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T_{cc} from finite volume energy levels: the left-hand cut problem

Lu Meng (孟 璐)

Ruhr-Universität Bochum

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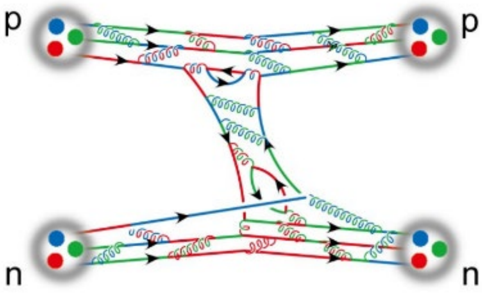
Base on JHEP10(2021)051, PoS LATTICE2022 (2023) 201 and PRD109(2024), L071506

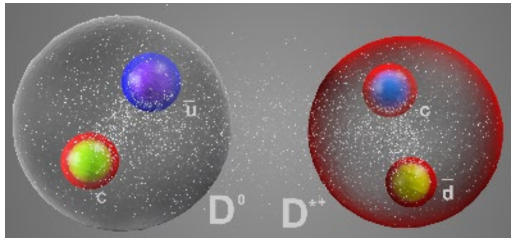
Together with V. Baru, E. Epelbaum, A. Filin, A.M. Gasparyan

Lattice QCD

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

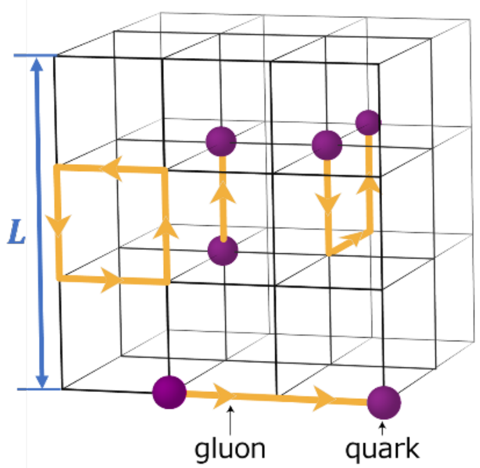


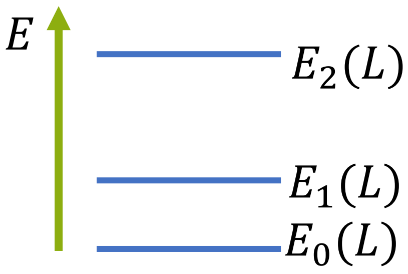
Nuclear force



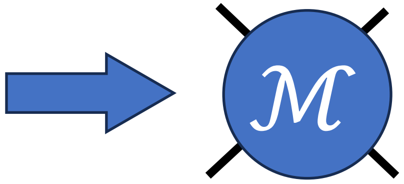
Hadronic molecules

- 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

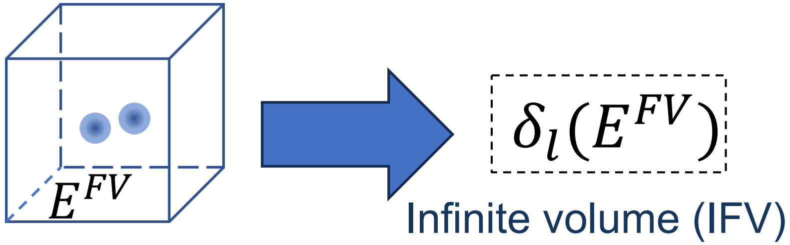
- Lüscher's formula:

Luscher:1990ux

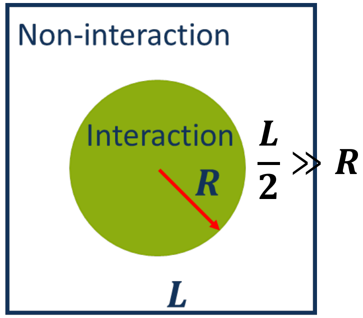
AKA : Lüscher Quantization conditions (LQCs)

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

Kinematical term K-matrix in IFV



- Derive it



Asymptotic behavior: for $r > R$

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

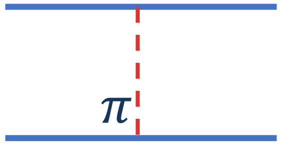
$$\psi_k(r) \sim \frac{e^{i\delta(k)}\sin[kr + \delta(k)]}{kr}.$$

Periodic Boundary condition:

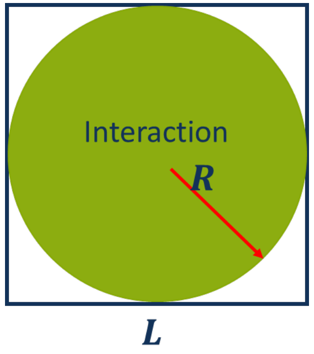
$$\boldsymbol{p} = \frac{2\pi}{L}\boldsymbol{n}, \qquad \boldsymbol{n} \in Z^3$$

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

    Require: $m_\pi L > 4 \Rightarrow L > 5.7$ fm
  - ▶ Left-hand cut (lhc) problem
  - ▶ Partial-wave mixing effects



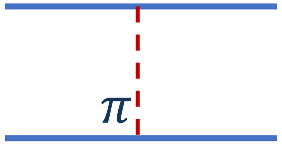
NN , D^*D systems…



Long-range interaction and small box???

Left-hand cut

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



Left-hand cut

on-shell pion

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

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

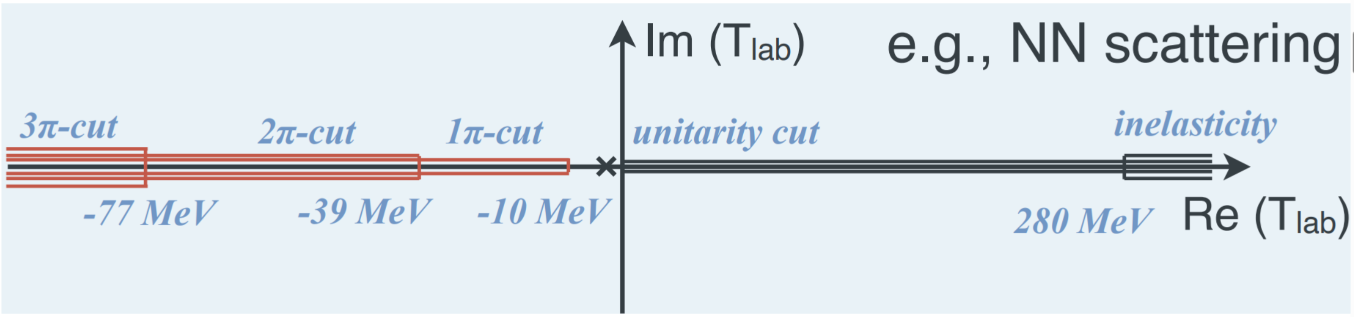
$$V_{l=0}(p, p') = \int_{-1}^{1} dz \frac{1}{p^2 + p'^2 - 2pp'z + m^2} = -\frac{1}{2pp'} \log\left(\frac{(p-p')^2 + m^2}{(p+p')^2 + m^2}\right)$$

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

$$V_{l=0}(k, k) = \int_{-1}^{1} dz \frac{1}{2k^2(1-z) + m^2}, \qquad 2k^2(1-z) + m^2 = 0 \Rightarrow z = \frac{m^2}{2k^2} + 1, \qquad -1 < z < 1 \Rightarrow k^2 < -\frac{m^2}{4}$$

on-shell pion

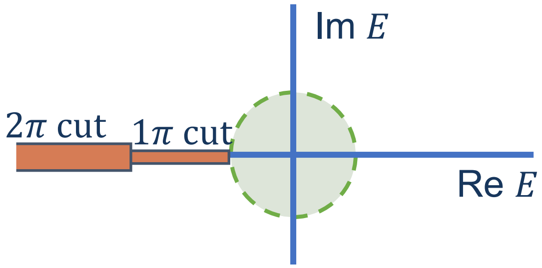
- ▶ Branch point: $k^2 < -\frac{m^2}{4}$



Left-hand cut problem

- lhc in the IFV
  - ▶ Effective range expansion (ERE):

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



  - ▶ Radius of convergence of ERE

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

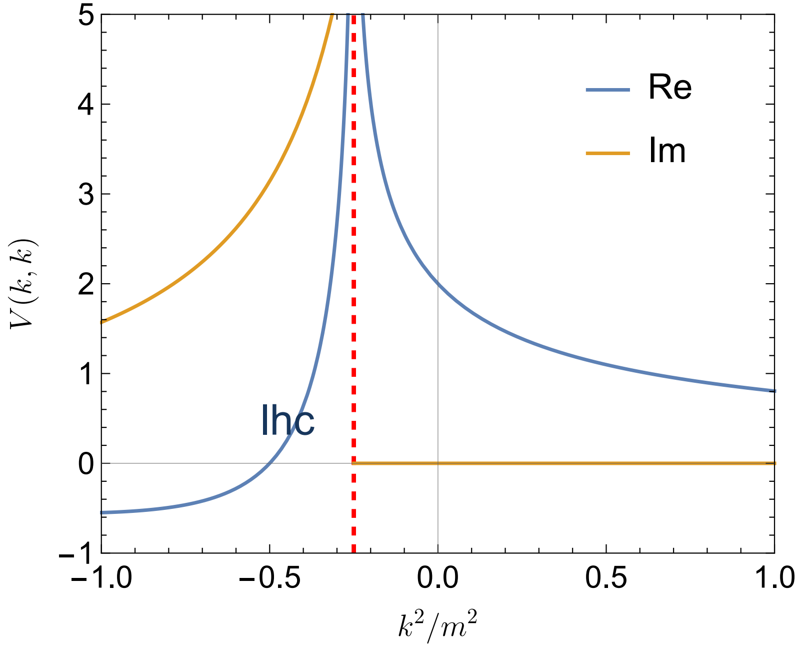
- lhc problem of Lüscher formula

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

Real — K-matrix in the IFV

$$K = V + VG^{\mathcal{P}}K$$

  - ▶ For $k^2 > -\frac{m^2}{4}$, K-matrix is real
  - ▶ For $k^2 < -\frac{m^2}{4}$, $\text{Im}\,K \neq 0$



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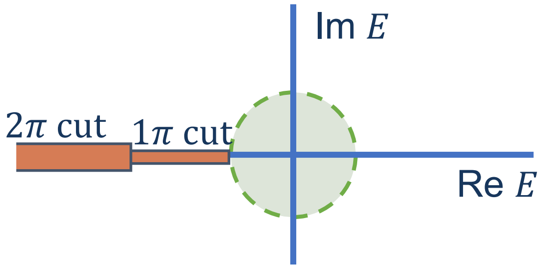

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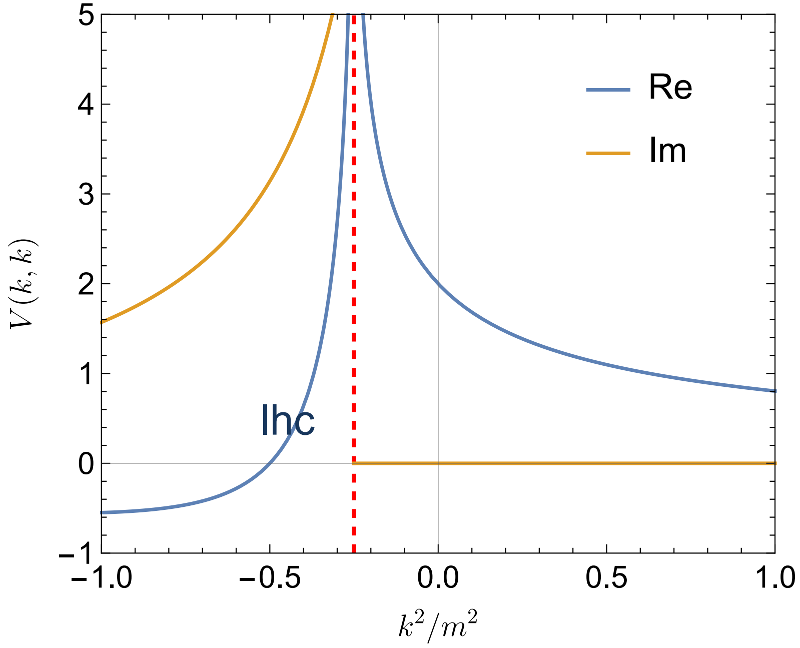
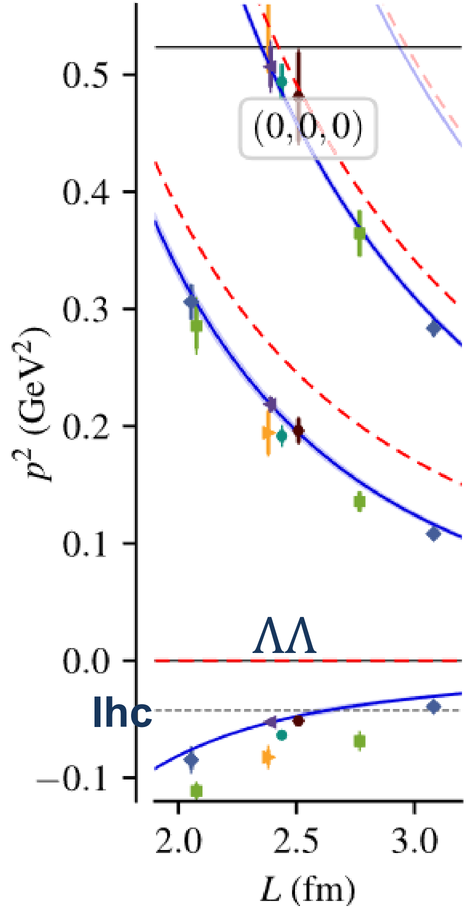


Left-hand cut problem in LQCD

Green:2021qol

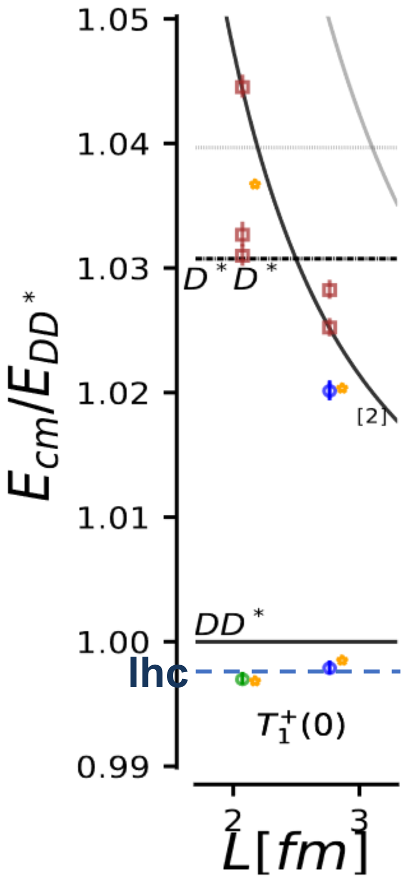
$m_\pi = m_K \approx 420$ MeV



H-dibaryons ($udsuds$)

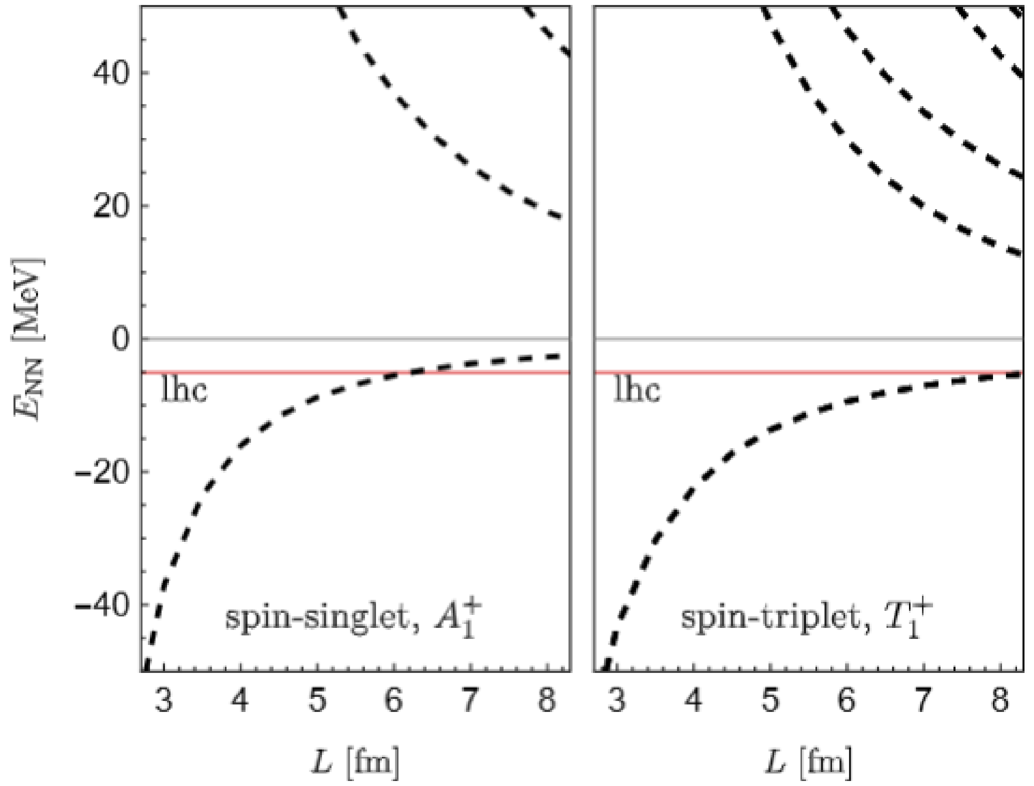
Padmanath:2022cvl

$m_\pi = 280$ MeV



DD^* (T_{cc})

$m_\pi = 137$ MeV



NN systems

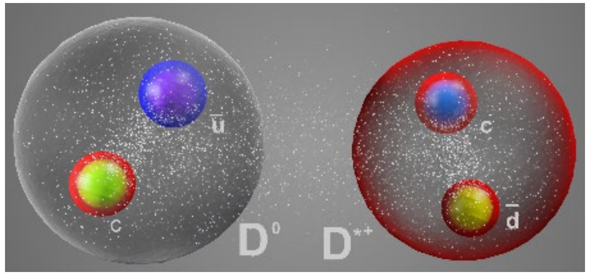
$L > 8$ fm to get rid of the lhc problem

T_{cc} state

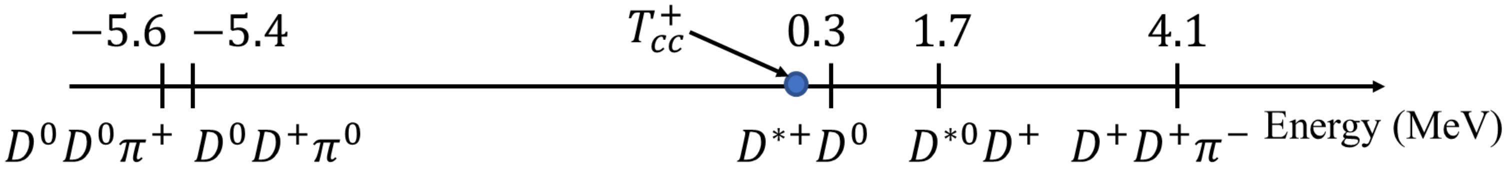
$T_{cc}(3875)^+$ state

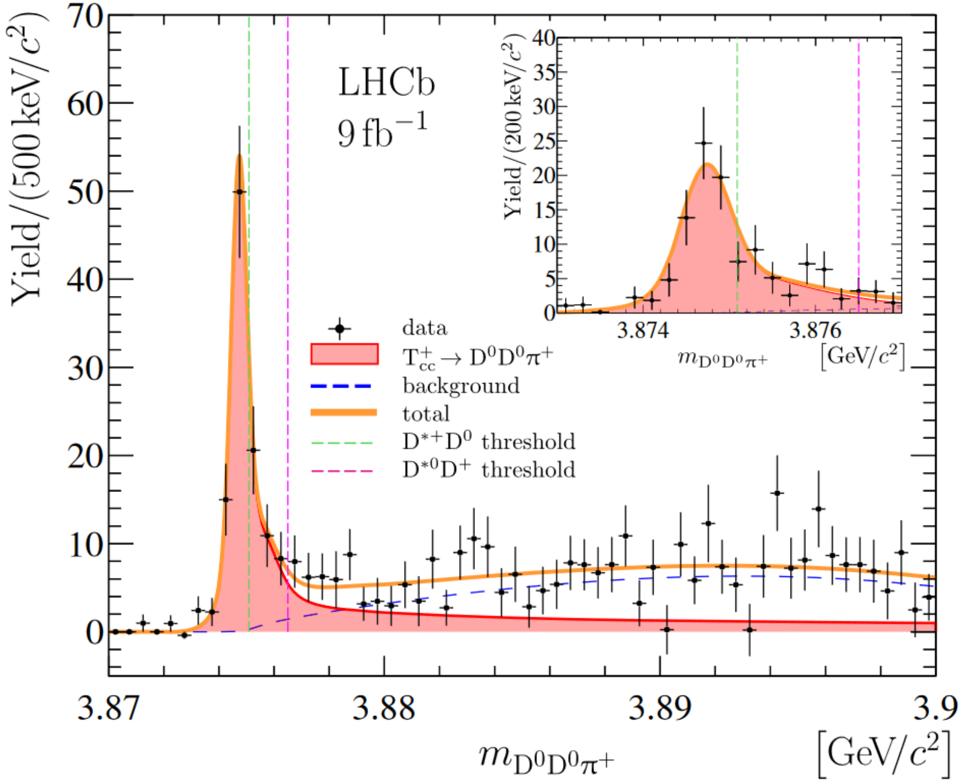
- $T_{cc}(3875)^+$ was observed in 3-body final states: $D^0D^0\pi^+$
- Very close to D^0D^{*+} thresholds: $\delta m_U \approx -360$keV, $\Gamma \approx 48$ keV
- Exotic hadrons: minimal quark content: $cc\bar{u}\bar{d}$
- Good candidates of D^0D^{*+} molecule

LHCb Collaboration



- 3-body dynamics could be important



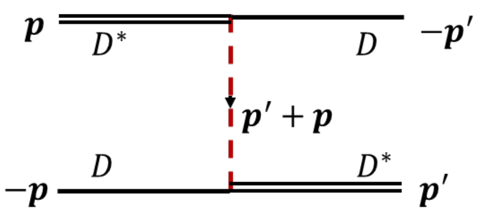


lhcb:2021vvq, lhcb:2021auc, Du:2021zzh, Meng:2021jnw…

T_{cc} lattice QCD simulations

Padmanath:2022cvl

- 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
  - ▶ $p_{\text{lhc}}^2 \approx -\left(\frac{m_{\text{eff}}}{2}\right)^2 = -(126\ \text{MeV})^2$
  - ▶ $p_{\text{rhc3}}^2 \approx 2\mu_{DD^*}(2m_D + m_\pi - m_D - m_{D^*}) \approx (560\ \text{MeV})^2$



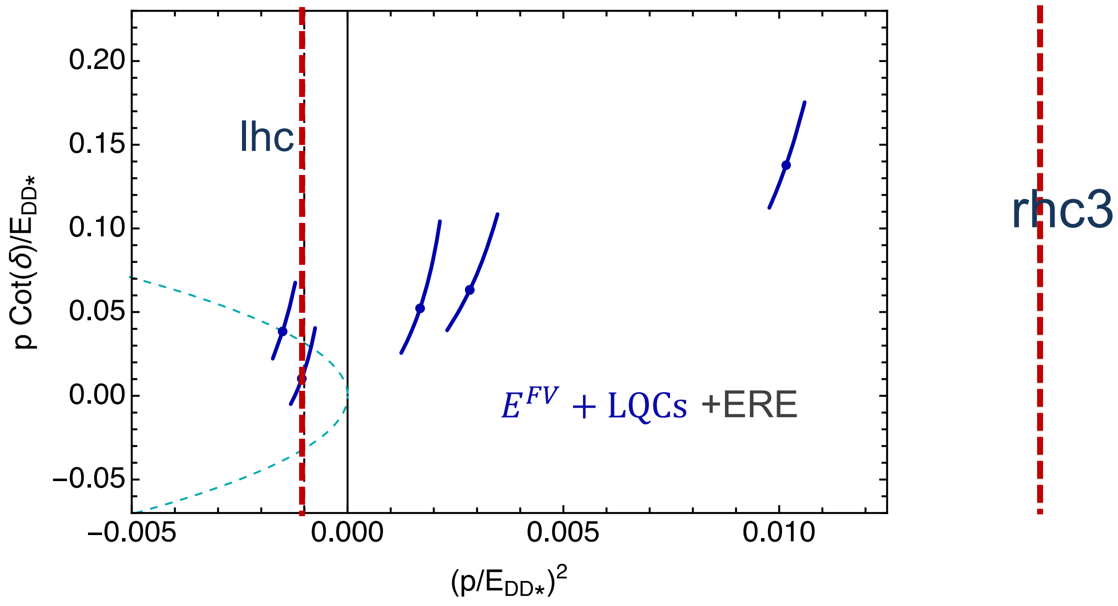
$$\frac{-1}{k^2 + m_\pi^2 - k_0^2 - i\epsilon} = \frac{-1}{k^2 + m_{\text{eff}}^2 - i\epsilon}$$

- 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, Lyu:2023xro, Whyte:2024ihh…

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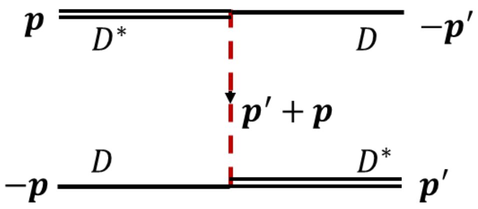

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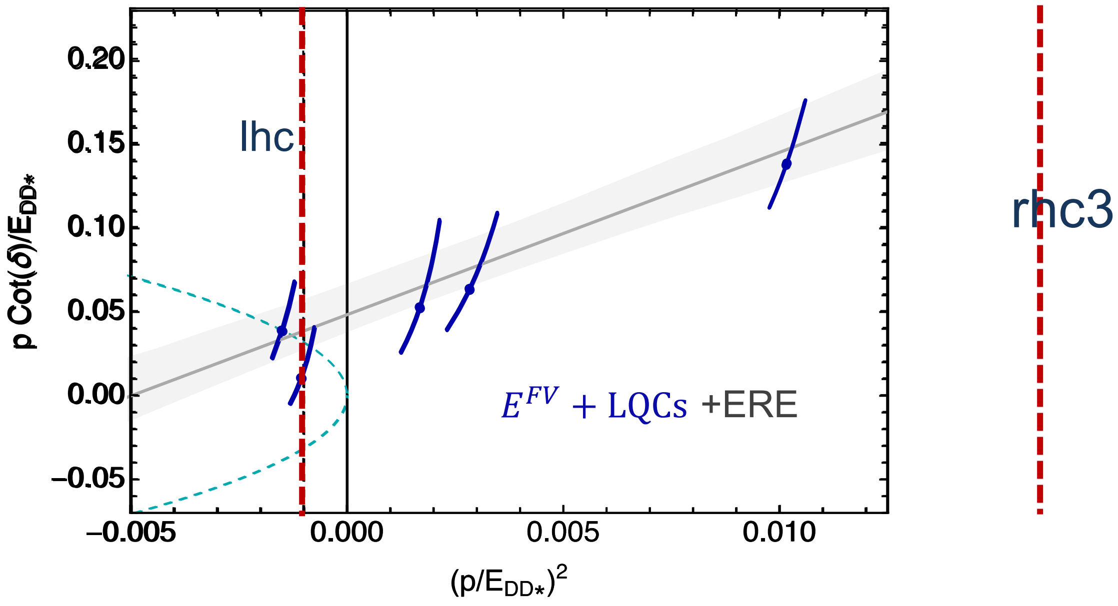
  ~~Lüscher formula~~, effective ~~range~~ expansion



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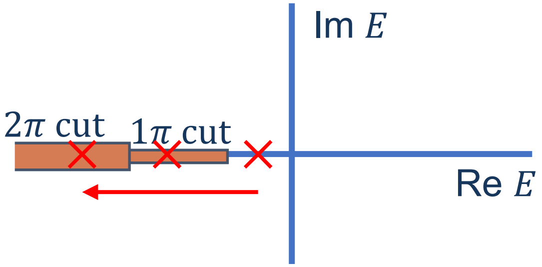
Our strategy

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

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

Off-shell, for $\mathrm{E} < 0$

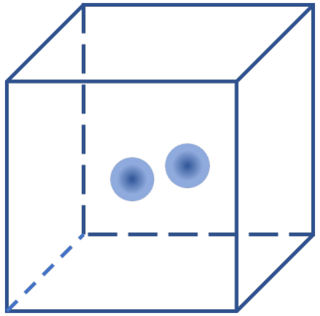


  - Works well even for $2\mu E < -\frac{m^2}{4}$
  - For the $p, p' > 0$, no lhc

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

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

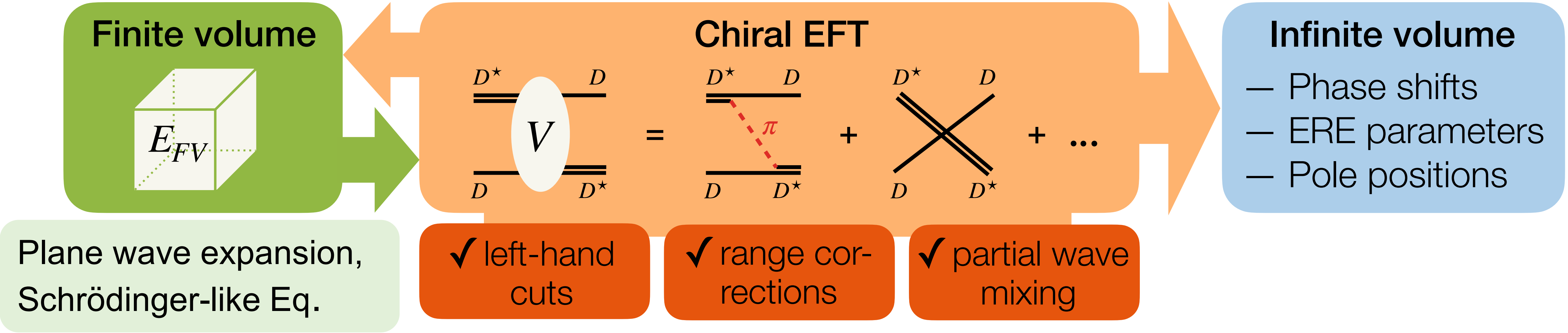
$$\int \frac{d^3\boldsymbol{p}}{(2\pi)^3} \to \frac{1}{L^3}\sum_{\boldsymbol{p}_n}$$



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

Our strategy

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



Chiral EFT

- Symmetry from QCD
  - ▶ Chiral symmetry and its spontaneous breaking
- Weinberg power counting
  - ▶ Systemic calculation, controllable truncation error

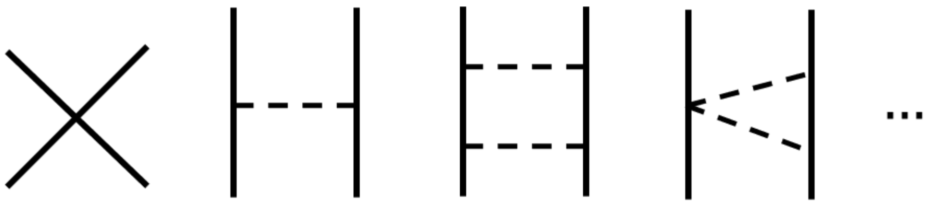
$$V(\vec{p}', \vec{p}) = V_{\text{contact}} + V_{1\pi} + V_{2\pi}$$

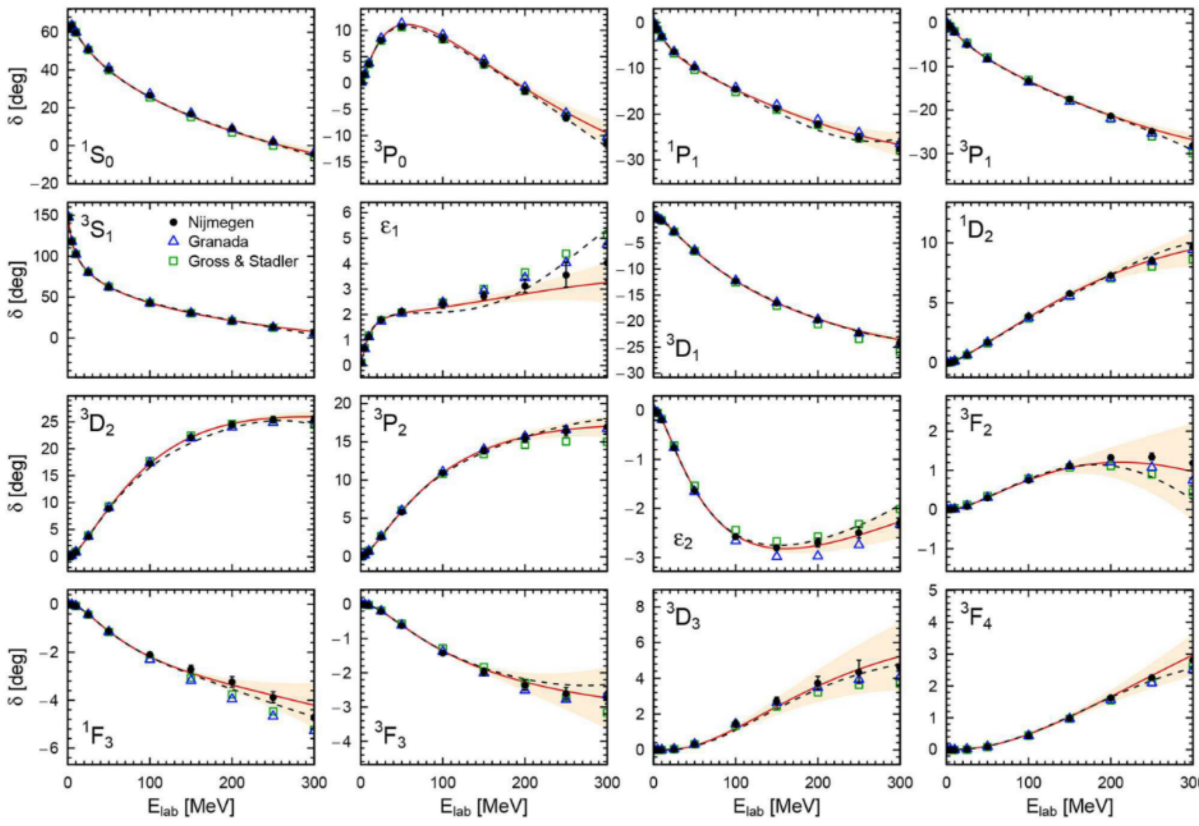
Reinert:2017usi

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

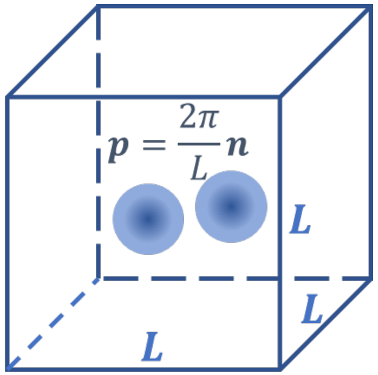
$$V_{1\pi}(\vec{p}', \vec{p}) = -\frac{g_A^2}{4F_\pi^2}\left(\frac{\vec{\sigma}_1 \cdot \vec{q}\vec{\sigma}_2 \cdot \vec{q}}{q^2 + m_\pi^2} + C(m_\pi)\vec{\sigma}_1 \cdot \vec{\sigma}_2\right) e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}$$

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





Hamiltonian method in plane wave basis



Periodic boundary condition

- 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

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

- Why not use the plane wave (with discrete momentum) basis directly
- $|\boldsymbol{p_n}, \boldsymbol{\eta}\rangle$: $\boldsymbol{p_n}$ discrete momentum, $\boldsymbol{\eta}$: polarization vector for $S = 1$

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

- $\{|\boldsymbol{p_n}, \boldsymbol{\eta}\rangle\}$ form the representation space of corresponding point group

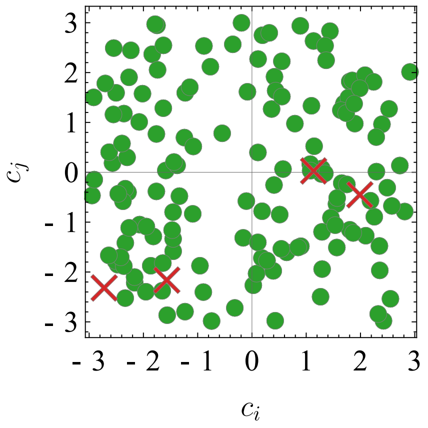
Hamiltonian method in plane wave basis

- 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

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

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

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

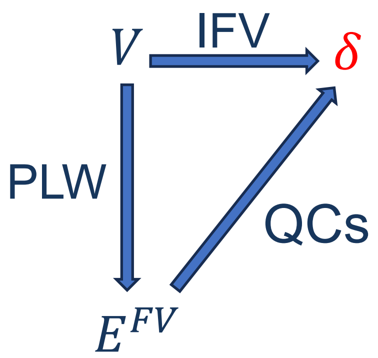


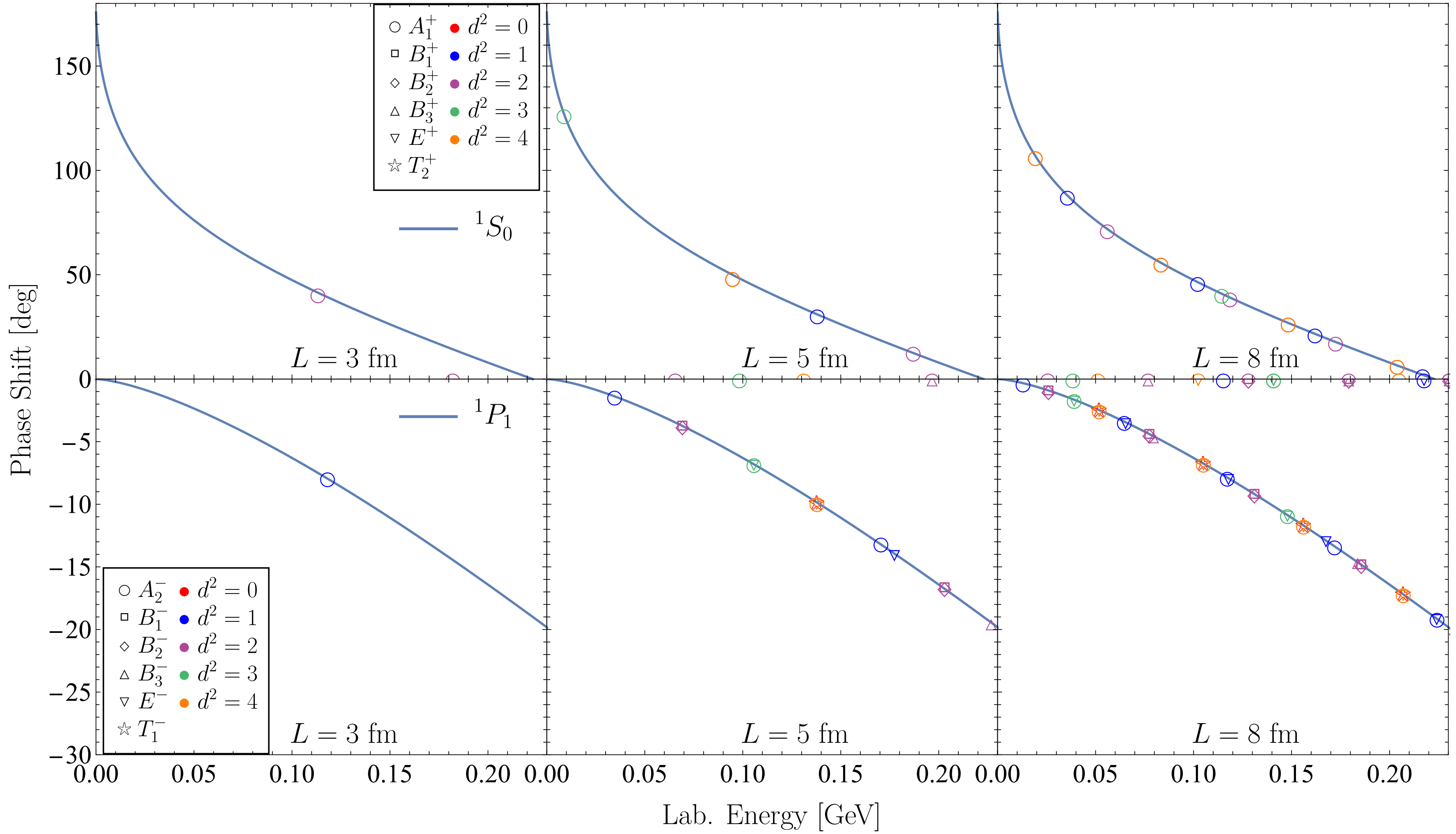
- Accelerate calculation: subspace learning
  - ► specifically **eigenvector continuation**
- For moving systems, elongated boxes, particles with arbitrary spin...

- 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**

Benchmark: contact interaction

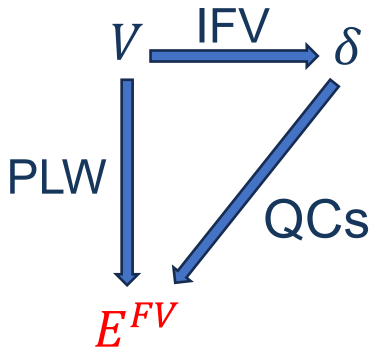
- Contact interaction: $V(\boldsymbol{p},\boldsymbol{p}') = C_S + C_1\boldsymbol{q}^2 + C_2\boldsymbol{k}^2$
- Only contribute to S-wave and P-wave

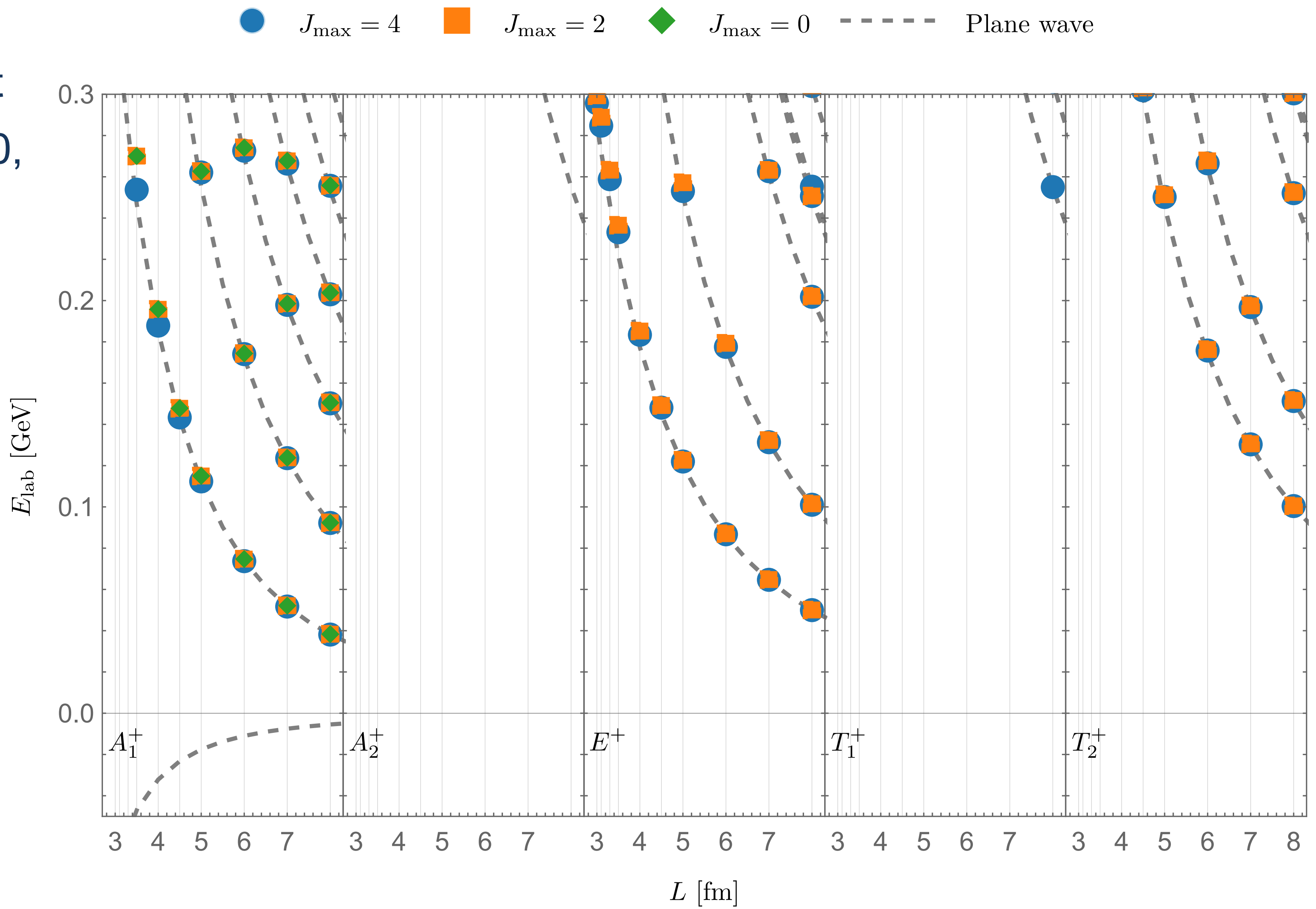




Benchmark: chiral EFT, partial wave mixing

- 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

Numerical calculation

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

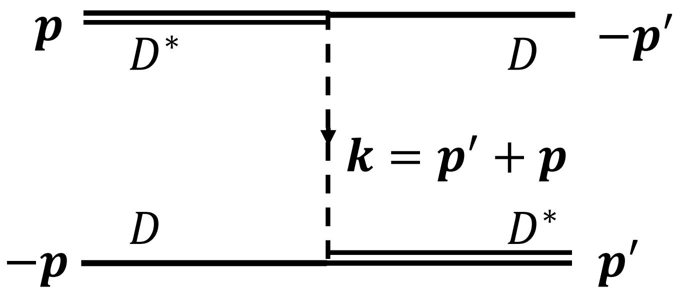
Li:2021mob

- Get the poles

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

Interaction: ChEFT

- Contact terms to NLO
  - ▶ 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



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

  - ▶ Semilocal momentum-space regularization

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

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

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

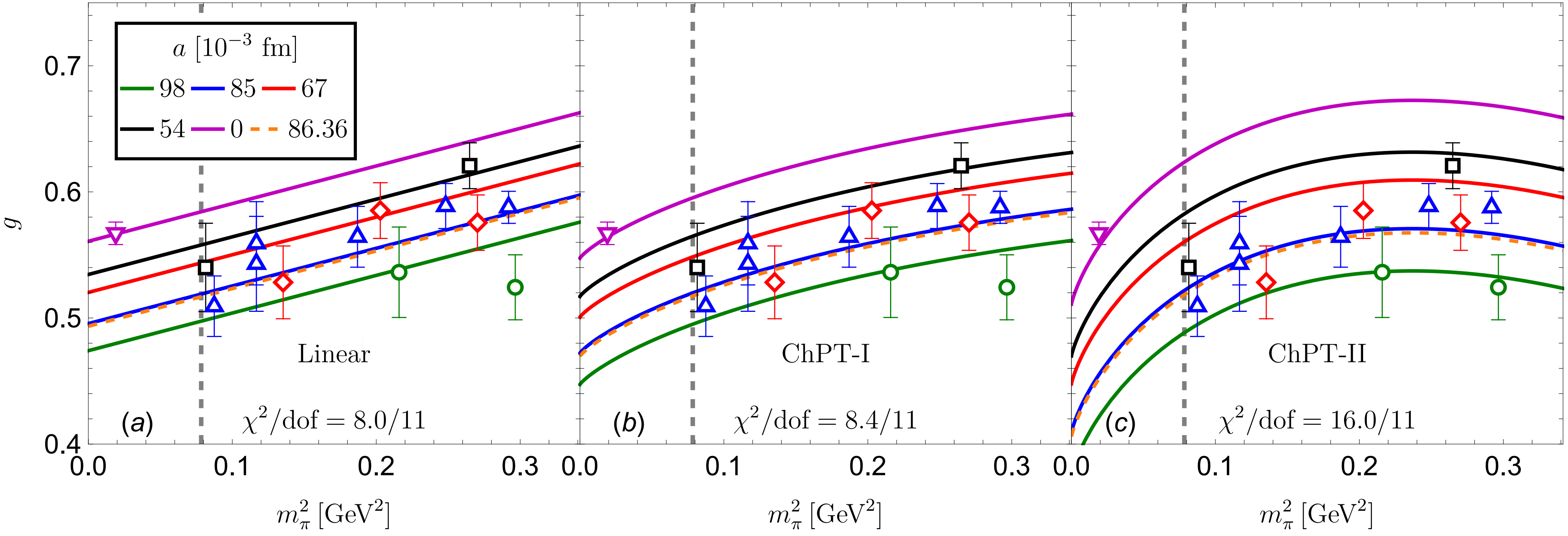
F_π and g

- 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, $\xi = m/m^{ph}$

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

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



$\Lambda = 0.9$ GeV, only contact terms

- Results using Lüscher's QCs Padmanath:2022cvl

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

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

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

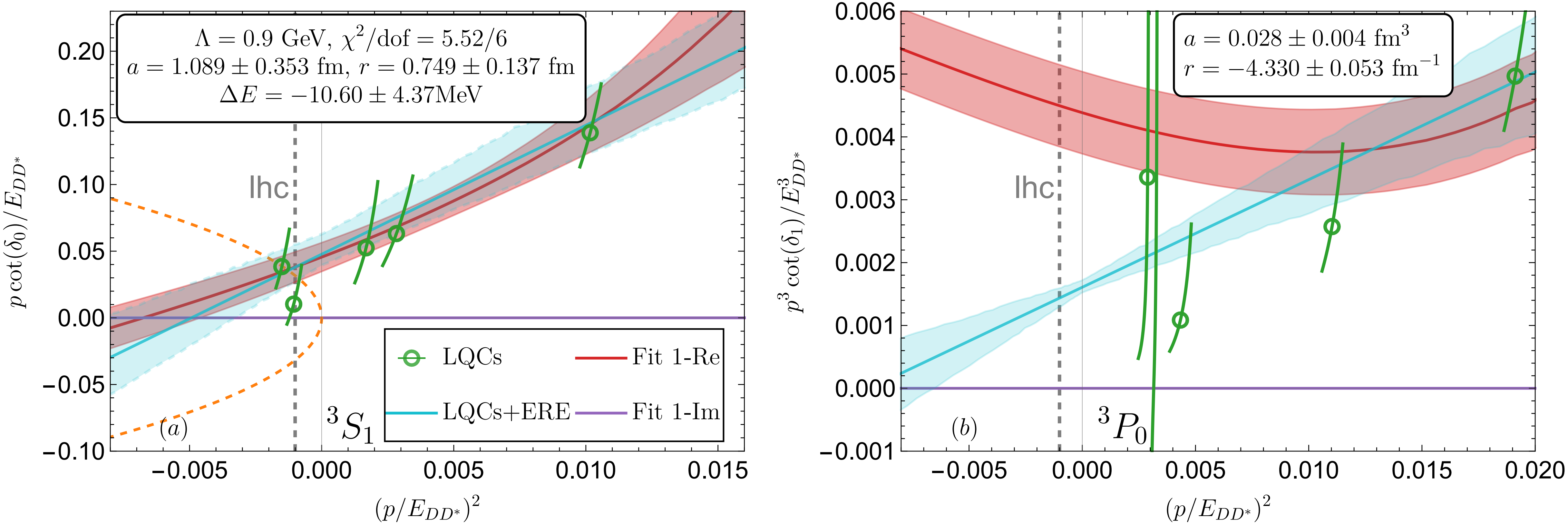
Four parameters:

$a_{\,{}^3S_1}, r_{\,{}^3S_1}, a_{\,{}^3P_0}, r_{\,{}^3P_0}$

- Our results

Three parameters:

LO and NLO ${}^3S_1$, NLO ${}^3P_0$ LECs



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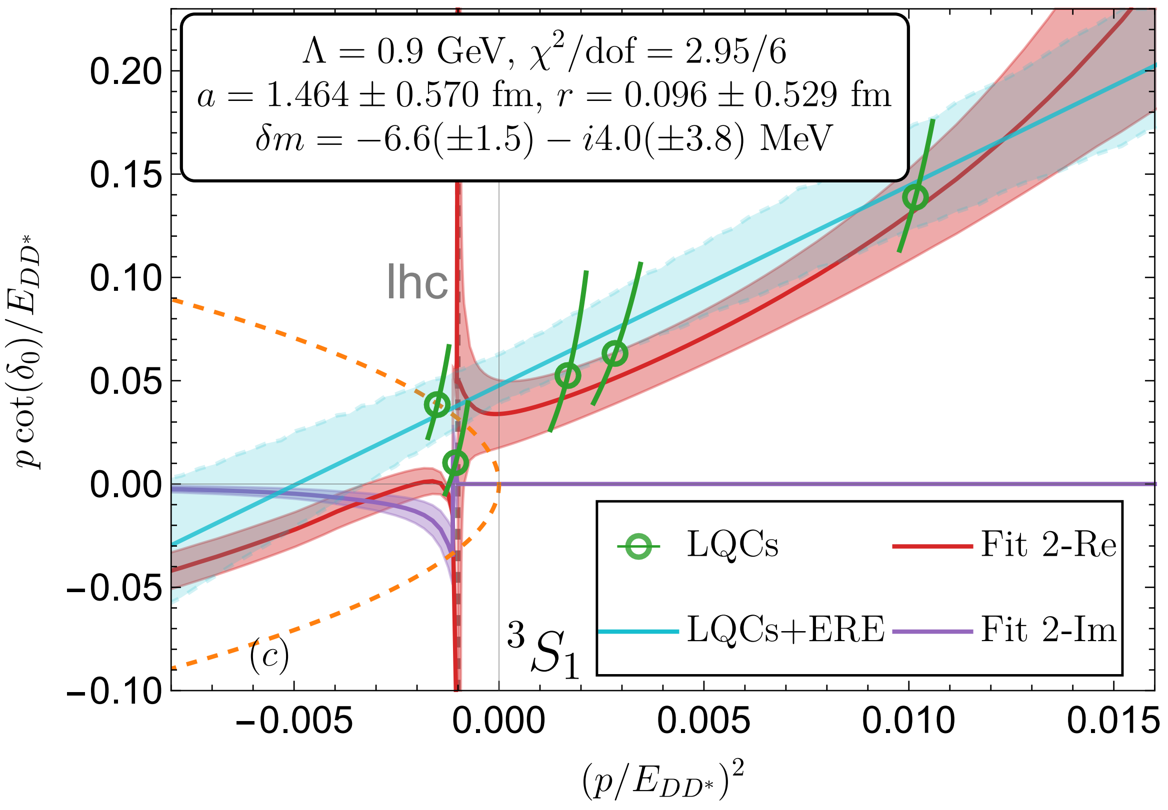
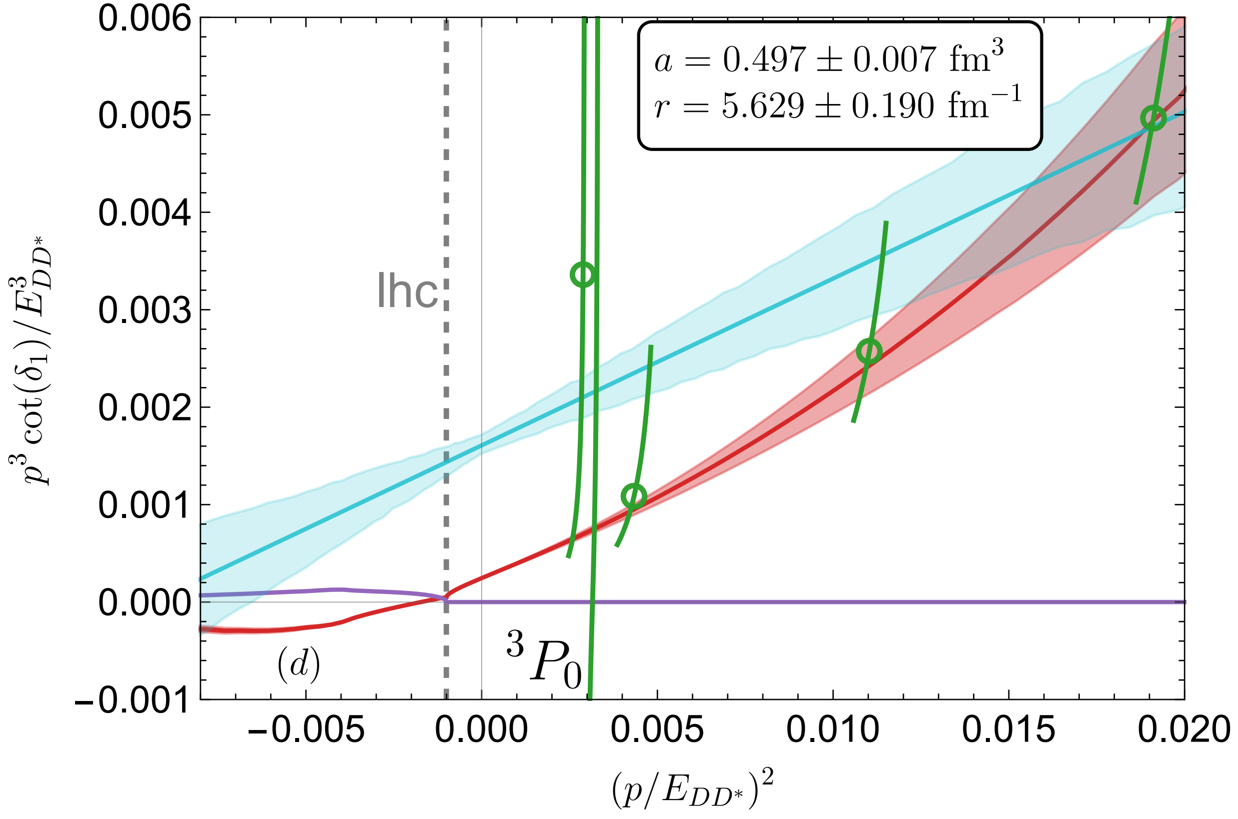
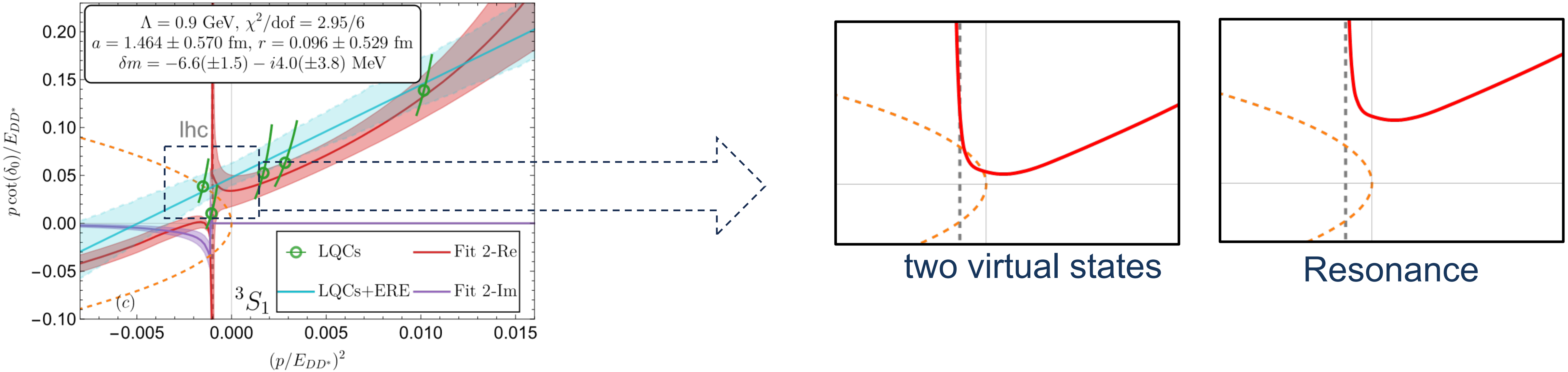




$\Lambda = 0.9$ GeV, contact terms+OPE

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



Other methods

- 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

- 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

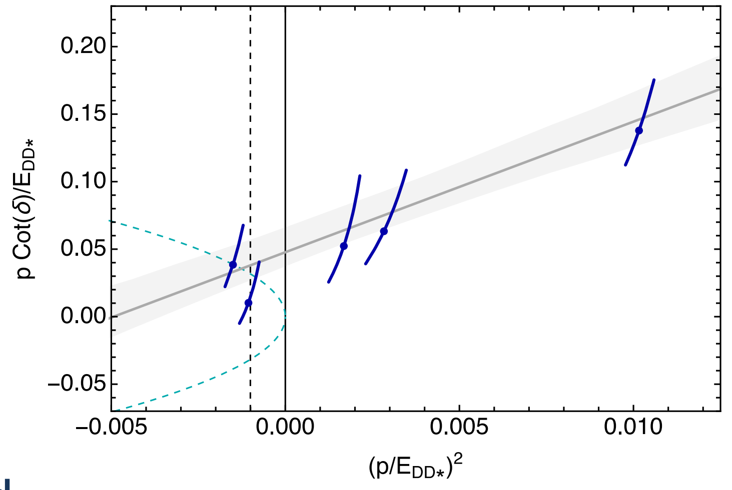
Model-(in)dependence

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

Model-independent *Model-dependent?*

Our answers：

FV Hamiltonian method / EFT **VS** Lüscher QCs / Parametrization of T-matrix



- 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 could be regarded as parametri. schemes of the T-matrix
  - ▸ 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^i_{FV} **separately**, $V_i = \lambda_i V_{short-range}$
  - ▸ Each V_i will give a phase shift $\delta(E^i_{FV})$ in the infinite volume

Summary and Outlook

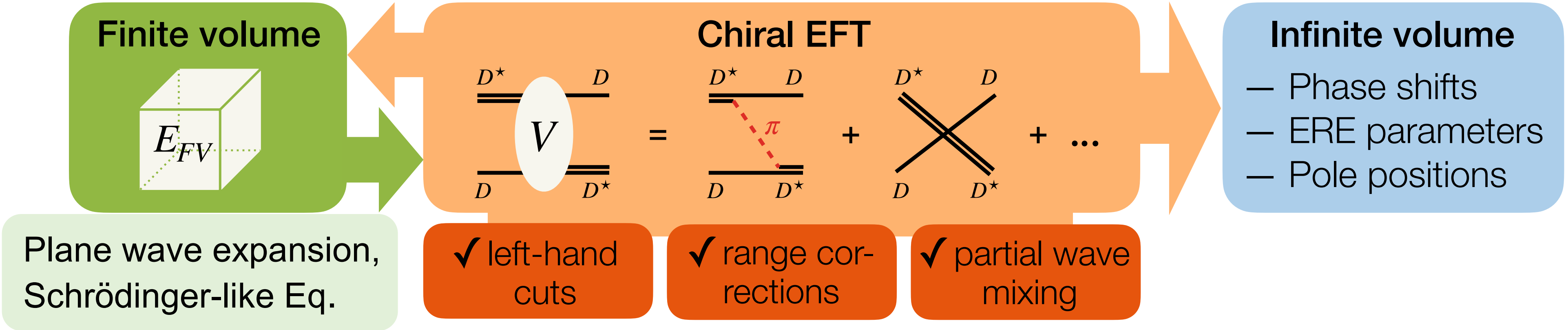
- Validation of Lüscher's formula

  ① e^{-mL} effect can be neglected
  ② Considering the PW mixing effect
  ③ E^{FV} well above lhc
  ④ERE works in IFV   Du:2023hlu

  Invalidate ←

One-pion-exchange interaction

- Our formalism



- T_{cc} lattice data
  - ▸ E^{FV} below the left-hand cut
  - ▸ Lattice T_{cc}, more likely resonance
  - ▸ The possible partial wave mixing effect
  - ▸ Important one-pion exchange interaction

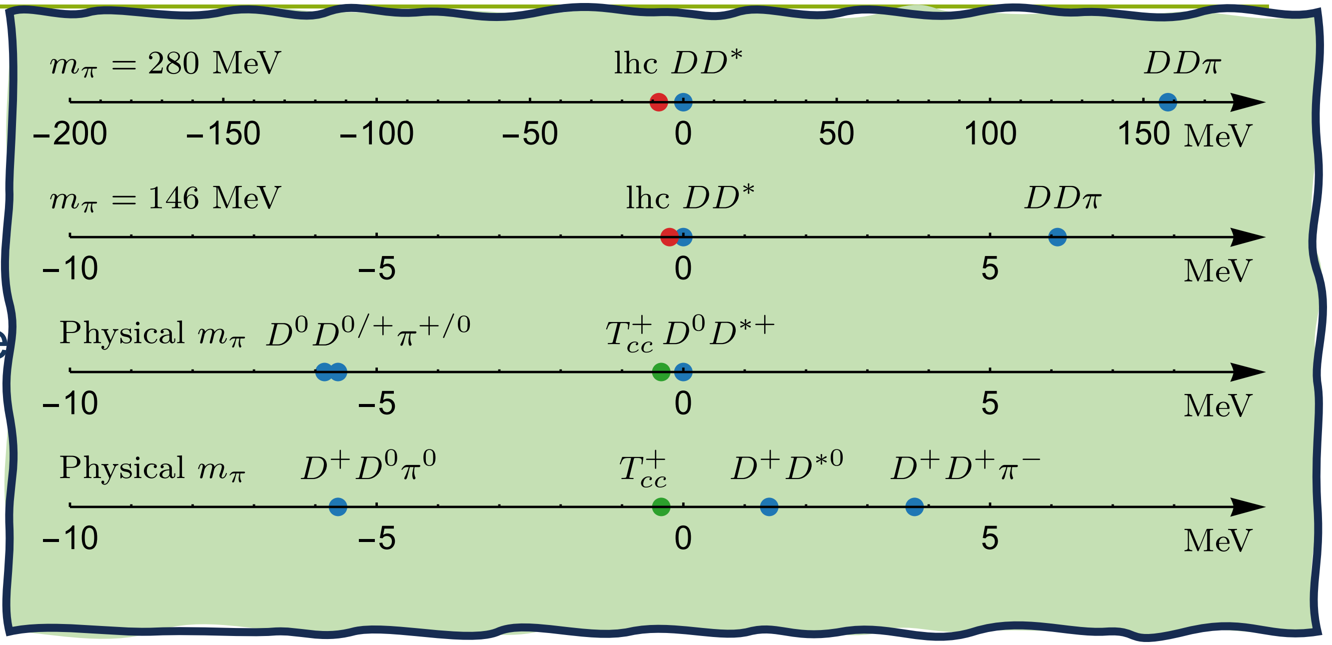
T_{cc} is a playground

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

Finite volume

Infinite volume

2407.04649



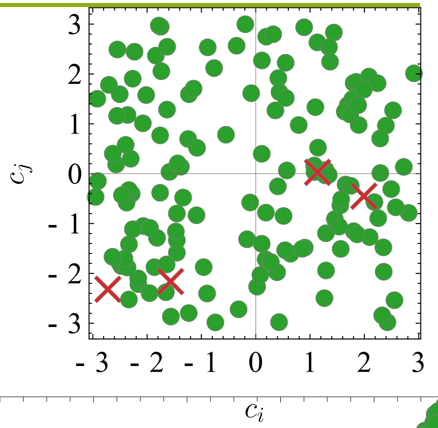
Thanks for your attentions!

Back up

Towards a practical approach: eigenvector continuation

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

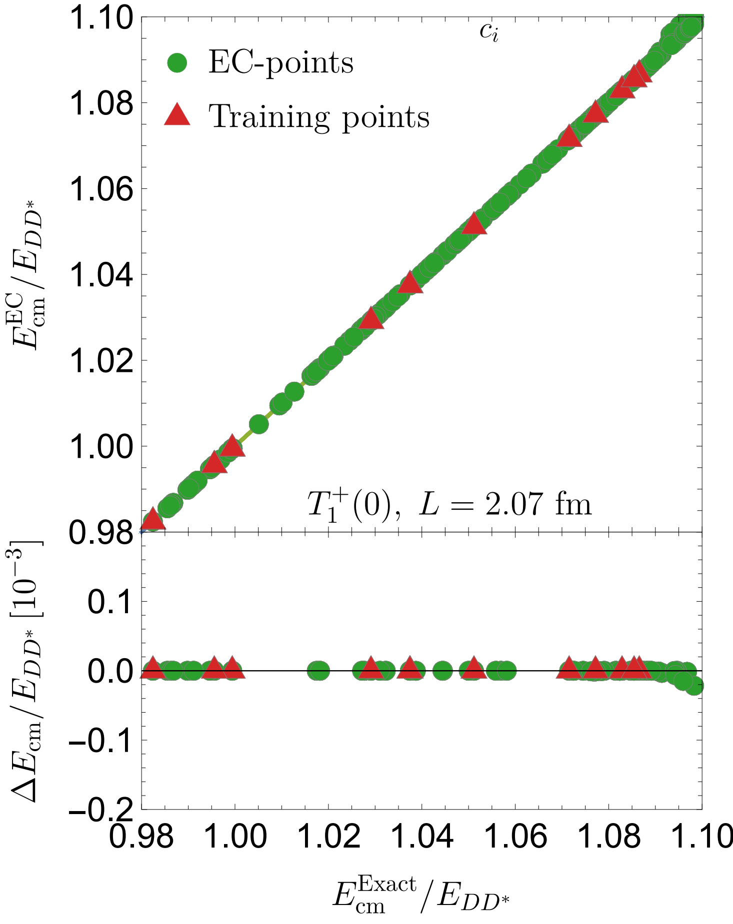
Frame:2017fah,Demol:2019yjt, Furnstahl:2020abp,Yapa:2022nnv



- 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 LEC in EFT (~ 1) makes the EC more reliable
- dim is linear function

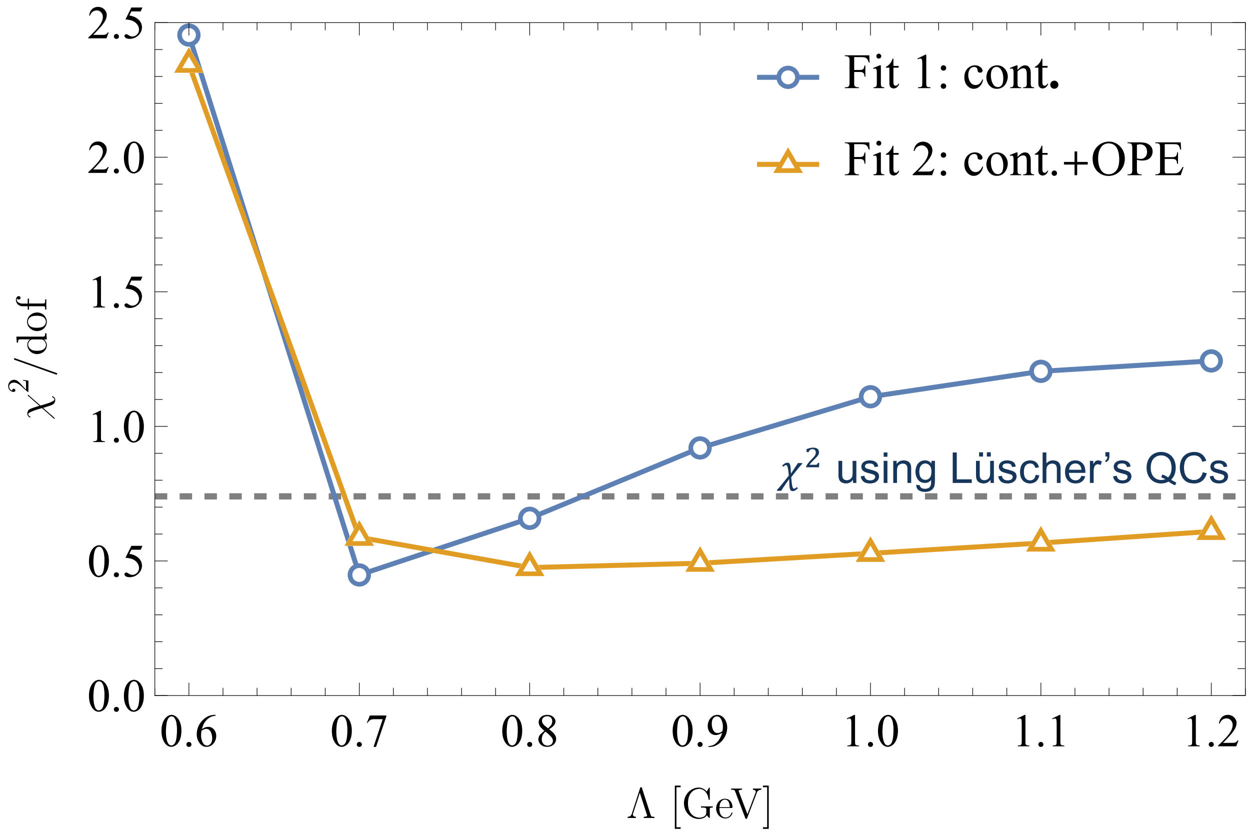
$$\dim^{EC} = \frac{p_{max}}{2\pi/L} \sim \mathcal{O}(10), \quad p_{max} \approx 0.6 \text{ GeV}$$

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



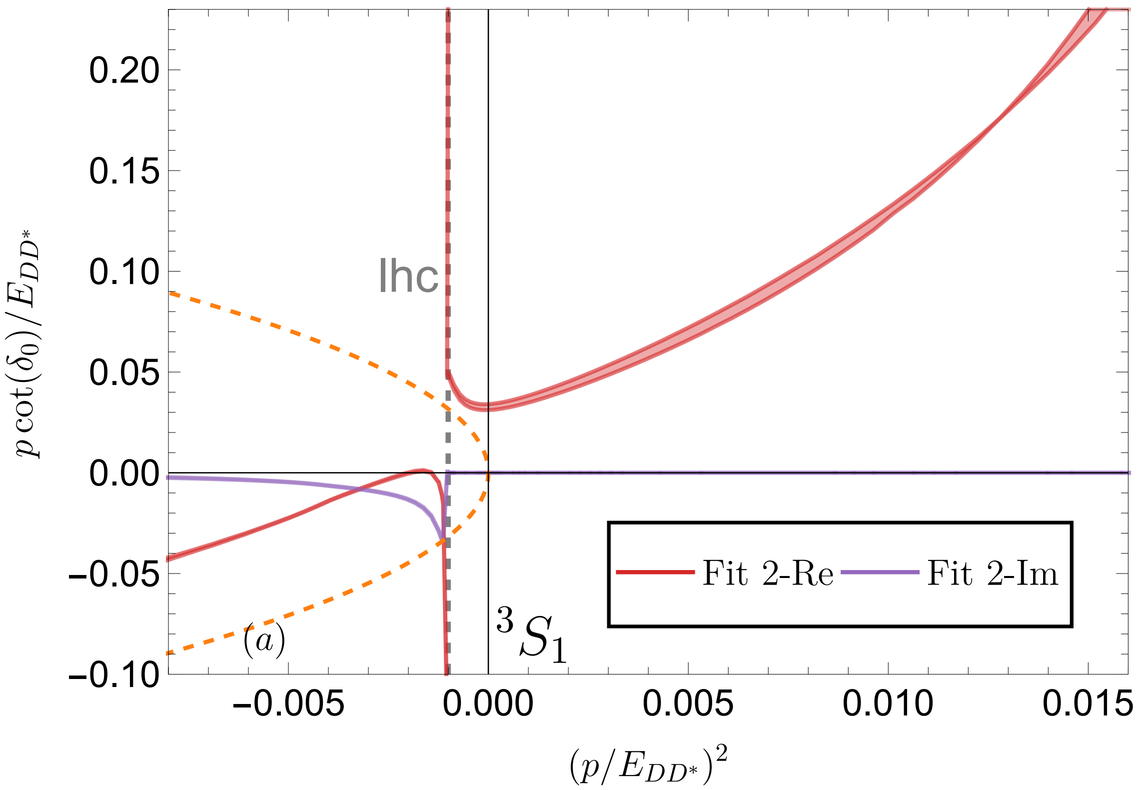
Cutoff dependence of χ^2

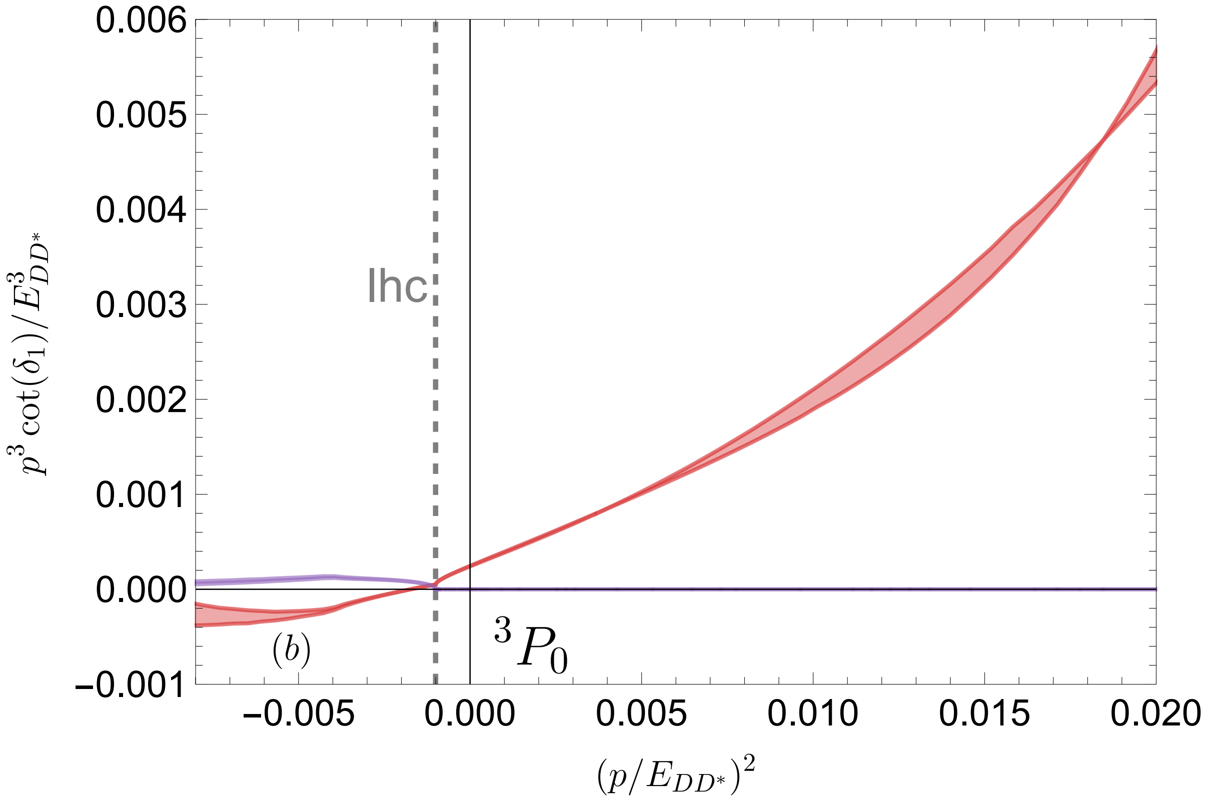
- 3 LECs: LO and NLO $^3S_1$ contact terms, NLO $^3P_0$
- In $V_{\rm ctc}$ fit, the P-wave dominate states control Λ-dependence of the χ^2
  - The shape of the of $k^3 \cot\delta_1$ is determined by regulator and cutoff
  - Sensitive to Λ
- The $V_{\rm ctc}$+ $V_{1\pi}$ fit is stable with Λ
- The $V_{\rm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



Cutoff dependence of phase shift

$\Lambda = 0.7 - 1.2$ GeV





Two approaches

- **Hansen's approach** Raposo:2023oru
  - ▶ FV: lattice data fix $\overline{\mathcal{K}}^{os}$

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

  - ▶ IFV: solve a integral equation

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

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

$$S_{\boldsymbol{k}^\star \ell m, \boldsymbol{k}'^\star \ell' m'}(P,L) = \frac{1}{2L^3}\,\frac{4\pi\, Y_{\ell m}(\hat{\boldsymbol{k}}^\star)\, Y^*_{\ell' m'}(\hat{\boldsymbol{k}}^\star)\, \delta_{\boldsymbol{k}^\star \boldsymbol{k}'^\star}\, |\boldsymbol{k}^\star|^{\ell+\ell'}\, e^{-\alpha[(\boldsymbol{k}^\star)^2 - (k^\star_{\rm os})^2]}}{4\omega_N(\boldsymbol{k})\left[(k^\star_{\rm os})^2 - (\boldsymbol{k}^\star)^2\right]},$$

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

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

$\xi = 1$

Model-independent?
You have to choose a parameterization of $\overline{\mathcal{K}}^{os}$: ERE
To some how, the ERE is equivalent to the contact EFT

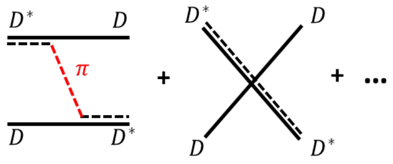
- **Our approach**
  - ▶ FV: lattice data fix contact terms

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

  - ▶ IFV: solve a integral equation

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

$V_{EFT} =$



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

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

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:: $\det\left[M^{(\Gamma,\boldsymbol{P})}_{ln,l'n'} - \delta_{ll'}\delta_{nn'}\cot\delta_l\right] = 0$
- Example $\Gamma = A_1^+$, w_{lm} depends on E but independent on V

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

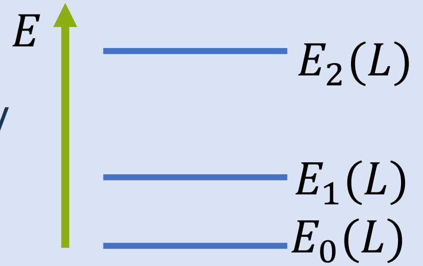
Bernard:2008ax

- 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. $\{E_1^{FV}, E_2^{FV}\} \nRightarrow \{\delta_S(E_1^{FV}), \delta_S(E_2^{FV}), \delta_D(E_1^{FV}), \delta_D(E_2^{FV}) \ldots\}$
  - ▶ 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,...

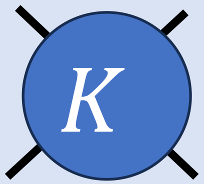
Requirements of a practical Lüscher method

FV energy spectrum



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

① e^{-mL} effect can be neglected
② Considering the PW mixing effect
③ E^{FV} well above lhc

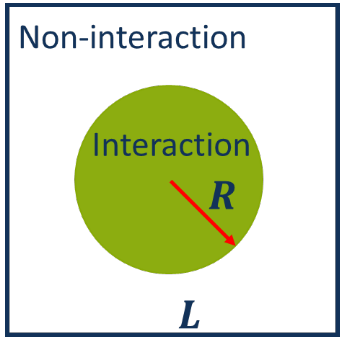


IFV K-matrix

④ERE works

Du:2023hlu

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



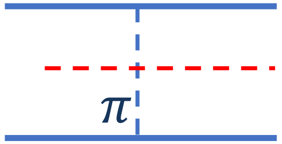
Requirement: $\frac{L}{2} \gg R$

Typically: $m_\pi L > 3$

High partial wave suppression

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

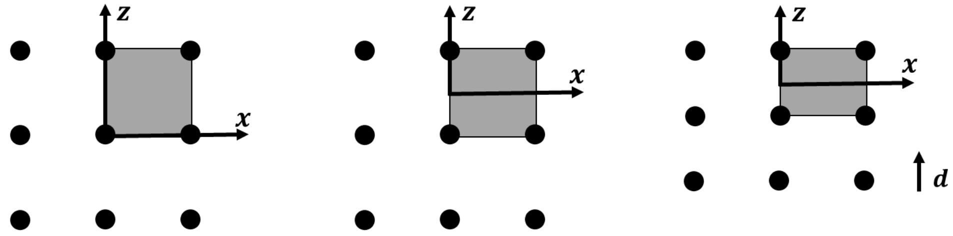
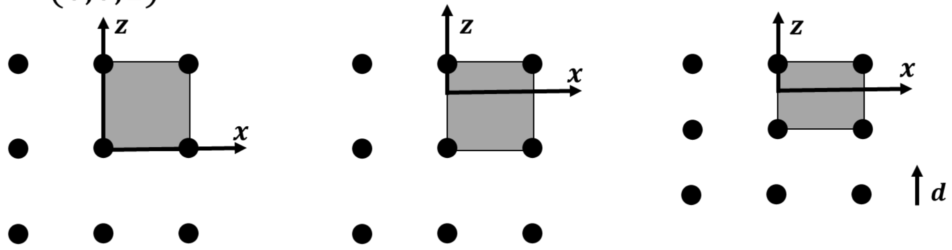
Taylor's textbook P197



Left-hand cut

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

Moving systems

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

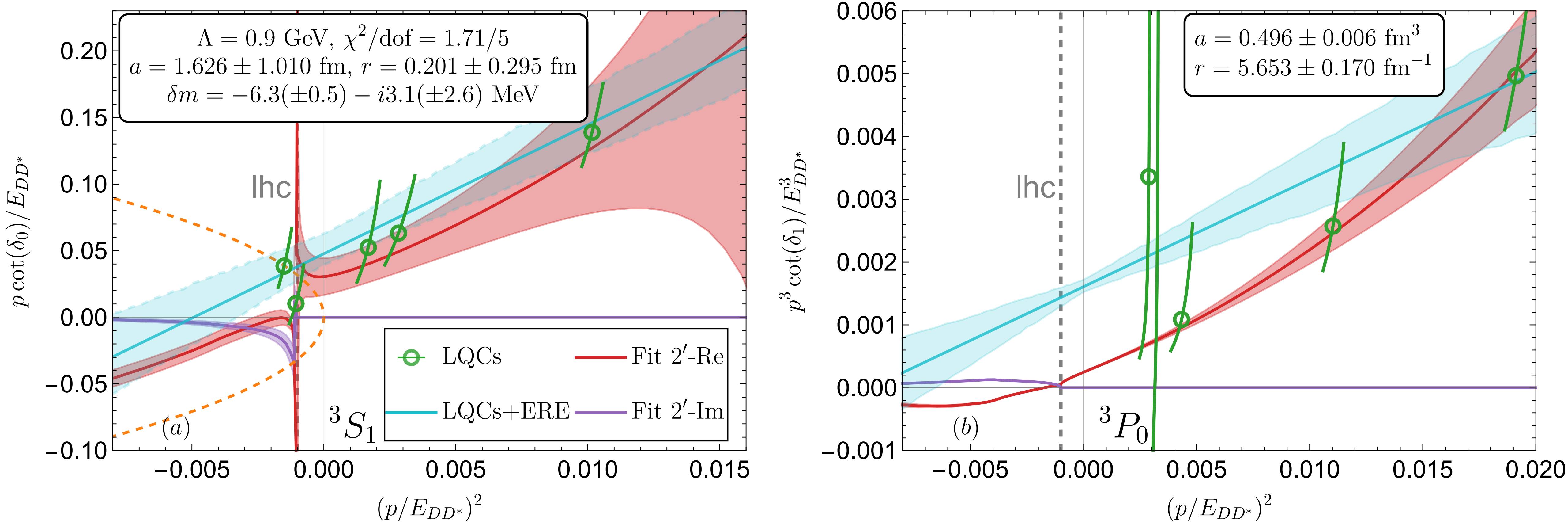
Space inversion invariance is broken

- 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

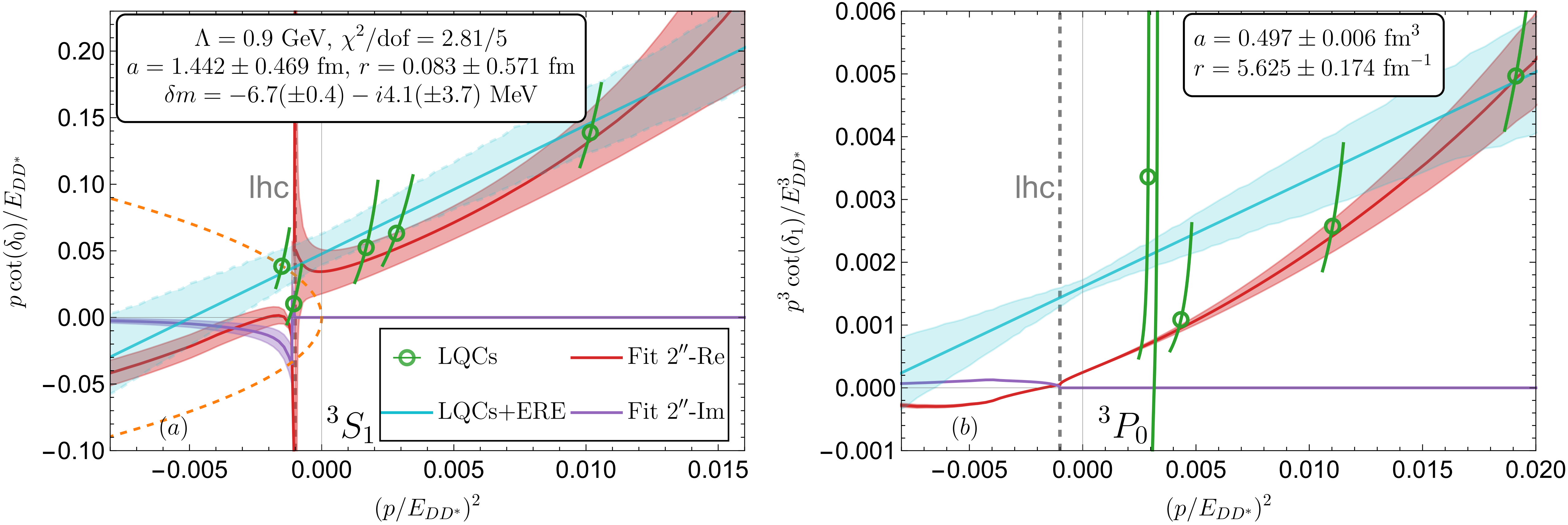
Rummukainen:1995vs,Leskovec:2012gb

- 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 $m_1 \neq m_2$
- $\boldsymbol{d} = (1,1,0)$, ...

Including SD transition terms



Including 3P2 term



Lüscher's formula

- Lippmann-Schwinger equation in the finite volume   Luscher:1990ux,Polejaeva:2012ut

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

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

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

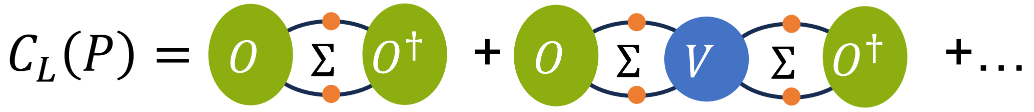
- The "=" relation is valid up to the exponentially suppressed terms in L
- K matrix in the infinite volume: $K = V + VG_K K$

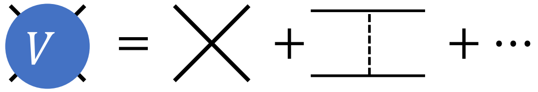
$$T^L = V + V(G_K + G_F)T^L = K + KG_F T^L$$

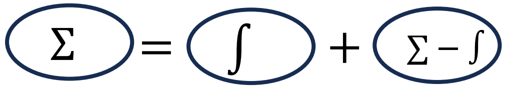
- E^{FV} corresponding to poles of T^L : interaction-independent form

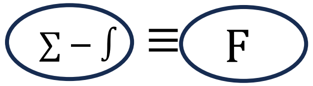
$$\det[1 - KG_F] = 0, \text{ or } \det[G_F - K^{-1}] = 0$$

Detailed derivation of Lüscher's formula





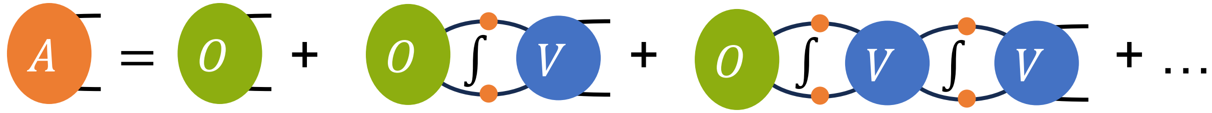




$$\left[\frac{1}{L^3}\sum_{\boldsymbol{k}} - \int \frac{d^3\boldsymbol{k}}{(2\pi)^3}\right] f(k) = \begin{cases} \mathcal{O}(e^{-mL}) & \text{smooth } f(k) \\ \text{power of } L & \text{otherwise} \end{cases}$$

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.

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

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

- 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}

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