

Left-hand cut problem in lattice QCD and an EFT-based solution

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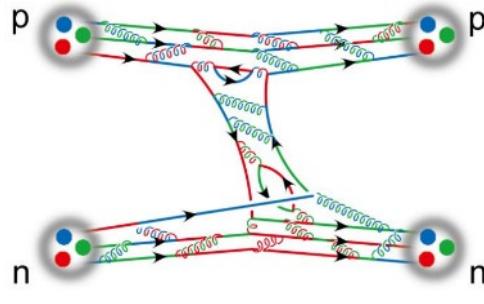
27 Aug. 2024, Bochum

Base on [JHEP10\(2021\)051](#), [PoS LATTICE2022 \(2023\) 201](#) and [PRD109\(2024\), L071506](#)

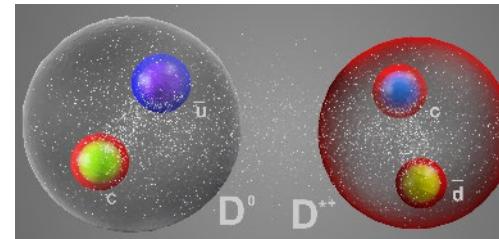
Together with V. Baru, E. Epelbaum, A. Filin, A.M. Gasparyan

Lattice QCD

- QCD is the fundamental theory of the strong interaction
- To get the hadron-hadron interaction from the first principle?

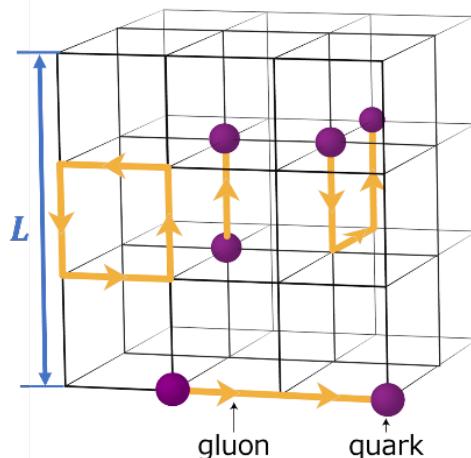


Nuclear force

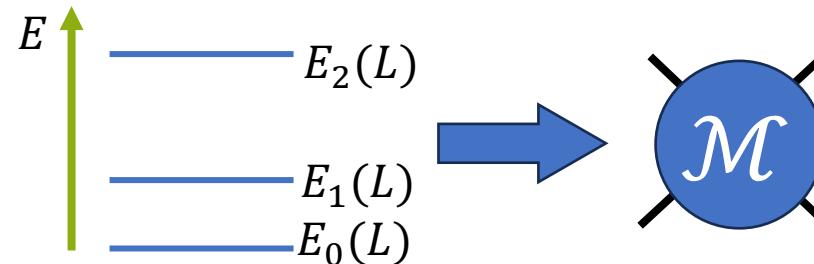


Hadronic molecules

- Lattice QCD: on a lattice of points in space and time in a **finite volume (FV)**



Raw data from lattice: FV energy levels



Observables in the infinite volume (IFV)

Lüscher's formula

- Lüscher's formula:

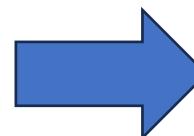
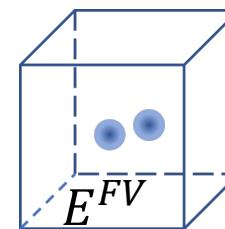
Luscher:1990ux

AKA : Lüscher Quantization conditions (LQCs)

$$\det [G_F^{-1}(L, E^{FV}) - K(E^{FV})] = 0$$

Kinematical term

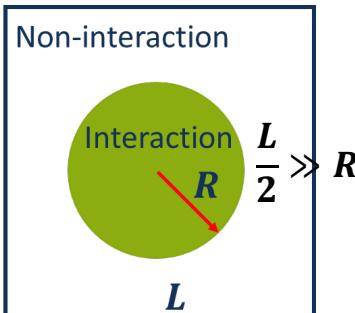
K-matrix in IFV



$$\delta_l(E^{FV})$$

Infinite volume (IFV)

- Derive it



Asymptotic behavior: for $r > R$

$$(\nabla^2 + k^2)\psi_k(r) = 0,$$

$$\psi_k(r) \sim \frac{e^{i\delta(k)} \sin[kr + \delta(k)]}{kr}.$$

Periodic Boundary condition:

$$\mathbf{p} = \frac{2\pi}{L}\mathbf{n}, \quad \mathbf{n} \in \mathbb{Z}^3$$

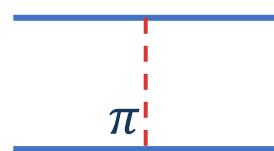
- Limitations:

► Exponentially suppressed effect: $e^{-L/R} \sim e^{-m_\pi L}$

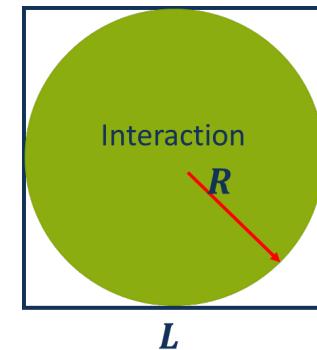
Require: $m_\pi L > 4 \Rightarrow L > 5.7 \text{ fm}$

► Left-hand cut (lhc) problem

► Partial-wave mixing effects



NN , D^*D systems...



Long-range interaction and small box???

Left-hand cut

- Left-hand cut (lhc) from the one-pion exchange interaction



$$V(r) = \frac{e^{-mr}}{r}, \quad V(\vec{p}, \vec{p}') = \frac{1}{(\vec{p}' - \vec{p})^2 + m^2}$$

- Partial wave decomposition, e.g. S-wave

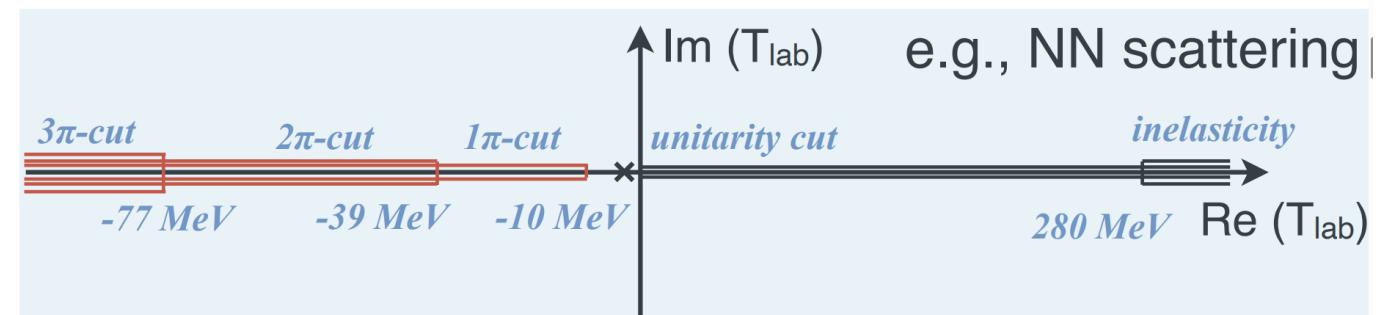
$$V_{l=0}(p, p') = \int_{-1}^1 dz \frac{1}{p^2 + p'^2 - 2pp'z + m^2} = -\frac{1}{2pp'} \log \left(\frac{(p - p')^2 + m^2}{(p + p')^2 + m^2} \right)$$

Multivalued function with cuts

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

$$V_{l=0}(k, k) = \int_{-1}^1 dz \frac{1}{2k^2(1-z) + m^2}, \quad 2k^2(1-z) + m^2 = 0 \Rightarrow z = \frac{m^2}{2k^2} + 1, \quad \text{on-shell pion}$$

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

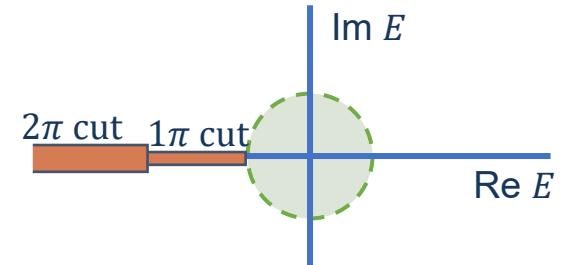


Left-hand cut problem

- Ihc in the IFV

► Effective range expansion (ERE):

$$K^{-1}(p) = p \cot\delta(p) = \frac{1}{a} + \frac{1}{2} rp^2 + \dots$$



► Radius of convergence of ERE
Meng-Lin's talk

NN: Baru:2015ira, Baru:2016evv
DD*: Du:2023hlu

- Ihc problem of Lüscher formula

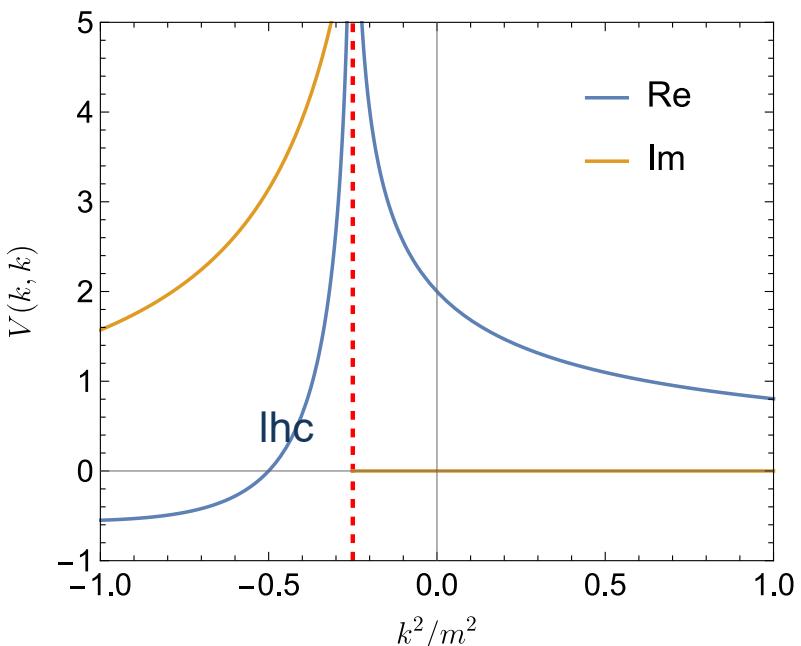
$$\det [G_F^{-1}(L, E) - K(E)] = 0$$

Real
K-matrix in the IFV

$$K = V + VG^P K$$

► For $k^2 > -\frac{m^2}{4}$, K-matrix is real

► For $k^2 < -\frac{m^2}{4}$, $\text{Im } K \neq 0$



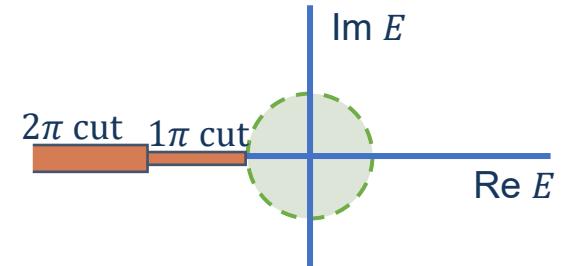
Maxwell, Akaki, Sebastian's talks

Left-hand cut problem

- Ihc in the IFV

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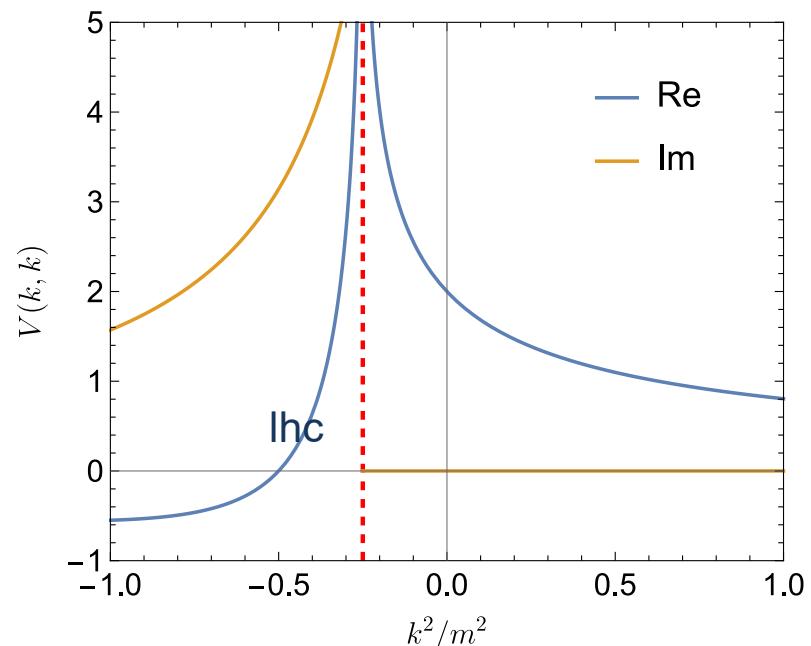
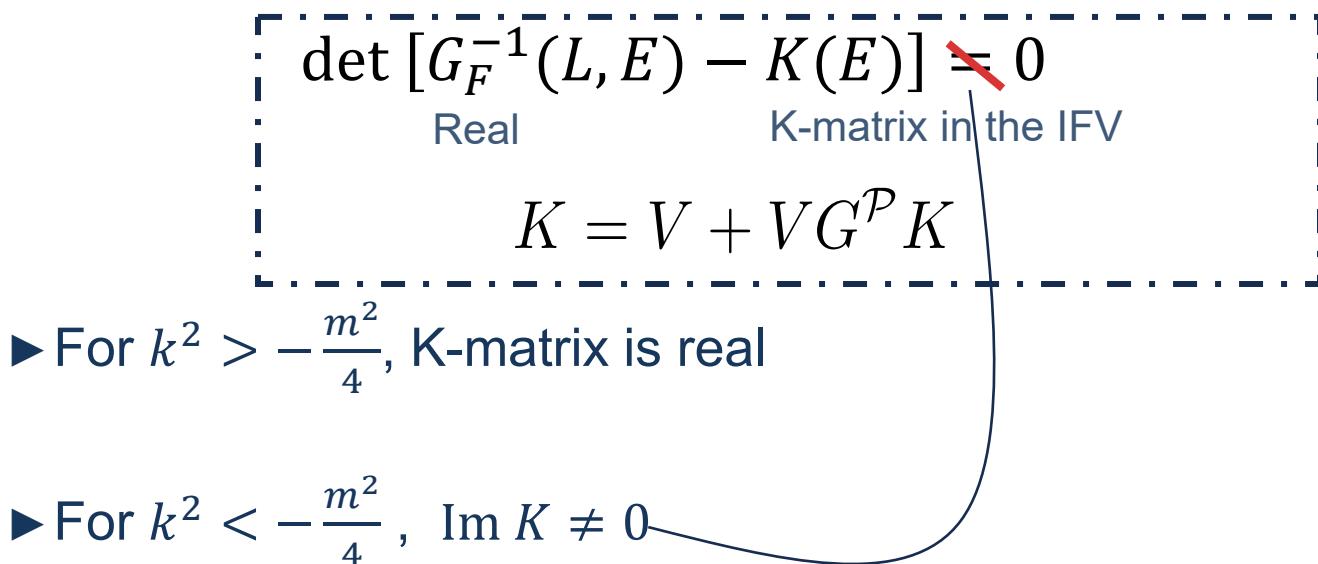


 - Radius of convergence of ERE
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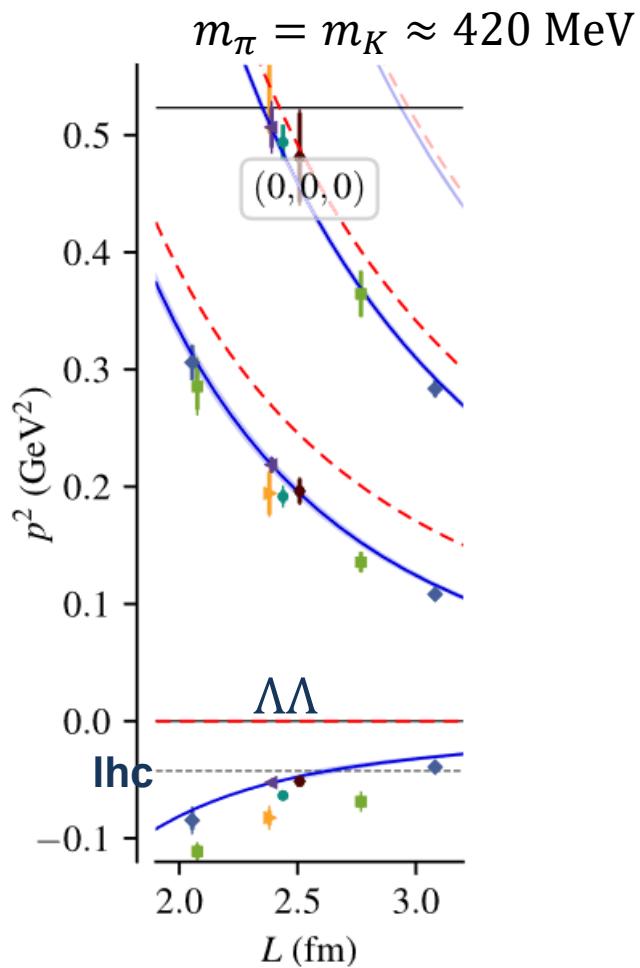
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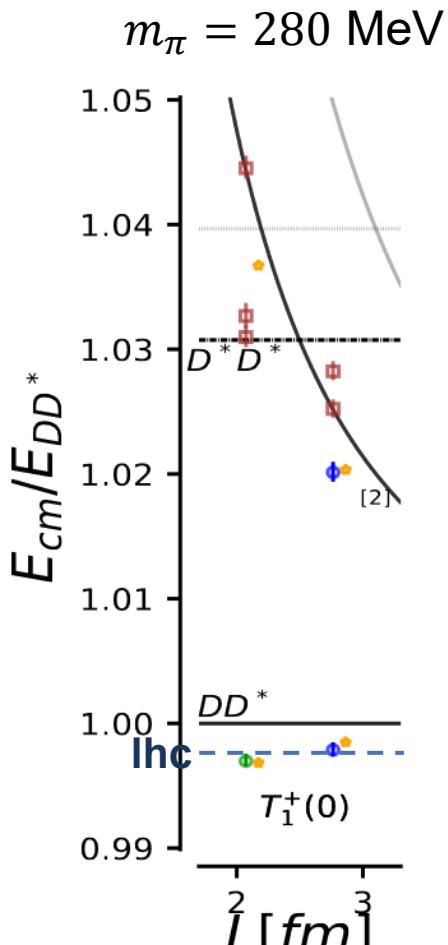
Left-hand cut problem in LQCD

Green:2021qol



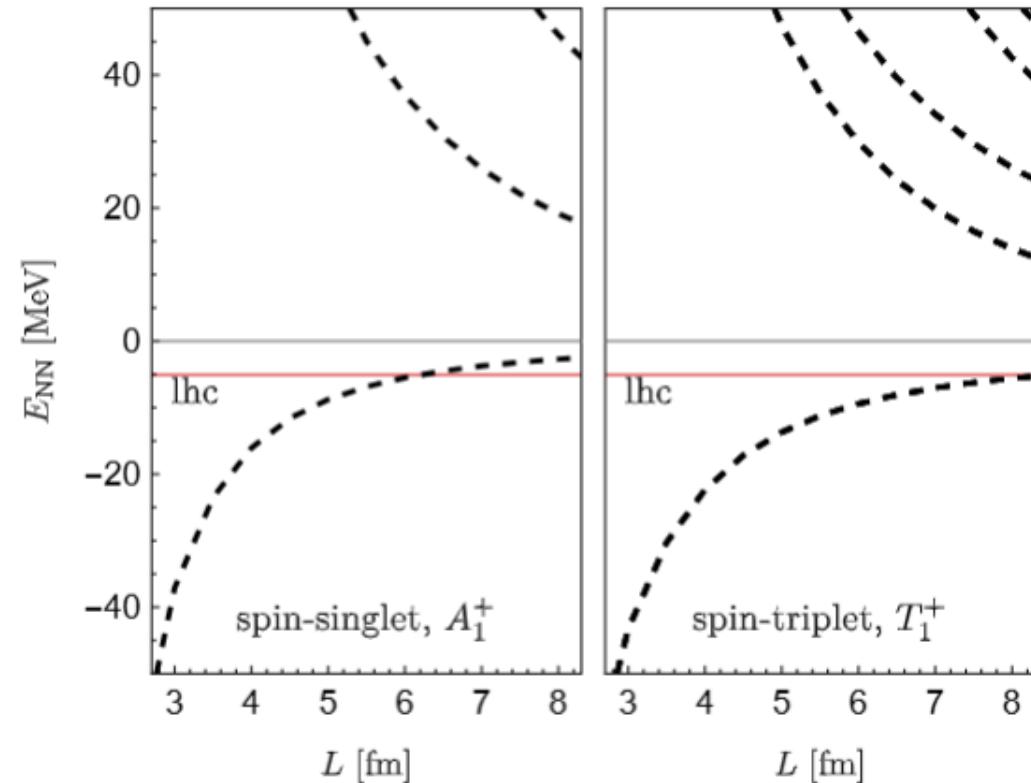
H-dibaryons ($udsuds$)

Padmanath:2022cvl



DD^* (T_{cc})

$m_\pi = 137$ MeV



NN systems

$L > 8$ fm to get rid of the Ihc problem

T_{cc} state in lattice QCD

T_{cc} lattice QCD simulations

Padmanath:2022cwl

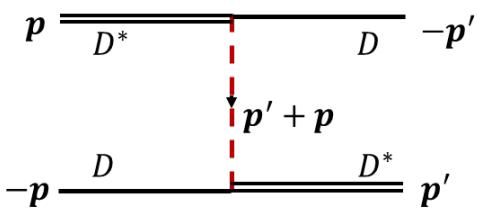
- LQCD setting: $m_\pi \approx 280$ MeV, $m_D \approx 1927$ MeV, $m_{D^*} \approx 2049$ MeV, $L \approx 2.07, 2.76$ fm, $a \approx 0.086$ fm

- Some quick estimations

► $m_{\text{eff}}^2 = m_\pi^2 - (m_{D^*} - m_D)^2 > 0$, $m_{\text{eff}} \approx 252$ MeV

► $p_{\text{lhc}}^2 \approx -\left(\frac{m_{\text{eff}}}{2}\right)^2 = -(126 \text{ MeV})^2$

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



$$\frac{-1}{k^2 + m_\pi^2 - k_0^2 - i\epsilon} = \frac{-1}{k^2 + m_{\text{eff}}^2 - i\epsilon}$$

- A conventional procedure to the IFV:

- Using Lüscher formula to get phase shift
- Use ERE to parameterize K -matrix

- Conclusion: virtual states

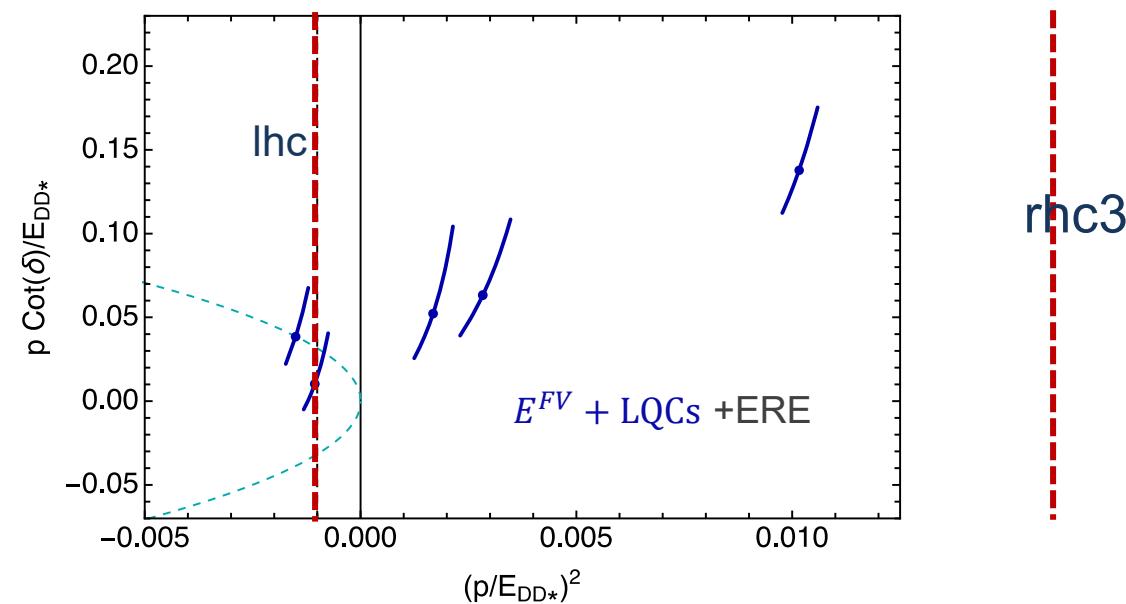
- Limitations

► $m_{\text{eff}}L = 2.6, 3.5$

exponential effect can be important

► left-hand cut

~~Lüscher formula, effective range expansion~~



Other lattice results: Cheung:2017tnt, Junnarkar:2018twb, Chen:2022vpo, Lv:2023xro, Whyte:2024ihh...

T_{cc} lattice QCD simulations

Padmanath:2022cwl

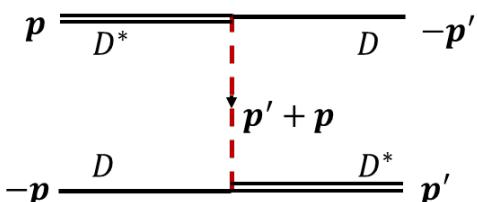
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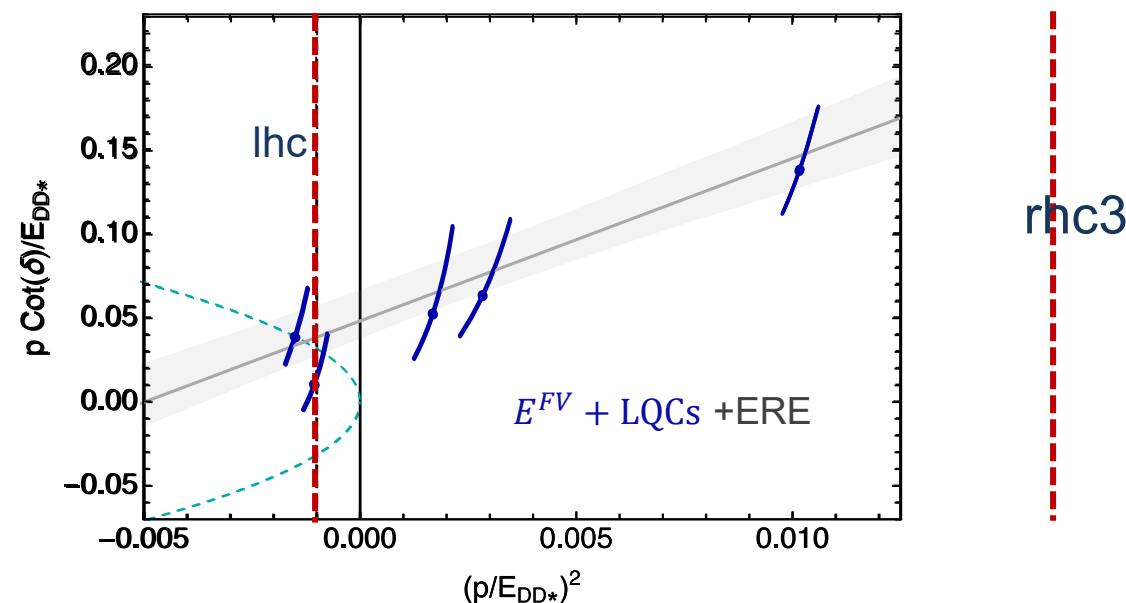
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~~Lüscher formula, effective range expansion~~



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Our strategy

Key point: off-shell effect

- Lüscher formula:
 - ▶ The E_{FV} s are only related to the **on-shell** T-matrix
 - ▶ **The off-shell** effect is exp. suppr. and thus neglectable
- The lhc problem of the Lüscher formula: off-shell effect, exp. suppr. effect
- Schrödinger Eq. in the IFV to get the **bound state** solutions

$$\frac{\mathbf{p}^2}{2\mu} \psi(\mathbf{p}) + \int \frac{d^3\mathbf{p}'}{(2\pi)^3} V(\mathbf{p}, \mathbf{p}') \psi(\mathbf{p}') = E \psi(\mathbf{p})$$

Off-shell, for $E < 0$

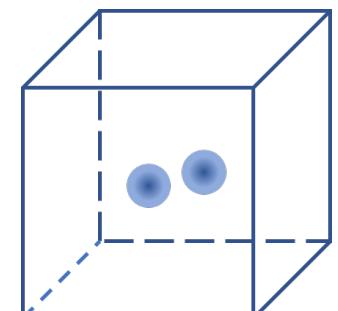
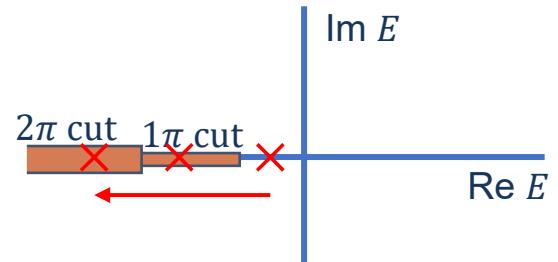
- ▶ Works well even below the left-hand cut
- ▶ For the $p, p' > 0$, no lhc in potential

$$V_{l=0}(p, p') = \int_{-1}^1 dz \frac{1}{p^2 + p'^2 - 2pp'z + m^2} = -\frac{1}{2pp'} \log \left(\frac{(p - p')^2 + m^2}{(p + p')^2 + m^2} \right)$$

- FV energy levels are “bound states” trapped by the potential well

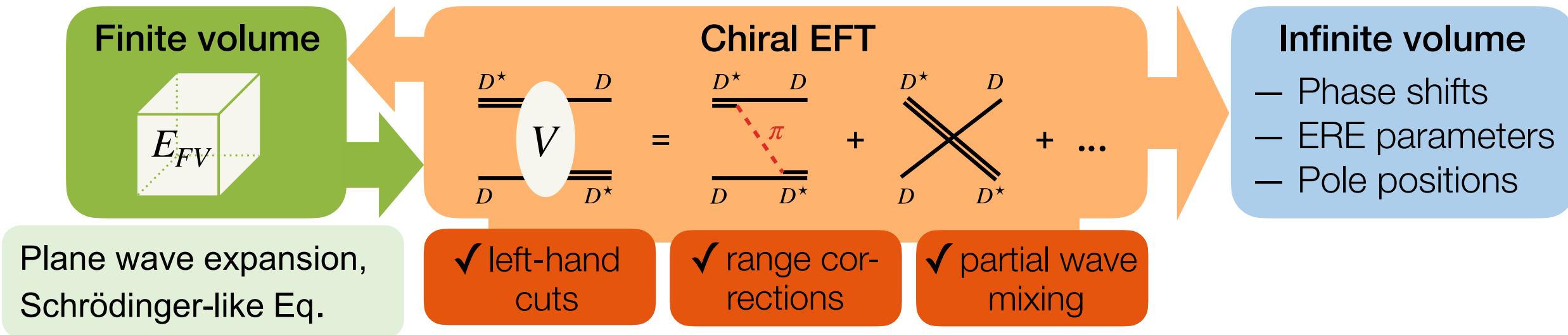
$$\int \frac{d^3\mathbf{p}}{(2\pi)^3} \rightarrow \frac{1}{L^3} \sum_{\mathbf{p}_n}$$

- Basic idea: using V to connect FV and IFV; FV effect: Schrödinger-like Eq.



Our strategy

- Hamiltonian method in plane wave basis + Chiral effective field theory



- Symmetry from QCD
 - ▶ Chiral symmetry and its spontaneous breaking

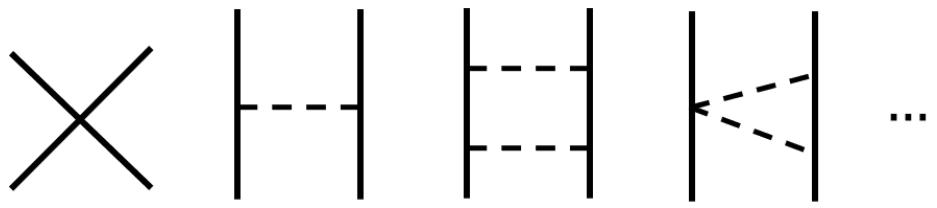
- Weinberg power counting
 - ▶ Systemic calculation, controllable truncation error

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

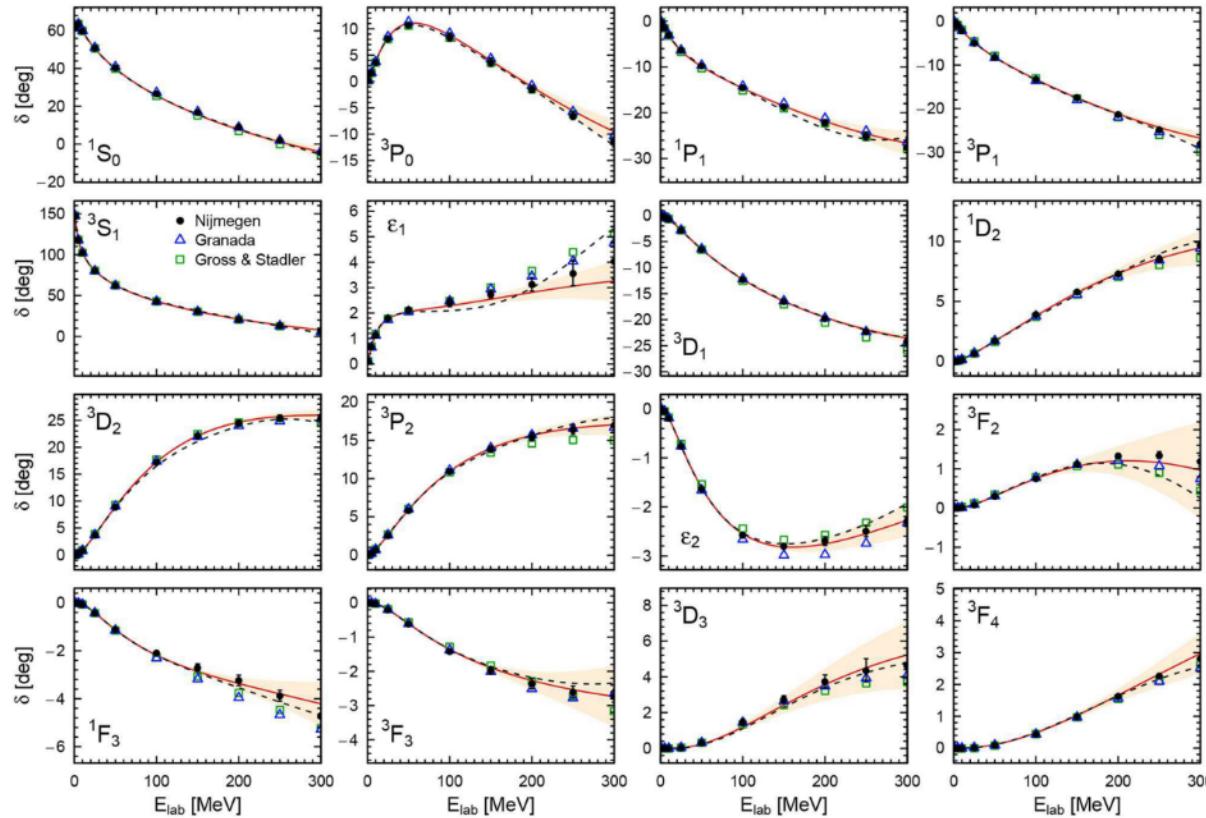
- Great success in the nuclear force
- Semilocal momentum-space regularization

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

- Long-range interaction: $V_{1\pi}$ is known
- Short-range interaction: contact interaction
 - ▶ Unknown low energy constants (LECs)
 - ▶ fitting lattice QCD data



Reinert:2017usi



Hamiltonian method in plane wave basis

- Boundary conditions in the cubic box

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

$$p_1 + p_2 = P, \quad p_1 = \frac{2\pi}{L} n, \quad P = \frac{2\pi}{L} d, \quad n, d \in \mathbb{Z}^3$$

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

- $\{l, m\}$ 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 from lattice: irreducible representations (irreps.) of O_h

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

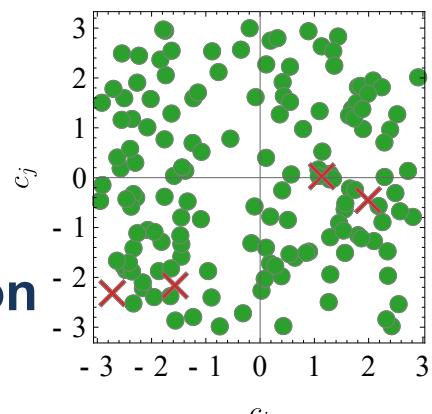
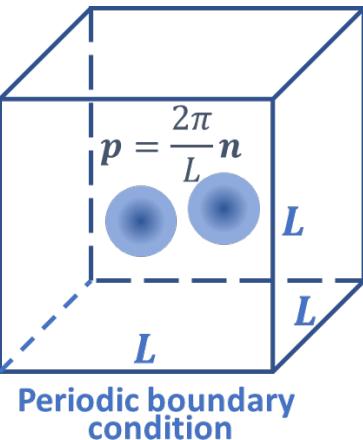
- Why not use the **plane wave (with discrete momentum)** basis directly?

- Finite volume energy levels

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

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

- Accelerate calculation: subspace learning, specifically **eigenvector continuation**
- Extra advantage: **partial wave mixing effect**

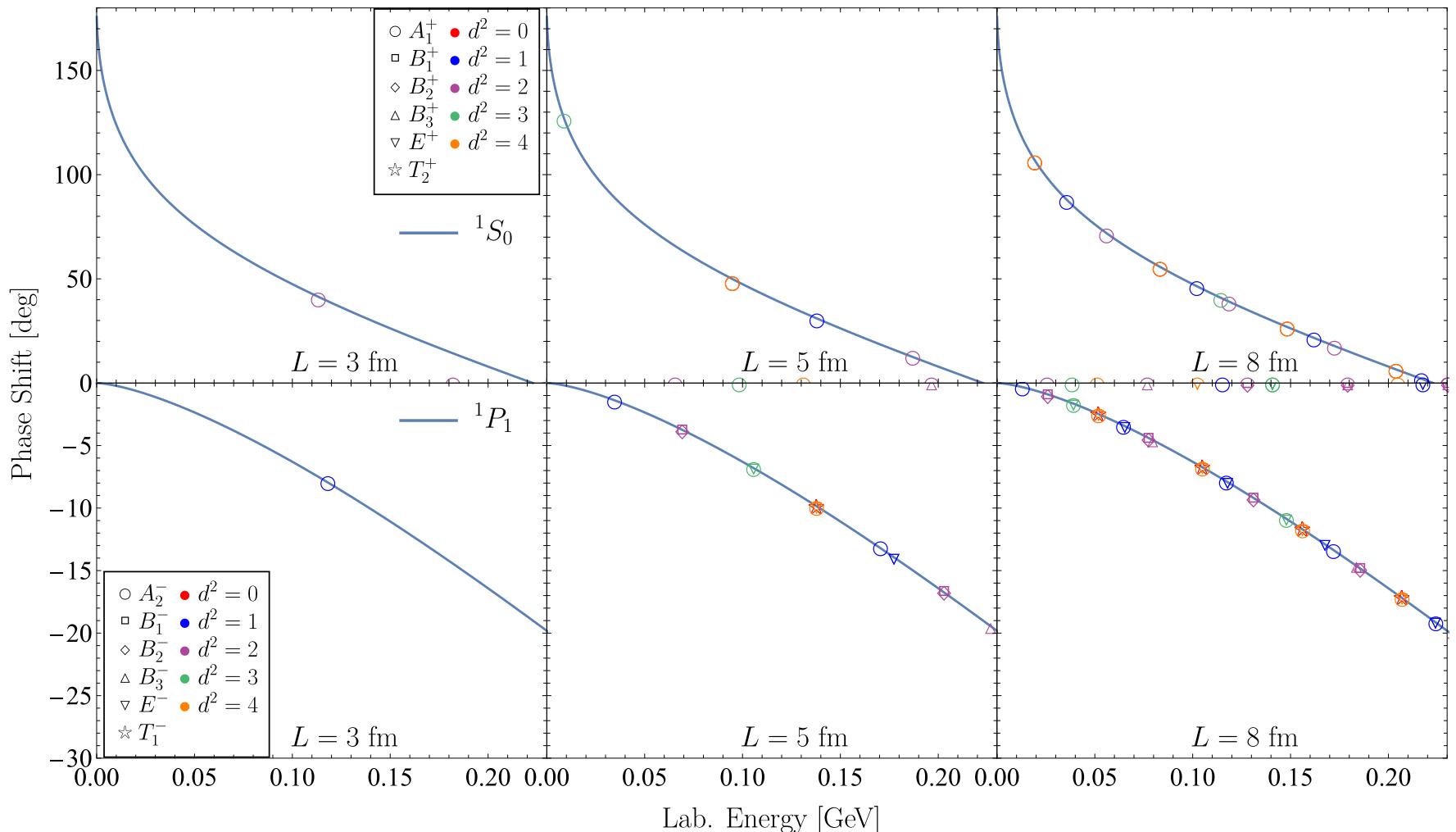
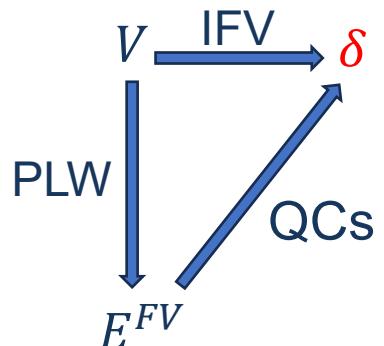


Frame:2017fah

Benchmark: contact interaction

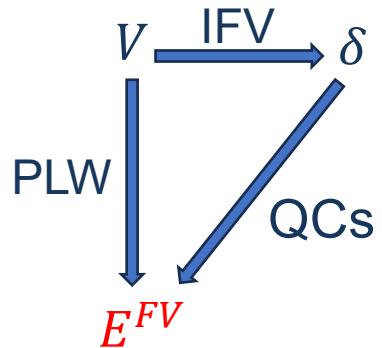
- Contact interaction: $V(\mathbf{p}, \mathbf{p}') = C_S + C_1 q^2 + C_2 k^2$

- Only contribute to S-wave and P-wave

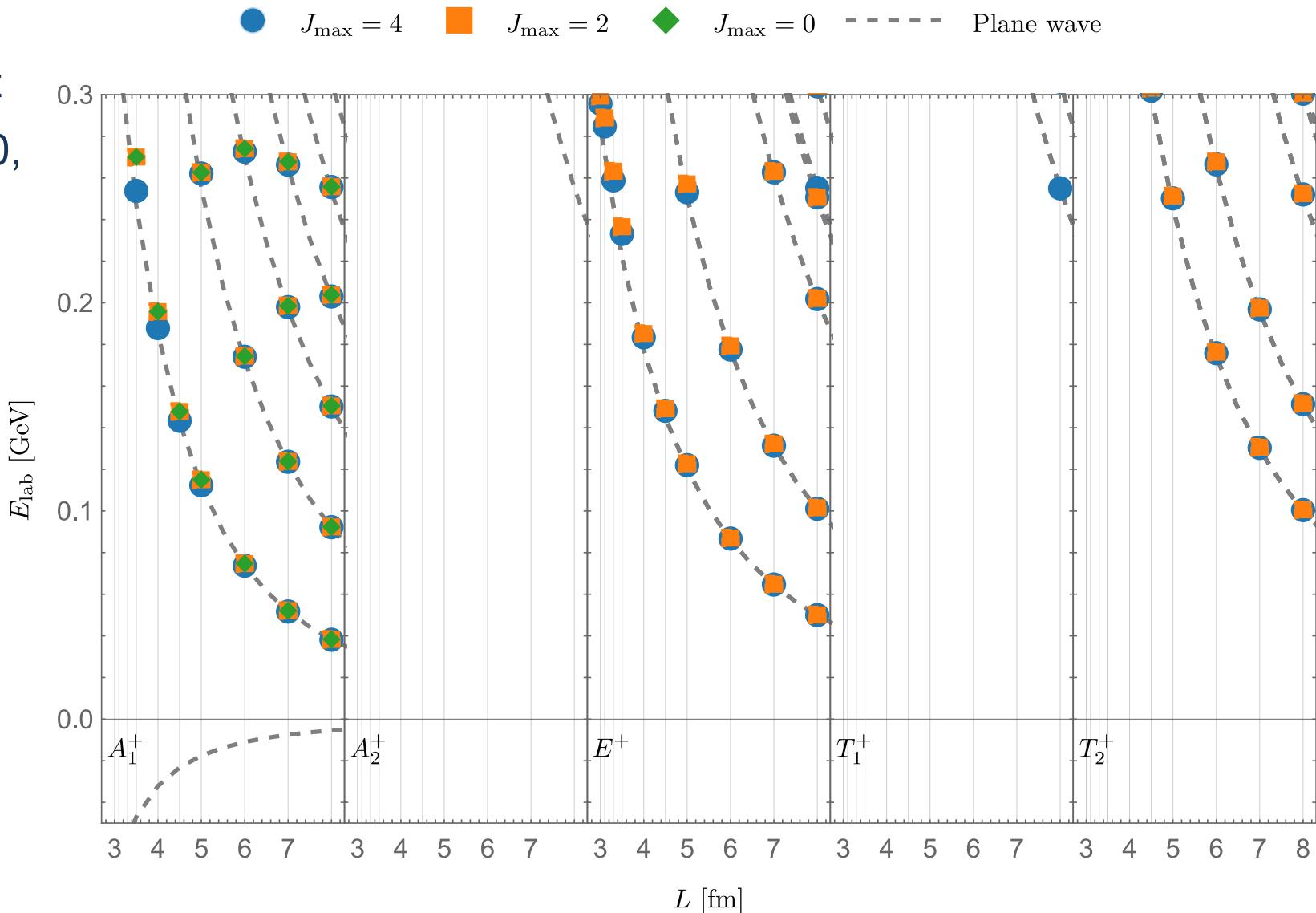


Benchmark: chiral EFT, partial wave mixing

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



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

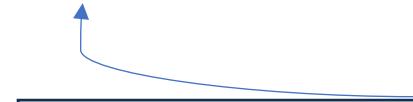


Numerical calculation

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

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

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



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

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

$$\int \frac{d^3\mathbf{q}}{(2\pi)^3} \rightarrow \mathcal{J} \int \frac{d^3\mathbf{q}_{box}}{(2\pi)^3} \rightarrow \mathcal{J} \sum_n \frac{1}{L^3}$$

Li:2021mob

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

- Get the poles

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

- Contact terms to NLO

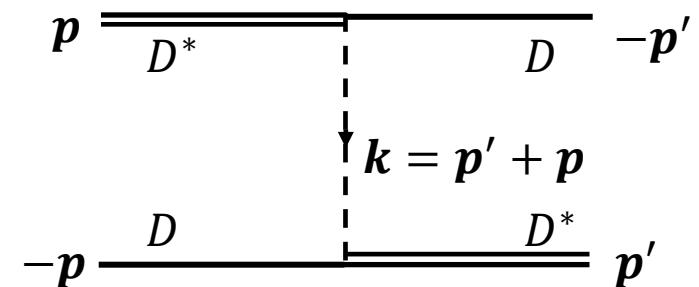
- ▶ In present calculation: LO and NLO 3S_1 contact terms, NLO 3P_0
- ▶ 3S_1 - 3D_1 transition term and 3P_2 are included to estimate the systemic uncertainties
- ▶ Separable regulator: $e^{-\frac{p^n + p'^n}{\Lambda^n}}$, $n = 2, 4, 6$

- One-pion exchange interaction

- ▶ Pion propagator: static approximation

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

- ▶ Semilocal momentum-space regularization



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

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

The regulator will not change the long-range behavior

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

Reinert:2017usi

F_π and g

- F_π 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

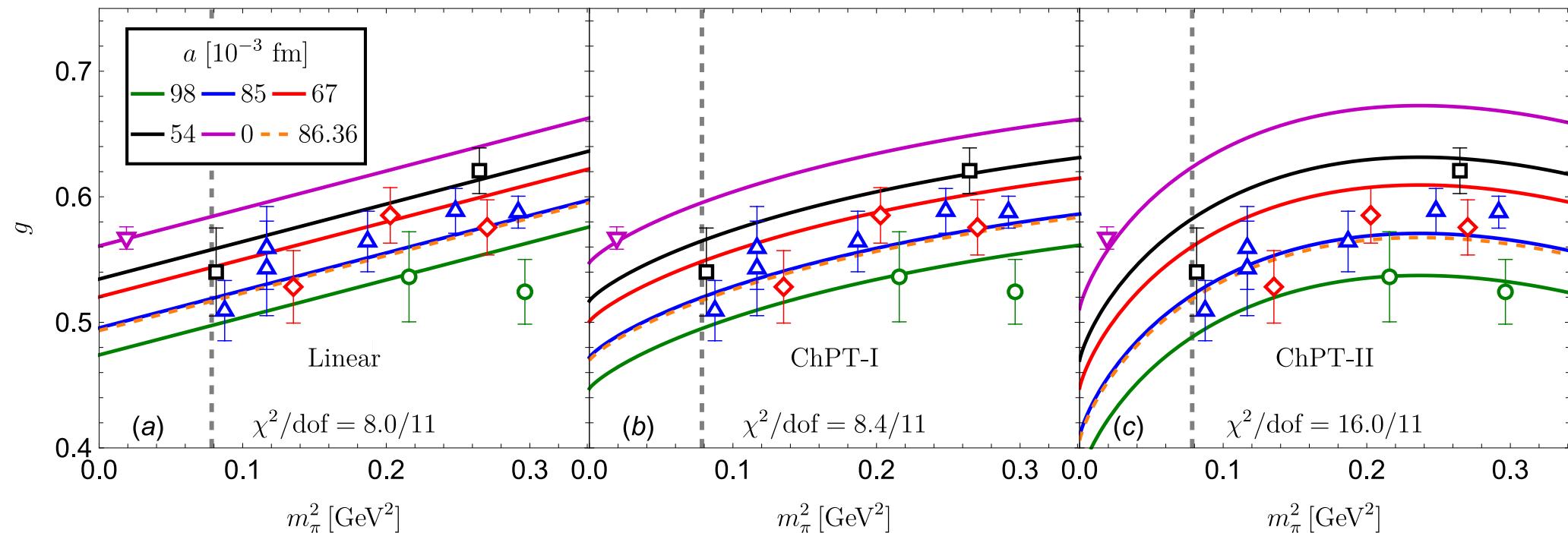
- $F_{ph} = 92.1$ MeV, $F_0 = 85$ MeV, chiral extrapolation, $\xi = m/m^{ph}$

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

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



- Results using Lüscher's QC

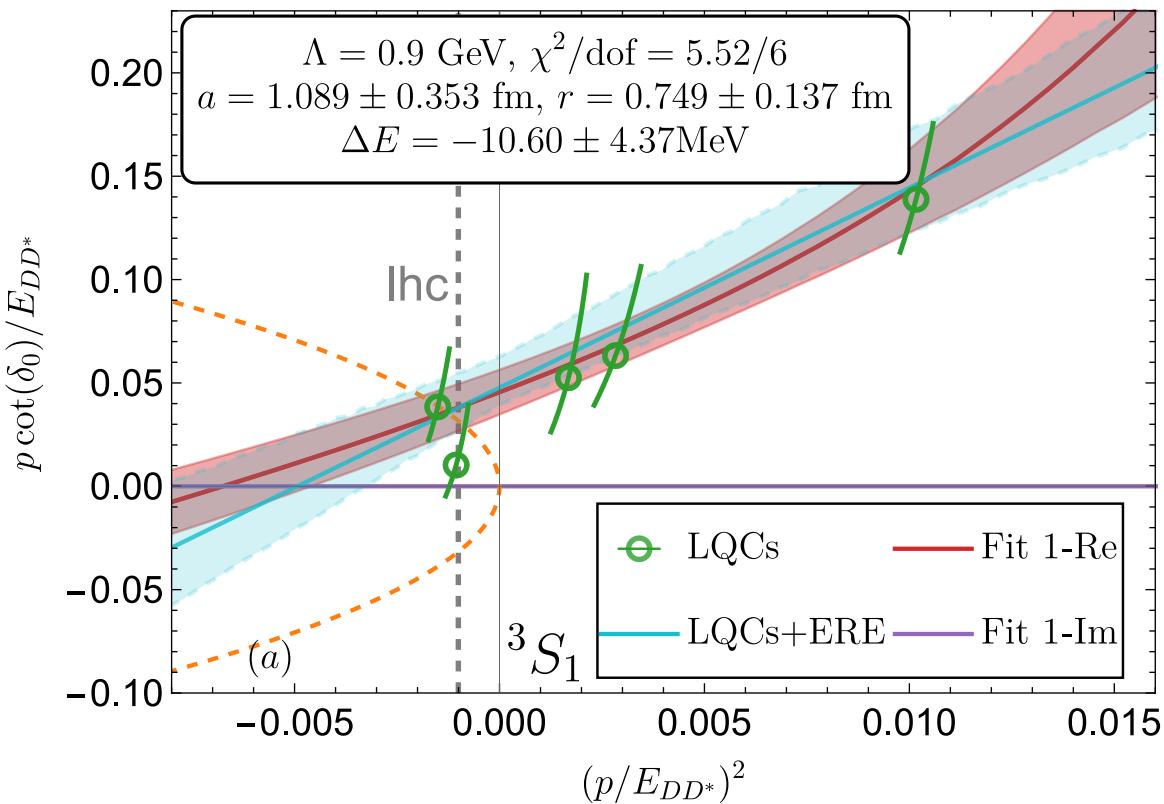
Padmanath:2022cvl

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

$$a^{^3S_1} = 1.04(29) \text{ fm}, \quad r^{^3S_1} = 0.96^{+0.18}_{-0.20} \text{ fm}$$

$$a^{^3P_0} = 0.076^{+0.008}_{-0.009} \text{ fm}^3, \quad r^{^3P_0} = 6.9(2.1) \text{ fm}^{-1}$$

- Our results

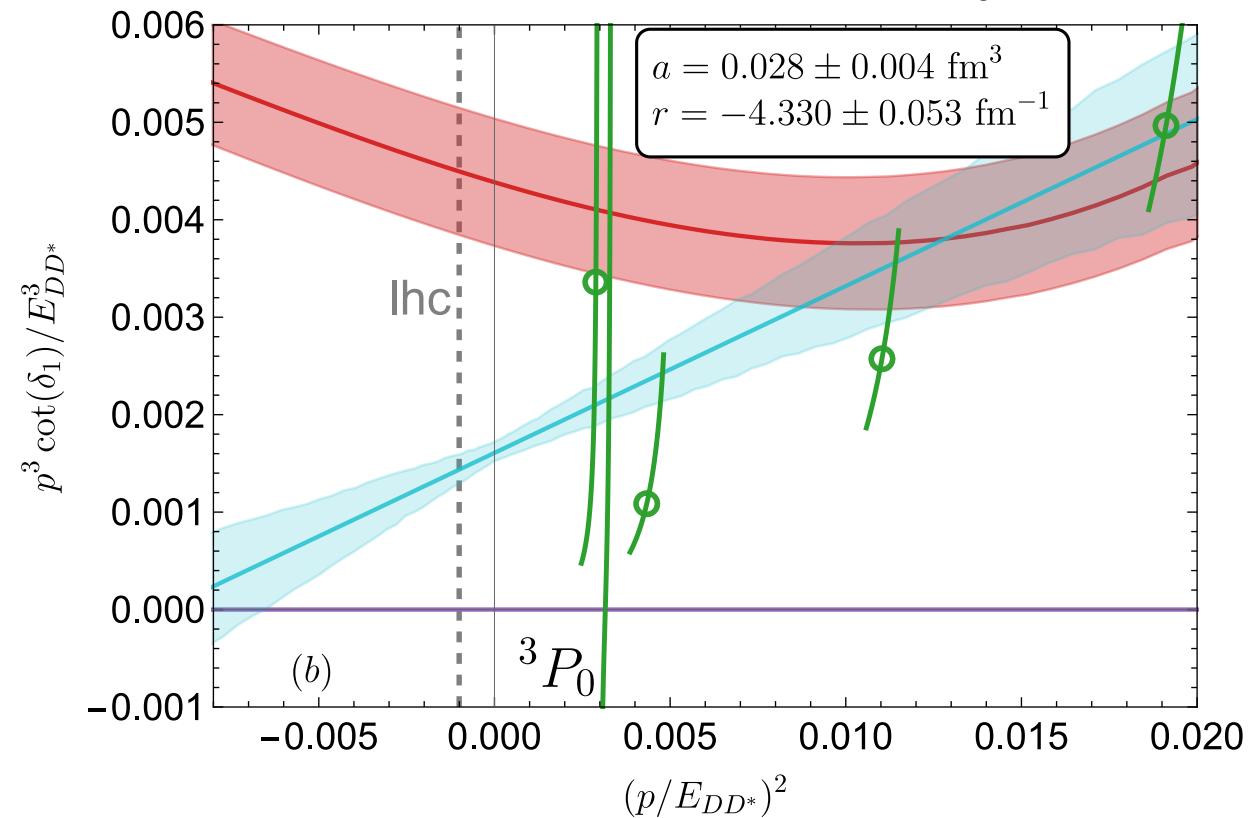


Four parameters:

$$a^{^3S_1}, r^{^3S_1}, a^{^3P_0}, r^{^3P_0}$$

Three parameters:

LO and NLO 3S_1 , NLO 3P_0 LECs



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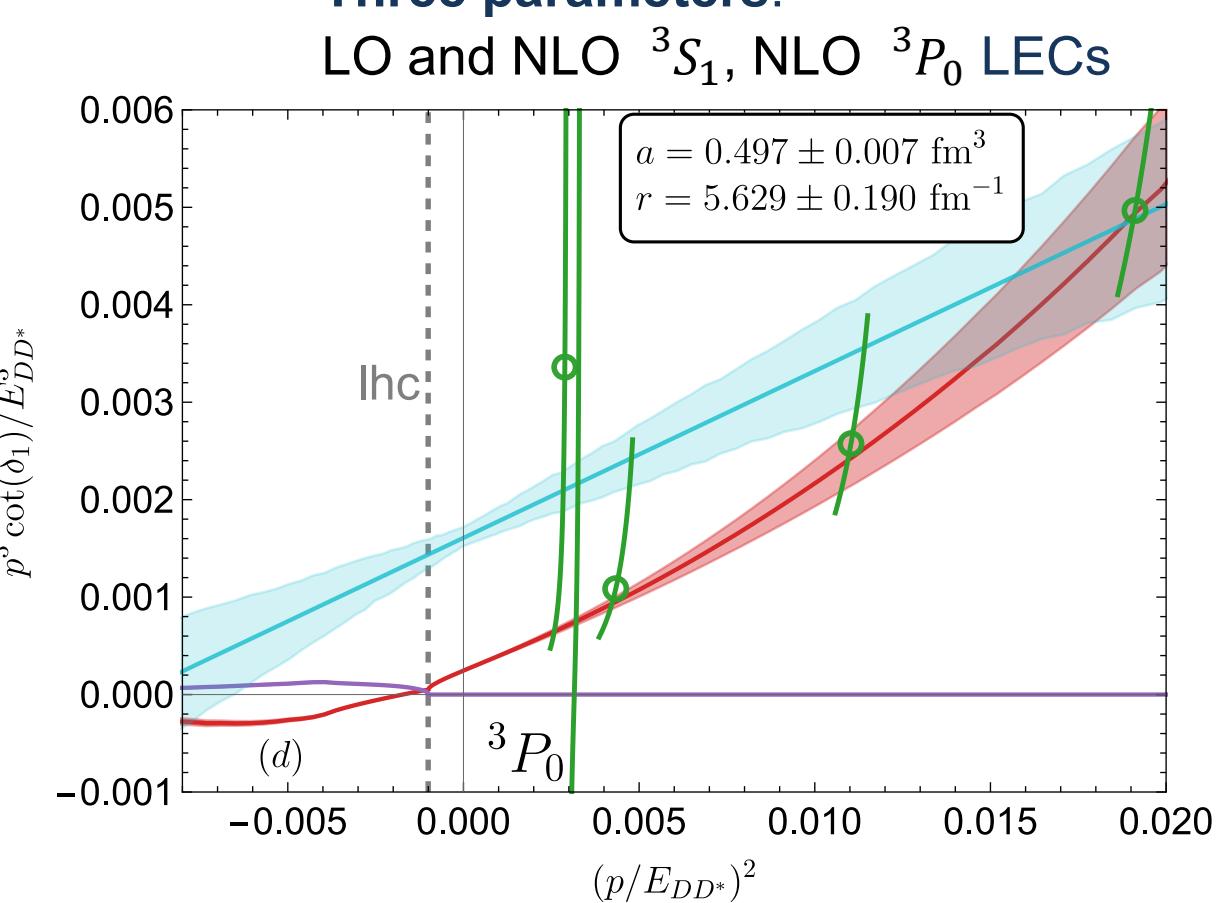
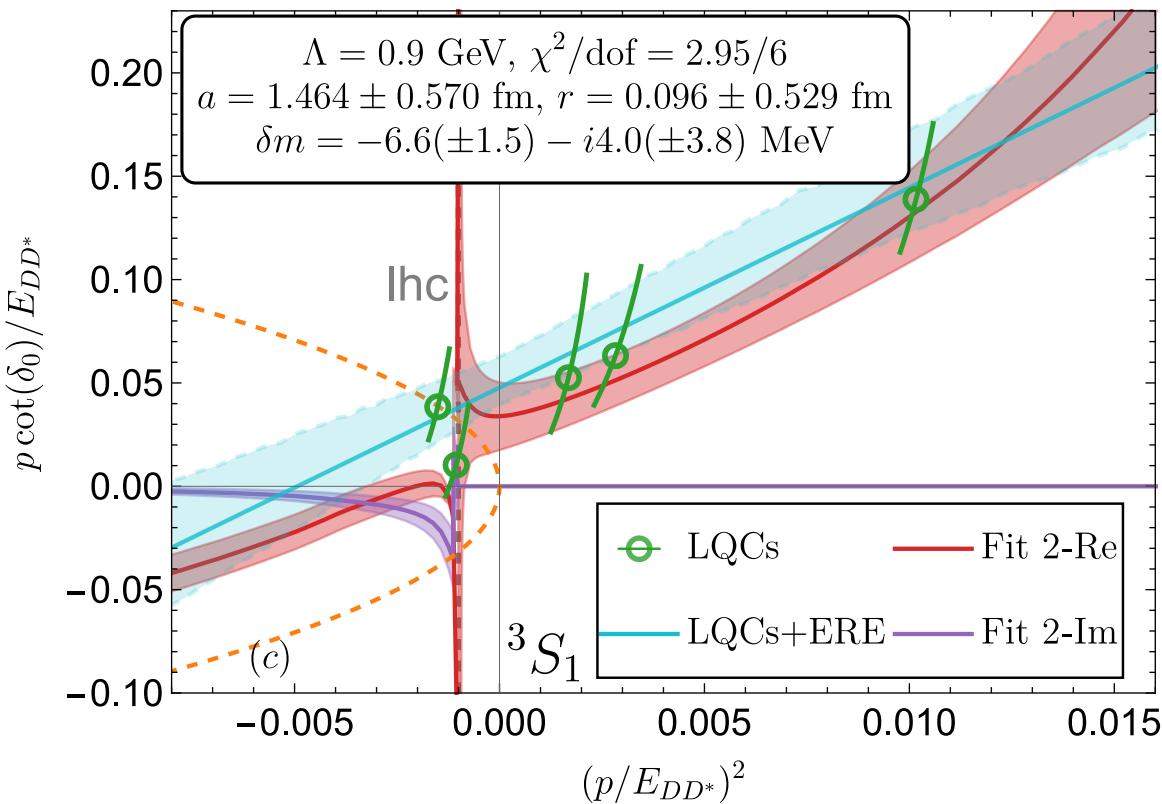
Padmanath:2022cvl

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

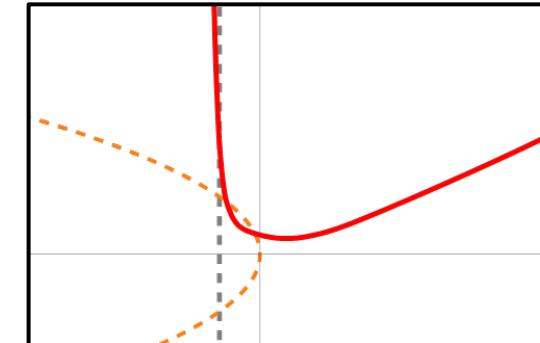
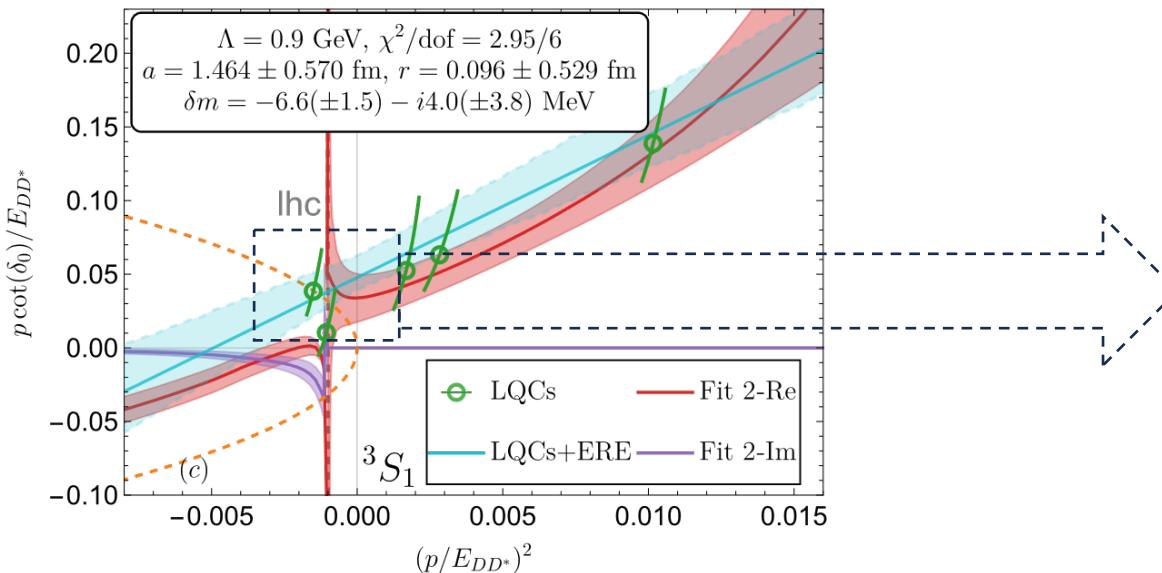
$$a^{^3S_1} = 1.04(29) \text{ fm}, \quad r^{^3S_1} = 0.96^{+0.18}_{-0.20} \text{ fm}$$

$$a^{^3P_0} = 0.076^{+0.008}_{-0.009} \text{ fm}^3, \quad r^{^3P_0} = 6.9(2.1) \text{ fm}^{-1}$$

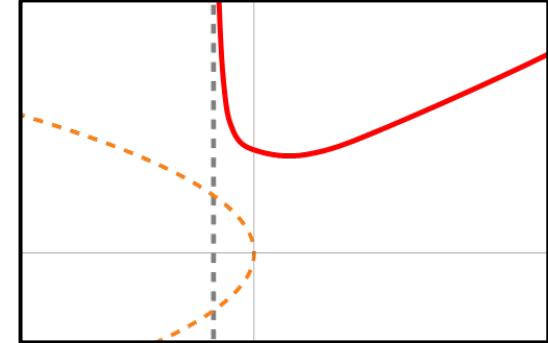
- Our results



- Resonance with 85% probability within the 1σ uncertainty
 - Rather than the virtual state from Lüscher QC+ERE



two virtual states



Resonance

- Modified effective range expansion

- ▶ R. Bubna, H-W. Hammer, F. Müller, J-Y. Pang, A. Rusetsky and J-J. Wu,
JHEP 05 (2024) 168
- ▶ [Talk of Rusetsky in lattice2024](#)

- Modified Lüscher quantization condition

- ▶ A. Raposo and M. Hansen, *JHEP* 08 (2024) 075
- ▶ [Talk of Raposo in lattice2024](#)

Maxwell, Akaki,
Sebastian's talks

- Using three-particle formalism

- ▶ M. Hansen, F. Romero-López and S. Sharpe, *JHEP* 06 (2024) 051
- ▶ [Talk of S. Dawid in lattice2024](#)

- HAL QCD approach

- ▶ Lyu et al, *PhysRevLett.* 131.161901,
- ▶ [Talk of S.Aoki in lattice2024](#)

Also working with Schrodinger-type equation
No lhc problem

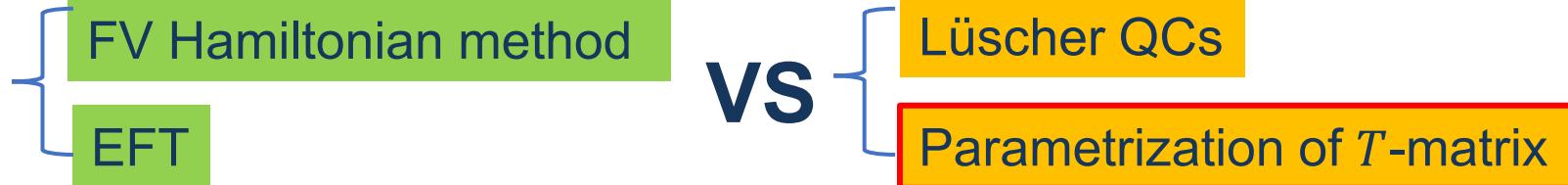
Model-(in)dependence

- Question: (modified) Lüscher formula **VS** FV Hamiltonian methods + EFTs

Model-independent

Model-dependent?

Our answers:



- Parametrization of T -matrix: model dependence

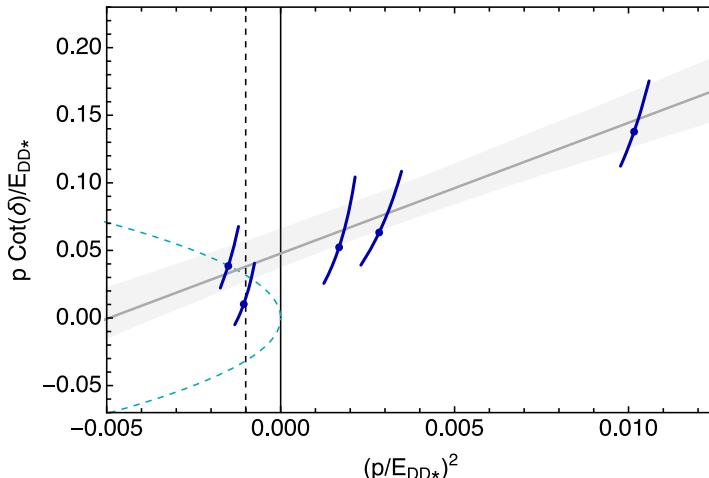
- ▶ Without PW mixing: one-to-one relation, $E_{FV} \sim \delta_l(E_{FV})$
- ▶ Phase shift over continue energy: T -matrix parametri.. is needed
- ▶ PW mixing effect: T -matrix parametri. is needed

- EFTs: also parametri. of the T -matrix with following advantages

- ▶ Clear breaking down scale
- ▶ Powering counting, controllable and knowable systemic uncertainties

- FV Hamiltonian method without PW mixing could also provide the one-to-one relation

- ▶ Define short-range interaction for each E_{FV}^i **separately**, $V_i = \lambda_i V_{\text{short-range}}$
- ▶ Each V_i will give a phase shift $\delta(E_{FV}^i)$ in the infinite volume



Summary and Outlook

● Validation of Lüscher's formula

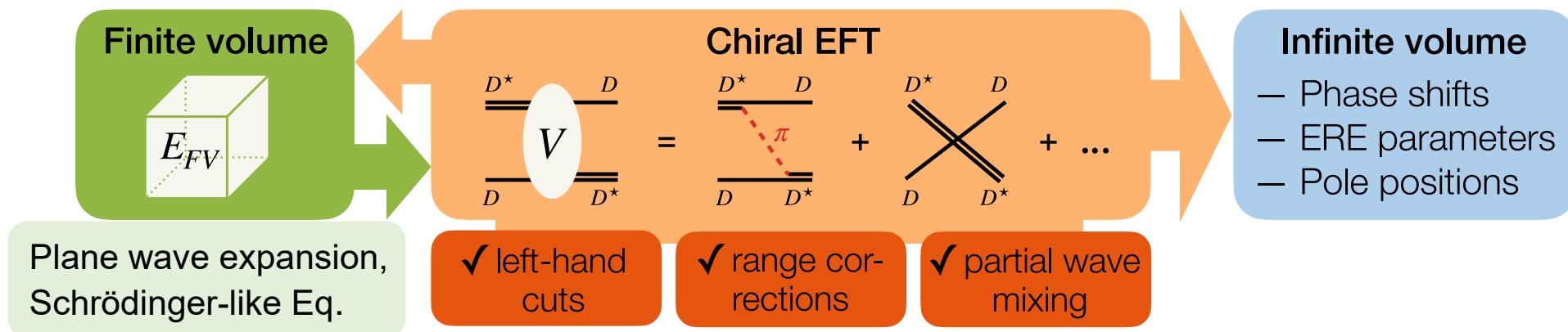
- ① e^{-mL} effect can be neglected
- ② Considering the PW mixing effect
- ③ E^{FV} well above Ihc
- ④ ERE works in IFV

Du:2023hlu

Invalidate



● Our formalism



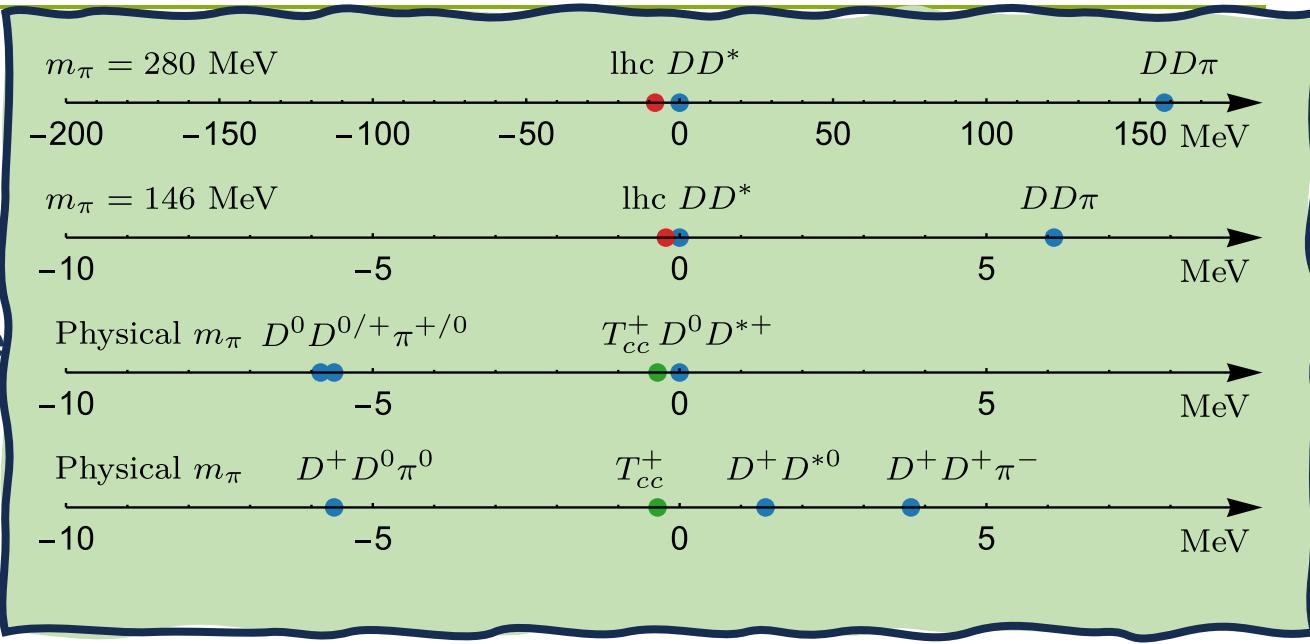
● T_{cc} lattice data

- E^{FV} below the left-hand cut
- Lattice T_{cc} at $m_\pi = 280$ MeV, more likely resonance
- The possible partial wave mixing effect
- Important one-pion exchange interaction, **Chiral dynamics**

T_{cc} is a playground

- Left-hand cut
- Three-body effect
- Isospin violation effect
- Light quark mass (pion mass) dependence
- Heavy quark mass dependence
- ...

Michael Abolnikov's talk 2407.04649



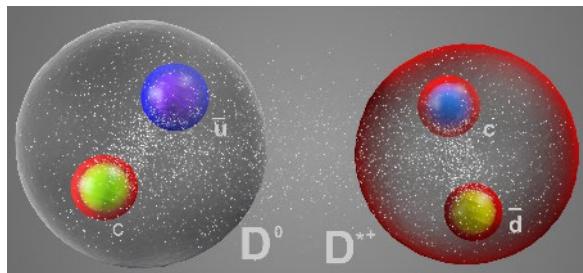
Thanks for
your attentions!

Back up

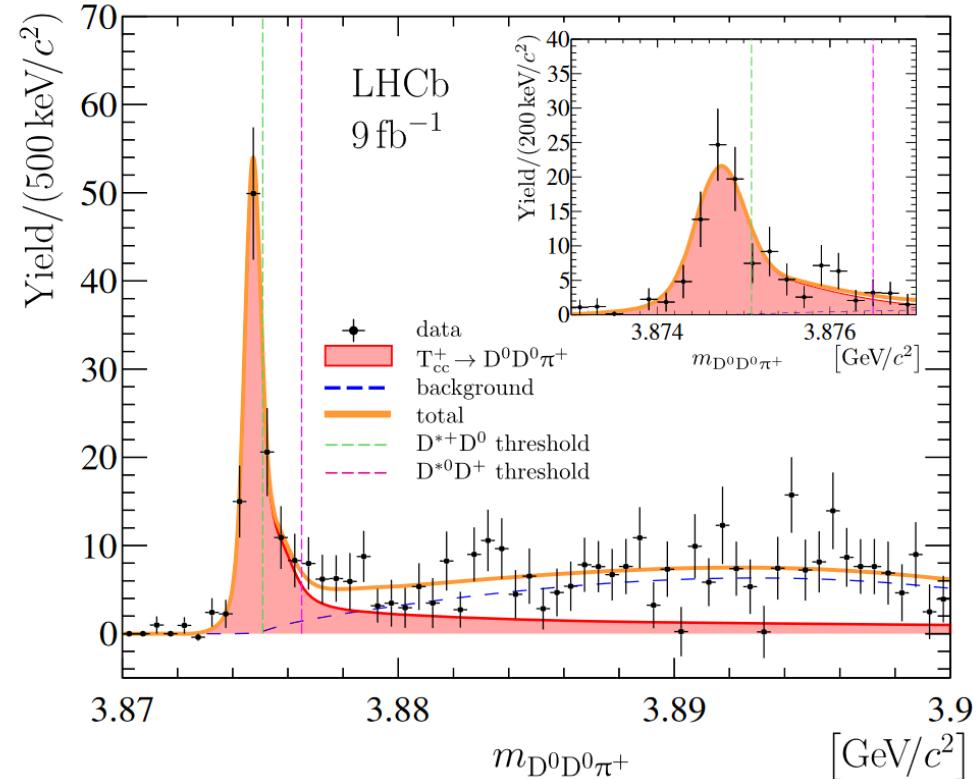
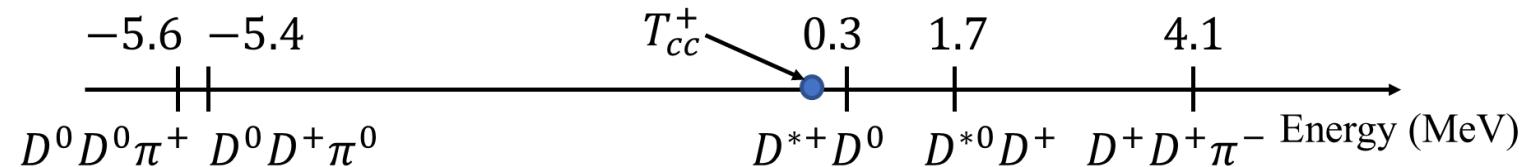
$T_{cc}(3875)^+$ state

- $T_{cc}(3875)^+$ was observed in 3-body final states: $D^0 D^0 \pi^+$
- Very close to $D^0 D^{*+}$ thresholds: $\delta m_U \approx -360\text{keV}$, $\Gamma \approx 48\text{ keV}$
- Exotic hadrons: minimal quark content: $cc\bar{u}\bar{d}$
- Good candidates of $D^0 D^{*+}$ molecule

LHCb Collaboration



- 3-body dynamics could be important



lhcb:2021vvq, lhcb:2021auc, Du:2021zzh, Meng:2021jnw...

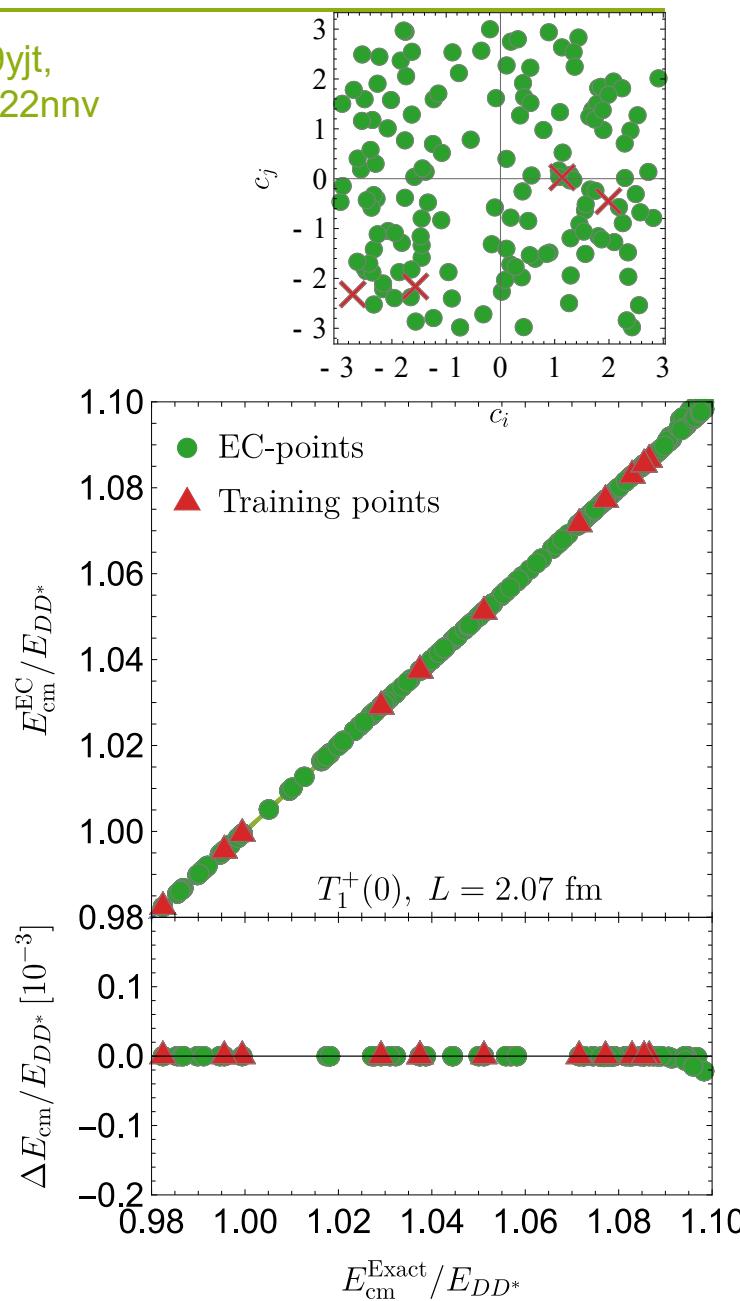
Towards a practical approach: eigenvector continuation

- Plane wave basis+Eigenvector continuation
 - ▶ Eigenvector continuation (EC) with subspace learning
- To fit or quantify uncertainty: solve eigenvalue problem with different $\{c_i\}$ repeatedly
- EC basis: eigenvectors from a selection of parameter sets $\{c_i\}_1, \{c_i\}_2, \dots$ (training point)
- Naturalness of LEC in EFT (~ 1) makes the EC more reliable
- dim is linear function

$$\dim^{EC} = \frac{p_{max}}{2\pi/L} \sim \mathcal{O}(10), \quad p_{max} \approx 0.6 \text{ GeV}$$

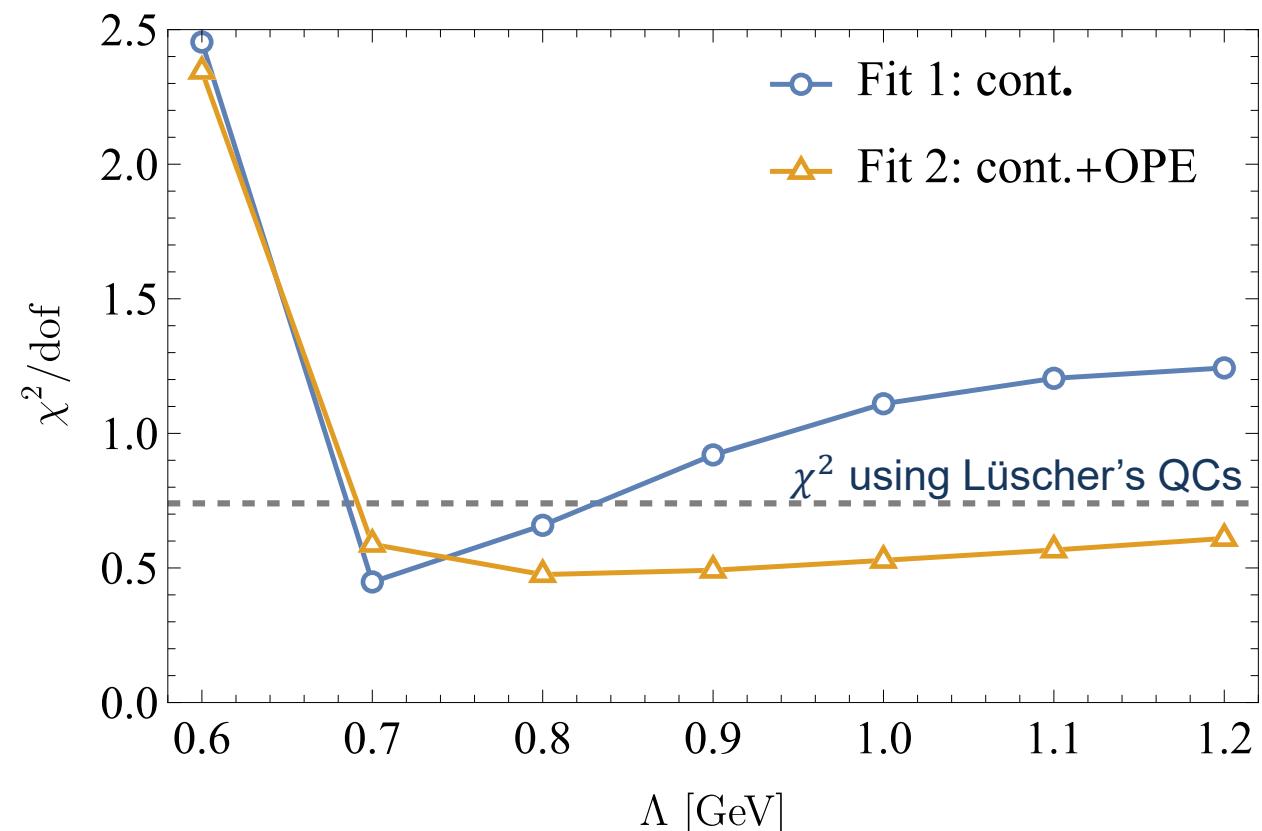
- The subspace learning is the one-time cost
- Make the calculation fast and accurate

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



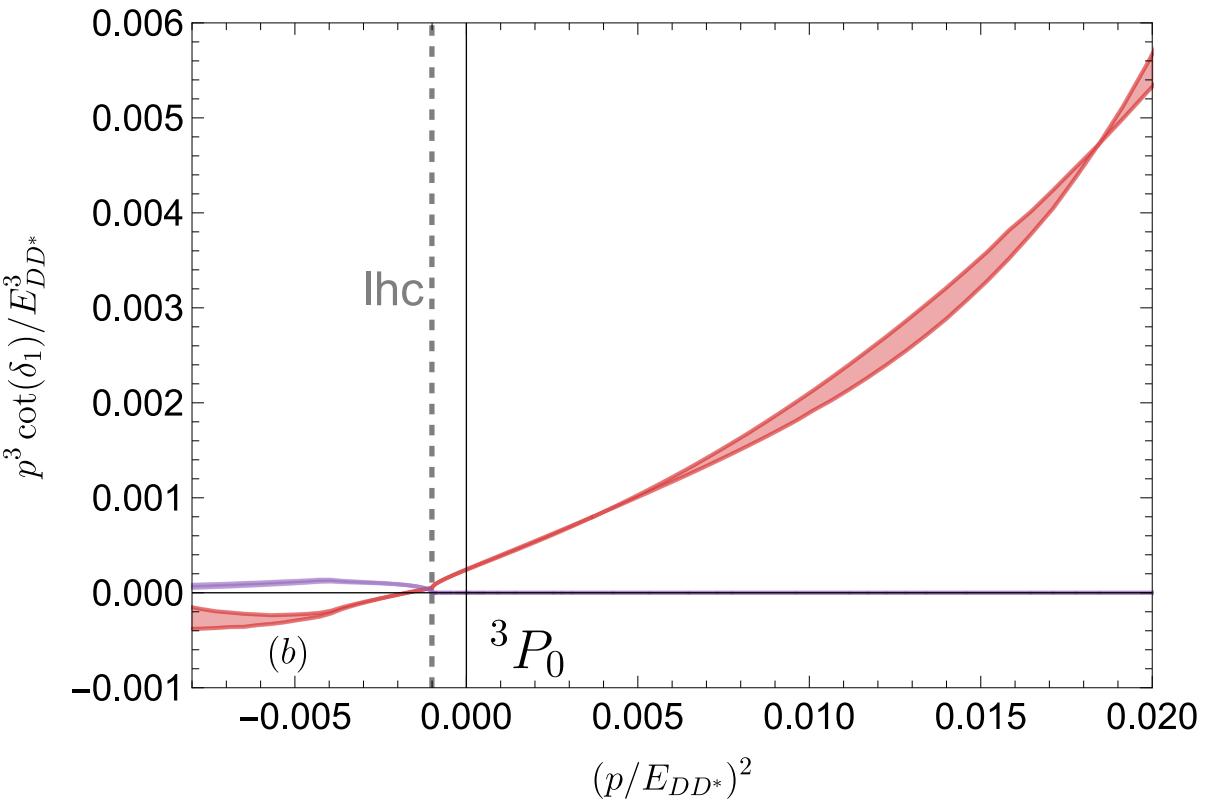
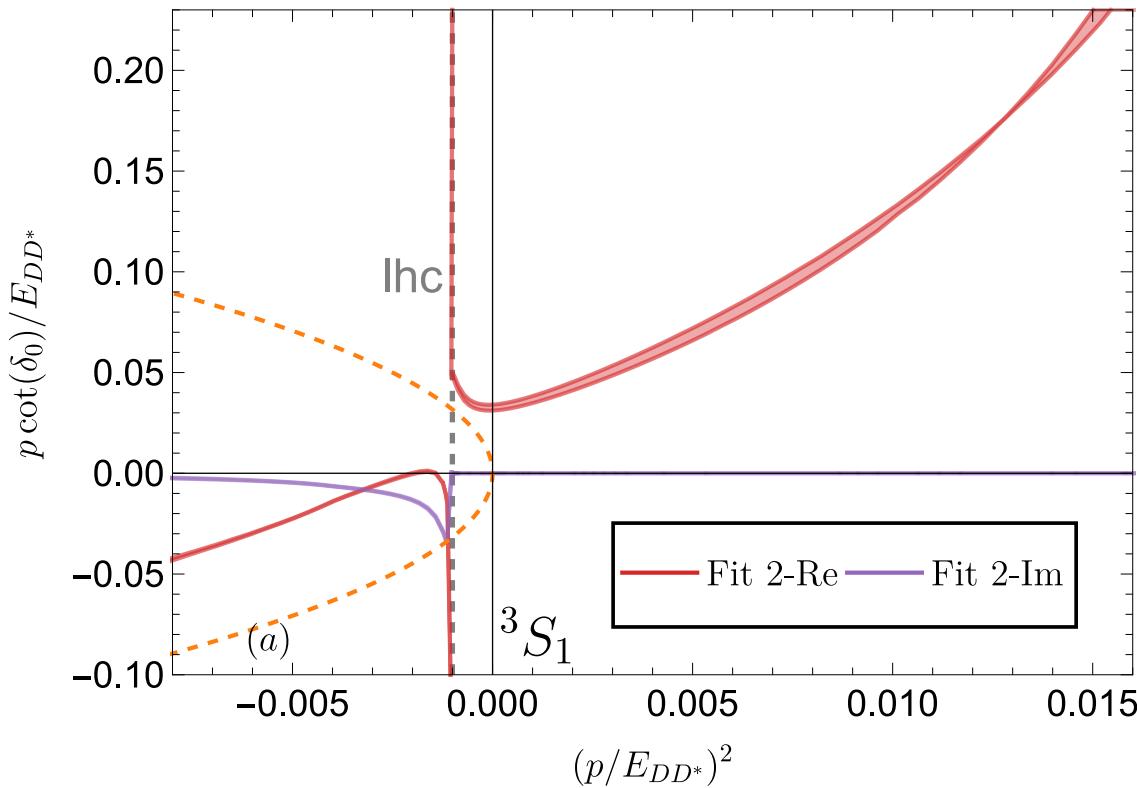
Cutoff dependence of χ^2

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



Cutoff dependence of phase shift

$\Lambda = 0.7 - 1.2 \text{ GeV}$



Two approaches

- Hansen's approach Raposo:2023oru

► FV: lattice data fix $\bar{\mathcal{K}}^{os}$

$$\det_{\mathbf{k}^* \ell m} \left[S(P_j, L)^{-1} + \xi^\dagger \bar{\mathcal{K}}^{os}(P_j) \xi + 2g^2 \mathcal{T}(P_j) \right] = 0$$

► IFV: solve a integral equation

$$\mathcal{M}^{aux}(P, p, p') = \mathcal{K}^T(P, p, p') - \frac{1}{2} \int \frac{d^3 k^*}{(2\pi)^3} \frac{\mathcal{M}^{aux}(P, p, k) H(k^*) \mathcal{K}^T(P, k, p')}{4\omega_N(k^*) [(k_{os}^*)^2 - (k^*)^2 + i\epsilon]},$$

$$\mathcal{K}^T(P, p, p') = \bar{\mathcal{K}}^{os}(P, p, p') + 2g^2 \mathcal{T}(P, p, p'),$$

$$S_{\mathbf{k}^* \ell m, \mathbf{k}'^* \ell' m'}(P, L) = \frac{1}{2L^3} \frac{4\pi Y_{\ell m}(\hat{\mathbf{k}}^*) Y_{\ell' m'}^*(\hat{\mathbf{k}}^*) \delta_{\mathbf{k}^* \mathbf{k}'^*} |\mathbf{k}^*|^{\ell + \ell'} e^{-\alpha[(\mathbf{k}^*)^2 - (k_{os}^*)^2]}}{4\omega_N(\mathbf{k}) [(k_{os}^*)^2 - (\mathbf{k}^*)^2]},$$

$$\mathcal{T}_{\mathbf{k}^* \ell m, \mathbf{k}'^* \ell' m'}(P) = -\frac{1}{4\pi |\mathbf{k}^*|^\ell |\mathbf{k}'^*|^{\ell'}} \int d\Omega_{\hat{\mathbf{k}}^*} d\Omega_{\hat{\mathbf{k}}'^*} Y_{\ell m}(\hat{\mathbf{k}}^*) Y_{\ell' m'}^*(\hat{\mathbf{k}}'^*) \times \frac{1}{(p' - p)^2 - M_\pi^2}$$

$$\omega_N(\mathbf{p})^2 = m_N^2 + \mathbf{p}^2, \quad p = (\omega_N(\mathbf{k}^*), \mathbf{k}^*), \quad p' = (\omega_N(\mathbf{k}'^*), \mathbf{k}'^*)$$

$\xi = 1$ Model-independent?

You have to choose a parameterization of $\bar{\mathcal{K}}^{os}$: ERE

To some how, the ERE is equivalent to the contact EFT

- Our approach

► FV: lattice data fix contact terms

$$\det[\mathbb{G}^{-1}(E) - \mathbb{V}] = 0.$$

► IFV: solve a integral equation

$$T(\mathbf{p}, \mathbf{p}', E) = V(\mathbf{p}, \mathbf{p}') + \int \frac{d^3 q}{(2\pi)^3} V(\mathbf{p}, \mathbf{q}) G(\mathbf{q}, E) T(\mathbf{q}, \mathbf{p}', E).$$

$$V_{EFT} = \begin{array}{c} D^* \\ \diagdown \quad \diagup \\ D \end{array} + \begin{array}{c} D^* \\ \diagup \quad \diagdown \\ D \end{array} + \dots$$

$$\mathbb{G}(E) = \frac{\mathcal{J}(\mathbf{q}_n)}{L^3} G(\mathbf{q}_n, E) \delta_{\mathbf{n}', \mathbf{n}}, \quad \mathbb{V} = V(\mathbf{q}_n, \mathbf{q}_{n'})$$

$$\begin{aligned} G(\mathbf{q}, E) &= i \int \frac{dq^0}{2\pi} \frac{1}{(P - q)^2 - m_1^2 + i\epsilon} \frac{1}{q^2 - m_2^2 + i\epsilon} \\ &= \frac{1}{4\omega_1 \omega_2} \left(\frac{1}{E - \omega_1 - \omega_2} - \frac{1}{E + \omega_1 + \omega_2} \right) \\ &= \frac{1}{2\omega_1 \omega_2} \frac{(\omega_1 + \omega_2)}{E^2 - (\omega_1 + \omega_2)^2 + i\epsilon}, \end{aligned}$$

Lüscher's formula: partial wave mixing effect

- Expanding it in partial wave (PW) 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. Γ_i of point group:: $\det [M_{ln,l'n'}^{(\Gamma,P)} - \delta_{ll'}\delta_{nn'} \cot \delta_l] = 0$

- Example $\Gamma = A_1^+$, w_{lm} depends on E but independent on V

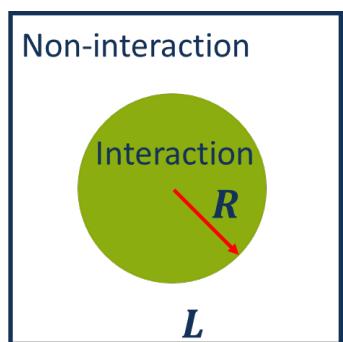
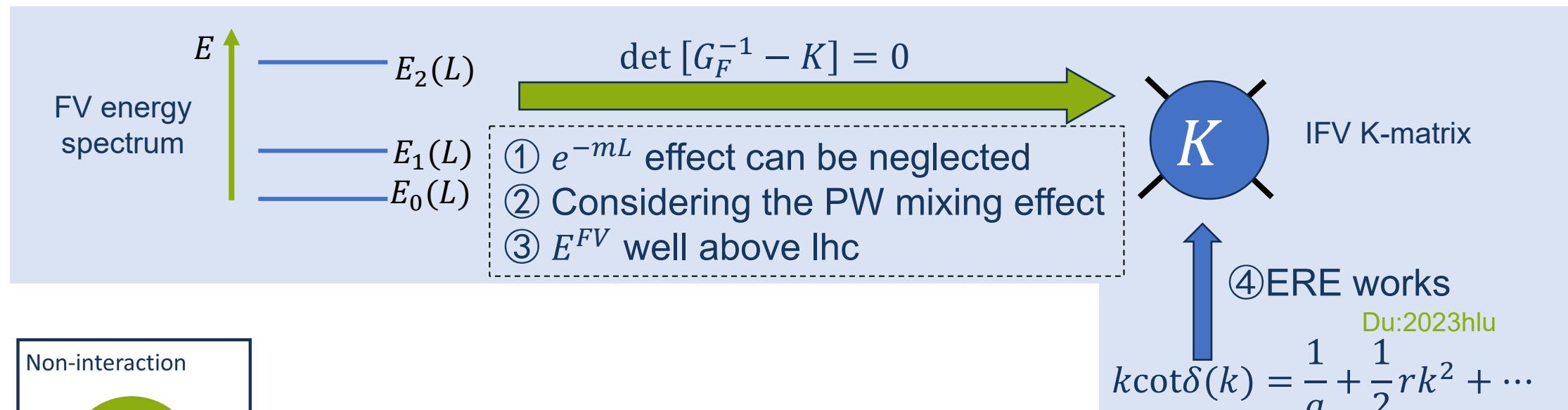
$$\det [M_{ln,l'n'}^{(\Gamma,P)} - \delta_{ll'}\delta_{nn'} \cot \delta_l] = 0, \quad M^{(A_1^+, d)} = \begin{bmatrix} w_{00} & -\sqrt{5}w_{20} & \cdots \\ -\sqrt{5}w_{20} & w_{00} + \frac{10}{7}w_{20} + \frac{18}{7}w_{40} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

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. $\{E_1^{FV}, E_2^{FV}\} \not\Rightarrow \{\delta_S(E_1^{FV}), \delta_S(E_2^{FV}), \delta_D(E_1^{FV}), \delta_D(E_2^{FV}) \dots\}$
 - ▶ 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, ...

Requirements of a practical Lüscher method



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

Typically: $m_\pi L > 3$

High partial wave suppression

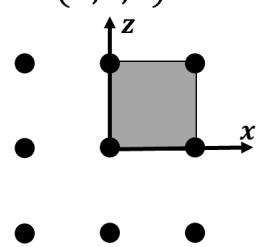
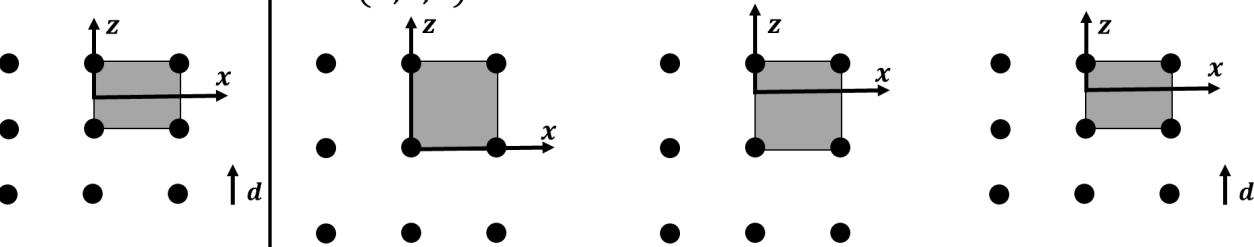
- Threshold effect: $T_l(p) \sim p^{2l}$
- The large scale: m_π

Taylor's textbook P197



All four requirements constrained by the $V_{1\pi}$

Moving systems

$m_1 = m_2, \quad A = 1$	$m_1 \neq m_2, \quad A = 1 + \frac{m_1^2 - m_2^2}{E^*}$
$\mathbf{n} \in Z$ $\mathbf{n} - \frac{1}{2}\mathbf{d}$ $\gamma^{-1} \left(\mathbf{n}_{\parallel} - \frac{\mathbf{d}}{2} \right) + \mathbf{n}_{\perp}$	$\mathbf{n} \in Z$ $\mathbf{n} - \frac{A}{2}\mathbf{d}$ $\gamma^{-1} \left(\mathbf{n}_{\parallel} - \frac{A}{2}\mathbf{d} \right) + \mathbf{n}_{\perp}$
$\mathbf{d} = (0,0,1)$ 	$\mathbf{d} = (0,0,1)$ 

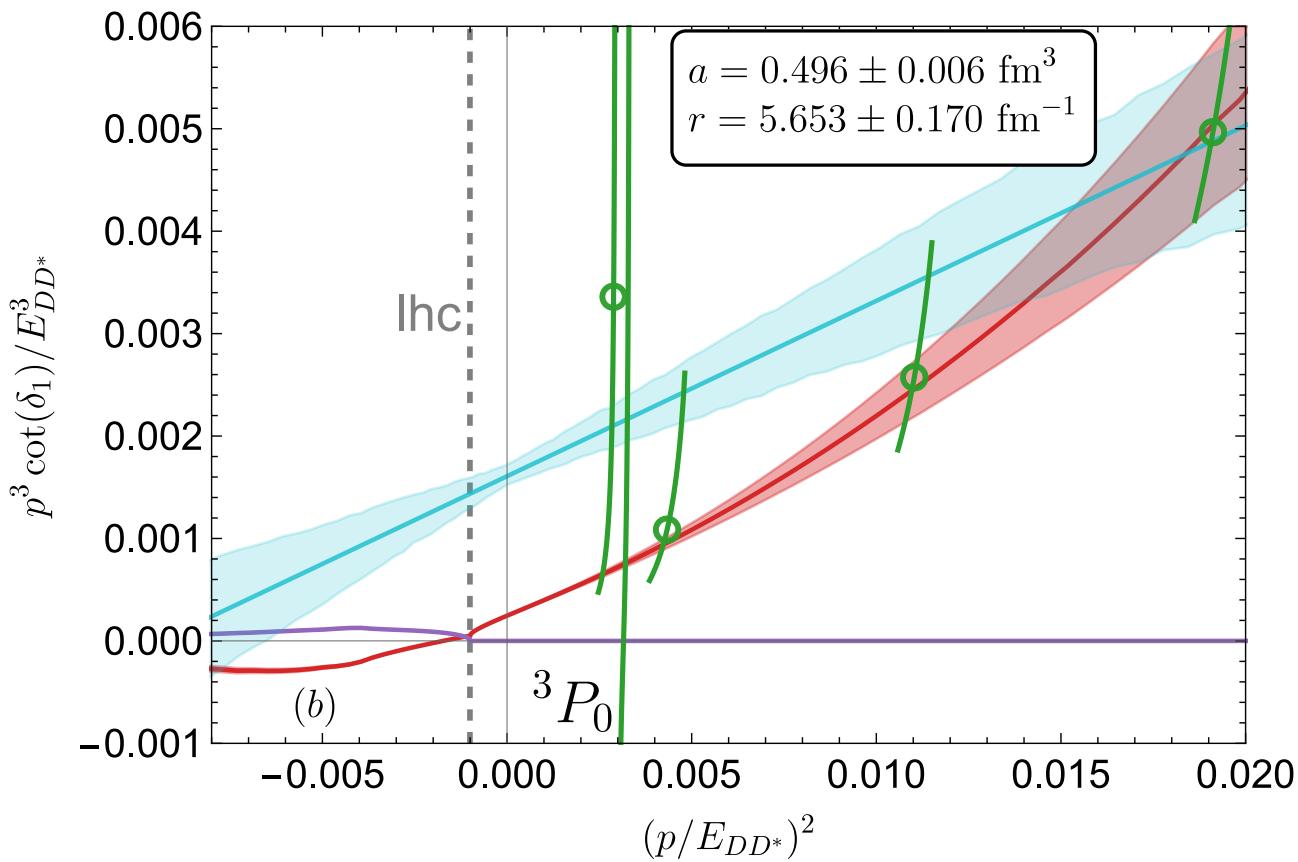
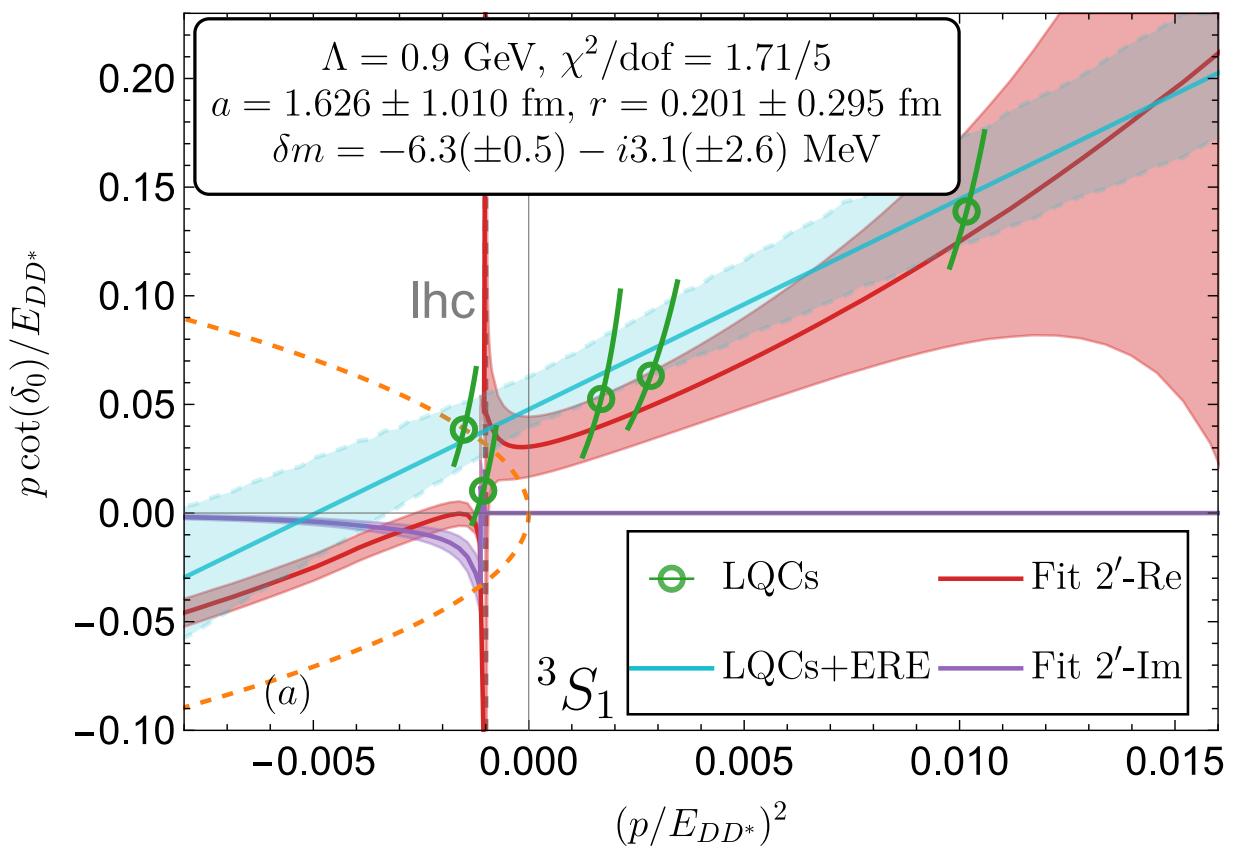
Space inversion invariance is broken

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

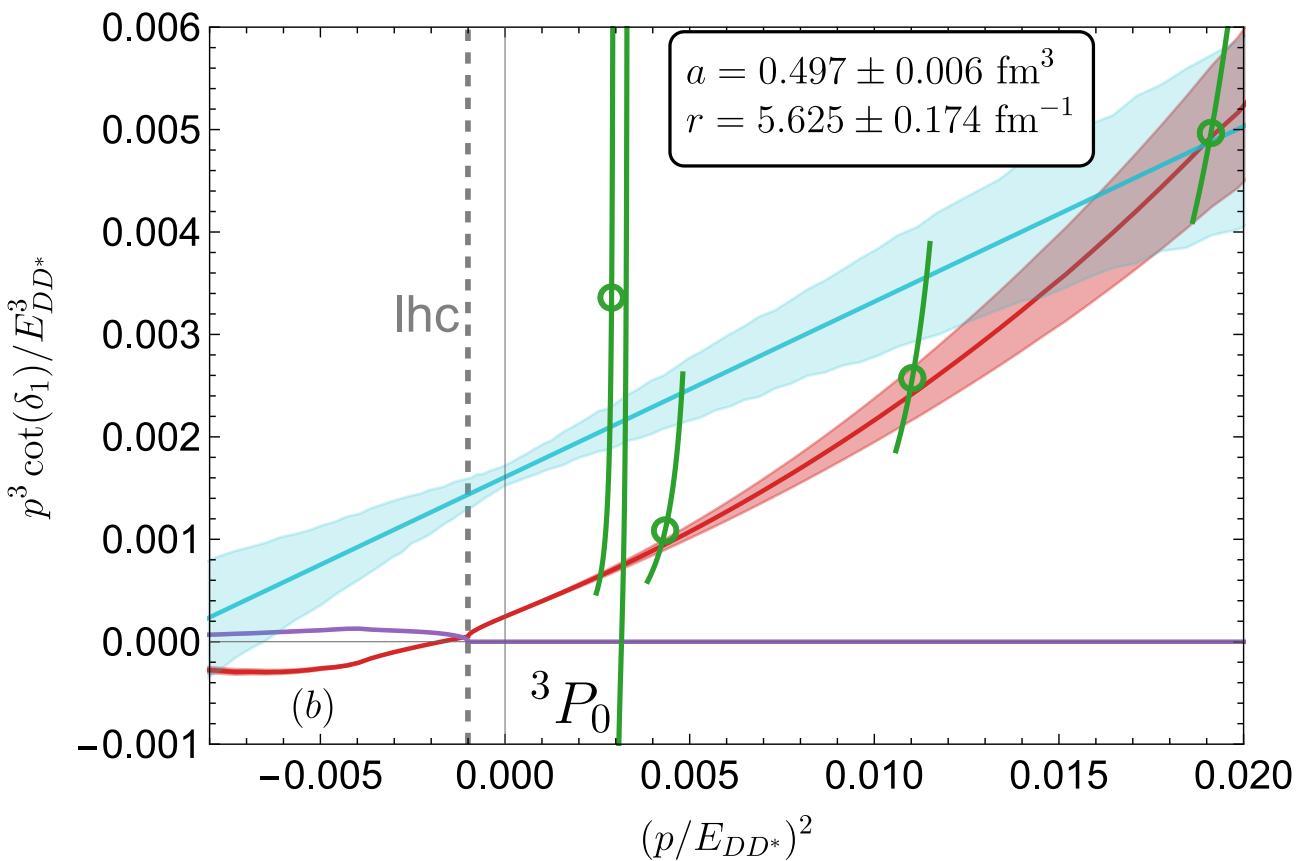
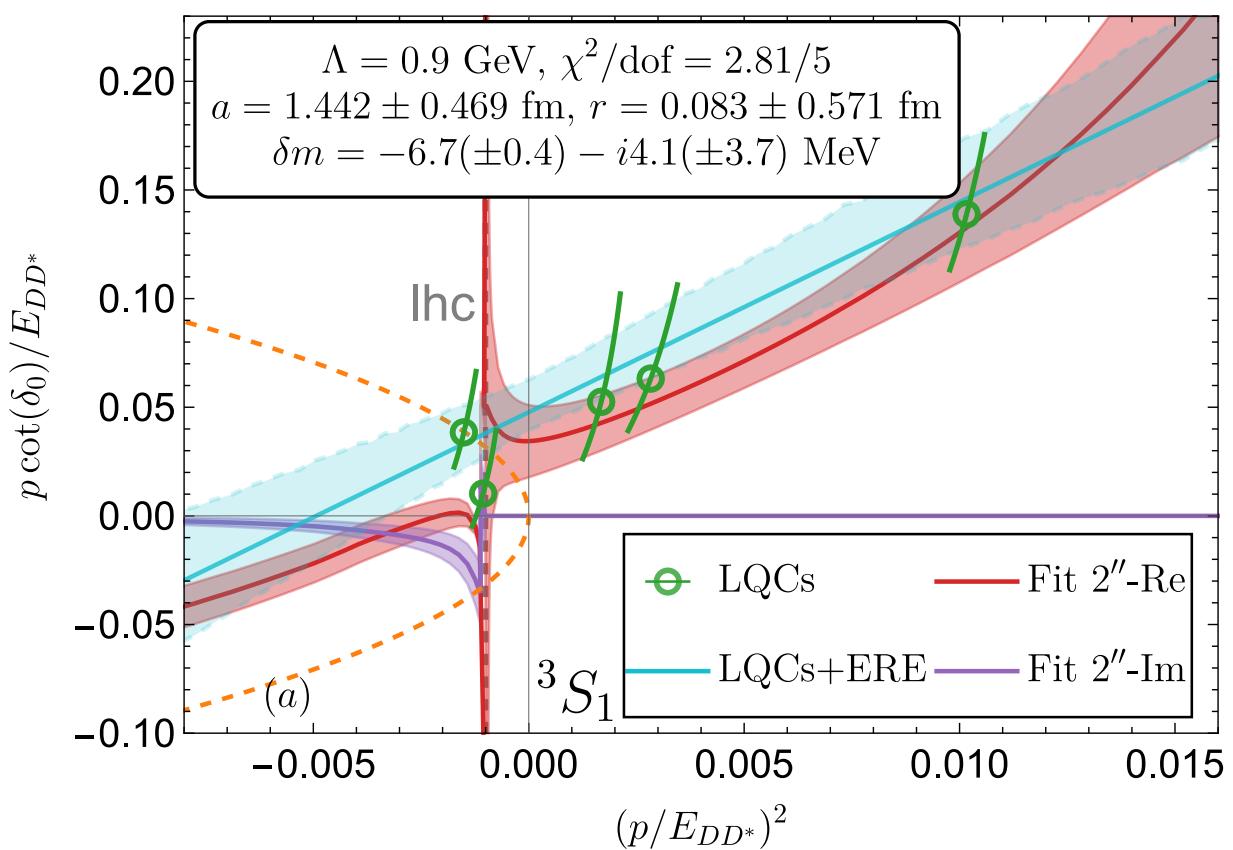
Rummukainen:1995vs,Leskovec:2012gb

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

Including SD transition terms



Including 3P2 term



Lüscher's formula

- Lippmann-Schwinger equation in the finite volume

Luscher:1990ux,Polejaeva:2012ut

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

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

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

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

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

- 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

$$C_L(P) = \text{---} + \text{---} + \dots$$

Diagram: A series of terms showing the operator \mathcal{O} (green circle) connected by a double line to its adjoint \mathcal{O}^\dagger (green circle). The first term has a self-energy loop Σ between them. Subsequent terms add a vertex V (blue circle) and another self-energy loop Σ .

$$V = \text{---} + \text{---} + \dots$$

$$\Sigma = \text{---} + \text{---}$$

$$\Sigma - \text{---} \equiv F$$

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

$$C_L(P) = C_\infty(P) + \text{---} + \text{---} + \dots$$

Diagram: The expression for $C_L(P)$ includes the infinite volume limit $C_\infty(P)$ plus terms involving the operator \mathcal{O} (orange circle), the function F (orange circle), and the kernel K (purple circle).

Within on-shell approximation:

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

$$A = \text{---} + \text{---} + \text{---} + \dots$$

Diagram: The definition of A (orange circle) as a sum of terms. The first term is the operator \mathcal{O} (green circle). Subsequent terms involve the operator \mathcal{O} (green circle) connected by a double line to the function V (blue circle), and the function V (blue circle) connected by a double line to itself.

$$K = \text{---} + \text{---} + \dots$$

Diagram: The definition of K (purple circle) as a sum of terms. The first term is the function V (blue circle). Subsequent terms involve the function V (blue circle) connected by a double line to itself.

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

Hamiltonian method in plane wave basis

- Finite volume levels

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

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

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

- Accelerate calculation: subspace learning

- ▶ specifically **eigenvector continuation**

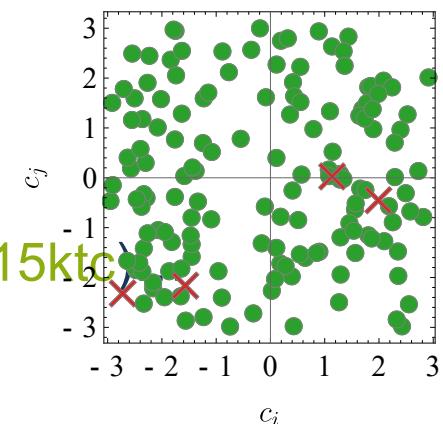
- For moving systems, elongated boxes, particles with arbitrary spin...

- Similar approaches:

- ▶ Momentum lattice ([Doring:2011ip](#)), Hamiltonian EFT([Wu:2014vma](#), [Liu:2015ktc](#))

- **Using plane wave + reducing to irreps of point group +EC** is unique

- Extra advantage: **partial wave mixing effect**



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: $\{0, 0, a\}_{6 \times 3} = 2T_1^+ \oplus T_2^+ \oplus A_1^- \oplus E_1^- \oplus T_1^- \oplus T_2^-$
- For moving systems, elongated boxes, particles with arbitrary spin...

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

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

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