- Pion propagator

$$D = q^2 - m_\pi^2 + i\epsilon\,, q^2 = (p_3 - p_2)^2 = (p_4 - p_1)^2$$

$$M_1 = M_D, M_2 = M_{D^*}$$

- Approximation

$$p_1 = (M_2, \boldsymbol{p}), p_3 = (M_2, \boldsymbol{p'}), p_2 = (M_1, -\boldsymbol{p}), p_4 = (M_1, -\boldsymbol{p}')$$

$$D \approx -\boldsymbol{q}^2 - [m_\pi^2 - (M_{D^*} - M_D)^2] + i\epsilon$$

- Semilocal momentum-space regularization

Reinert:2017usi

$$\mathcal{V}(q) = -\frac{g^2}{4F_\pi}\left[\frac{\boldsymbol{q}\cdot\boldsymbol{\epsilon}'^*\boldsymbol{q}\cdot\boldsymbol{\epsilon}}{\boldsymbol{q}^2 + u^2} + C_{sub}\boldsymbol{\epsilon}'^*\cdot\boldsymbol{\epsilon}\right] e^{-\frac{q^2+u^2}{\Lambda^2}}$$

$$C_{sub} = -\frac{\Lambda(\Lambda^2 - 2u^2) + 2\sqrt{\pi}u^3 e^{\frac{u^2}{\Lambda^2}}\operatorname{erfc}(\frac{u}{\Lambda})}{3\Lambda^3}$$

► The regulator will not change the long-range behavior

► The short-range part of OPE is subtracted: $V_{\epsilon\cdot\epsilon}(r=0) = 0$

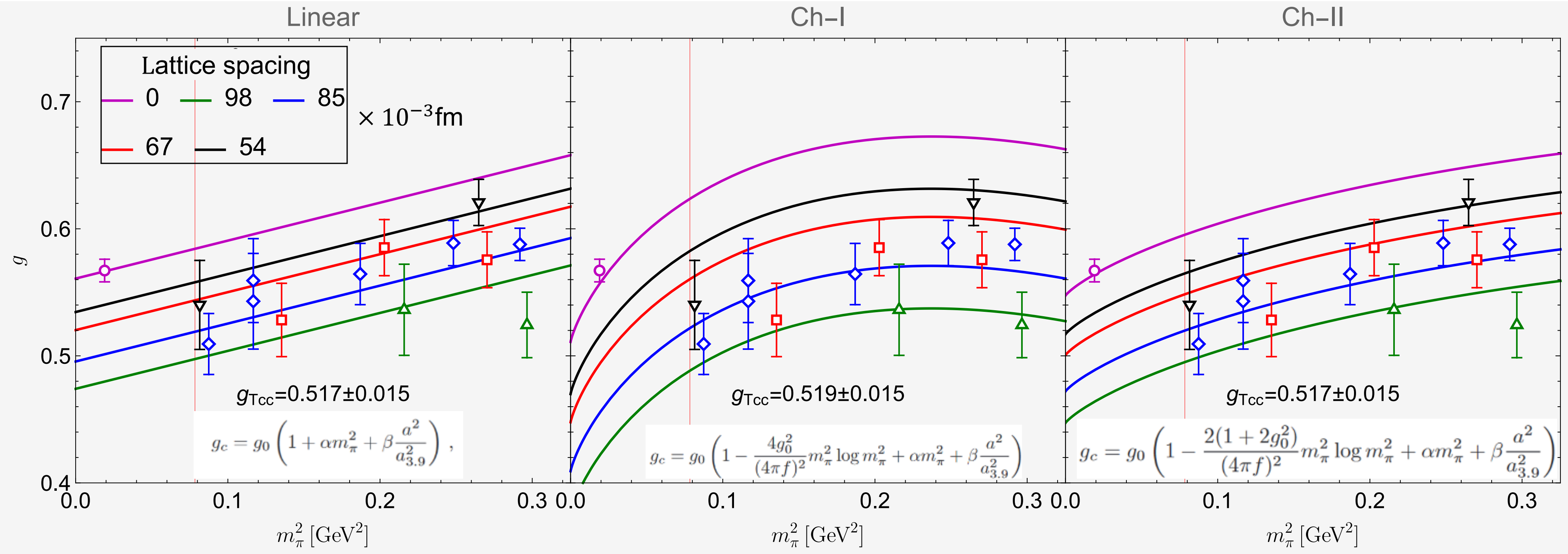
# $F_\pi$ and $g$

- $F_\pi$ and $g_{D^*D\pi}$ at $m_\pi = 280$ MeV are determined by lattice QCD data, physical values by either linear extrapolation or chiral extrapolation
- $F_{ph} = 92.1$ MeV, $F_0 = 85$ MeV, chiral extrapolation, $\xi = m/m^{ph}$

$$f_\pi(\xi) = f_\pi^{\rm ph}\left[1 + \left(1 - \frac{f_0}{f_\pi^{\rm ph}}\right)(\xi^2 - 1) - \frac{(m_\pi^{\rm ph})^2}{8\pi^2 f_0^2}\xi^2 \log \xi\right]$$

Du:2023hlu,Becirevic:2012pf

- Three extrapolations give the consistent results
  - ► The $g$ is slightly smaller than the value in Ref. [Du:2023hlu]
  - ► $g = 0.517 \pm 0.015$ for $a = 0.086$ fm



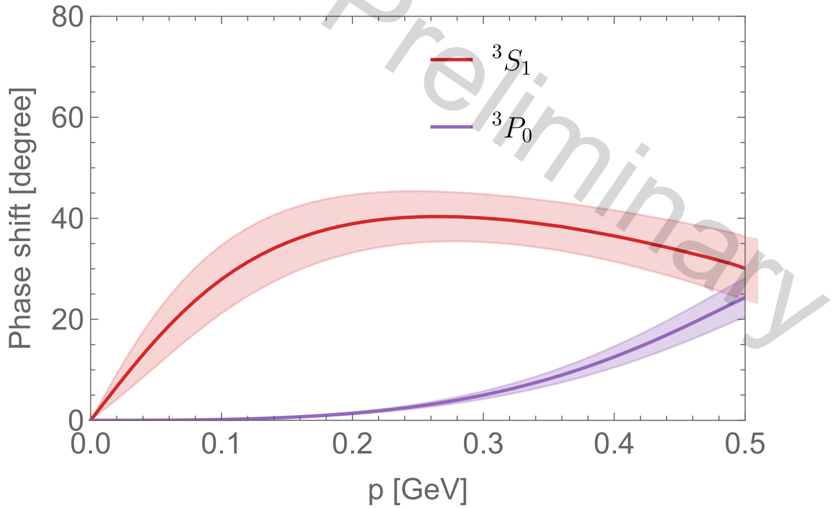
# $\Lambda = 1.1$ GeV, only contact terms

- Results using Lüscher's QCs   Padmanath:2022cvl

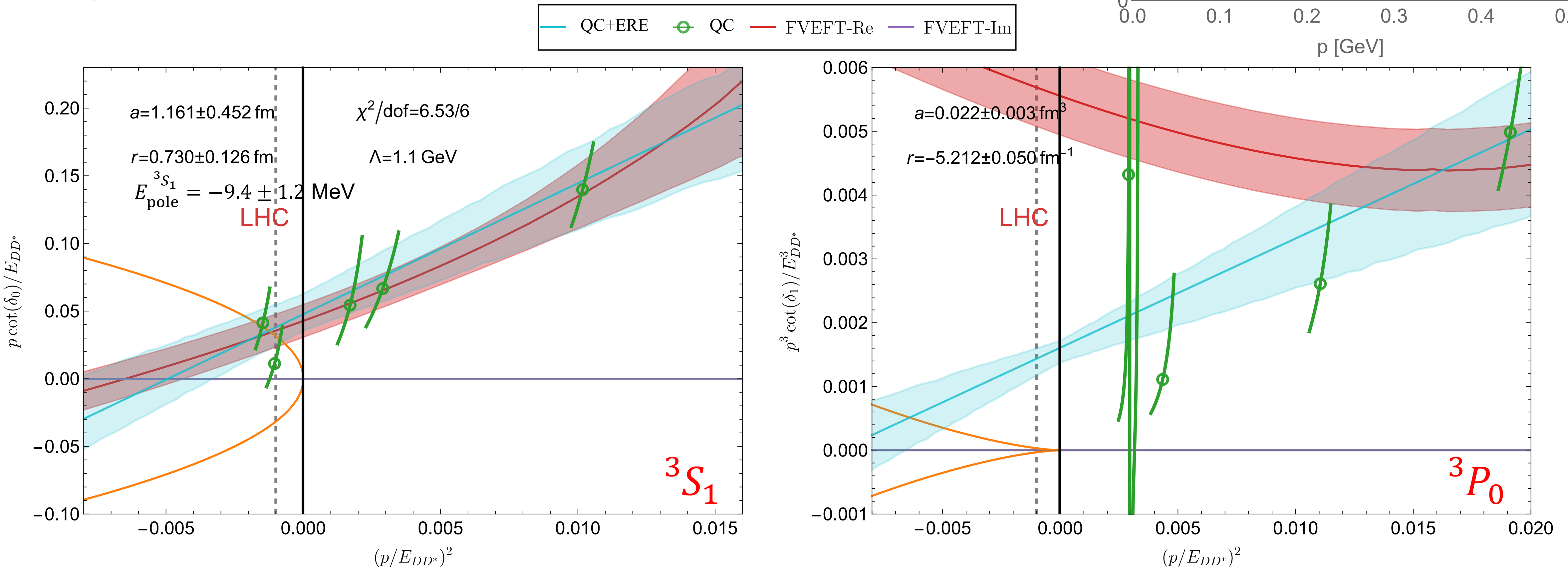
$$\chi^2/\text{dof}=3.7/5,\; E_{\text{pole}}^{^3S_1} = -9.9^{+3.6}_{-7.2}\ \text{MeV}$$

$$a_{^3S_1} = 1.04(29)\text{fm},\qquad r_{^3S_1} = 0.96^{+0.18}_{-0.20}\text{fm}$$

$$a_{^3P_0} = 0.076^{+0.008}_{-0.009}\text{fm}^3,\; r_{^3P_0} = 6.9(2.1)\text{fm}^{-1}$$




- Our results



# $\Lambda = 1.1$ GeV, contact terms+OPE

- Results using Lüscher's QCs Padmanath:2022cvl

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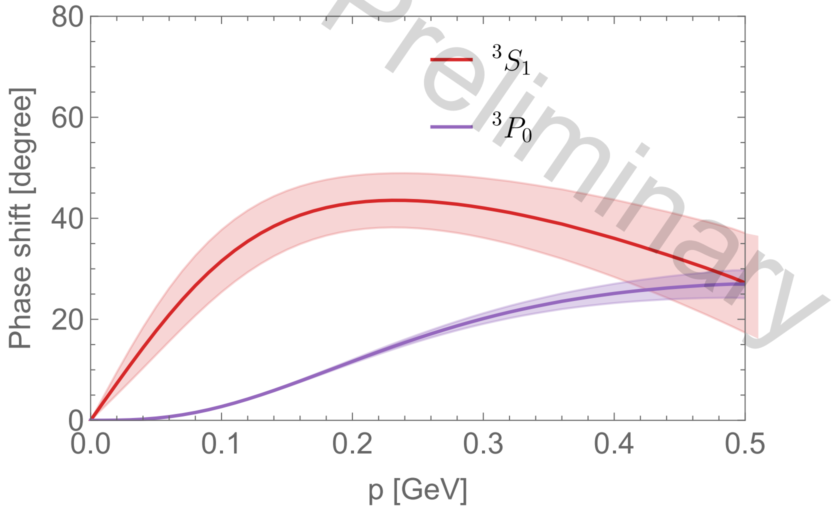


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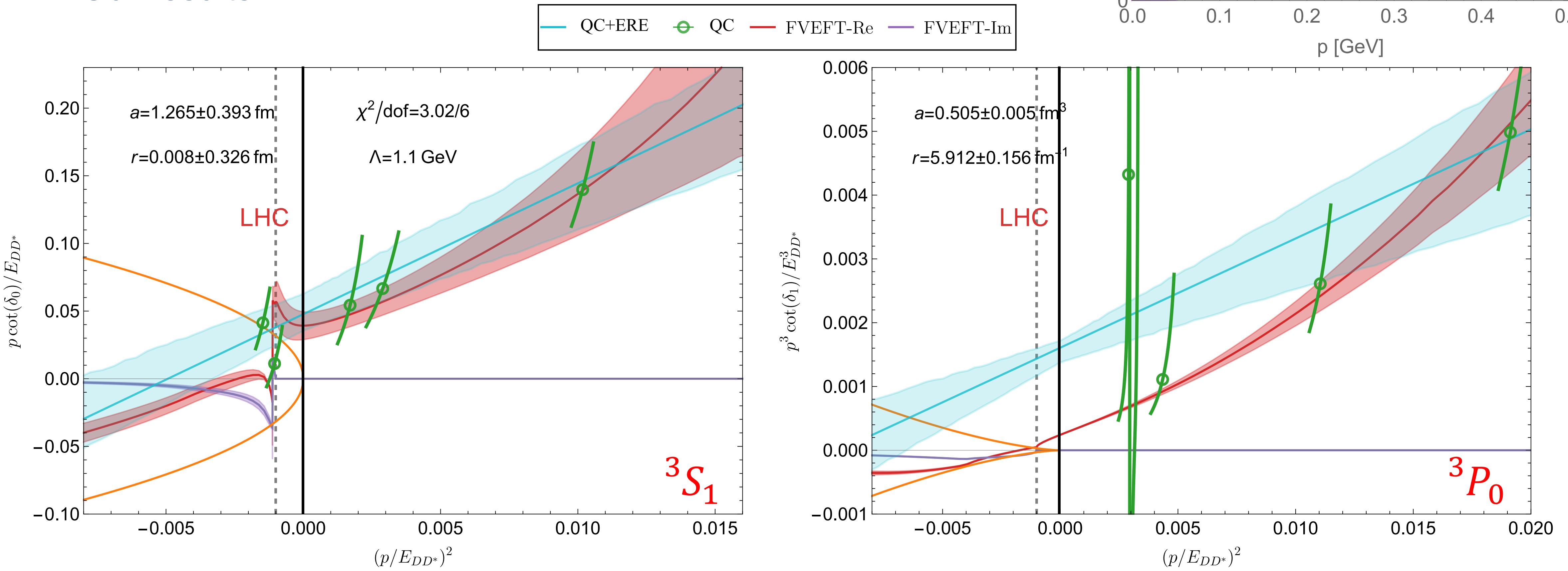
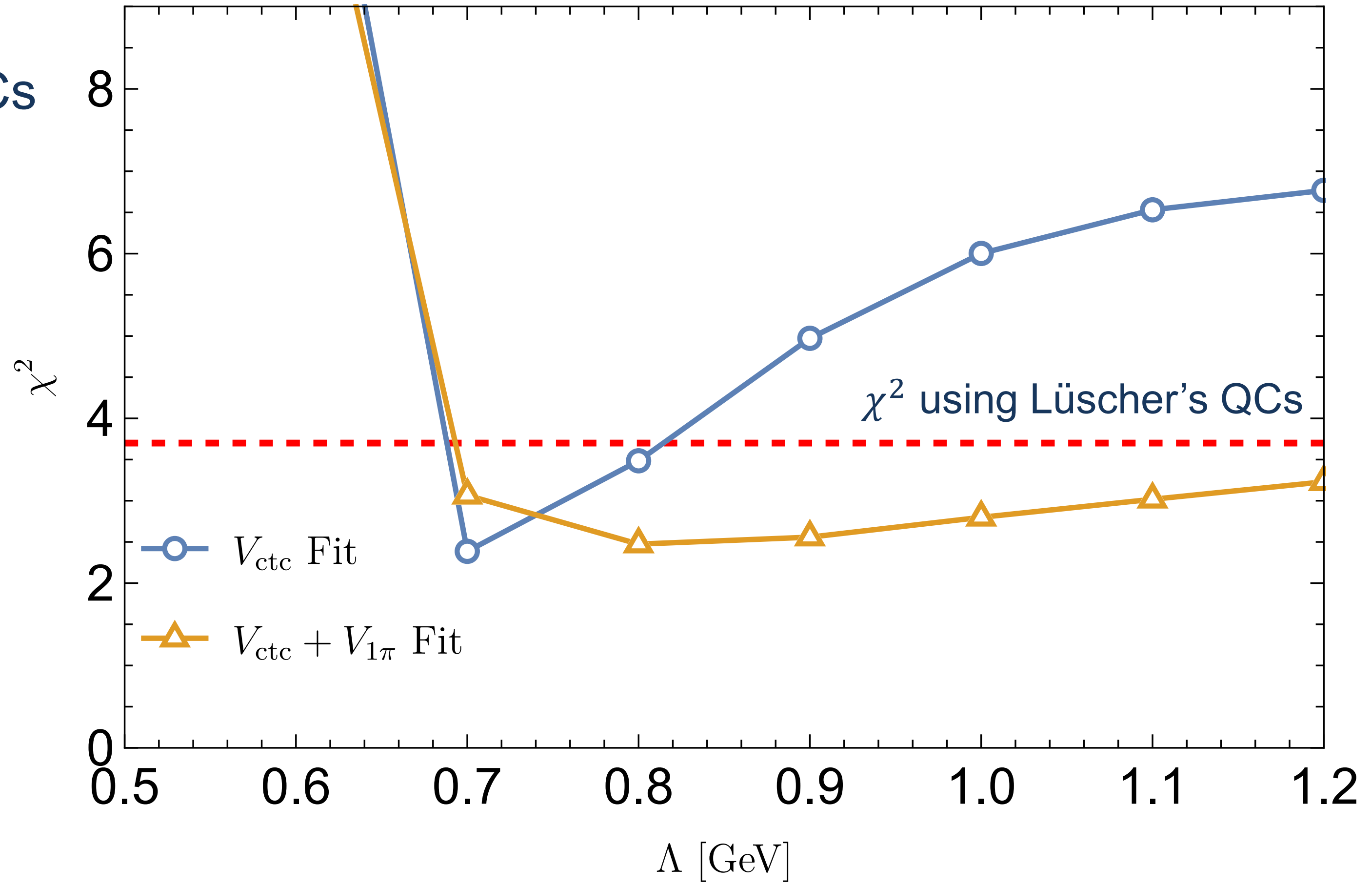


# Cutoff dependence of $\chi^2$

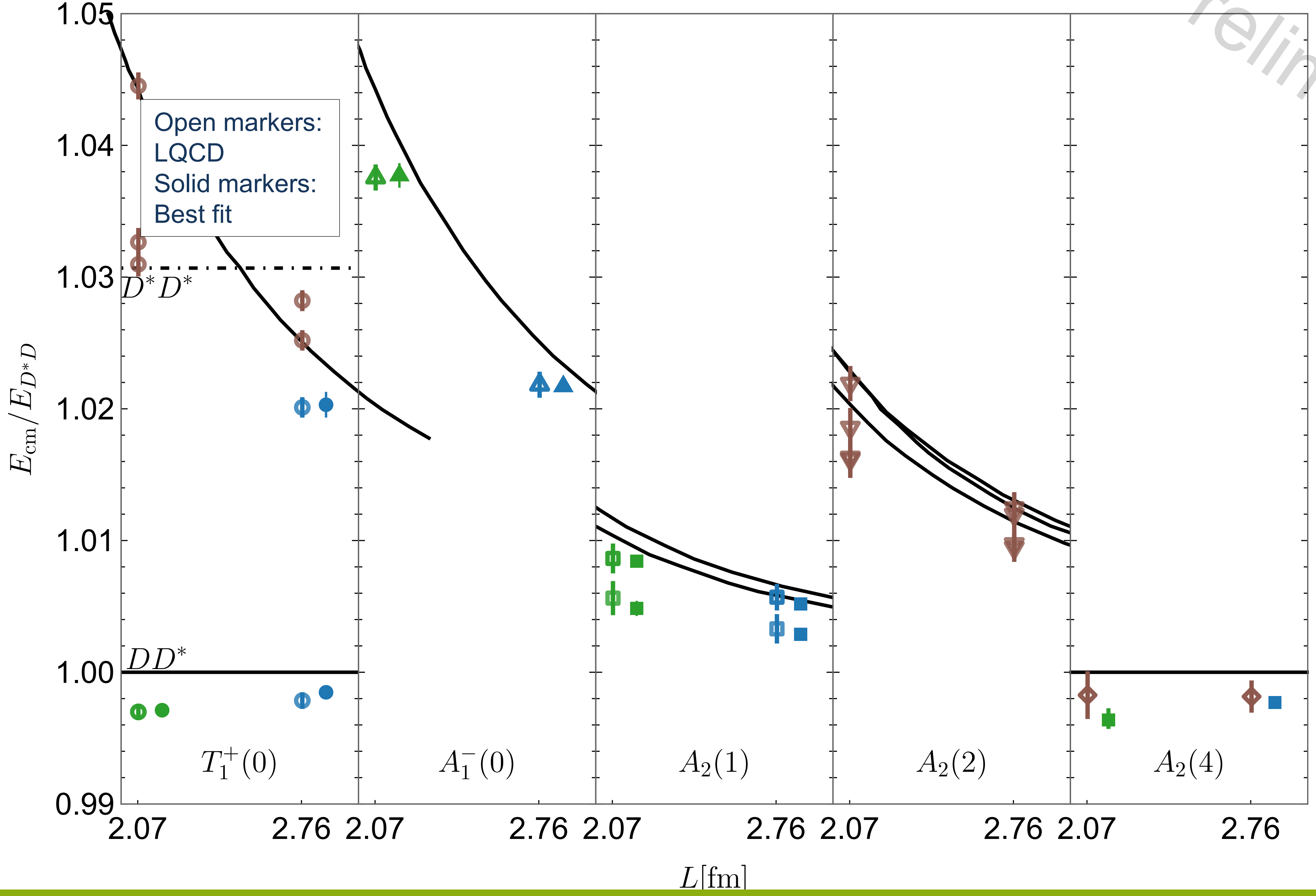


- 3 LECs: LO and NLO $^3S_1$ contact terms, NLO $^3P_0$
- In $V_{\rm ctc}$ fit, the P-wave dominate states control $\Lambda$-dependence of the $\chi^2$
  - ▶ The shape of the of $k^3 \cot \delta_1$ is determined by regulator and cutoff
  - ▶ Sensitive to $\Lambda$
- The $V_{\rm ctc}$+ $V_{1\pi}$ fit is stable with $\Lambda$
- The $V_{\rm ctc}$+ $V_{1\pi}$ fit is even better than QCs



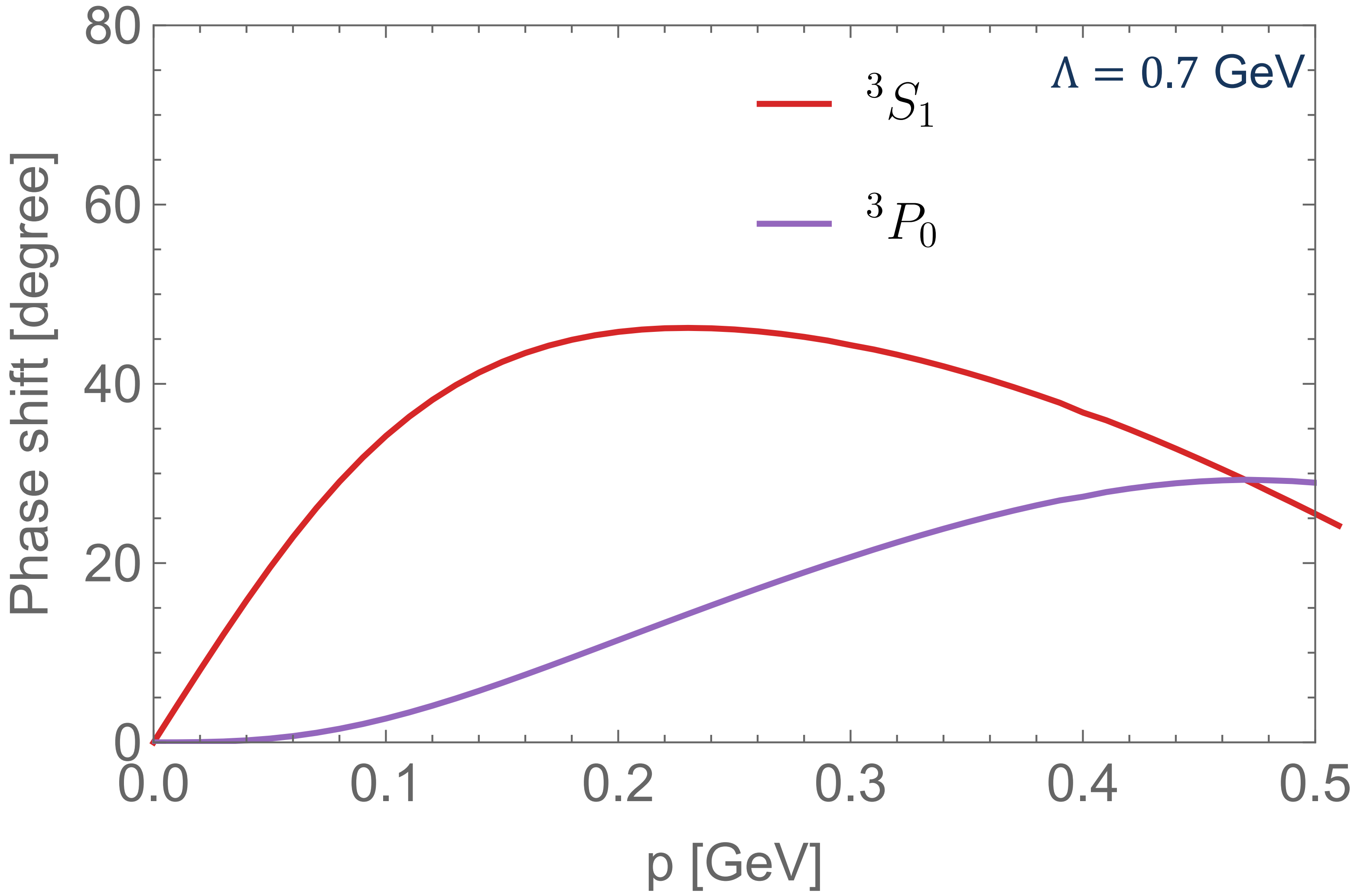
# Energy levels from the best fit





# Cutoff dependence of phase shift





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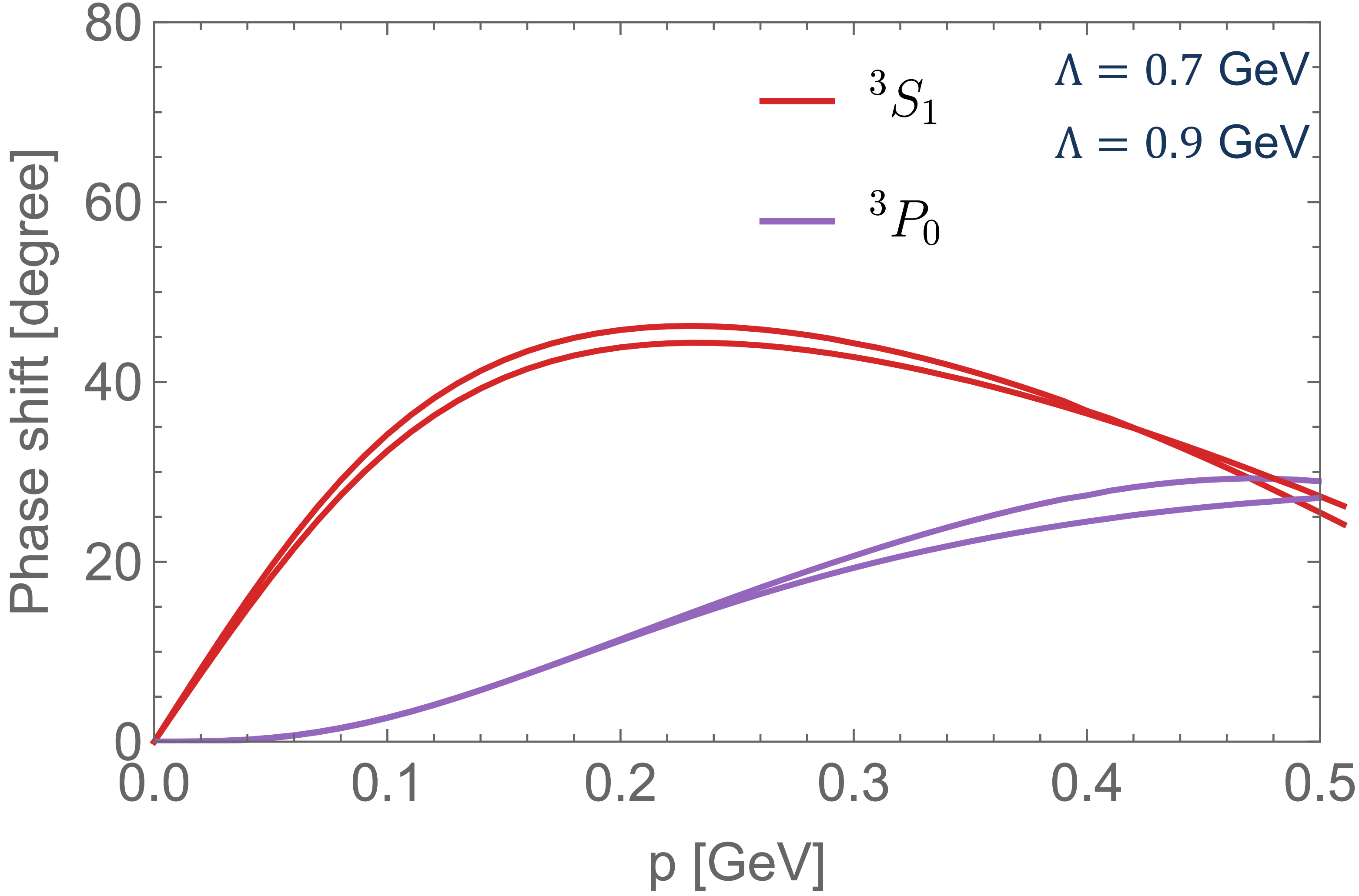

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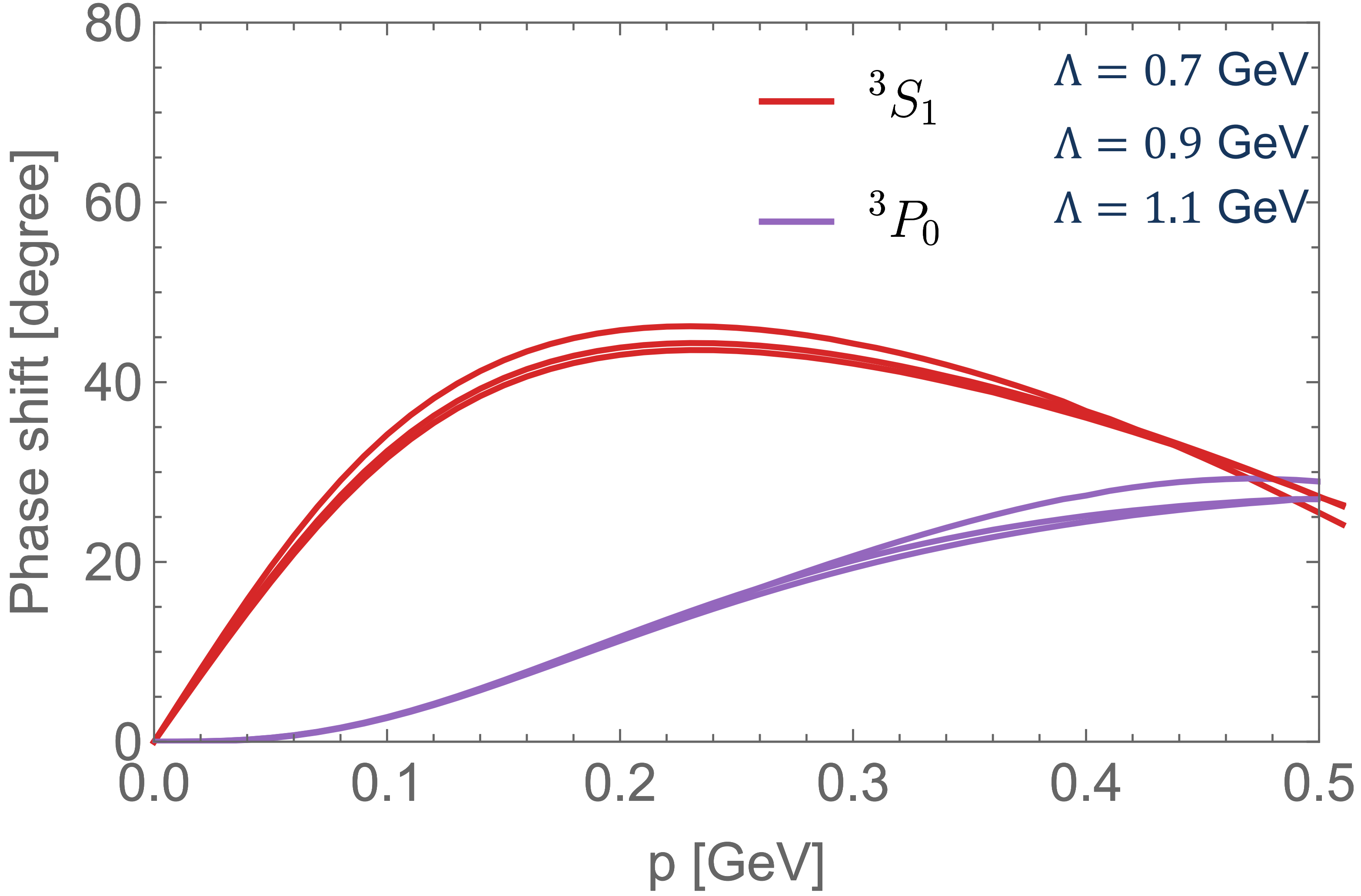


# Test consistency with Lüscher's formula

- Using the LECs of our best fitting
- $V_{\text{full}}$ and S-wave-projected $V_S$
- Obtain IFV T-matrix

Red solid VS red dashed; purple solid VS purple dashed

Physical S-D mixing effect

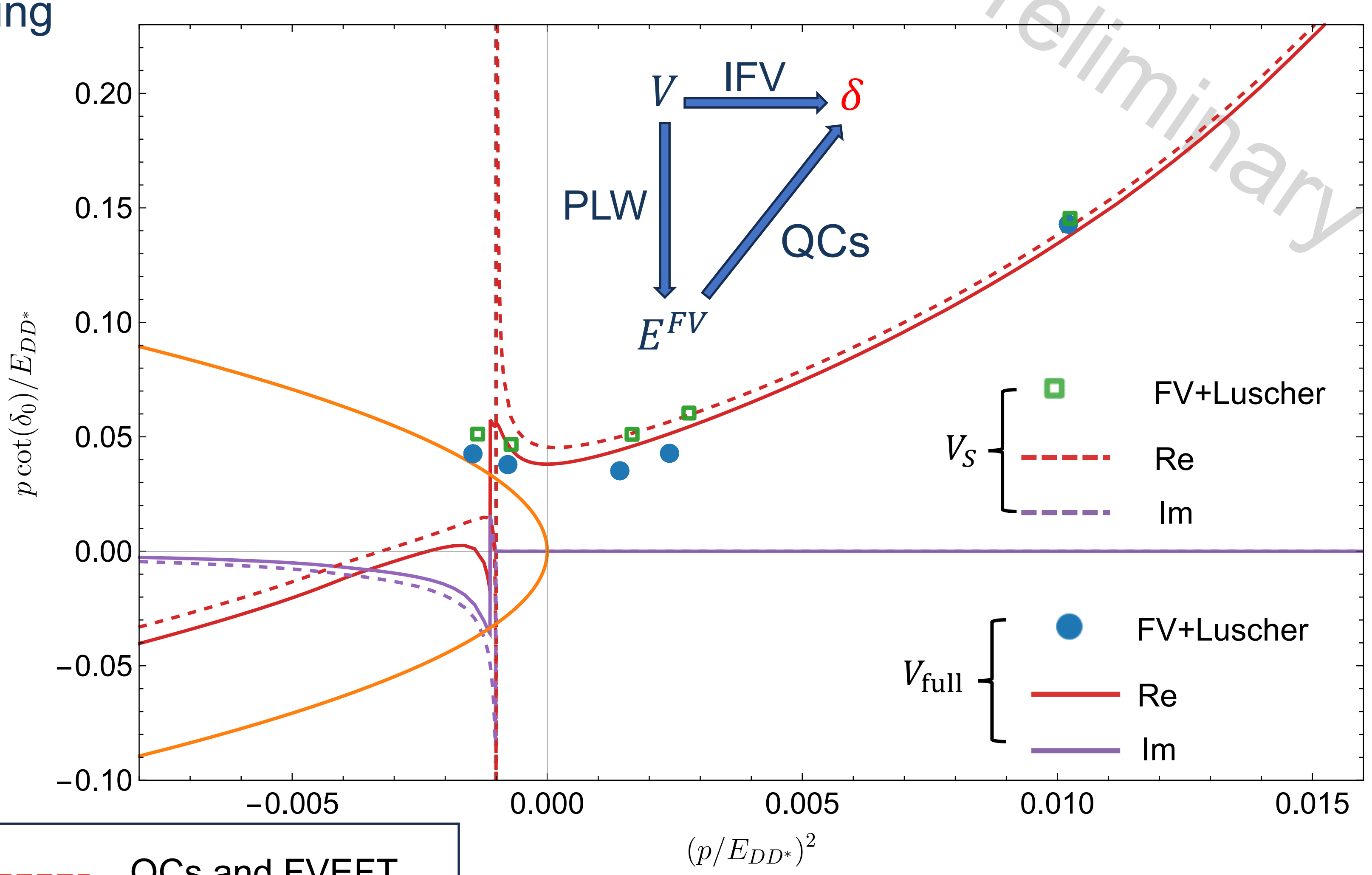
- Obtain the FV energy levels

Blue dot VS green square: S-D mixing, S-P mixing

- Using Lüscher's QCs to get $\delta$
  - ▶ Single partial wave QCs

Red solid line, blue dot: 1PW QCs fails

Red dashed line, green square: QCs and FVEFT Consistency




Red dashed line, green square: QCs and FVEFT inconsistency: LHC

# Summary and Outlook

- Validation of Lüscher's formula
  - ① $e^{-mL}$ effect can be neglected
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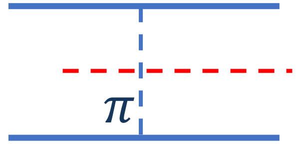
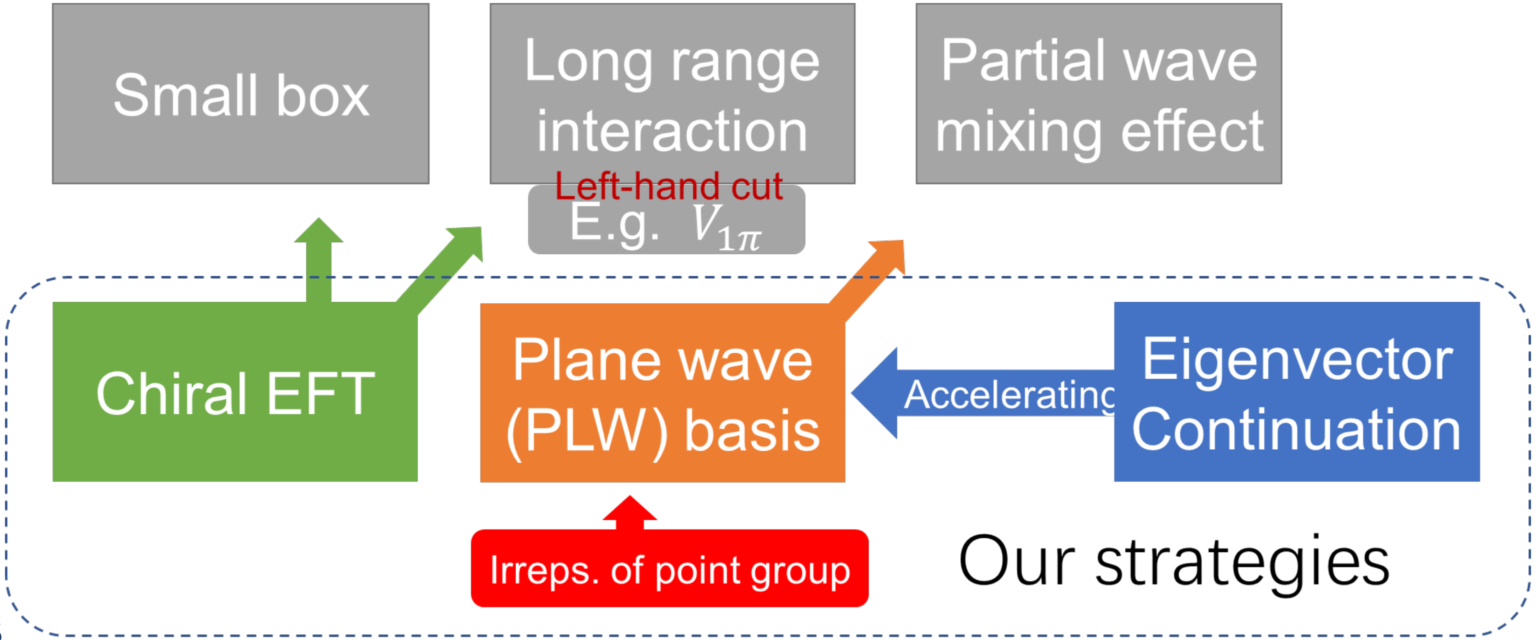
Invalidate



One-pion-exchange interaction

- Our formalism




- $T_{cc}$ lattice data
  - ▶ Better fit than QCs
  - ▶ The possible partial wave mixing effect
  - ▶ Left-hand cut fails the Lüscher's formula

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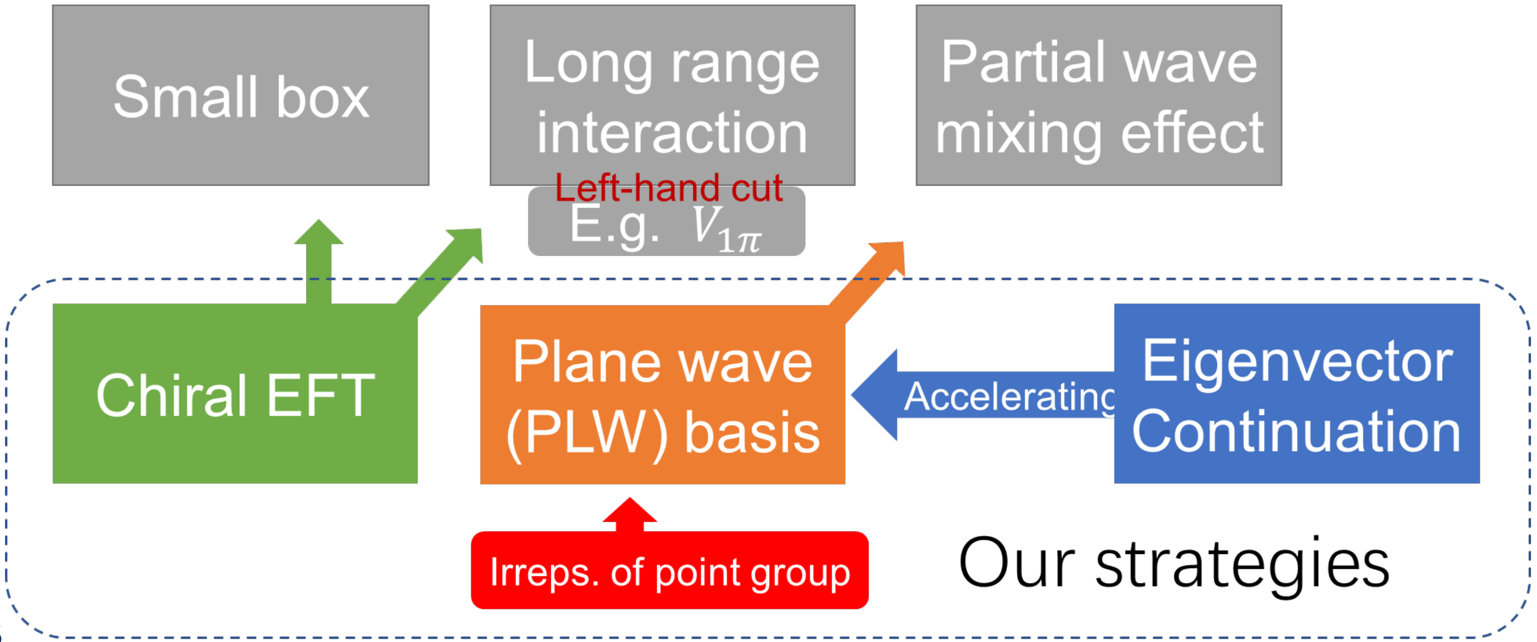


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Thanks for your attentions!

# Back up

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

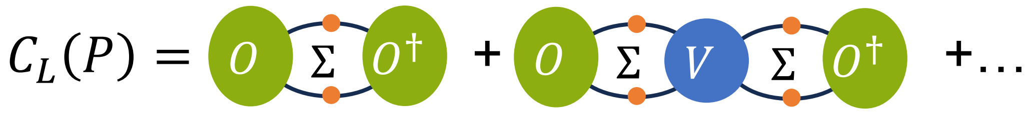
- The "$=$" relation is valid up to the exponentially suppressed terms in $L$
- $K$ matrix in the infinite volume: $K = V + VG_K K$

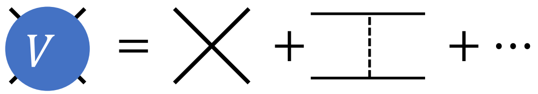
$$T^L = V + V(G_K + G_F)T^L = K + KG_F T^L$$

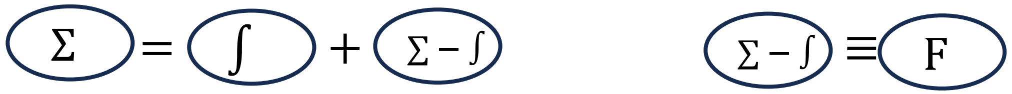
- $E^{FV}$ corresponding to poles of $T^L$ : interaction-independent form

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

# Detailed derivation of Lüscher's formula



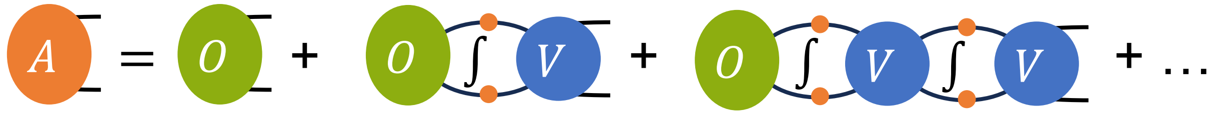




$$\left[\frac{1}{L^3}\sum_{\boldsymbol{k}} - \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\right] f(k) = \begin{cases} \mathcal{O}(e^{-mL}) & \text{smooth } f(k) \\ \text{power of } L & \text{otherwise} \end{cases}$$


Within on-shell approximation:

$$F + FKF + \cdots = F(1 - KF)^{-1} = (F^{-1} - K)$$





Note: all the $\int$ should be treated in the sense of P.V.

# Lüscher's formula: partial wave mixing effect

- Expanding it in partial wave basis

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

  - ▶ Determinate equation of a matrix with infinite dimensions.
  - ▶ Truncate at some $l_{\max}$

- Reduce to irreps. $\Gamma_i$ of point group

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

- Obtain the basis of the irreps. $|l,m\rangle \to |\Gamma, l, \alpha\rangle$ (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: partial wave mixing effect

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

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

- 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 relation
  - E.g. $\{E_1^{FV}, E_2^{FV}\} \neq \{\delta_S(E_1^{FV}), \delta_S(E_2^{FV}), \delta_D(E_1^{FV}), \delta_D(E_2^{FV})\}$
  - One has to parameterize the K-matrix
  - Effective range expansion
- Lüscher's formula: quantization conditions in partial wave basis
- Why not quantization conditions in plane wave basis + Hamiltonian method?

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

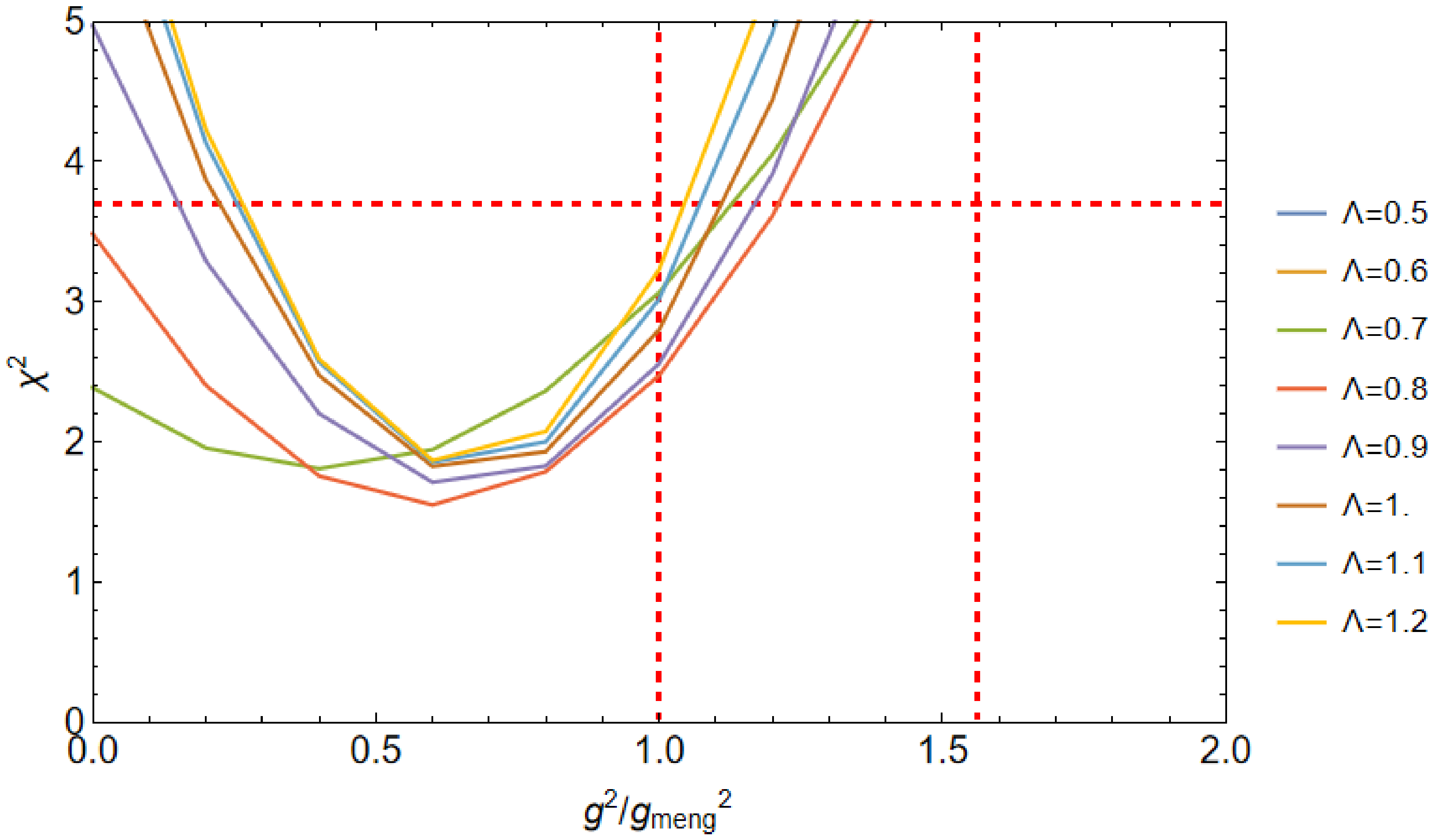
- For moving systems, elongated boxes, particles with arbitrary spin...

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

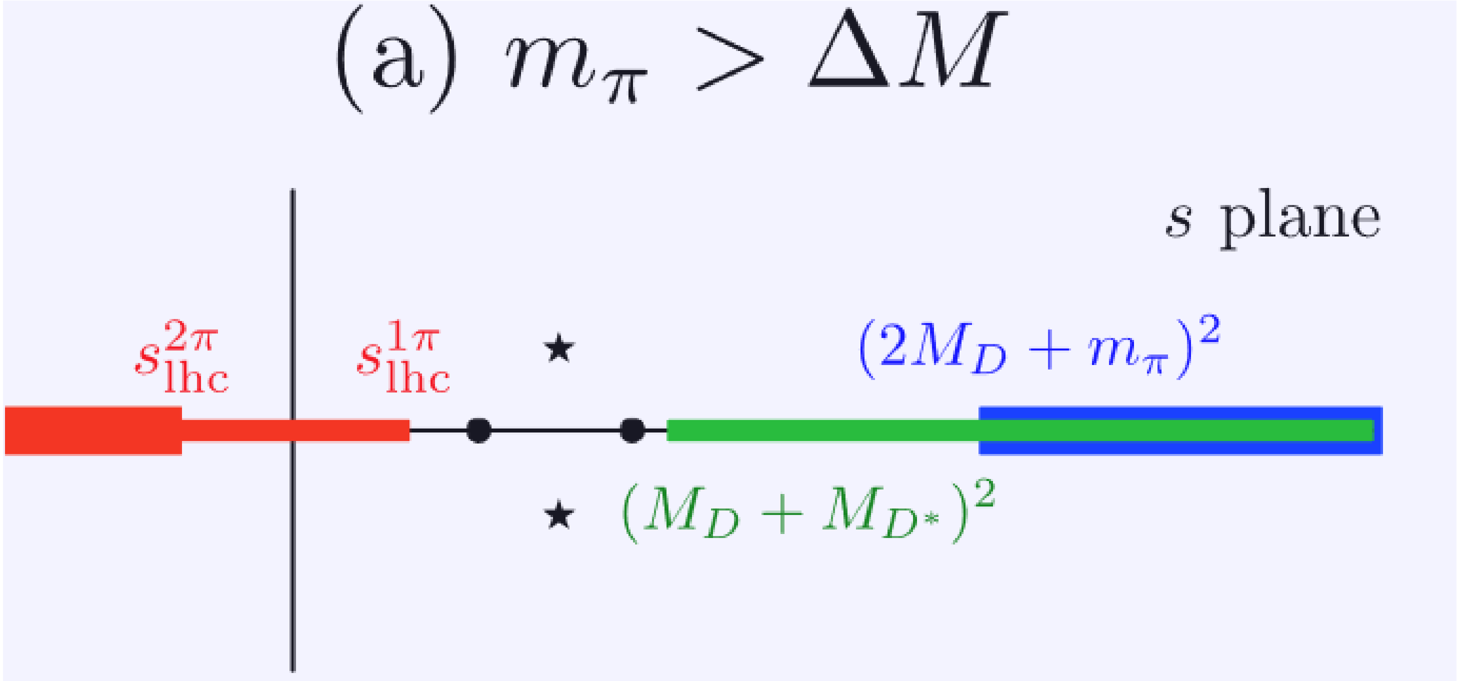
- dim of the $\mathbb{H}_\Gamma$ : cubic function of $L^{-1}$

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

# Tuning the g

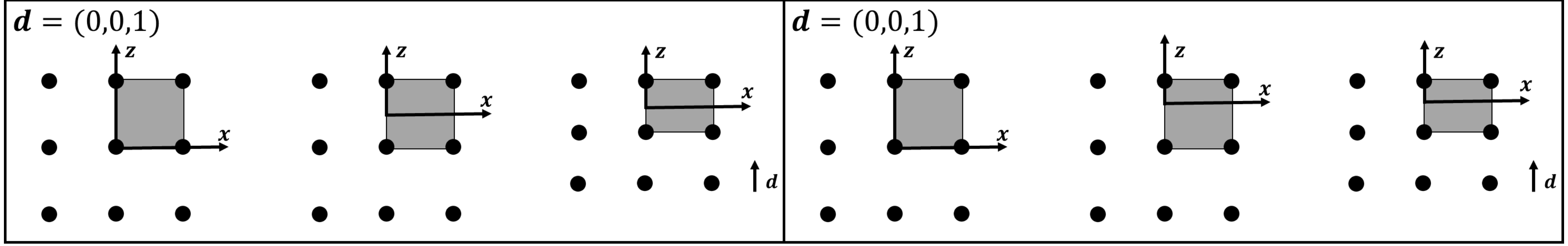


5
4
3
2
1
0
0.0
0.5
1.0
1.5
2.0
$\chi^2$
$g^2/g_{meng}^2$
Λ=0.5
Λ=0.6
Λ=0.7
Λ=0.8
Λ=0.9
Λ=1.
Λ=1.1
Λ=1.2


(a) $m_\pi > \Delta M$
$s$ plane
$s_{\rm lhc}^{2\pi}$
$s_{\rm lhc}^{1\pi}$
$(2M_D + m_\pi)^2$
$(M_D + M_{D^*})^2$

# Moving systems

| $m_1 = m_2, \quad A = 1$ | | | $m_1 \neq m_2, \quad A = 1 + \frac{m_1^2 - m_2^2}{E^*}$ | | |
|---|---|---|---|---|---|
| $\boldsymbol{n} \in Z$ | $\boldsymbol{n} - \frac{1}{2}\boldsymbol{d}$ | $\gamma^{-1}\left(\boldsymbol{n}_\parallel - \frac{\boldsymbol{d}}{2}\right) + \boldsymbol{n}_\perp$ | $\boldsymbol{n} \in Z$ | $\boldsymbol{n} - \frac{A}{2}\boldsymbol{d}$ | $\gamma^{-1}\left(\boldsymbol{n}_\parallel - \frac{A}{2}\boldsymbol{d}\right) + \boldsymbol{n}_\perp$ |




Space inversion invariance is broken

- Moving system in the box $\boldsymbol{P} = \frac{2\pi}{L}\boldsymbol{d} \neq 0$
  - ▶ For LQCD, changing box size is expensive
  - ▶ Calculate $E^{FV}$ of moving two-body systems in a box

Rummukainen:1995vs,Leskovec:2012gb

- Box frame (BF) $\boldsymbol{p}$ and center of mass frame (CMF) $\boldsymbol{p}^*$
  - ▶ BF: $\boldsymbol{p} = \frac{2\pi}{L}\boldsymbol{n}$; CMF: $\boldsymbol{p}^* = \gamma^{-1}\left(\boldsymbol{p}_\parallel - \frac{A}{2}\boldsymbol{P}\right) + \boldsymbol{p}_\perp$
  - ▶ For moving systems with $m_1 \neq m_2$, states with different parities could mix
- $\boldsymbol{d} = (0,0,1)$, $D_{4h}$ group for $m_1 = m_2$, $C_{4v}$ group for $m_1 \neq m_2$
- $\boldsymbol{d} = (1,1,0)$, ...

# Towards a practical approach: eigenvector continuation

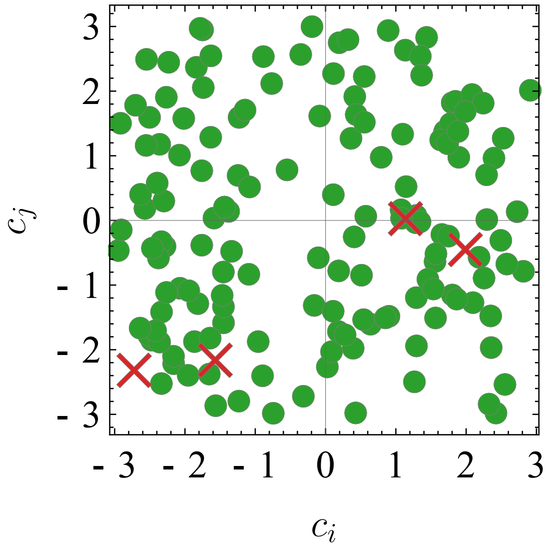
- Plane wave basis+Eigenvector continuation
  - ▶ Eigenvector continuation (EC) with subspace learning

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

- Rayleigh-Ritz variational principle:

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

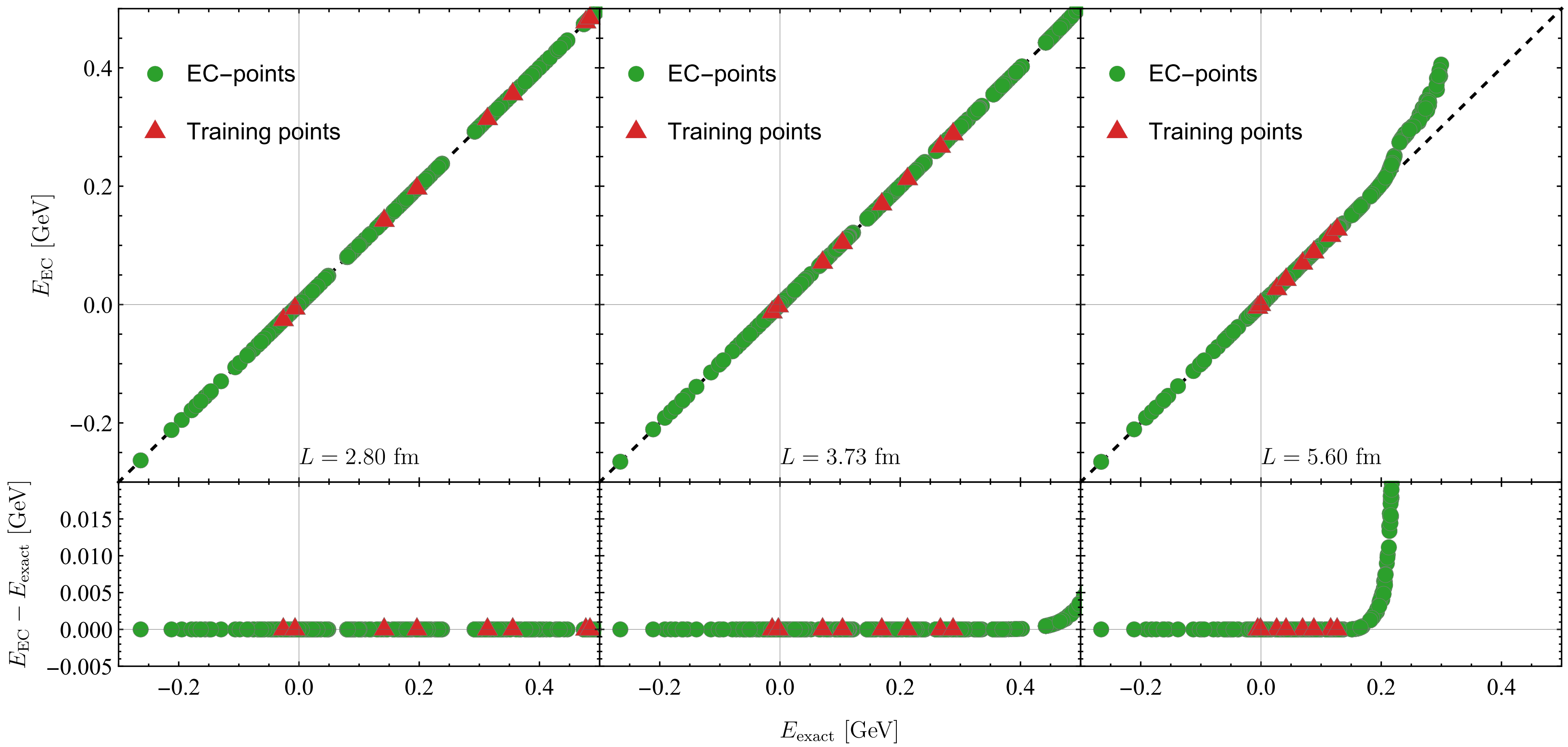
$$|\psi\rangle = a_m|\phi_m\rangle, \quad \langle\phi_m|H(c_i)|\phi_n\rangle a_n = \mathcal{E}\langle\phi_m|\phi_n\rangle a_n$$




  - ▶ 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 $\{c_i\}_1$, $\{c_i\}_2$ ,... (training point)
- Naturalness of low energy constants (LEC) of EFT ( ~ 1 ) make the EC more reliable

# Eigenvector continuation

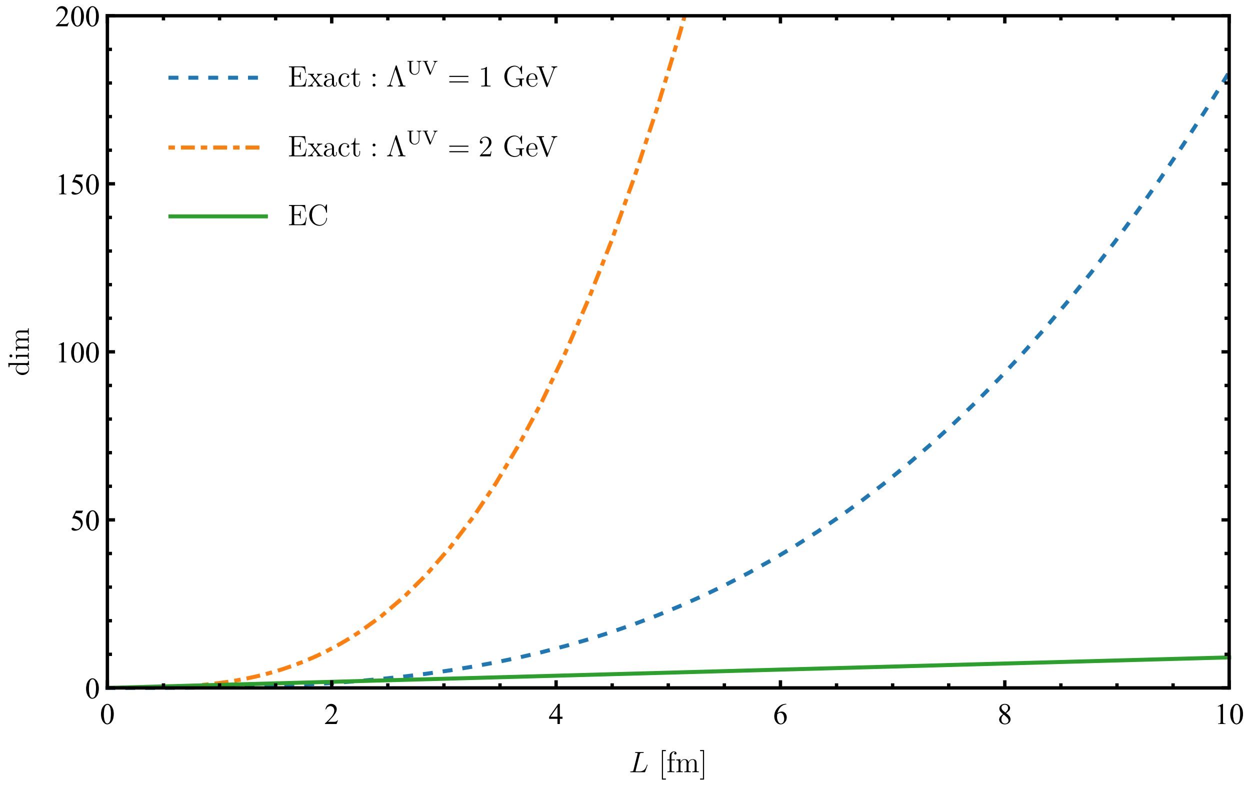



- Interaction: $V_{ctc}$ with 2 LECs $\{c_1, c_2\}$ + $V_{1\pi}$ in $L = \{2.70,3.73,5.60\}$ boxes
- Training points: $\{c_{1phy}, 0\}$, $\{0, c_{2phy}\}$ ; keep the first four energy levels as basis, dim=8

# Eigenvector continuation

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

- dim is linear function $L^{-1}$:
  - ▶ 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

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

  - ▶ Easy-to-use interface: no need to know the details of $\chi$EFT

## Approximation-II

$$p_1 = (w_2(\boldsymbol{p}), \boldsymbol{p}), p_3 = (w_2(\boldsymbol{p}'), \boldsymbol{p}'), p_2 = (w_1(\boldsymbol{p}), -\boldsymbol{p}), p_4 = (w_1(\boldsymbol{p}'), -\boldsymbol{p}')$$

$$w_i(\boldsymbol{p}) = \sqrt{M_i^2 + \boldsymbol{p}^2}$$

$$q^2 \approx \frac{[w_2(\boldsymbol{p}) - w_1(\boldsymbol{p}')]^2 + [w_2(\boldsymbol{p}') - w_1(\boldsymbol{p})]^2}{2} - \boldsymbol{q}^2$$