北京大学 | 12.06.2024

Extracting hadron potentials from HALQCD wave functions

Lu Meng（孟璐） | **RUHR-UNIVERSITÄT** BOCHUM

Based on papers in preparation

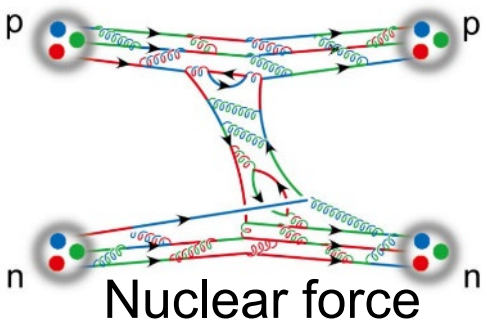
Together with Evgeny Epelbaum (RUB)

From QCD to nuclei and neutron stars

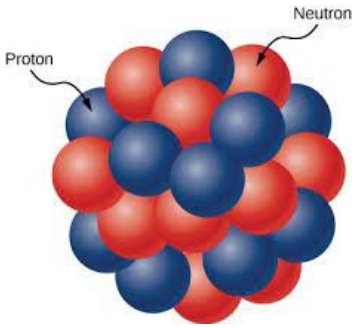
QCD: $\mathcal{L}_{QCD} = \sum_f \bar{q}_f (i\not{D} - \mathcal{M} q_f) - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu,a}$

Phenomenological model

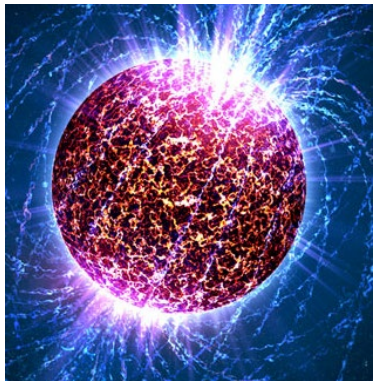
Chiral effective field theory



Nuclear force



nucleus



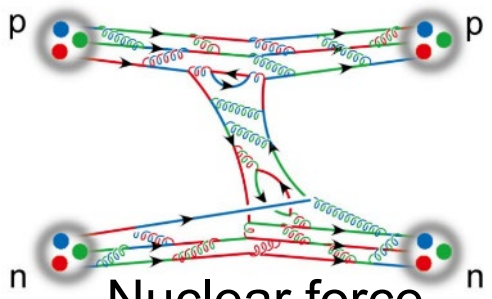
neutron star

From QCD to nuclei and neutron stars

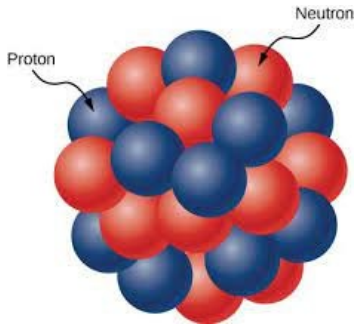
QCD: $\mathcal{L}_{QCD} = \sum_f \bar{q}_f (i\not{D} - \mathcal{M} q_f) - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu,a}$

Phenomenological model

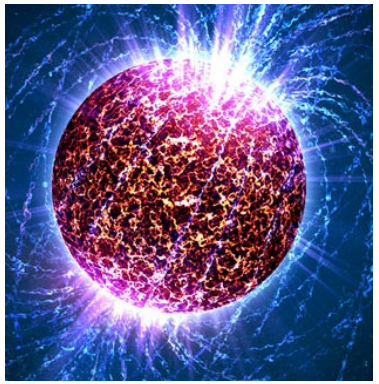
Chiral effective field theory



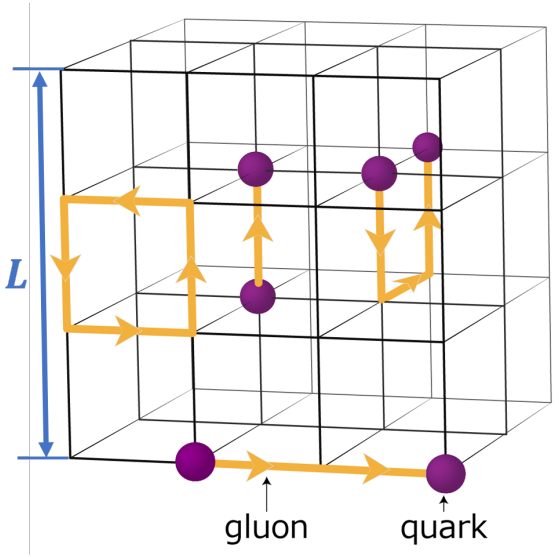
Nuclear force



nucleus



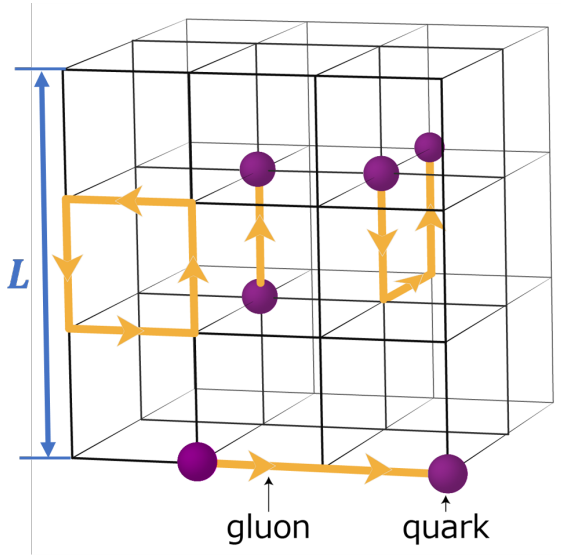
neutron star



Lattice QCD

Hadronic molecule

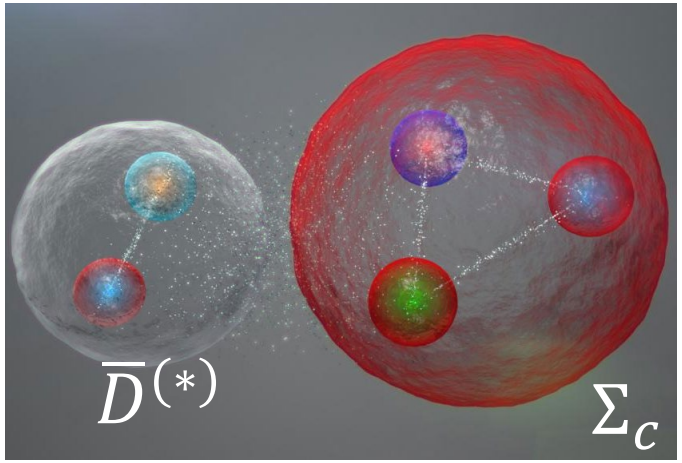
QCD: $\mathcal{L}_{QCD} = \sum_f \bar{q}_f (i\not{D} - \mathcal{M} q_f) - \frac{1}{4} G^a_{\mu\nu} G^{\mu\nu,a}$



Lattice QCD

Phenomenological model

Chiral effective field theory



hadronic molecule

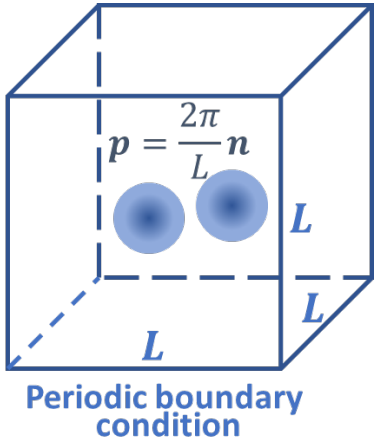
LHCb:2015yax

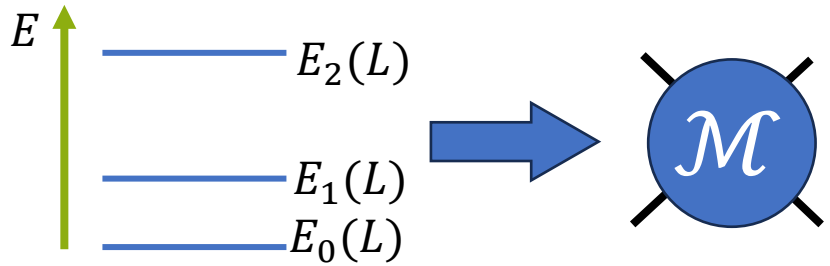
Energy level method

- Raw data: finite volume energy levels E^{FV}
- Get observables: Lüscher's formula
  - $E^{FV} \sim \delta(E^{FV})$

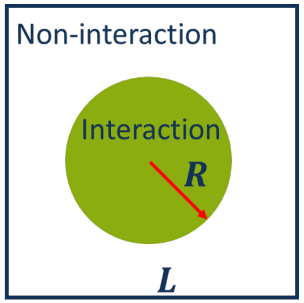
Luscher:1990ux

AKA: Lüscher method





- Requirement: larger box and short interaction $\frac{L}{2} \gg R$



- Derivation example of Lüscher's formula
  - The $(\nabla^2 + k^2)\psi(r) = 0$ for $r > R$
  - Asymptotic behavior: $\psi_k(r) \sim \frac{e^{i\delta(k)} \sin[kr + \delta(k)]}{kr}$
  - 1-D example

$$\psi(x) \sim \sin(kx + \delta(k))$$

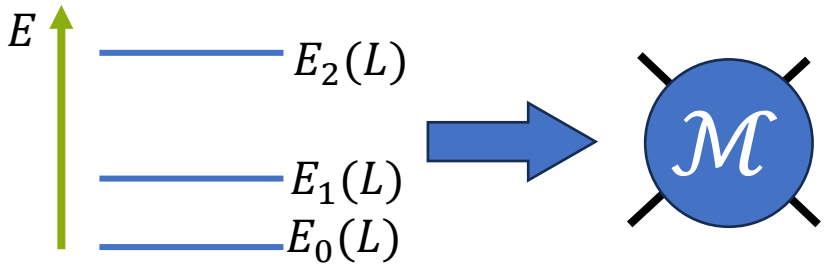
  - Quantization condition: $\sin\big(kL + \delta(k)\big) = 0 \Rightarrow kL + \delta(k) = n\pi$

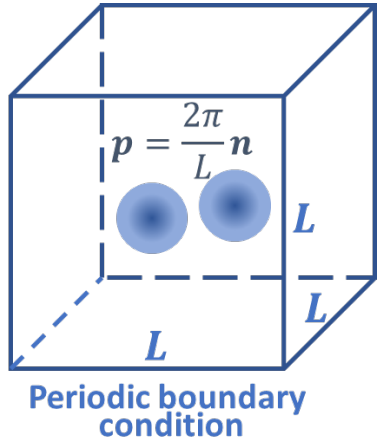
Energy level method

- Raw data: finite volume energy levels E^{FV}
- Get observables: Lüscher's formula
  - $E^{FV} \sim \delta(E^{FV})$

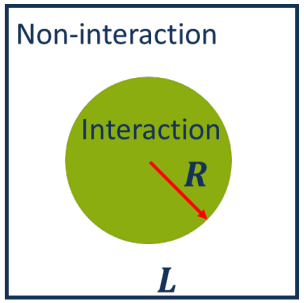
Luscher:1990ux

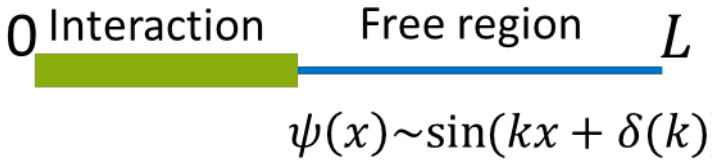
AKA: Lüscher method





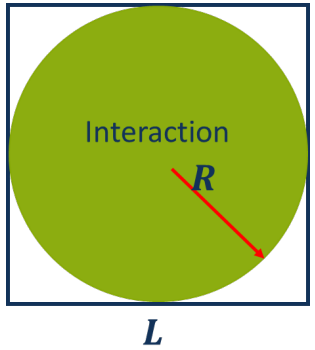
- Requirement: larger box and short interaction $\frac{L}{2} \gg R$
- Derivation example of Lüscher's formula
  - The $(\nabla^2 + k^2)\psi(r) = 0$ for $r > R$
  - Asymptotic behavior: $\psi_k(r) \sim \frac{e^{i\delta(k)} \sin[kr + \delta(k)]}{kr}$
  - 1-D example





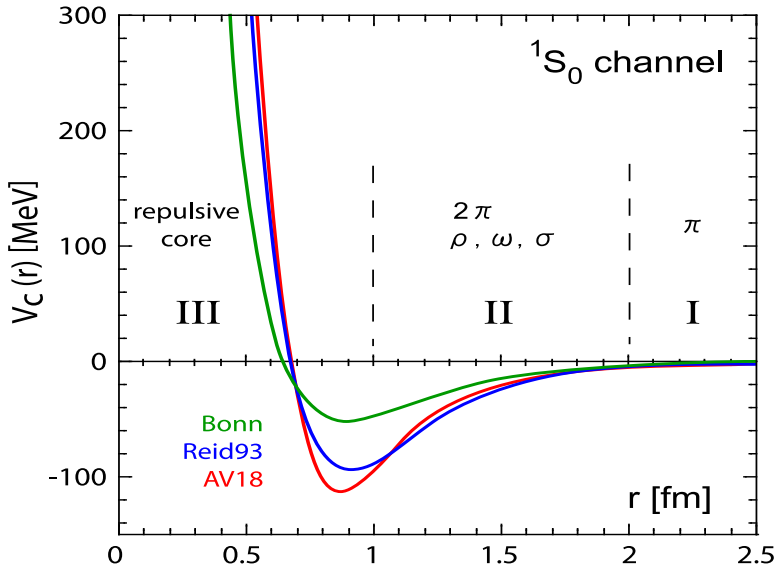
$$\psi(x) \sim \sin(kx + \delta(k))$$

  - Quantization condition: $\sin\big(kL + \delta(k)\big) = 0 \Rightarrow kL + \delta(k) = n\pi$

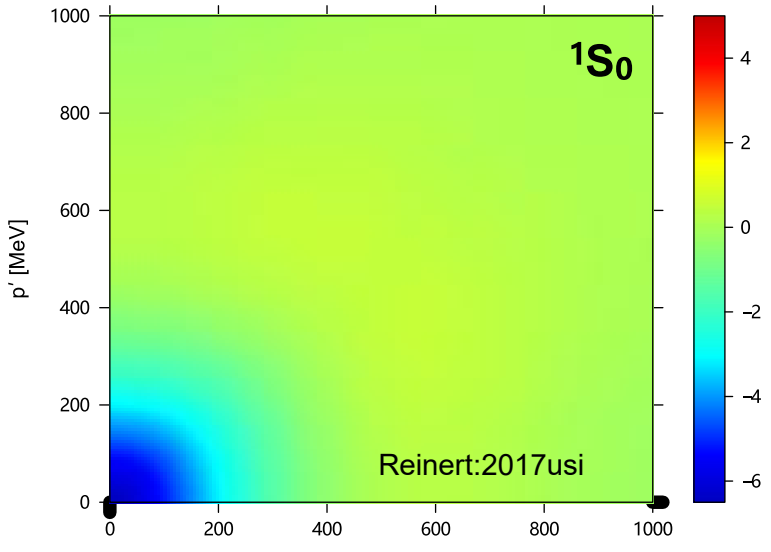


Long-range interaction and small box???
My talk in SDU

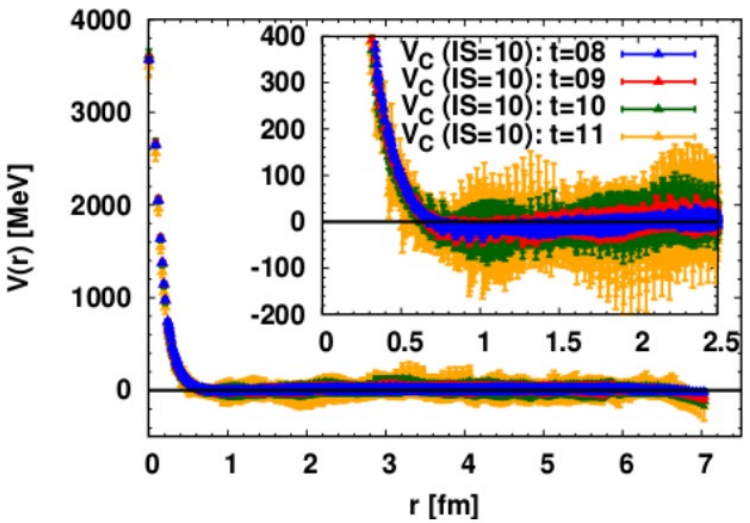
Potential methods



Phenomenological model



Chiral EFT



HALQCD

- Raw data: Nambu-Bethe-Salpeter wave function (NBS WFs) Ishii:2006ec,Aoki:2009ji,Aoki:2012tk
- Get observables

AKA: HALQCD (Hadrons to atomic nuclei from LQCD) method

NBS WFs → Potential → Observables

- ▶ Often criticized for **uncontrolled systematics**
- ▶ Potentials cannot determined by the observables (phase shifts etc)

To bind or not to bind

bind in both $^3S_1$ and $^1S_0$ channels

	With (deeply) bound NN			Without bound NN (or inconclusive)		
1	2006	NPLQCD	First dynamical calculations			
	2011	NPLQCD	$M_\pi \approx 390$ MeV			
	2012	Yamazaki et al.	$M_\pi \approx 510$ MeV	2012	HALQCD	$M_\pi \approx 710$ MeV
	2015	NPLQCD	$M_\pi \approx 800$ MeV	2012	HALQCD	$M_\pi \approx 469 - 1171$ MeV
	2015	Yamazaki et al.	$M_\pi \approx 310$ MeV			
2	2015	CalLat	$M_\pi \approx 800$ MeV+P,D,F waves			
	2015	NPLQCD	$M_\pi \approx 450$ MeV			
	2020	NPLQCD	$M_\pi \approx 450$ MeV			
				2019	"Mainz"	$M_\pi \approx 960$ MeV
3				2020	CoSMoN	$M_\pi \approx 714$ MeV
				2021	NPLQCD	$M_\pi \approx 800$ MeV

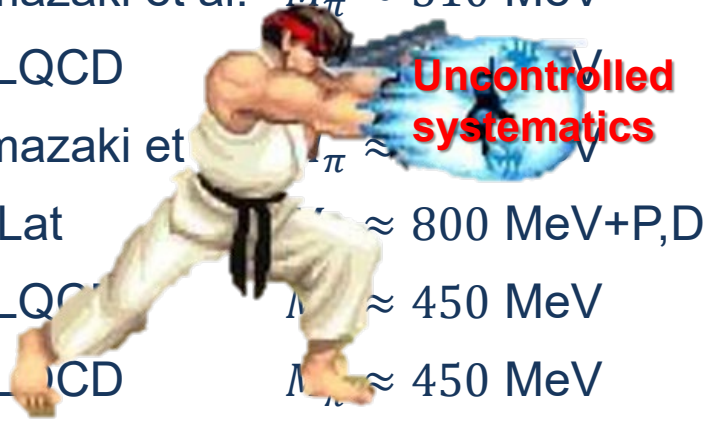
- However, we are observing a preponderance of evidence that the older methods with present statistics, are yielding qualitatively incorrect spectrum —
  I believe the old results are wrong (including those I was involved with)
  I believe the di-nucleon system unbinds at pion masses heavier than physical

Talk of A.Walker-Loud in lattice2023:https://indico.fnal.gov/event/57249/contributions/271301/

To bind or not to bind

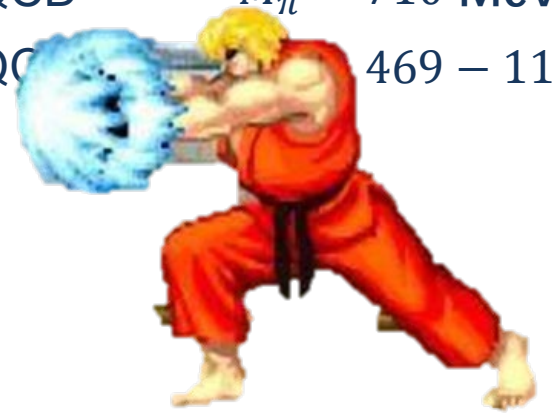
● With (deeply) bound NN

1	2006	NPLQCD	First dynamical calculations
	2011	NPLQCD	$M_\pi \approx 390$ MeV
	2012	Yamazaki et al.	$M_\pi \approx 510$ MeV
	2015	NPLQCD	V
	2015	Yamazaki et	$\pi \approx$ V
2	2015	CalLat	≈ 800 MeV+P,D,F waves
	2015	NPLQC	≈ 450 MeV
	2020	NPL CD	≈ 450 MeV
3			



● Without bound NN (or inconclusive)

2012	HALQCD	$M_\pi \approx 710$ **MeV**
2012	HALQC	$469 - 1171$ MeV
2019	"Mainz"	$M_\pi \approx 960$ MeV
2020	CoSMoN	$M_\pi \approx 714$ MeV
2021	NPLQCD	$M_\pi \approx 800$ MeV



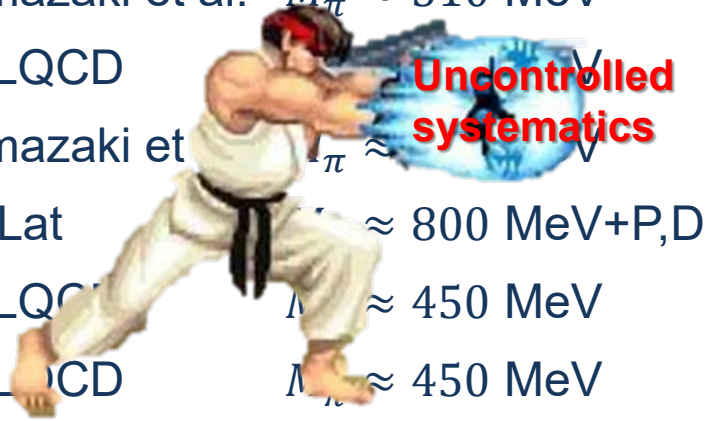
However, we are observing a preponderance of evidence that the older methods with present statistics, are yielding qualitatively incorrect spectrum —
I believe the old results are wrong (including those I was involved with)
I believe the di-nucleon system unbinds at pion masses heavier than physical

Talk of A.Walker-Loud in lattice2023:https://indico.fnal.gov/event/57249/contributions/271301/

To bind or not to bind

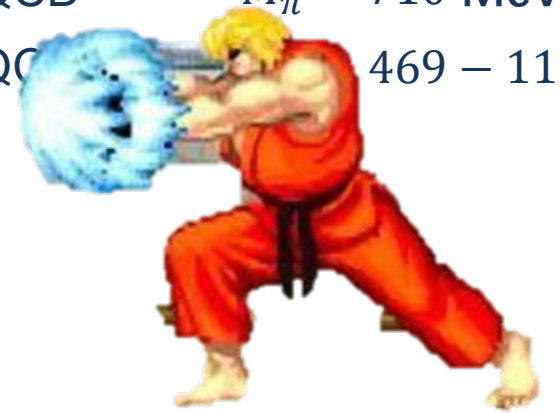
● With (deeply) bound NN

1	2006	NPLQCD	First dynamical calculations
	2011	NPLQCD	$M_\pi \approx 390$ MeV
	2012	Yamazaki et al.	$M_\pi \approx 510$ MeV
	2015	NPLQCD	$M_\pi \approx$ [illegible] MeV
	2015	Yamazaki et [illegible]	$M_\pi \approx$ [illegible] MeV
2	2015	CalLat	$M_\pi \approx 800$ MeV+P,D,F waves
	2015	NPLQC[illegible]	$M_\pi \approx 450$ MeV
	2020	NPL[illegible]CD	$M_\pi \approx 450$ MeV
3			



● Without bound NN (or inconclusive)

2012	HALQCD	$M_\pi \approx 710$ **MeV**
2012	HALQC[illegible]	$M_\pi \approx 469 - 1171$ MeV
2019	"Mainz"	$M_\pi \approx 960$ MeV
2020	CoSMoN	$M_\pi \approx 714$ MeV
2021	NPLQCD	$M_\pi \approx 800$ MeV



Significance of the HALQCD method
To improve the understanding of the systematics of HALQCD

Talk of A.Walker-Loud in lattice2023:https://indico.fnal.gov/event/57249/contributions/271301/

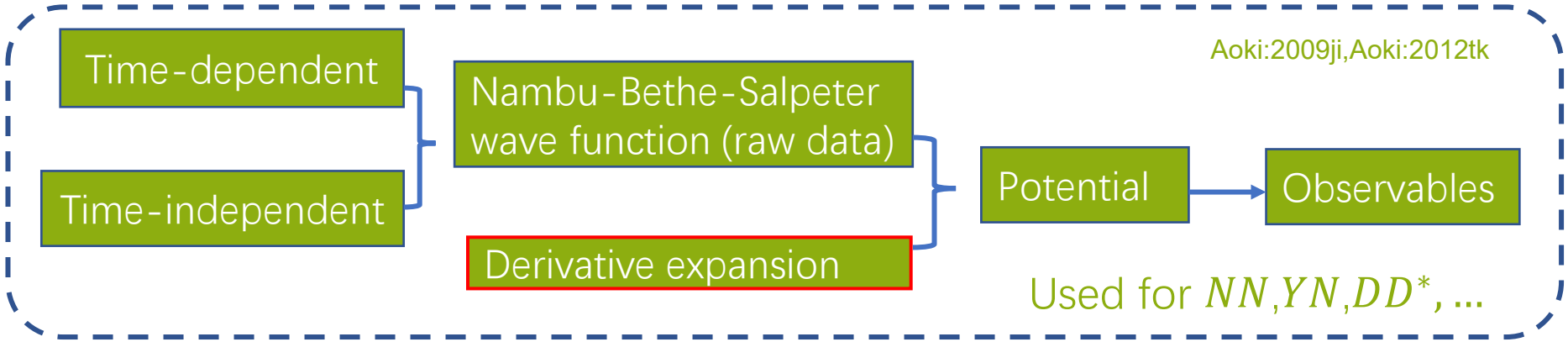
HALQCD method

Disclaimers:

- I am not the member of the HALQCD group
- I will try my best to be fair

Aoki:2009ji,Aoki:2012tk

HALQCD method



- The raw data of HAL QCD simulations are Nambu-Bethe-Salpeter (NBS) wave functions
- The derivative expansion (DE) method is often questioned by some people
  - ▶ Converge fast for NN
  - ▶ Converge slowly for $\pi\pi$
- In this talk, I will first illustrate some concepts and then provide an alternative way of DE method

Ishii:2006ec

Time-independent HAL QCD

- The equal-time BS amplitude (BS wave function, BSWF) CP-PACS:2005gzm

$$\psi(\vec{x};\vec{k}) = \langle 0|\pi_1(\vec{x}/2)\pi_2(-\vec{x}/2)|\pi_1(\vec{k}),\pi_2(-\vec{k});in\rangle$$

- Asymptotic behavior of BS wave function

$$\psi(\vec{x};\vec{k}) = e^{i\vec{k}\cdot\vec{x}} + \int \frac{d^3p}{(2\pi)^3}\frac{T(p;k)}{p^2-k^2-i\epsilon}e^{i\vec{p}\cdot\vec{x}}$$

  - $T(p;k)$ is the half-on-shell T-matrix
  - $\psi(\vec{x};\vec{k})$ satisfy the Lippmann-Schwinger eq. as the non-relativistic scattering wave function
  - Using Nishijima, Zimmermann and Haag (NZH) reduction formula for composite local operators
  - No non-relativistic approximation, just a formal resemblance

- The BSWF at different energies $\{k_i\}$ in the lattice are the raw data of t-independent HAL QCD

- The general problem: $\psi_{k_i}(\vec{x}) \Rightarrow V$ from Schrodinger-like equations

Time-independent HAL QCD

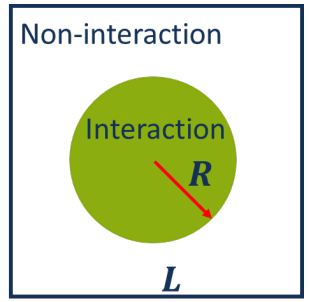
- The general problem (set $m = 1$, 1D case as an example)

$$\int dr' V(r,r')\psi_{k_i}(r') = (\frac{d^2}{dr^2} + k_i^2)\psi_{k_i}(r) \Rightarrow \int dr' V(r,r')R^{(i)}(r) = K^{(i)}(r)$$

  - ▶ Determined the potential $V(r,r')$ once $\{\Psi_{k_i}(r)\}$ are given
  - ▶ $R^{(i)}(r)$ and $K^{(i)}(r)$ are known
  - ▶ **Note: the # of wave functions is small, 2 or 3**
- In general, the potential is **nonlocal.** No reason to reject the nonlocal potentials
  - ▶ Definition of Local potential: $V(r,r') = V(r)\delta(r-r')$
- Regions of potential
  - ▶ Inner region (interacting region): $V(r,r') \neq 0 \ \ (r,r' < R)$
  - ▶ outer region (asymptotic region): $V(r,r') = 0 \ \ (r,r' > R)$
  - ▶ The raw data is $\psi_{k_i}(\vec{x})$ in the **interacting region +** outer region
  - ▶ In principle, one can get the $\delta(k_i)$ from $\psi_{k_i}(\vec{x})$

Asymptotic properties

  - ▶ The Lüscher's method only concerns on the asymptotic region
  - ▶ Could we get **more information than $\delta(k_i)$** from the $\psi_{k_i}(\vec{x})$?



Time-dependent HAL QCD

- ψ_{k_i} with fixed energies are projected from the correlation function after ground state saturation

$$R(r,t) = \sum_n a_n \psi_{k_n}(r) e^{-(2\sqrt{m_N^2+k_n^2}-2m_N)t}$$

Ishii:2012ssm

- For large box, it is expensive to get the ground state saturation
- Time-dependent Schrödinger-type equation

$$\left(-\frac{\partial}{\partial t} + \frac{1}{4m_N}\frac{\partial^2}{\partial t^2}\right) R(r,t) = \left(\hat{H}_0 + \hat{V}\right) R(r,t)$$

- Time-dependent strategy without ground state saturation makes simulations with large box and small pion mass available
  - ▶ $m_\pi = 146$ MeV, $a \simeq 0.0846$ fm, $L^4 = 96^4$, $L = 8.1$ fm

Doi:2017zov, Lyu:2022imf,Lyu:2023xro…

- The general problem

$$\int dr' V(r,r') R(r',t) = K(r,t) \qquad K(r,t) = \left(-\frac{\partial}{\partial t} + \frac{1}{4m_N}\frac{\partial^2}{\partial t^2} - \frac{1}{m_N}\frac{d^2}{dr^2}\right) R(r',t)$$

- **Note: the # of wave functions is small, 2 or 3**

Modern views of potential

Local potential VS nonlocal potential

- There is no reason to rule out the nonlocal potential either in principle or phenomenologically Bogner:2009bt
- Potential is not observable
  - ▶ Cannot be determined uniquely by scattering experiments
  - ▶ Observable-equivalent potentials are related by unitary trans. (UT) or field redefinition

$$H|\psi\rangle = E|\psi\rangle \Rightarrow UHU^{\dagger}U|\psi\rangle = EU|\psi\rangle \Rightarrow \tilde{H}|\tilde{\psi}\rangle = EU|\tilde{\psi}\rangle$$

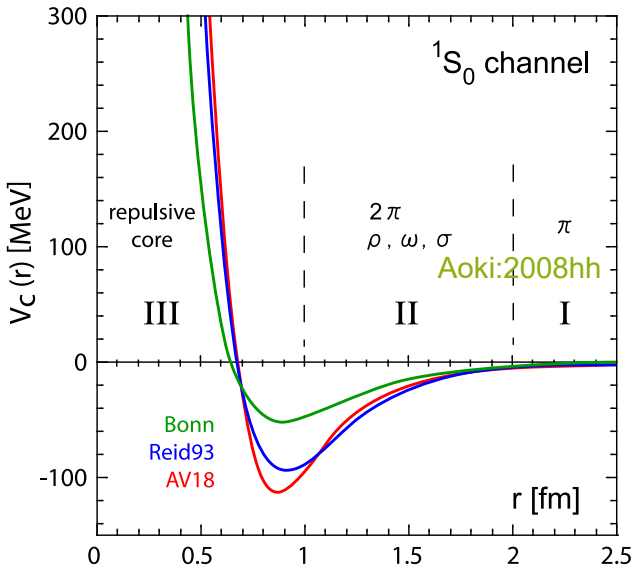
  - ▶ UT can relate local potentials to nonlocal potentials Ekstein:1960xkd
- Inverse scattering problem: given phase shifts, find the potential
  - ▶ To make the potential unique: local potential is assumed (no physical reason)
- Local potentials are an advantage or even a necessity for some methods of solving the nuclear many-body problem.
- There are still methods for nonlocal potentials: no-core shell model
- Sometimes, the nonlocal potential are advantage for
  - ▶ Separable interaction: $V = v_{ij}|i\rangle\langle j|$, or $V(r,r') = v_{ij}\varphi_i(r)\varphi_j(r')$ for the three body problem (Fadeev function)

Phase-equivalent potentials

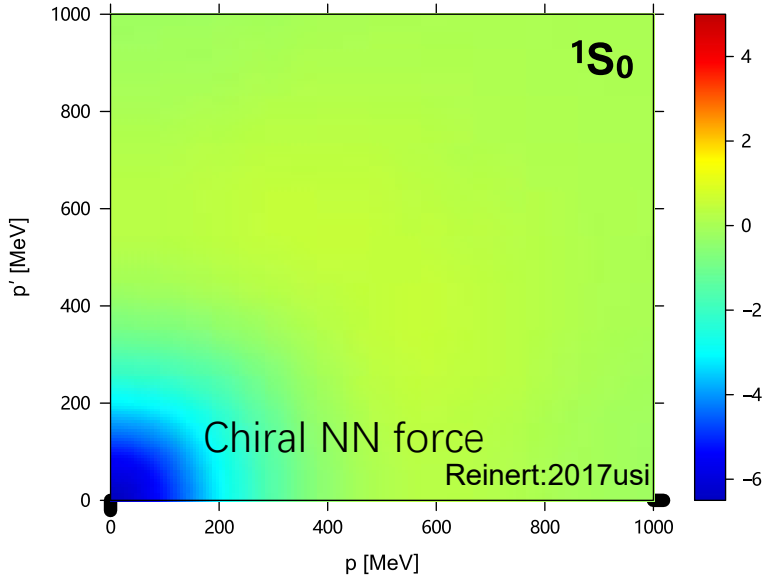
- Different nuclear forces are phase-equivalent potentials
- Similarity renormalization group (SRG) are used to soften the short-range interaction and increase the convergence of the many-body problems
  - ▶ $H_s = U(s)HU^{\dagger}(s)$, choose a specific $U(s)$ gives the flow equation

Bogner:2009bt

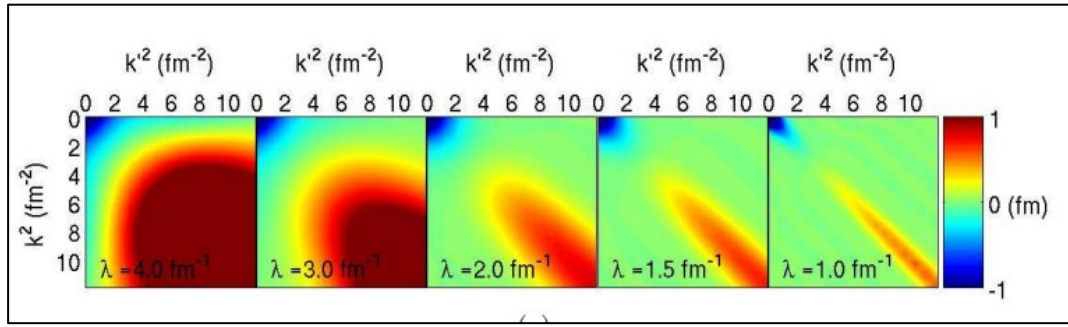
$$\frac{dH_s}{ds} = [[T_{rel}, H_s], H_s]$$



Local NN force



Nonlocal NN force

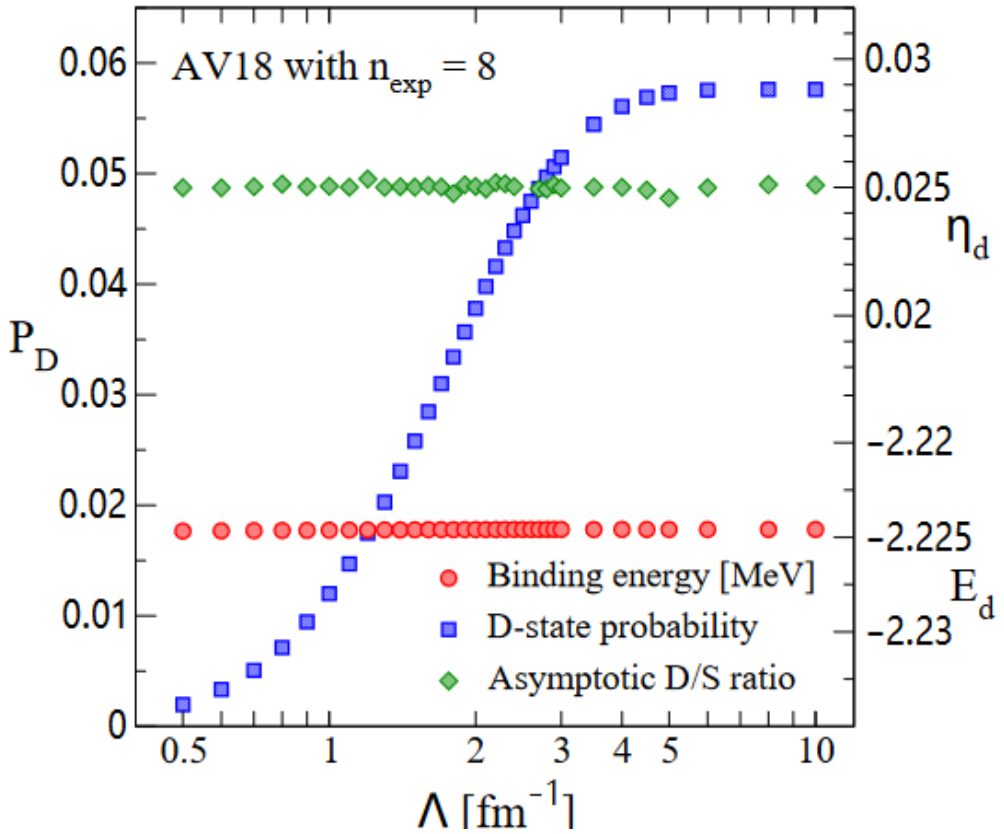


SRG evolution

Modern views of potential

- Non-observables
  - ▶ Non-asymptotic behavior of ψ, e.g. the deuteron D-state probability
  - ▶ Off-shell T-matrix
  - ▶ Potential
- Observables
  - ▶ Asymptotic behavior of ψ
  - ▶ Phase shift
  - ▶ On-shell T-matrix

Amghar:1995av



Interpolating operator VS potential

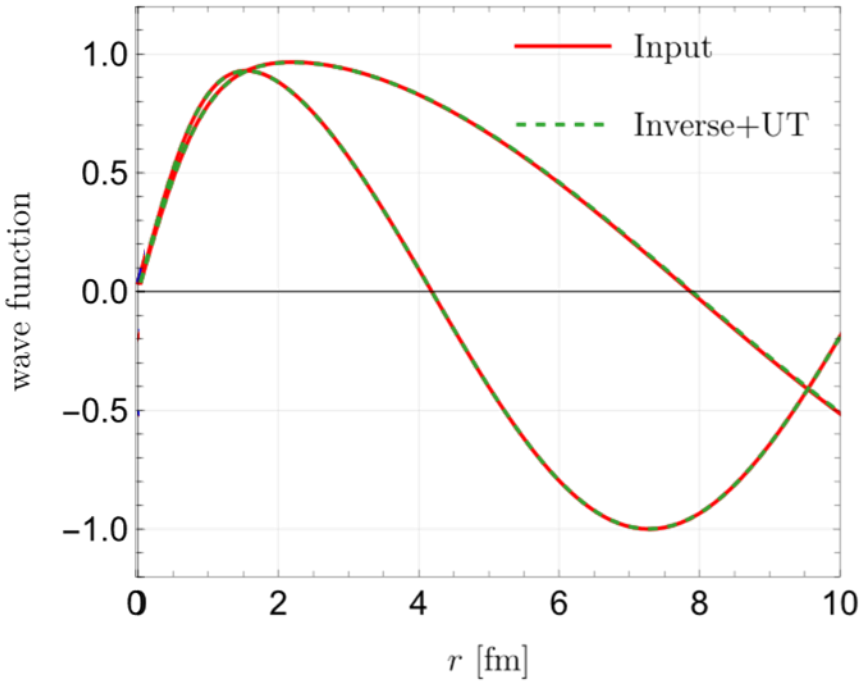
- In principle one may choose any composite operators with the same quantum numbers as the hadron to define the BS wave function
- Different operators give different BS wave functions and different hadron potentials
  - ▶ They are related by UT
  - ▶ We anticipate they lead to the same observables such as the δ and E_b
- **In the HAL QCD simulations: once the setting of interpolating operators (its smearing) are fixed, the "underlying" potential is fixed in principle**
- The "underlying" potential cannot be extracted from only a small number of the wave functions

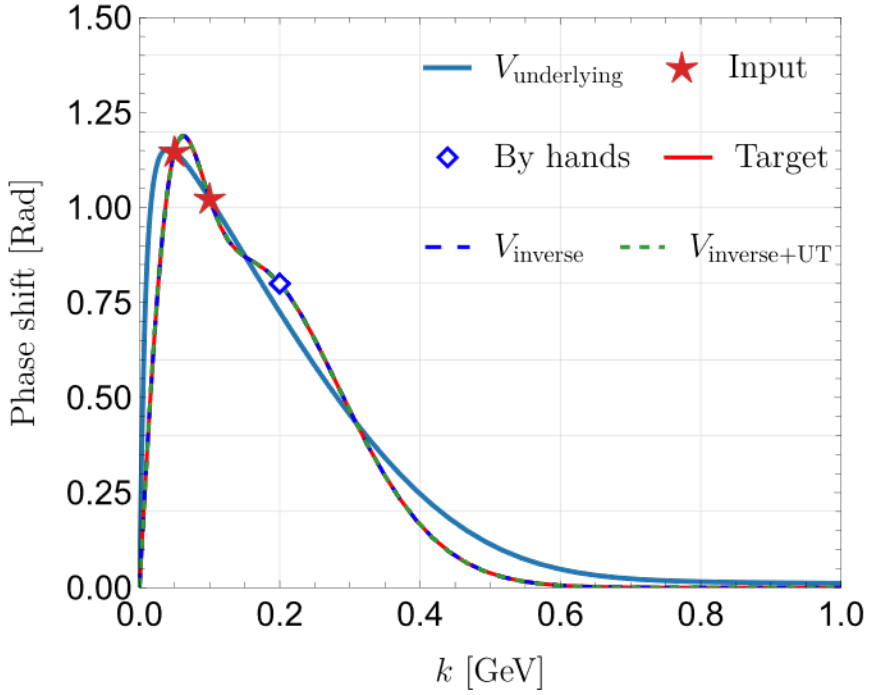
Interpolating operator VS potential

- From a small number of the wave functions, the potential can not be determined uniquely
  - ▶ Think it in a discrete way

$$\int dr' V(r,r') R^{(i)}(r) = K^{(i)}(r) \Rightarrow \mathbb{V}_{N\times N} R^{(i)}_{N\times 1} = K^{(i)}_{N\times 1}$$

  - ▶ One need N wave functions to fix potential matrix $\mathbb{V}_{N\times N}$
  - ▶ N: several tens, typical order of # quadrature points
  - ▶ In practices, only 2 or 3 wave functions are accessible



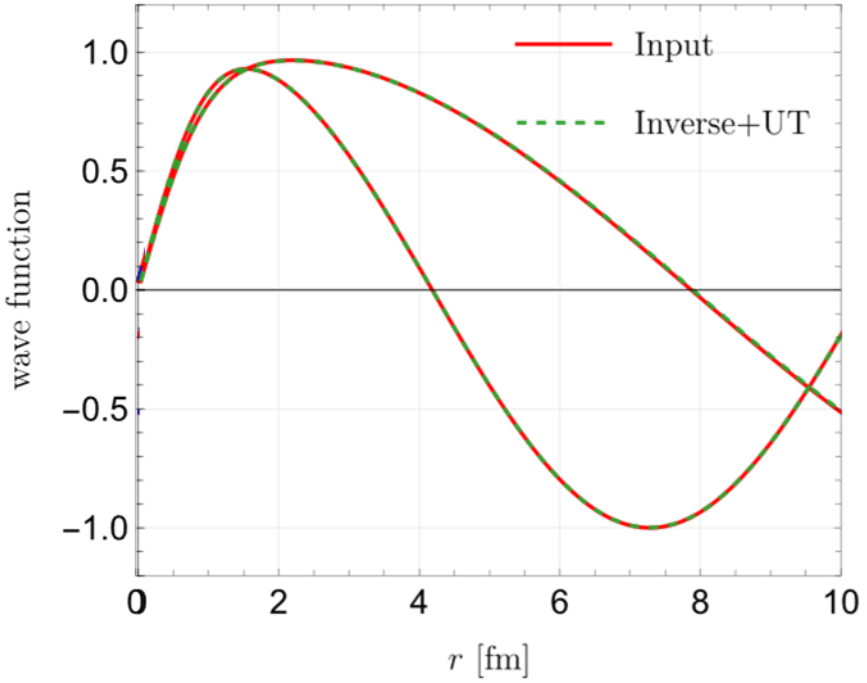


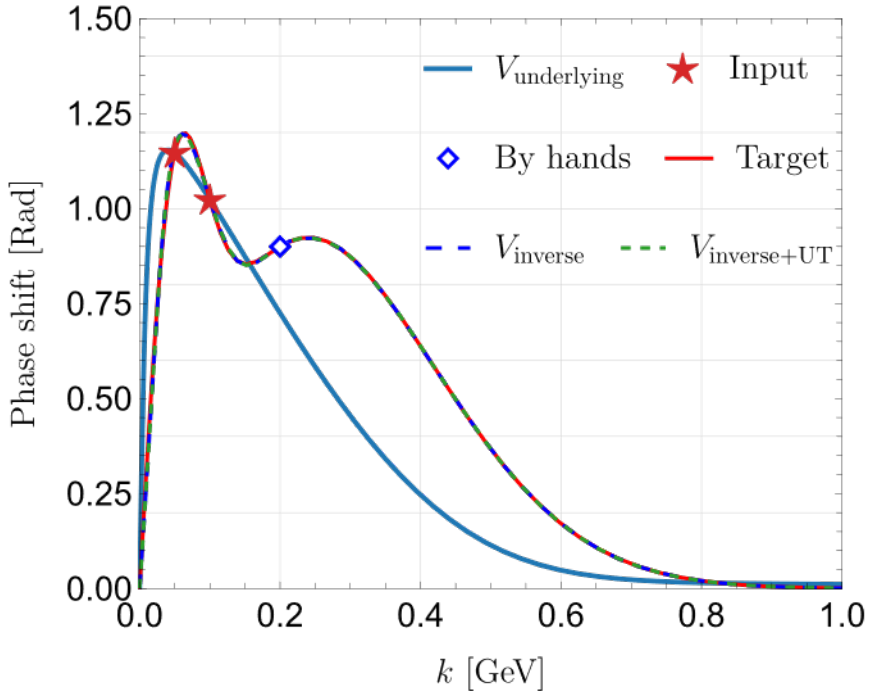
Interpolating operator VS potential

- From a small number of the wave functions, the potential can not be determined uniquely
  - ▶ Think it in a discrete way

$$\int dr' V(r,r') R^{(i)}(r) = K^{(i)}(r) \Rightarrow \mathbb{V}_{N\times N} R^{(i)}_{N\times 1} = K^{(i)}_{N\times 1}$$

  - ▶ One need N wave functions to fix potential matrix $\mathbb{V}_{N\times N}$
  - ▶ N: several tens, typical order of # quadrature points
  - ▶ In practices, only 2 or 3 wave functions are accessible



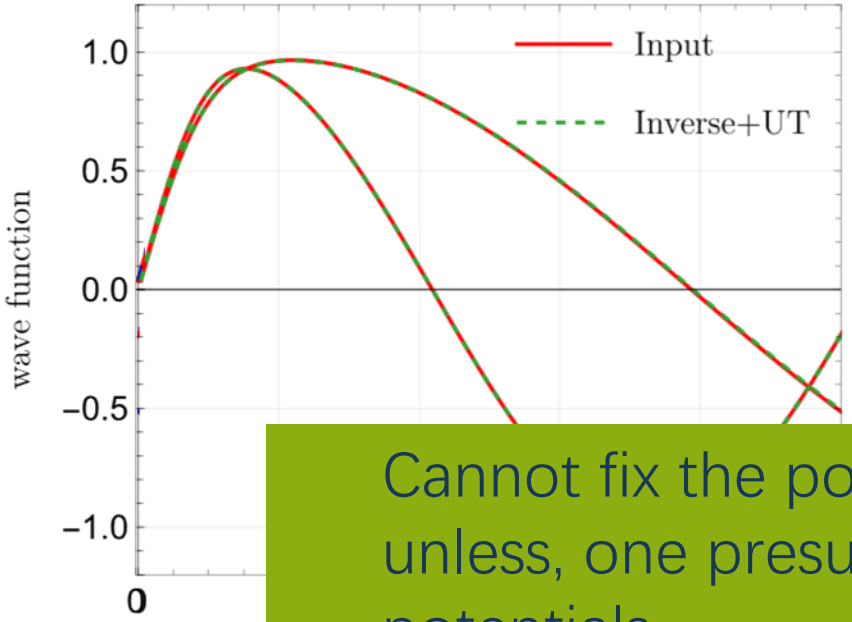


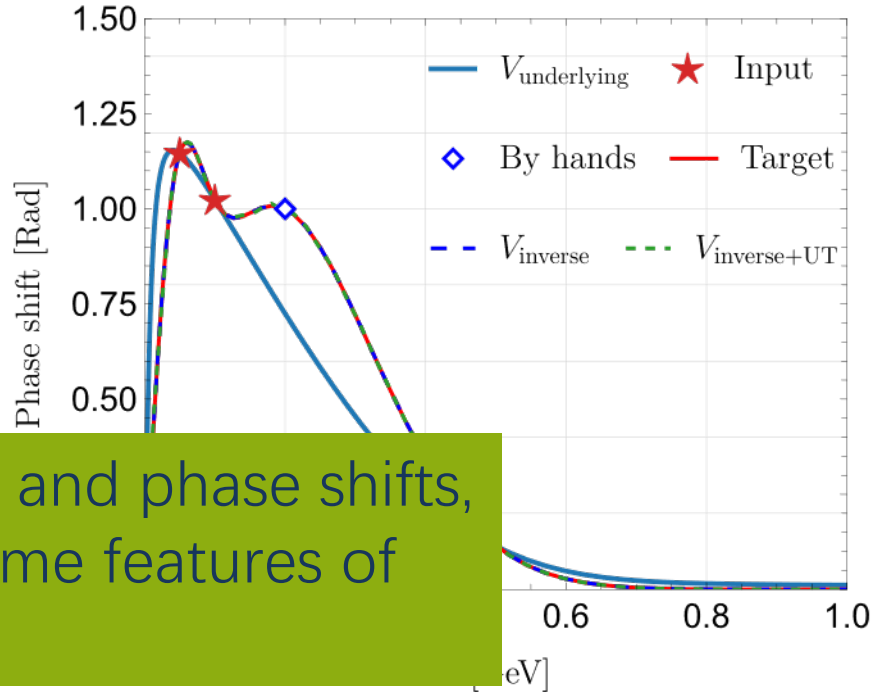
Interpolating operator VS potential

- From a small number of the wave functions, the potential can not be determined uniquely
  - ▶ Think it in a discrete way

$$\int dr' V(r,r') R^{(i)}(r) = K^{(i)}(r) \Rightarrow \mathbb{V}_{N\times N} R^{(i)}_{N\times 1} = K^{(i)}_{N\times 1}$$

  - ▶ One need N wave functions to fix potential matrix $\mathbb{V}_{N\times N}$
  - ▶ N: several tens, typical order of # quadrature points
  - ▶ In practices, only 2 or 3 wave functions are accessible





Cannot fix the potentials and phase shifts, unless, one presumes some features of potentials

Derivative expansion VS EST expansion

Derivative expansion

- Derivative expansion

Aoki:2021ahj

$$V(r,r') = V_0(r)\delta(r-r') + V_1(r)\delta(r-r')\frac{d^2}{dr'^2} + V_2(r)\delta(r-r')\frac{d^4}{dr'^4} + \ldots$$

- LO

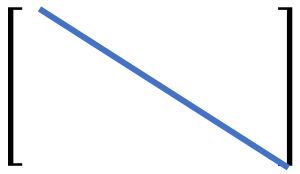
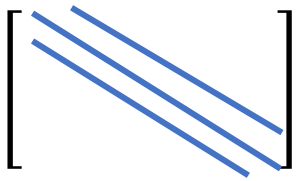
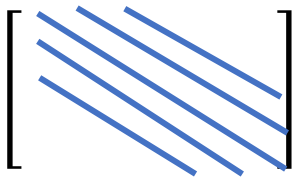
$$V_0(r)R^{(1)}(\vec{r}) = K^{(1)}(\vec{r}) \Rightarrow V_0(r) = \frac{K^{(1)}(\vec{r})}{R^{(1)}(\vec{r})}$$

- NLO

$$\begin{pmatrix} R^{(1)}(r) & \frac{d^2}{dr^2}R^{(1)}(r) \\ R^{(2)}(r) & \frac{d^2}{dr^2}R^{(2)}(r) \end{pmatrix} \begin{pmatrix} V_0(r) \\ V_1(r) \end{pmatrix} = \begin{pmatrix} K^{(1)}(r) \\ K^{(1)}(r) \end{pmatrix}$$

- It is not expansion about some definite small quantities
- Its convergence is tested self-consistently
- Think it in a discrete way,

$$\frac{d^2}{dr^2}\psi(x_n) \approx \frac{\psi(x_{n-1})+\psi(x_{n+1})-2\psi(x_n)}{h^2}$$

$V_0 =$  $, V_1 =$  $, V_2 =$  $, \ldots$

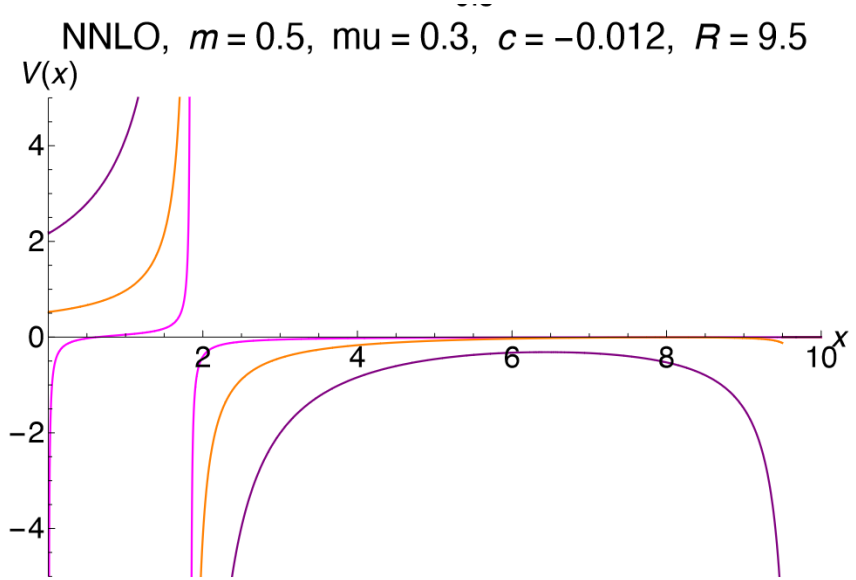
  - ▶ The band width become wider

Singular potential

- NLO derivative expansion

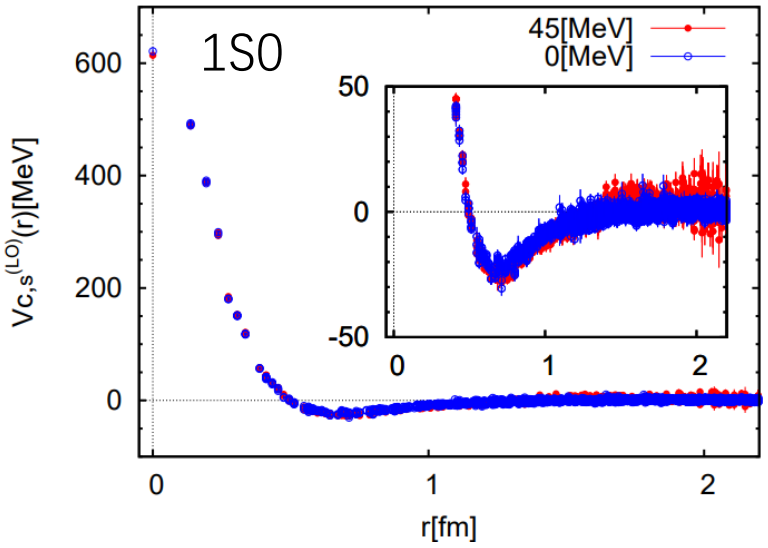
$$\begin{pmatrix} R^{(1)}(r) & \frac{d^2}{dr^2}R^{(1)}(r) \\ R^{(2)}(r) & \frac{d^2}{dr^2}R^{(2)}(r) \end{pmatrix} \begin{pmatrix} V_0(r) \\ V_1(r) \end{pmatrix} = \begin{pmatrix} K^{(1)}(r) \\ K^{(1)}(r) \end{pmatrix}$$

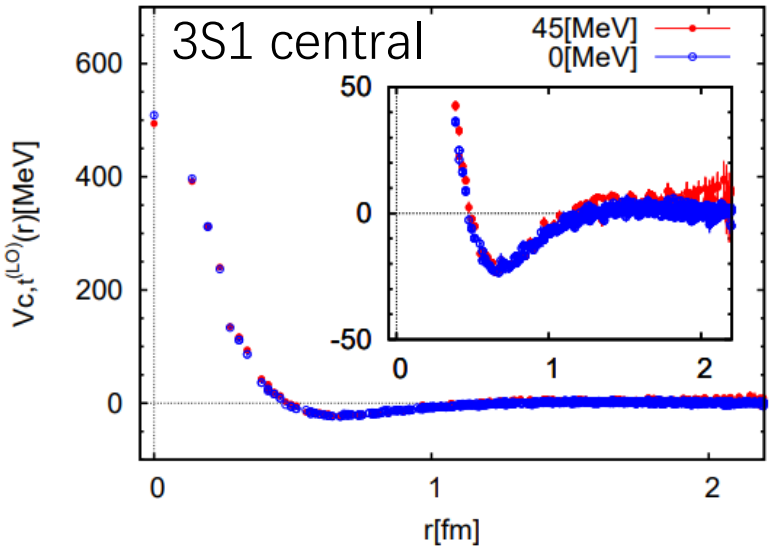
- The potential become singular at the zero of det of the coefficients matrix
- A example from toy model Aoki:2021ahj
  - ▶ In simulation, it is challenging to handle the singularity
  - ▶ Wave functions are obtained at discrete point.

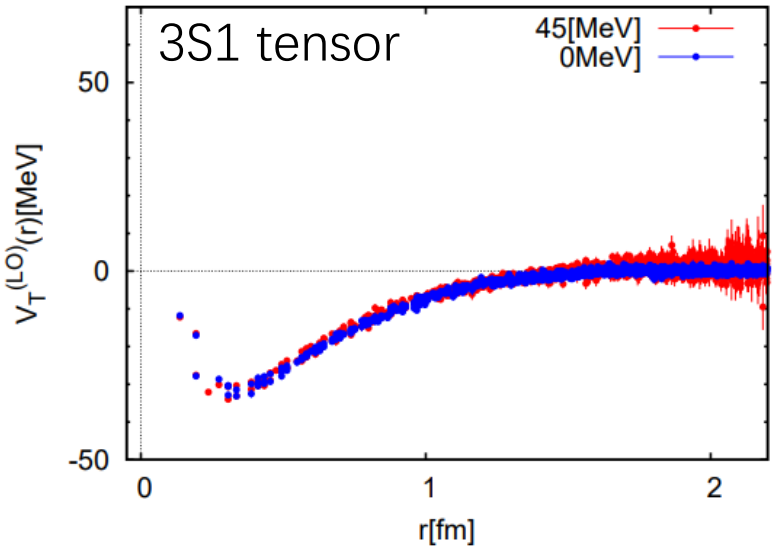


Locality of the potential

- Self-consistence test: LO NN potentials obtained at different energies (E ≃ 0 MeV and 45 MeV)
  - ▶ LO approximation of DE validates to E = 45 MeV. Murano:2011nz
  - ▶ Other test: optimized operators method Lyu:2022tsd







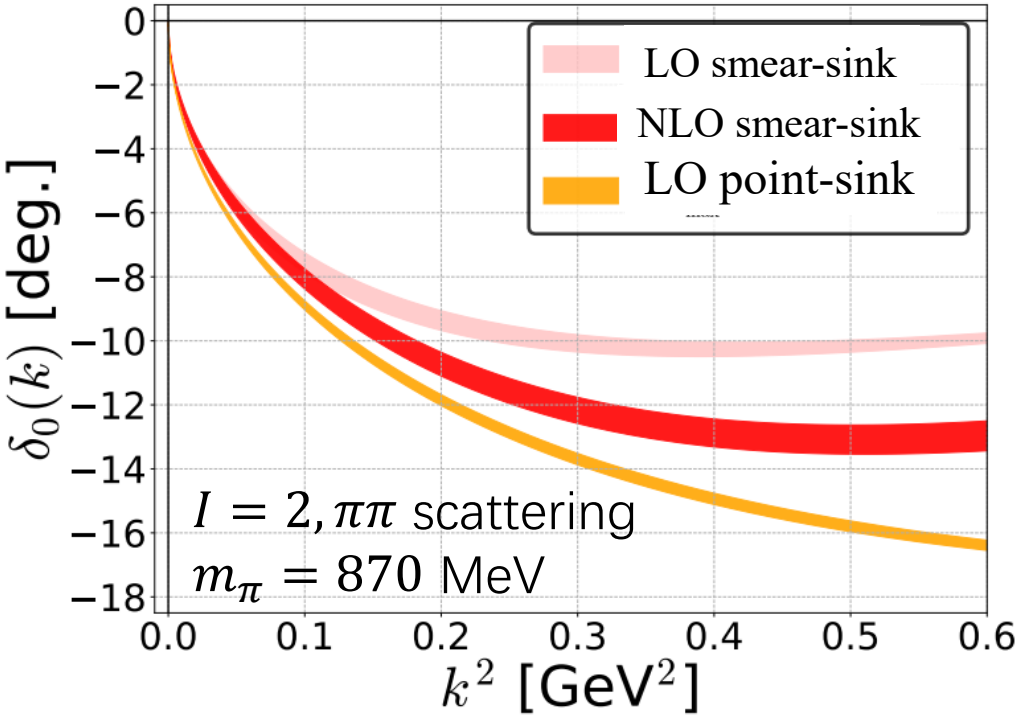
- Point-sink scheme used by HAL QCD group
  - ▶ Very local “underlying” potential, fast convergence of the DE

By experiences Murano:2011nz,HALQCD:2017xsa, Kurth:2013tua

DE VS EST

- In the case of two-particle scattering processes involving quark annihilation diagrams
  - ▶ smear-sink scheme
  - ▶ DE method does not converges as fast as point-sink scheme
  - ▶ The “underlying” potentials of the are more non-local than those of point-sink scheme

HALQCD:2017xsa



- To solve this problem, the HALQCD group has made extensive efforts to improve numerical computation methods while retaining the DE method. Akahoshi:2019klc, Akahoshi:2021sxc
- Local potentials do not possess any essential superiority over a non-local potentials.
- Perhaps, turning to another parameterization of the potentials will take less pains.
  - ▶ Separable parameterization

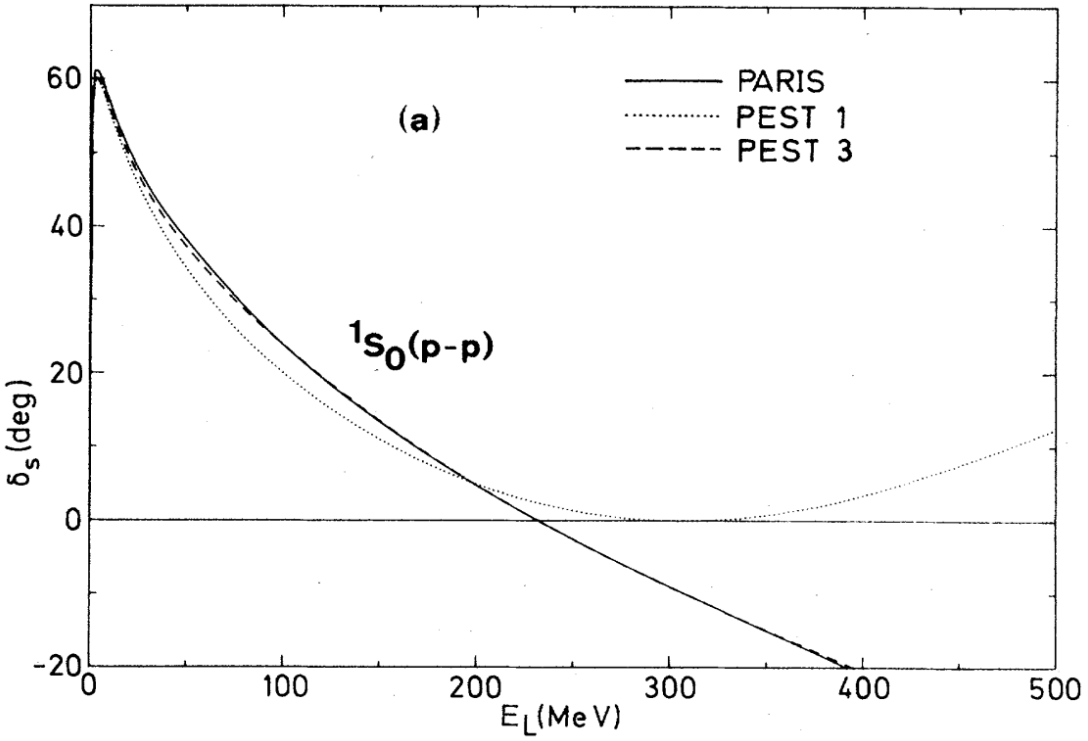
Separable representation

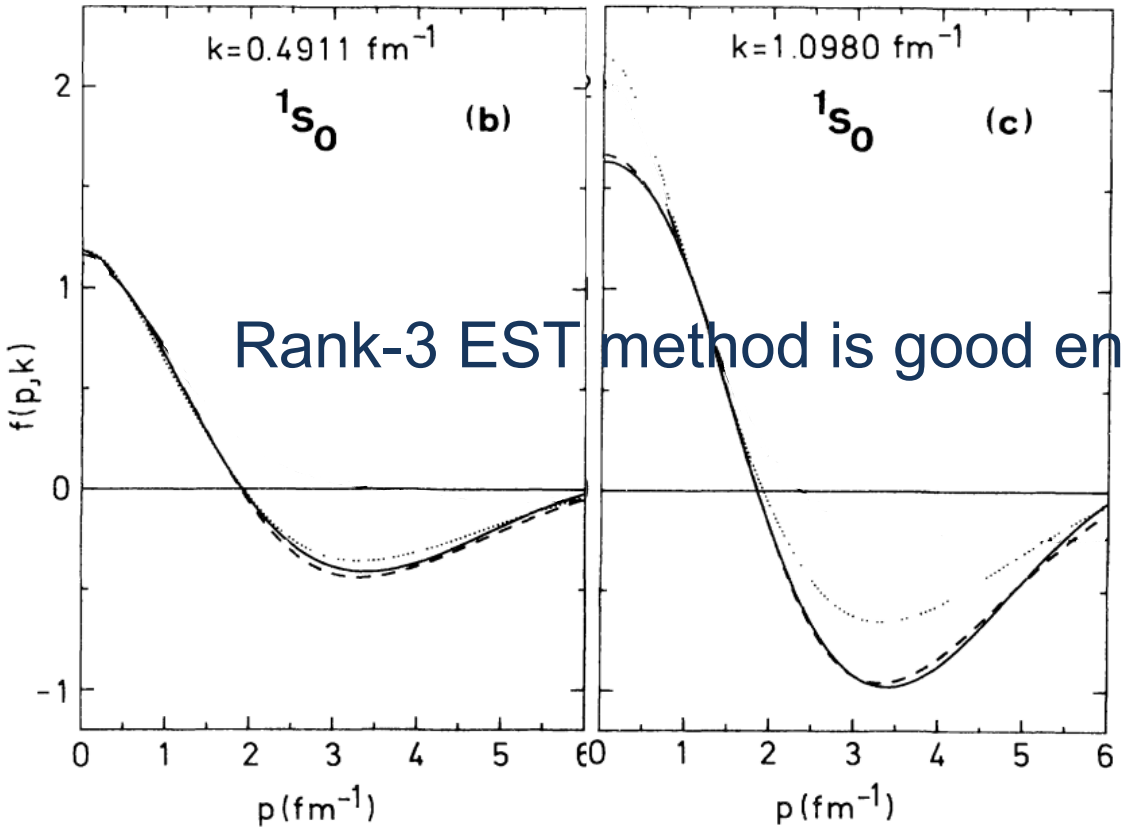
- The problem: $V|R^{(i)}\rangle = |K^{(i)}\rangle$ Ernst:1973zzb,Haidenbauer:1984dz
- Ernst-Shakin-Thaler (EST) method:
  - ▶ To solve the Fadeev function, find the equivalent separable potential of the high-precision nuclear force
  - ▶ on-shell and off-shell equivalent

$$V = \sum_{mn} |K^{(m)}\rangle \Lambda_{mn} \langle K^{(n)}|, \quad \Lambda_{mn} \langle K^{(n)}|R^{(i)}\rangle = \delta_{mi}$$

Separable representation

► Application: on-shell and off-shell equivalent separable potentials of Paris potentials





Rank-3 EST method is good enough

Ernst:1973zzb,Haidenbauer:1984dz

Numerical comparisons

Two underlying potentials

- Separable potential Aoki:2021ahj

$$V(\boldsymbol{r},\boldsymbol{r}') = \omega \frac{e^{-\mu r}}{r}\frac{e^{-\mu r'}}{r'}$$

- LO chiral nuclear force Reinert:2017usi

$$V_{ctc}(\boldsymbol{p},\boldsymbol{p}') = Ce^{-\frac{p^2+p'^2}{\Lambda^2}}, \quad V_{ope}(\boldsymbol{q}) = -\frac{g_A}{4F_\pi^2}\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{q}\boldsymbol{\sigma}_2\cdot\boldsymbol{q}}{\boldsymbol{q}^2+m_\pi^2} + C_{sub}\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\right)e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}$$

  - ▶ Separable contact interaction + local one-pion exchange interaction

- For simplicity: S-wave and ${}^1S_0$ NN interaction

- Solve the Time-(in)dependent Schrodinger equation to get wave functions
- Time-independent method
  - ▶ Choose $\{\psi_{k_i}\}$ as inputs
- Time-dependent method
  - ▶ Initial wave functions

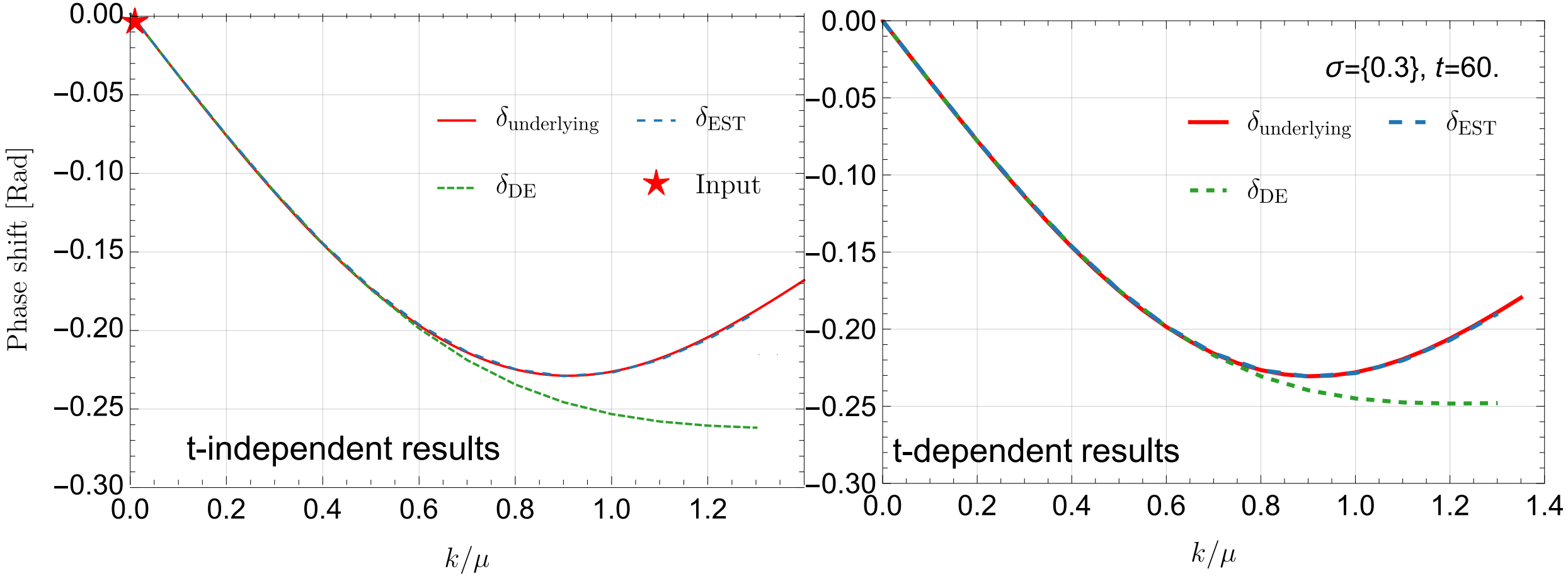
$$\tilde{R}(t=0,x) = \frac{\sigma^2 e^{-\sigma x}}{4\pi}$$

  - ▶ Evaluate t=60
  - ▶ Two $\sigma = \{0.3, 0.6\}$ as two inputs

Separatable interaction

- The EST methods give the accurate potential in LO
- The DE method is convergent

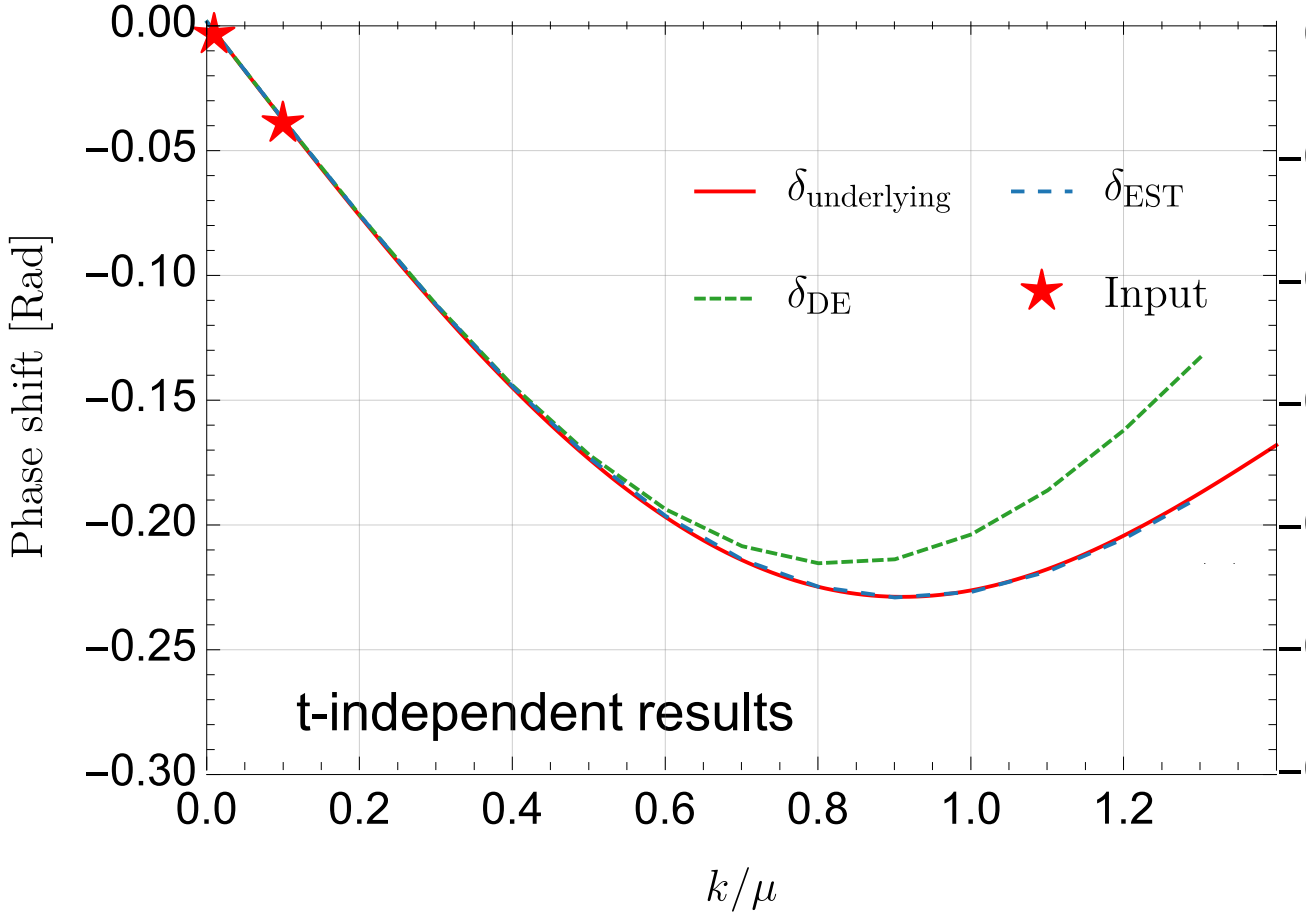
$$V(\boldsymbol{r},\boldsymbol{r}') = \omega \frac{e^{-\mu r}}{r} \frac{e^{-\mu r'}}{r'}$$

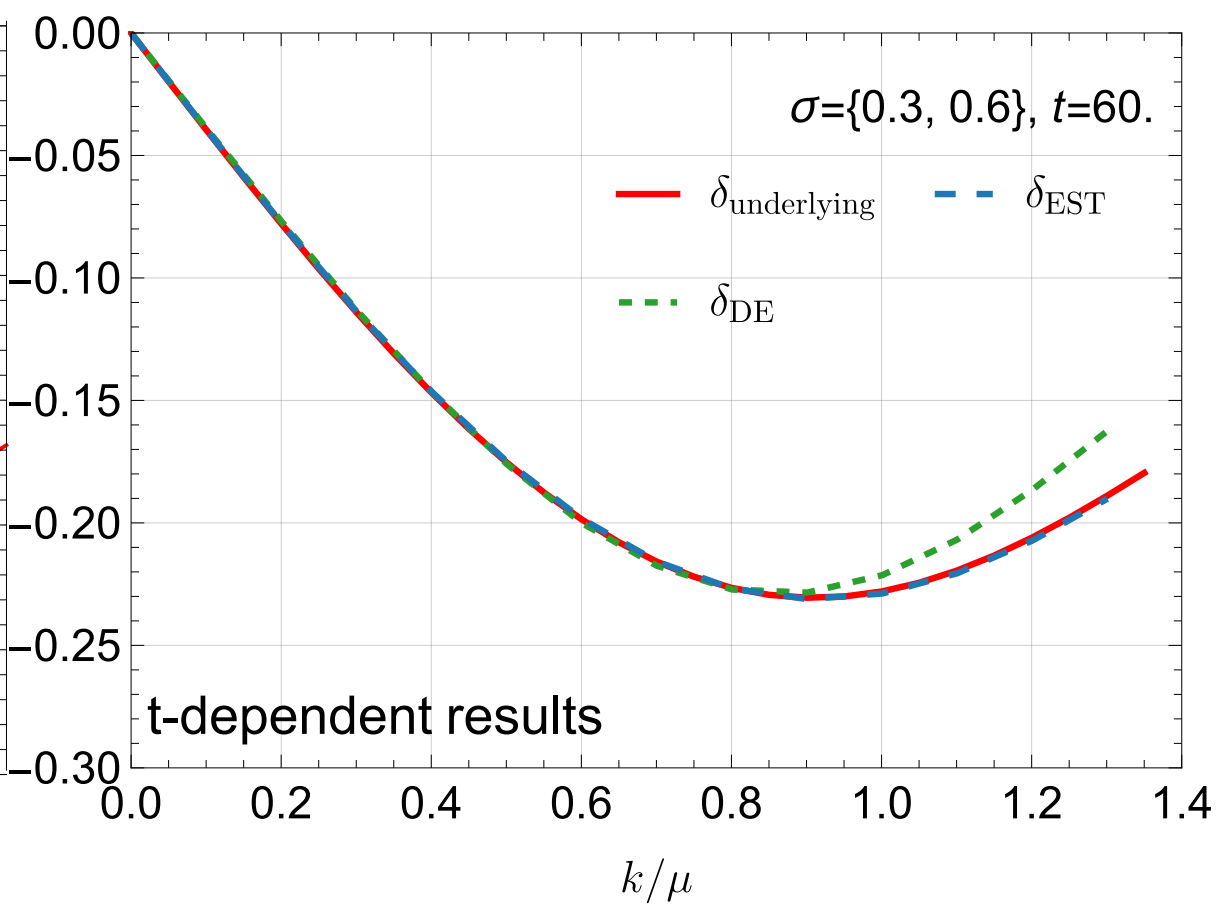


Separatable interaction

- The EST methods give the accurate potential in LO
- The DE method is convergent

$$V(\boldsymbol{r},\boldsymbol{r}') = \omega \frac{e^{-\mu r}}{r} \frac{e^{-\mu r'}}{r'}$$



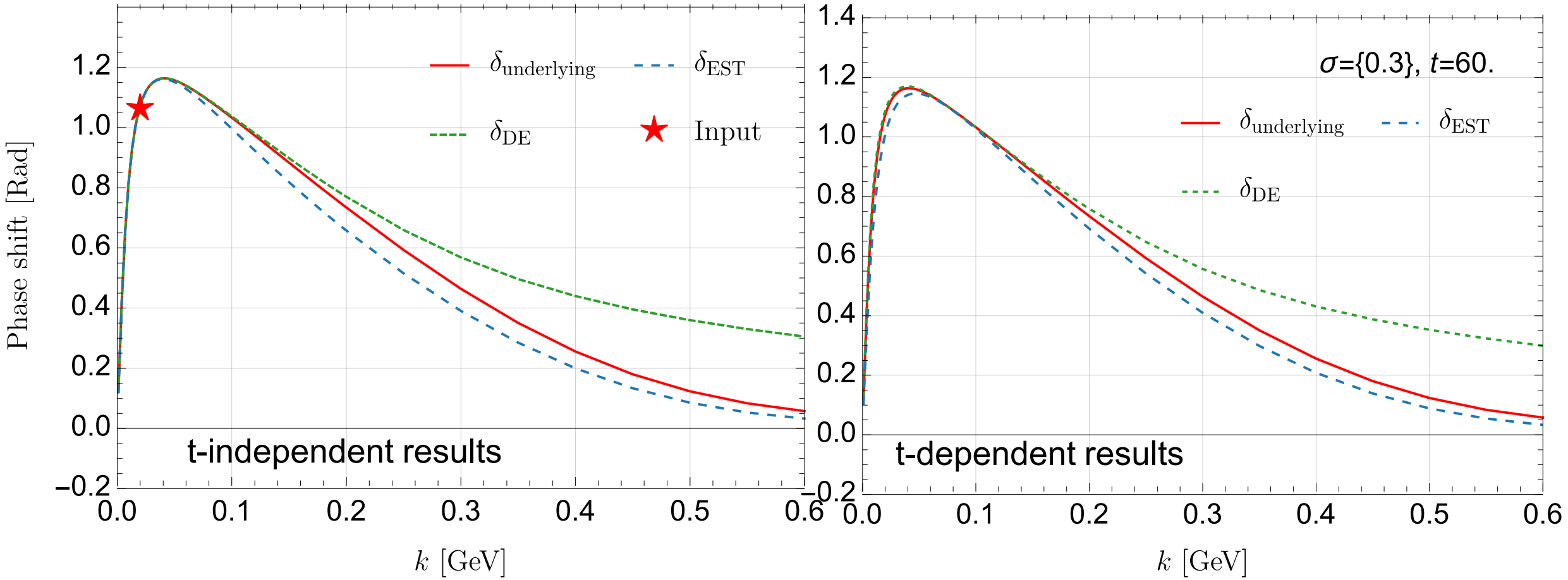


Physical interaction

- Including both separatable part and local part
- The performance of EST method is better
- In t-dependent methods, singular potential

$$V_{ctc}(\boldsymbol{p},\boldsymbol{p}') = Ce^{-\frac{p^2+p'^2}{\Lambda^2}},$$

$$V_{ope}(\boldsymbol{q}) = -\frac{g_A}{4F_\pi^2}\left(\frac{\boldsymbol{\sigma_1}\cdot\boldsymbol{q}\boldsymbol{\sigma_2}\cdot\boldsymbol{q}}{\boldsymbol{q}^2+m_\pi^2} + C_{sub}\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\right)e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}$$

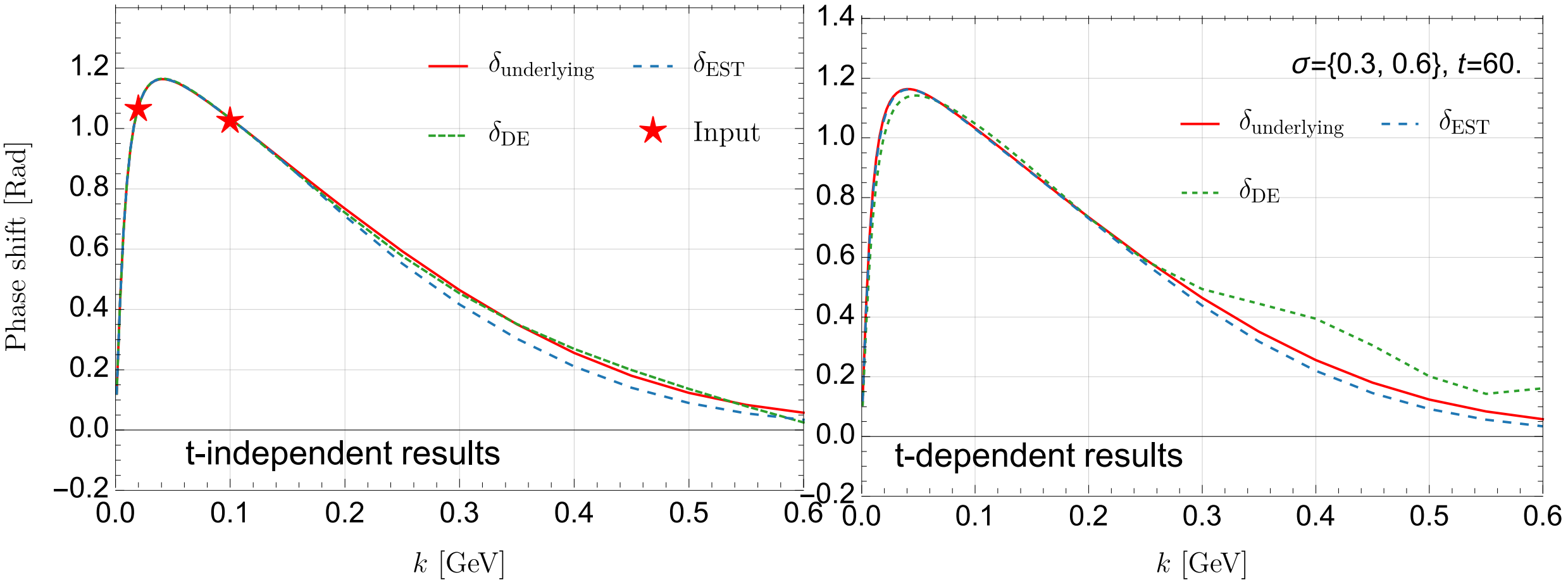


Physical interaction

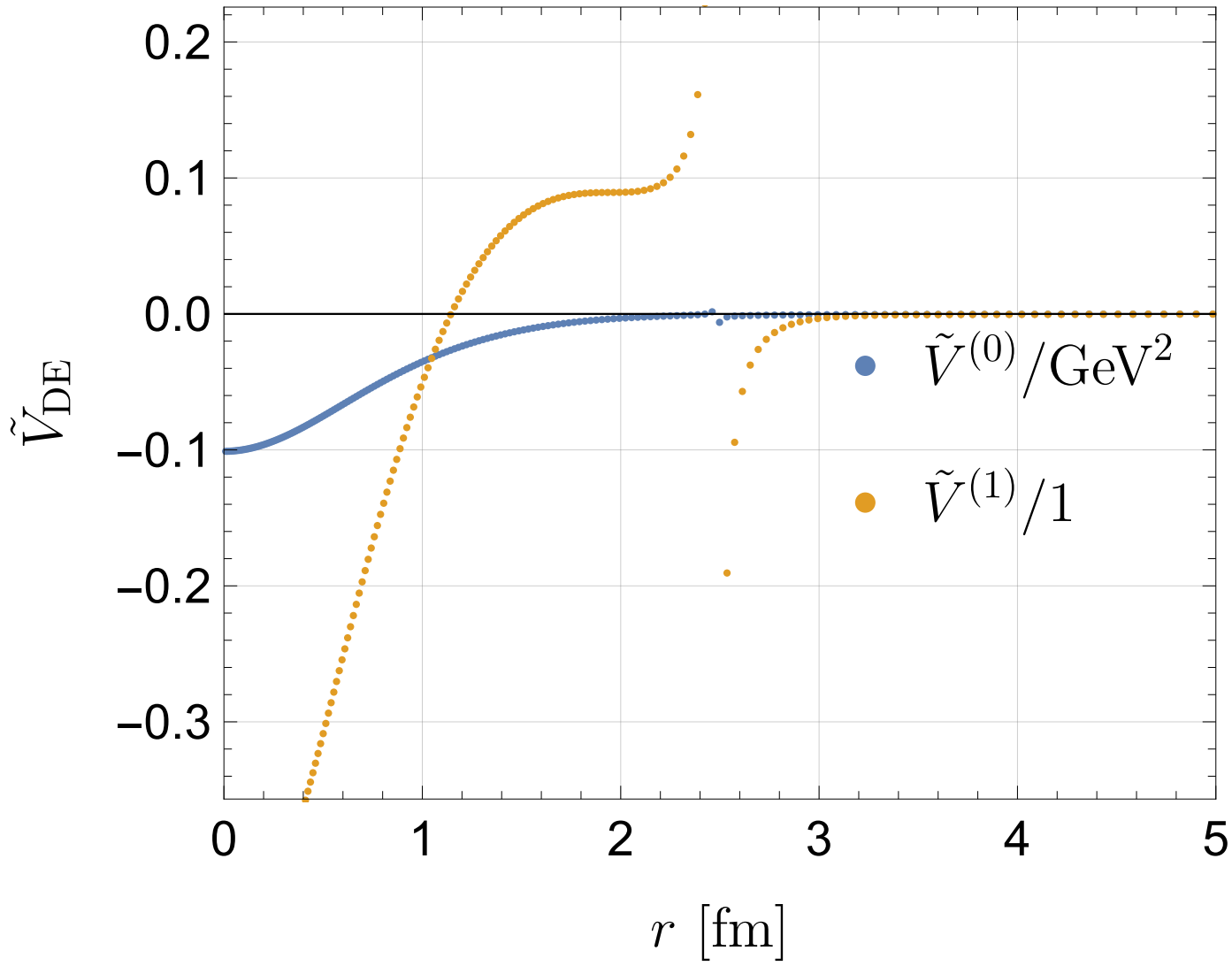
- Including both separatable part and local part
- The performance of EST method is better
- In t-dependent methods, singular potential

$$V_{ctc}(\boldsymbol{p},\boldsymbol{p}') = Ce^{-\frac{p^2+p'^2}{\Lambda^2}},$$

$$V_{ope}(\boldsymbol{q}) = -\frac{g_A}{4F_\pi^2}\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{q}\boldsymbol{\sigma}_2\cdot\boldsymbol{q}}{\boldsymbol{q}^2+m_\pi^2} + C_{sub}\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\right)e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}$$



Singularity in potential

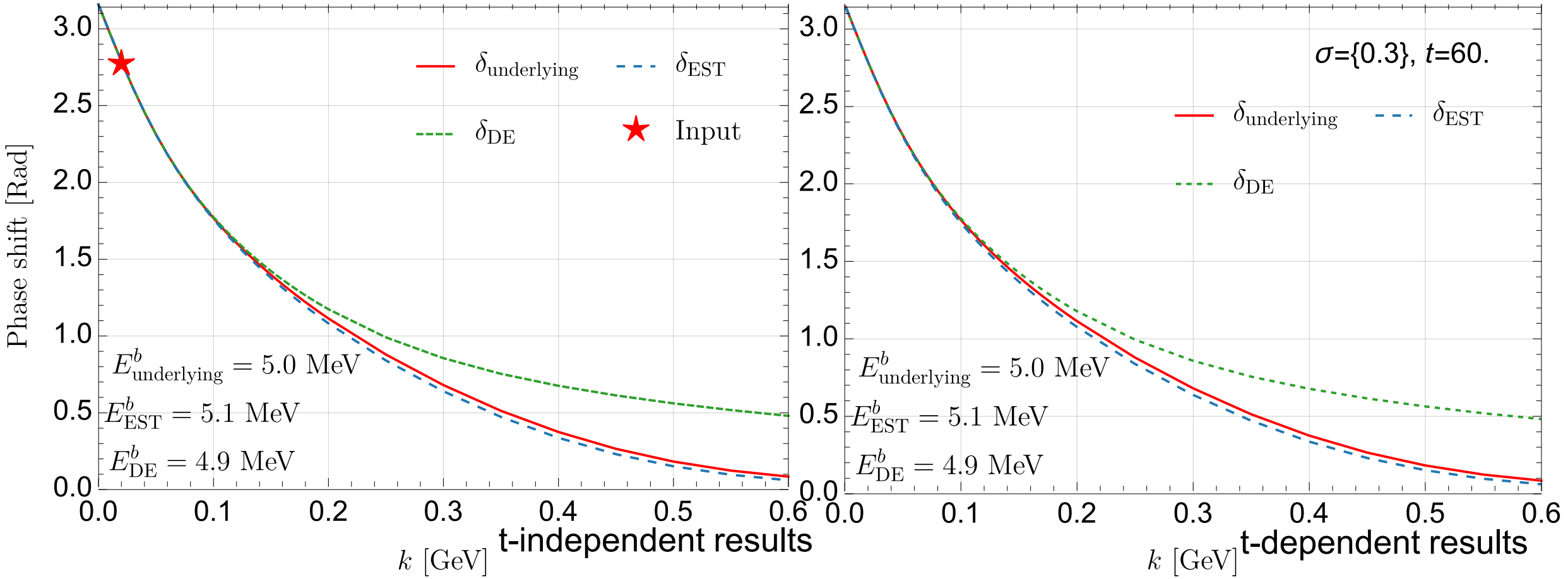


Bound state

- At LO, both EST and DE method give reasonable binding energy
- The EST method perform better in phase shift
- Singular potential in DE at NLO

$$V_{ctc}(\boldsymbol{p},\boldsymbol{p}') = Ce^{-\frac{p^2+p'^2}{\Lambda^2}},$$

$$V_{ope}(\boldsymbol{q}) = -\frac{g_A}{4F_\pi^2}\left(\frac{\boldsymbol{\sigma_1}\cdot\boldsymbol{q}\boldsymbol{\sigma_2}\cdot\boldsymbol{q}}{\boldsymbol{q}^2+m_\pi^2} + C_{sub}\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\right)e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}$$

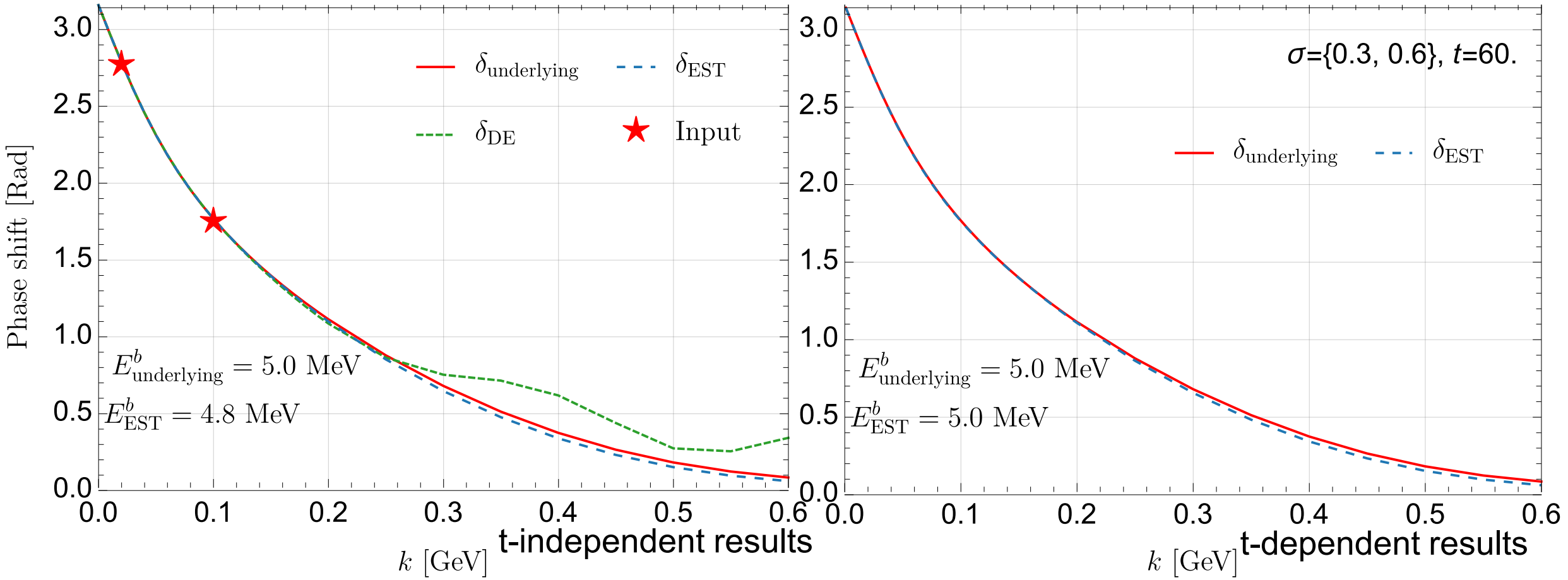


Bound state

- At LO, both EST and DE method give reasonable binding energy
- The EST method perform better in phase shift
- Singular potential in DE at NLO

$$V_{ctc}(\boldsymbol{p},\boldsymbol{p}') = Ce^{-\frac{p^2+p'^2}{\Lambda^2}},$$

$$V_{ope}(\boldsymbol{q}) = -\frac{g_A}{4F_\pi^2}\left(\frac{\boldsymbol{\sigma_1}\cdot\boldsymbol{q}\boldsymbol{\sigma_2}\cdot\boldsymbol{q}}{\boldsymbol{q}^2+m_\pi^2} + C_{sub}\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\right)e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}$$

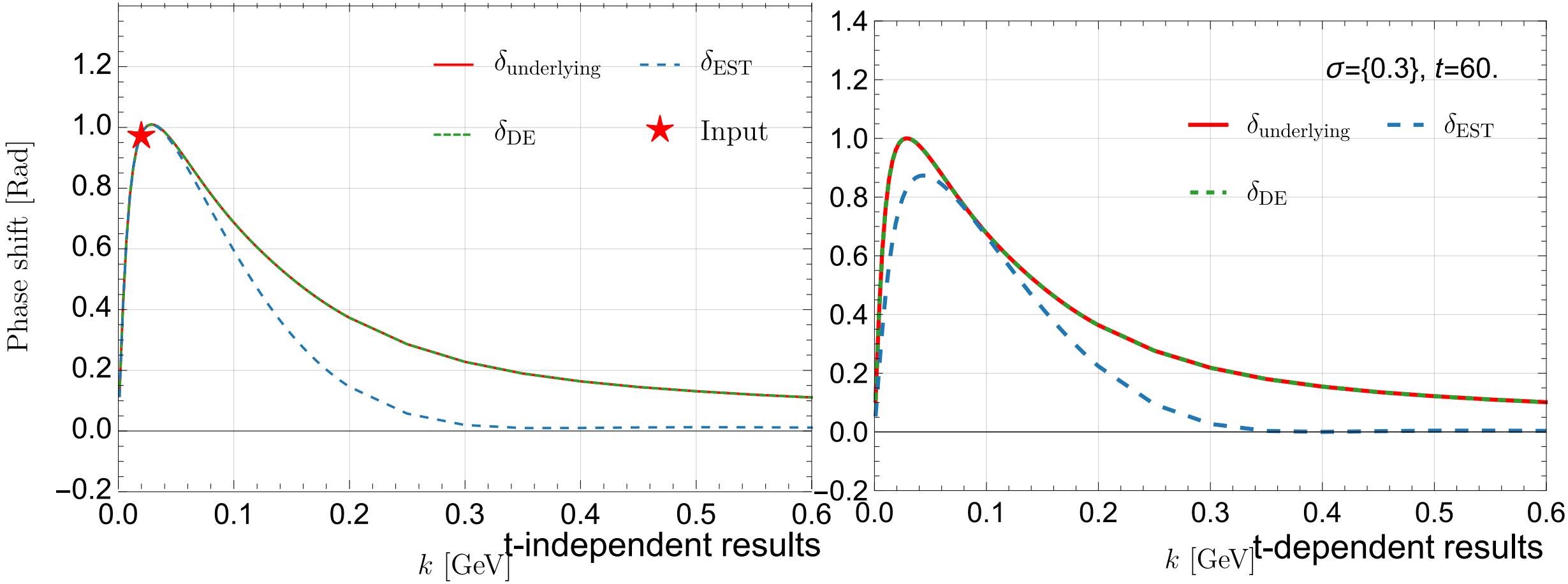


Local interaction

- The DE method gives the accurate results at LO
- Convergent EST results, not bad performance

$$V_{ctc}(\boldsymbol{p},\boldsymbol{p}') = Ce^{-\frac{p^2+p'^2}{\Lambda^2}},$$

$$V_{ope}(\boldsymbol{q}) = -\frac{g_A}{4F_\pi^2}\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{q}\boldsymbol{\sigma}_2\cdot\boldsymbol{q}}{\boldsymbol{q}^2+m_\pi^2} + C_{sub}\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\right)e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}$$

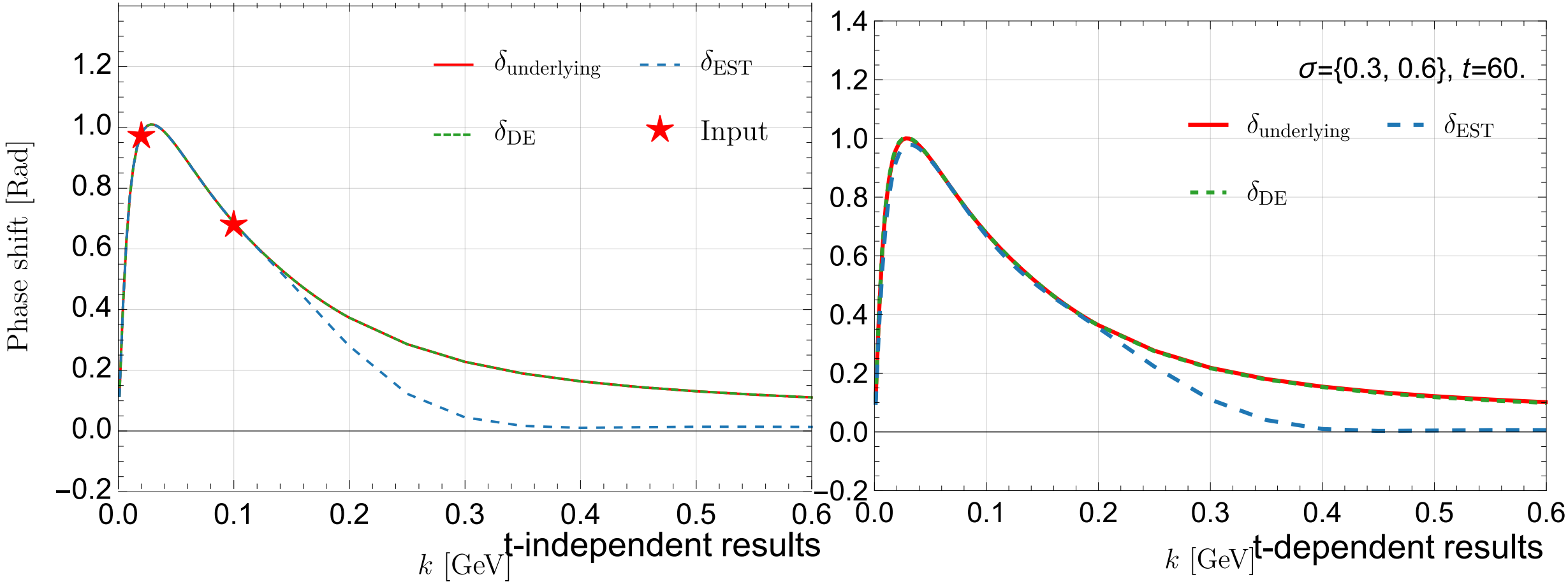


Local interaction

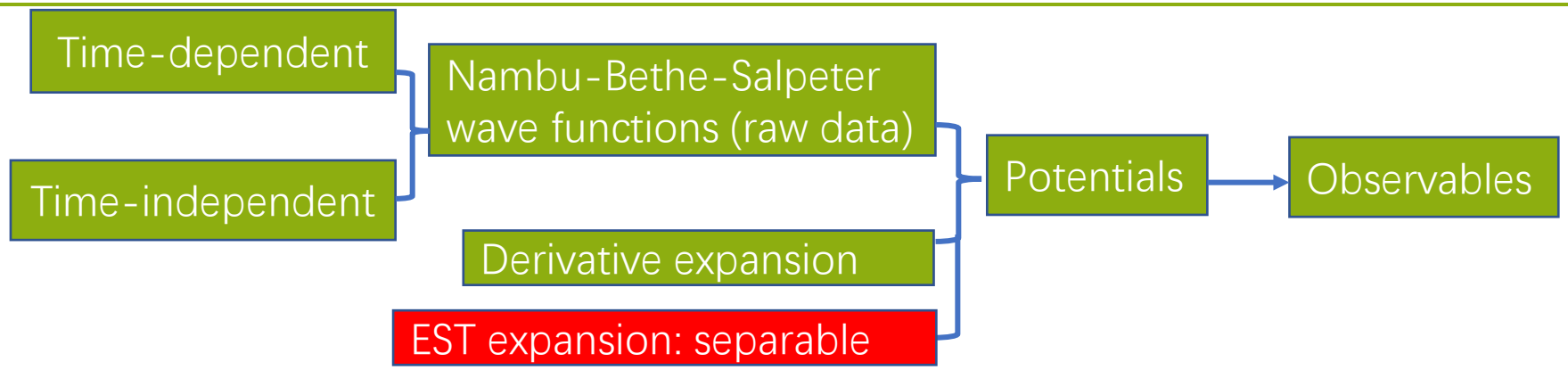
- The DE method gives the accurate results at LO
- Convergent EST results, not bad performance

$$V_{ctc}(\boldsymbol{p},\boldsymbol{p}') = Ce^{-\frac{p^2+p'^2}{\Lambda^2}},$$

$$V_{ope}(\boldsymbol{q}) = -\frac{g_A}{4F_\pi^2}\left(\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{q}\boldsymbol{\sigma}_2\cdot\boldsymbol{q}}{\boldsymbol{q}^2+m_\pi^2} + C_{sub}\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\right)e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}$$



Summary



- Re-emphasize some concepts
  - ▶ Potential and non-asymptotic wave function are not observable
  - ▶ The HALQCD potential is determined by the interpolating operators
  - ▶ A small number of wave functions can NOT determine the potential definitely
  - ▶ One cannot rule out the nonlocal potential either in principle or phenomenologically
- Derivative expansion VS EST expansion
  - ▶ For local potential, DE performs better, EST is not so bad (converge)
  - ▶ For separable potential EST perform better
  - ▶ For LO chiral nuclear force, EST perform better
- EST provide a alternative way to extract potential
  - ▶ Avoid possible singular potential
  - ▶ Changing potential representation takes less pains than changing operators to re-simulate
  - ▶ A way to estimate the systemic uncertainty
  - ▶ Combing EST and DE: short-range: EST, long-range: DE

Thanks for your attention!

Backup

TABLE 1 | Summary of binding energies [MeV] for $NN(^1S_0)$, $NN(^3S_1)$, and H-dibaryon in lattice QCD.

Collaboration	References	N_f	m_π	$-\Delta E(^1S_0)$	$-\Delta E(^3S_1)$	$-\Delta E(H)$
The direct method						
YKU2011	[35]	0	800	4.4 (1.2)	7.5 (1.0)	—
YIKU2012	[36]	2+1	510	7.4 (1.4)	11.5 (1.3)	—
NPL2015	[37]	2+1	450	12.5 $(^{+3.0}_{-5.0})$	14.4 $(^{+3.2}_{-2.6})$	—
NPL2012	[38]	2+1	390	7.1 (9.0)	11 (13)	13.2 (4.4)
YIKU2015	[39]	2+1	300	8.5 $(^{+1.7}_{-0.9})$	14.5 $(^{+2.5}_{-1.1})$	—
NPL2013	[40]	3	810	15.9 (3.8)	19.5 (4.8)	74.6 (4.7)
NPL2017	[41]	3	810	20.6 $(^{+3.3}_{-2.9})$	27.9 $(^{+3.8}_{-2.7})$	—
CalLat2017	[42]	3	810	21.8 $(^{+3.3}_{-5.8})$	30.7 $(^{+2.5}_{-3.0})$	—
		3		8.35 (1.1)*	3.3 $(^{+1.2}_{-0.9})$	—
Mainz2018	[43]	3†	960	0	—	19 (10)
		2+1†	440	—	—	18.8 (5.5)*
The HAL QCD method						
IAH2007	[26]	0	530	0	0	—
AHI2009	[23]	0	380, 530, 730	0	0	—
HAL2012	[44]	3	1171	0	0	49.1(6.5)
		3	1015	0	0	37.2(4.4)
		3	837	0	0	37.8(5.2)
		3	672	0	0	33.6(5.9)
		3	469	0	0	26.0(6.5)
HAL2012a	[34]	2+1	701	0	—	—
HAL2013	[45]	2+1	411, 570, 701	0	—	—

NPL2013, NPL2017, and CalLat2017 employed the same set of gauge configurations. CalLat2017 found two states in each channel. In Mainz2018, dynamical 2-flavor with quenched strange quark configurations are employed and N_f in the table (with † symbol) denotes the information in the valence quark sector. All values of ΔE correspond to those in the infinite volume limit except ones with $*$, which are values on the finite volumes. The number 0 in ΔE indicates the system is unbound in this channel.

the BS wave function in the "outer region" ($r > R$) satisfies the Helmholtz equation, $((W/2)^2 - \nabla^2 + m_N^2)\psi_{\alpha\beta}(\boldsymbol{r}) = -(\nabla^2 + k^2)\psi_{\alpha\beta}(\boldsymbol{r}) = 0$, up to an exponentially small correction. Here the "asymptotic momentum" k is related to the total energy W through the relation, $W = 2\sqrt{k^2 + m_N^2}$. To make a formal resemblance with the non-relativistic case, we introduce the "effective center of mass energy", $E = k^2/(2\mu) = k^2/m_N$.[15] As shown in Appendix A, using the unitarity of the

$$\left[\sqrt{p^2+m_1^2}+\sqrt{p^2+m_2^2}\right]\phi(p)+\frac{1}{(2\pi)^3}\int U(p,p')p'^2\phi(p')=E\phi(p)$$

$$\left[m_1+m_2+\frac{q^2}{2m_1}+\frac{q^2}{2m_2}\right]\psi(q)+\frac{1}{(2\pi)^3}\int V(q,p')p'^2\psi(p')=E\psi(q)$$

$$\sqrt{p^2+m_1^2}+\sqrt{p^2+m_2^2}=m_1+m_2+\frac{q^2}{2m_1}+\frac{q^2}{2m_2}$$

$$p^2dp=h(q)^2q^2dq$$

$$h(q)^2=\frac{p}{q}\frac{\omega_{12}}{\mu_{12}}$$

$$\left[m_1+m_2+\frac{q^2}{2m_1}+\frac{q^2}{2m_2}\right]\phi(p(q))+\frac{1}{(2\pi)^3}\int U(p(q),p'(q))h(q')^2q'^2\phi(p'(q'))=E\phi(p(q))$$

$$\left[m_1+m_2+\frac{q^2}{2m_1}+\frac{q^2}{2m_2}\right]h(q)\phi(p(q))+\frac{1}{(2\pi)^3}h(q)\int U(p(q),p'(q'))h(q')^2q'^2\phi(p'(q'))=Eh(q)\phi(p(q))$$

if $\psi(q)=h(q)\phi(p(q))$ and $h(q)U(p(q),p'(q'))h(q')=V(q,q')$

we can get

$$\left[m_1+m_2+\frac{q^2}{2m_1}+\frac{q^2}{2m_2}\right]\psi(q)+\frac{1}{(2\pi)^3}\int V(q,p')p'^2\psi(p')=E\psi(q)$$

Similarity renormalization group

$$H_s = U(s) H U^\dagger(s) \equiv T_{\rm rel} + V_s \ , \qquad (1)$$

$$\frac{dH_s}{ds} = [\eta(s), H_s] \ , \qquad (2)$$

with

$$\eta(s) = \frac{dU(s)}{ds} U^\dagger(s) = -\eta^\dagger(s) \ . \qquad (3)$$

Choosing $\eta(s)$ specifies the transformation. Here we make perhaps the simplest choice [10],

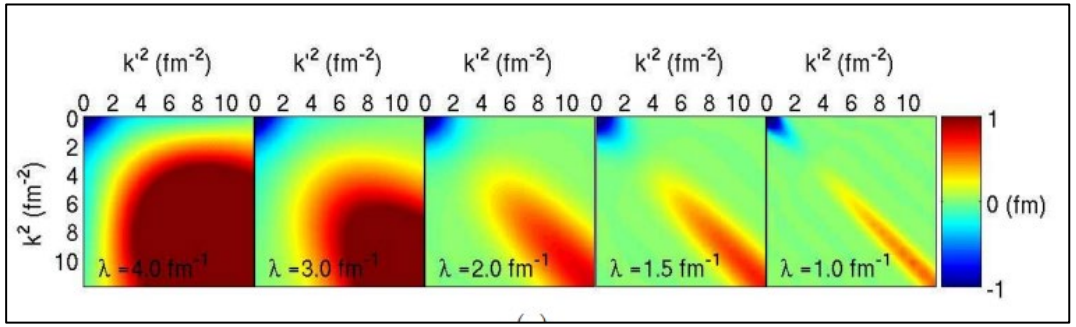
$$\eta(s) = [T_{\rm rel}, H_s] \ , \qquad (4)$$

which gives the flow equation,

$$\frac{dH_s}{ds} = [[T_{\rm rel}, H_s], H_s] \ . \qquad (5)$$

Other choices will be studied elsewhere [14].

$$\frac{dV_s(k,k')}{ds} = -(k^2 - k'^2)^2 \, V_s(k,k') + \frac{2}{\pi} \int_0^\infty q^2 \, dq \, (k^2 + k'^2 - 2q^2) \times V_s(k,q) \, V_s(q,k') \ . \qquad (6)$$



SRG evolution

- Soften the short range interaction
- Improve the convergence of the many-body probelm

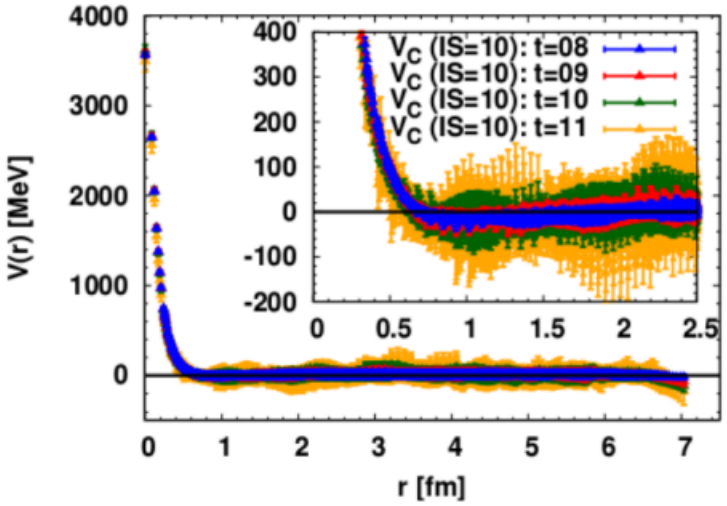
Highlight of HALQCD results: NN interaction

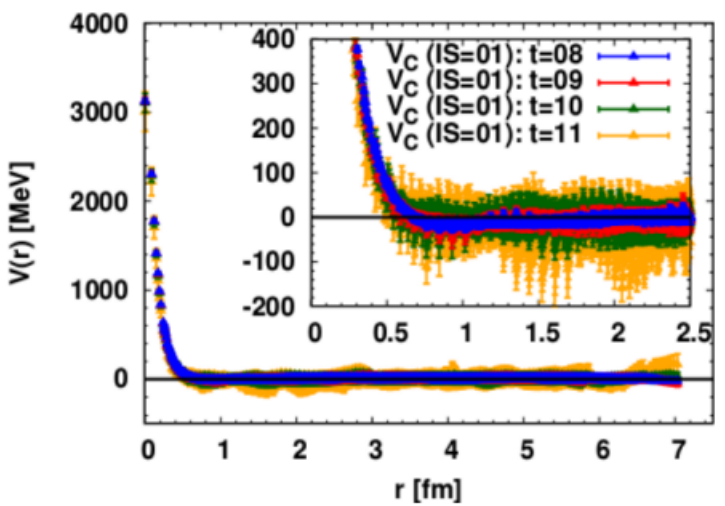
- lattice Setting: $m_\pi = 146$ MeV, $m_K = 525$ MeV, $a = 0.0846$fm, $L = 8.1$fm, 96^4

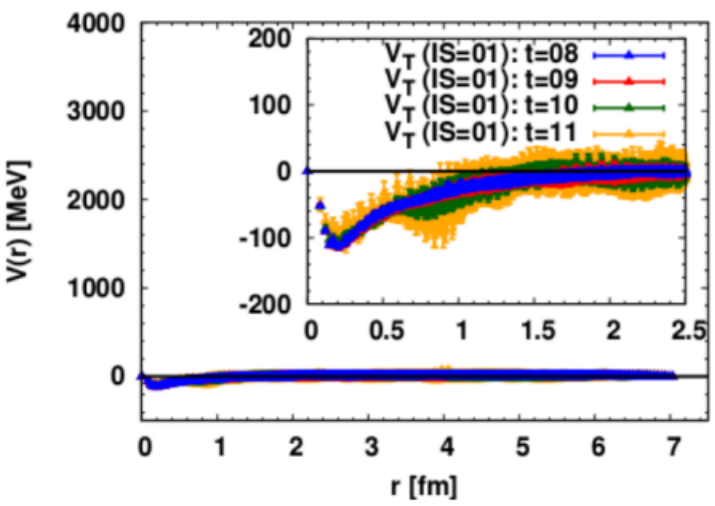
  $\Rightarrow$ Almost physical pion mass, very large box size, the finite volume effect is neglected

  $\Rightarrow$ NN: ${}^1S_0$ central potential, ${}^3S_1$ central potential, ${}^3S_1 - {}^3D_1$ tensor potential

Doi:2017zov







D^*D interaction: 2 pion tails

- lattice Setting: $m_\pi = 146$ MeV, $m_K = 525$ MeV, $a = 0.0846$fm, $L = 8.1$fm, 96^4
- D^*D, ϕN interaction...

Lyu:2022imf,Lyu:2023xro

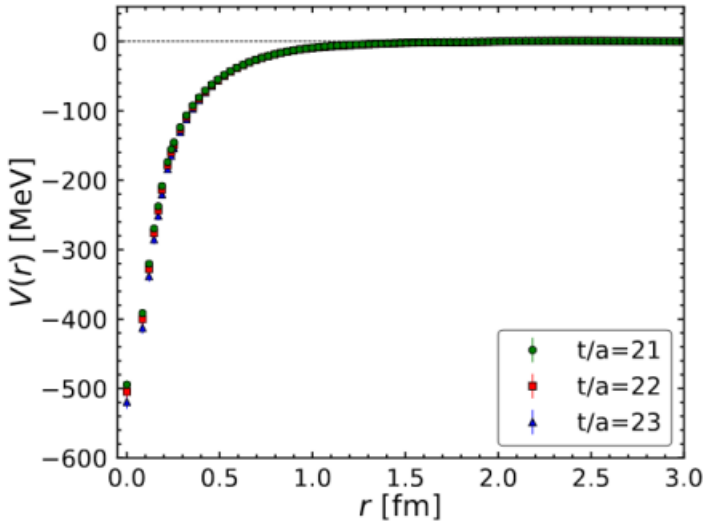
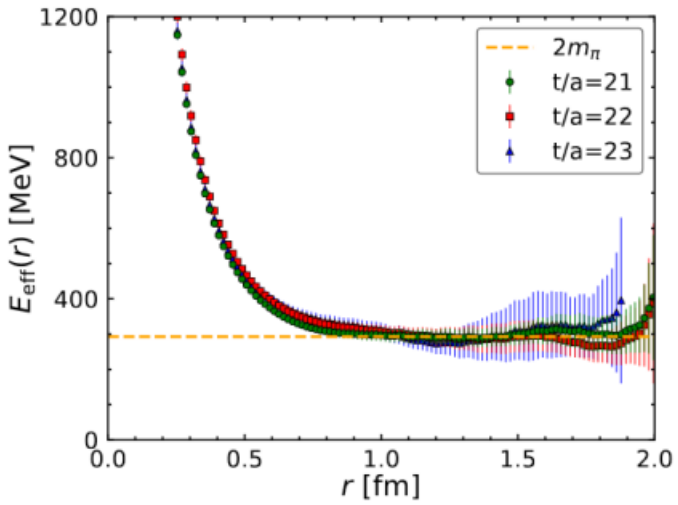


FIG. 2. The D^*D potential $V(r)$ in the $I = 0$ and S-wave channel at Euclidean time $t/a = 21$ (green circles), 22 (red squares), and 23 (blue triangles).



D^*D interaction: 2 pion tails

Fitiing the potential with:

$$V_{fit}(r) = \sum_{i=1,2} a_i e^{-r^2/b_i^2} + a_3 \frac{e^{-2mr}}{r^2} \tag{65}$$

once a_3 is determined

define

$$E_{eff}(r) = -\frac{\ln[-V(r)r^2/a_3]}{r} \tag{66}$$

one get a plateau at $E_{eff} = 2m$

- No one-pion exchange interaction: $\frac{1}{u} = 4.1$ fm

An example

HALQCD:2017xsa

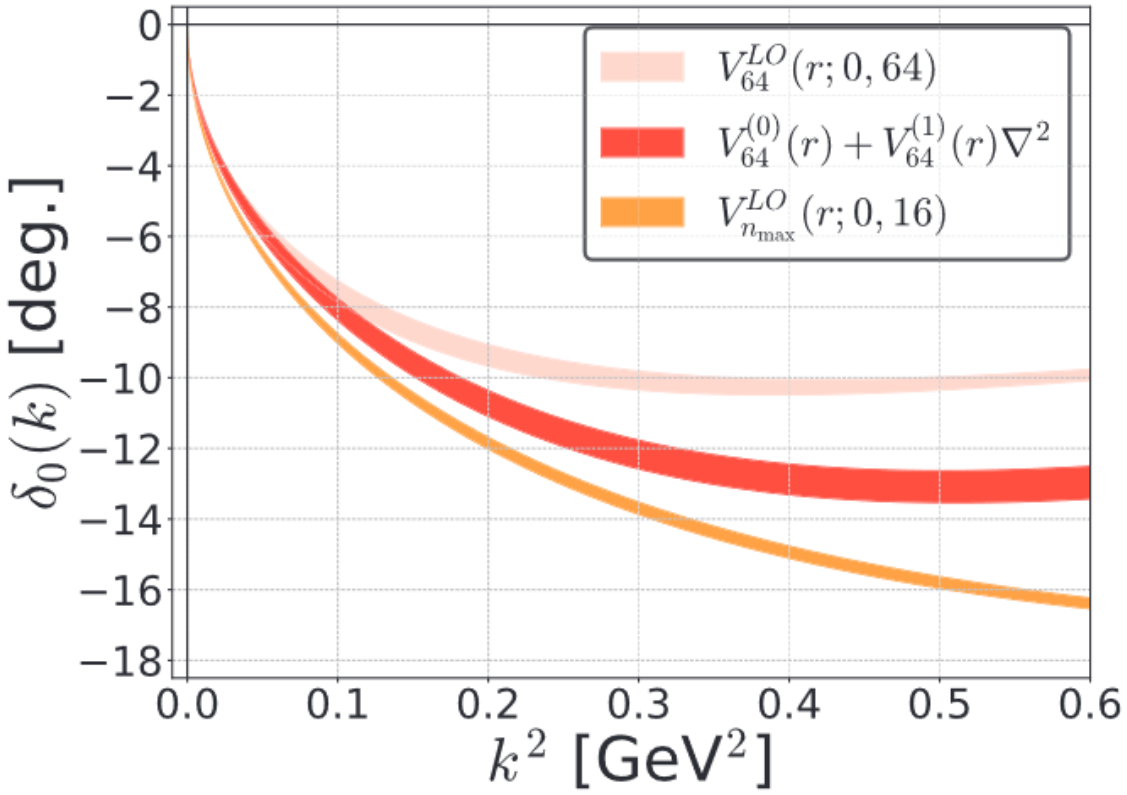


Fig. 5. The phase shifts of the S-wave $I = 2$ $\pi\pi$ scattering from the potential in the point-sink scheme (LO: orange) and the smeared-sink scheme (LO: pink, NLO: red) as a function of k^2.

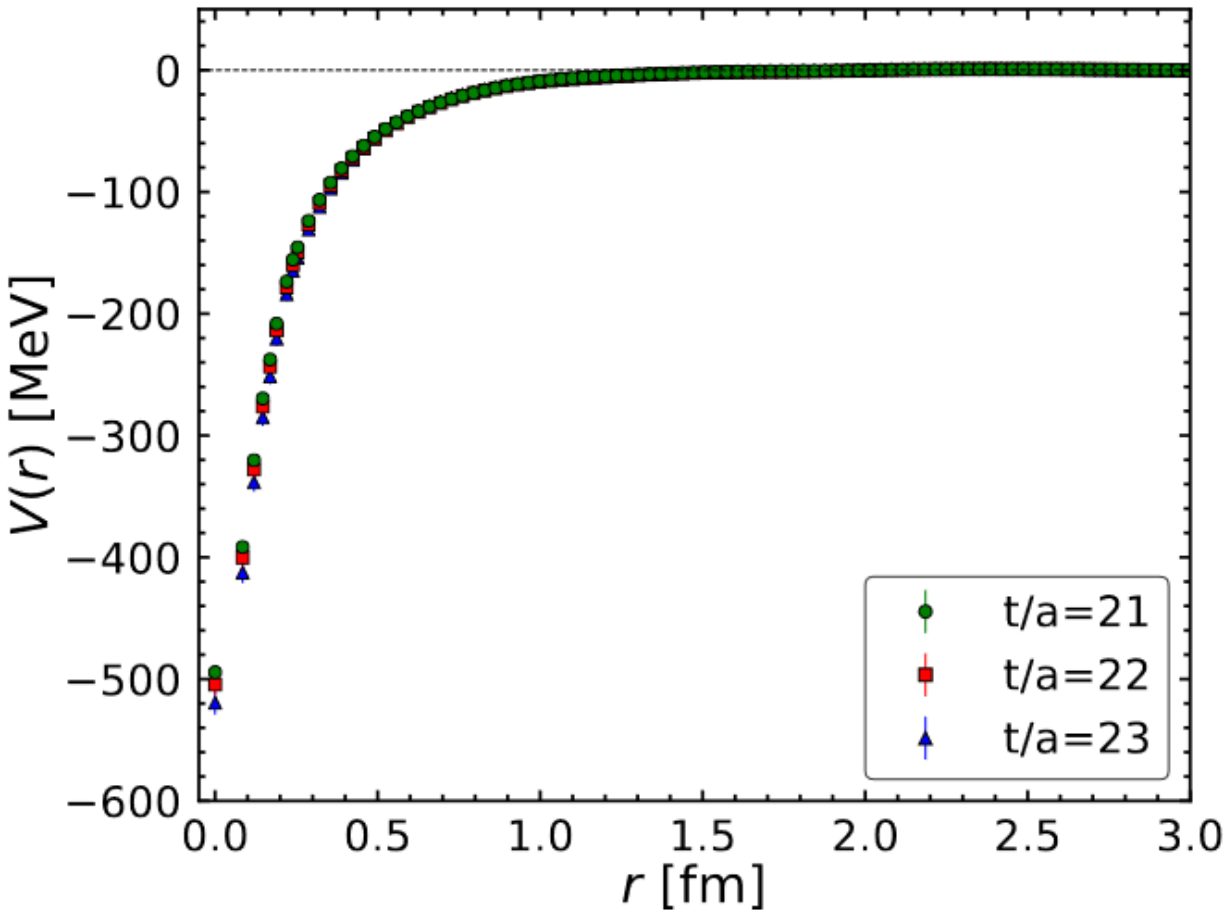
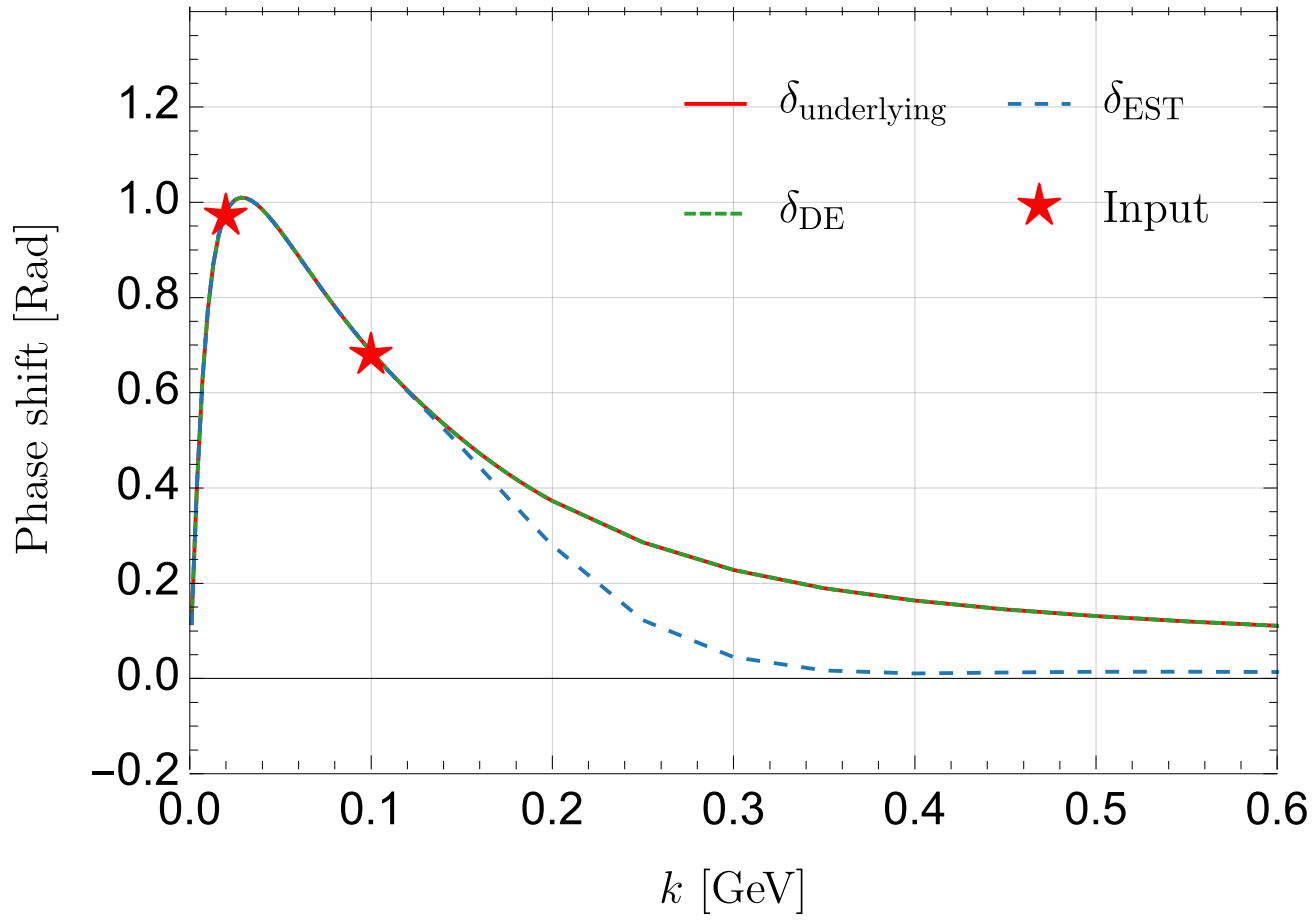


FIG. 2. The D^*D potential $V(r)$ in the $I = 0$ and S-wave channel at Euclidean time $t/a = 21$ (green circles), 22 (red squares), and 23 (blue triangles).

- Extracting potential from NBS is not a expansion of small quantities
- It is more like a interpolating and extrapolating
- Self-consistence test also make sense

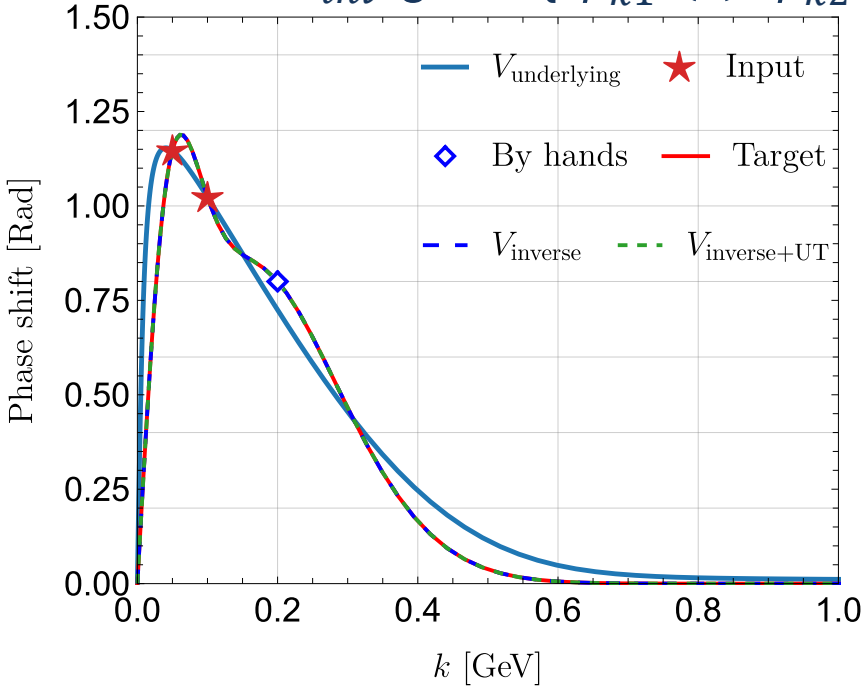


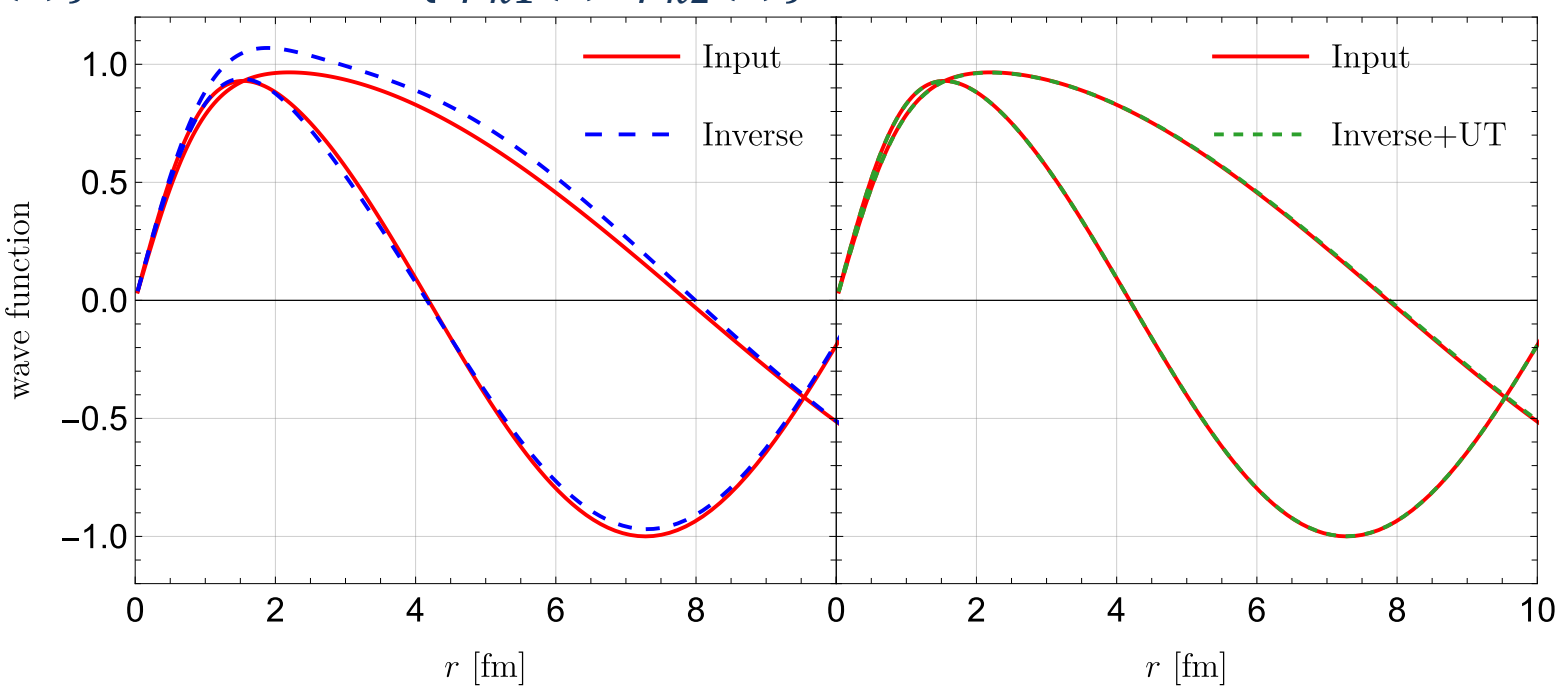
A small number of wave functions

1. Underlying potential $V_{underlying}$ give its phase shift $\delta(k)$
2. Using two wave functions as input $\{\psi_{k1}(r), \psi_{k2}(r)\}$ with phase shifts $\{\delta(k_1), \delta(k_2)\}$
3. Find a $\delta_{tar}(k)$ go thorough $\{\delta(k_1), \delta(k_2)\}$ and the third phase shift $\delta_{by-hand}(k_3)$ assigned by hand
4. Find a potential $V_{inverse}$ permit $\delta_{tar}(k)$
   ► many choices: i.e. a separable potential

Tabakin:1969mr

5. The V_{inv} gives $\{\psi^{inv}_{k1}(r), \psi^{inv}_{k2}(r)\}$ different with $\{\psi_{k1}(r), \psi_{k2}(r)\}$





A small number of wave functions

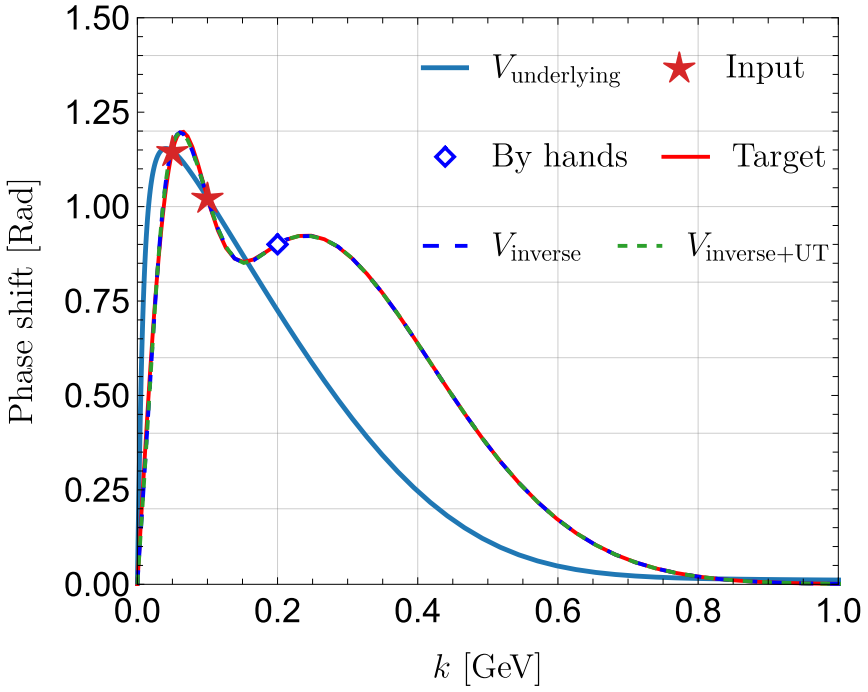
6. Construct an unitary trans. (UT): $U\left|\psi_{\mathrm{k}_i}^{inv}\right\rangle = \left|\psi_{k_i}\right\rangle$

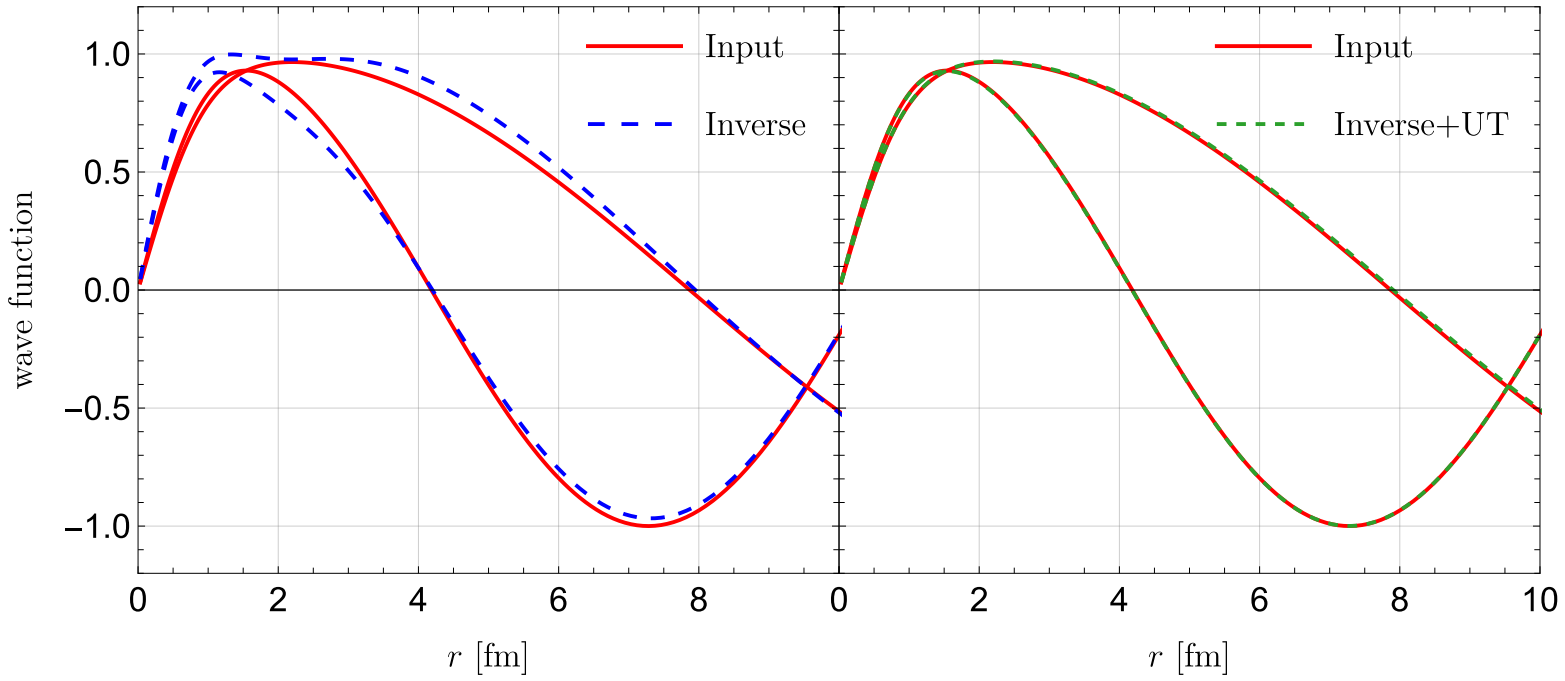
Ernst:1973utx

$$|f_i\rangle = |\psi_{k_i}\rangle - |\psi_{k_i}^{inv}\rangle, \quad U - 1 \equiv \sum_{mn} |f_m\rangle \Lambda_{mn} \langle f_n|, \quad \Lambda_{mn}\langle f_n|\psi_i\rangle = \delta_{mi}$$

7. V^{inv+UT} permit the $\{\psi_{k1}(r), \psi_{k2}(r)\}$

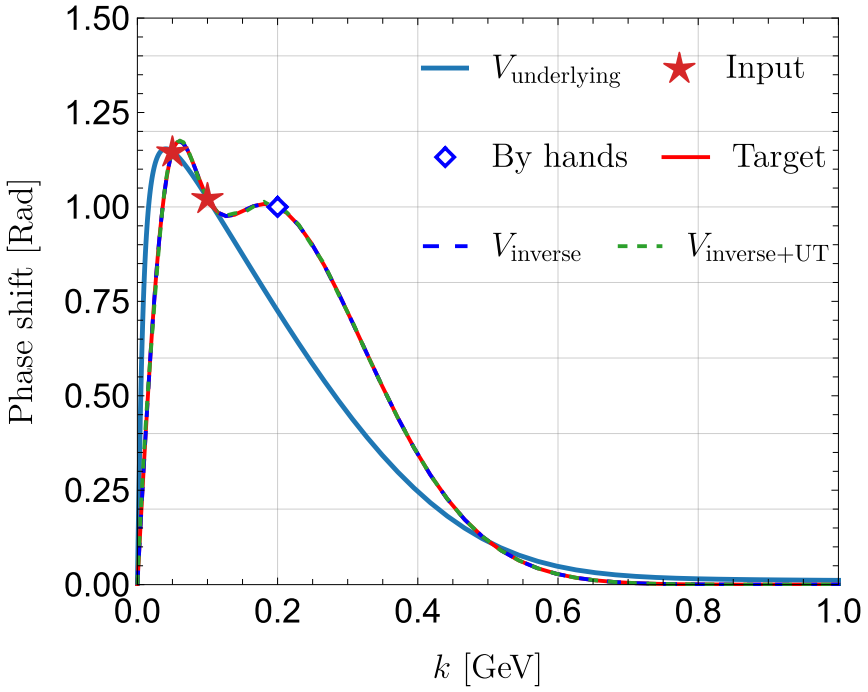
$$V^{inv+UT} = UV^{inv}U^{\dagger} + UH_0U^{\dagger} - H_0$$

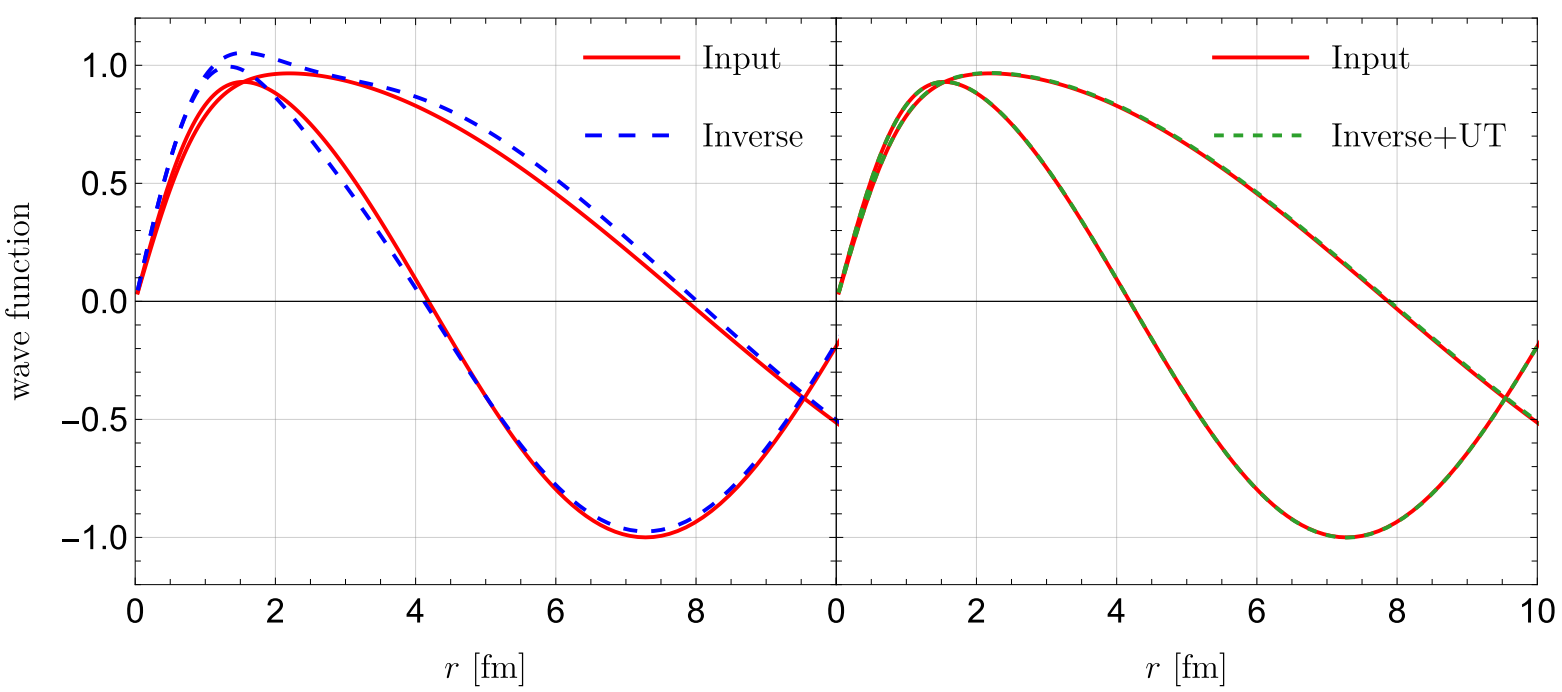


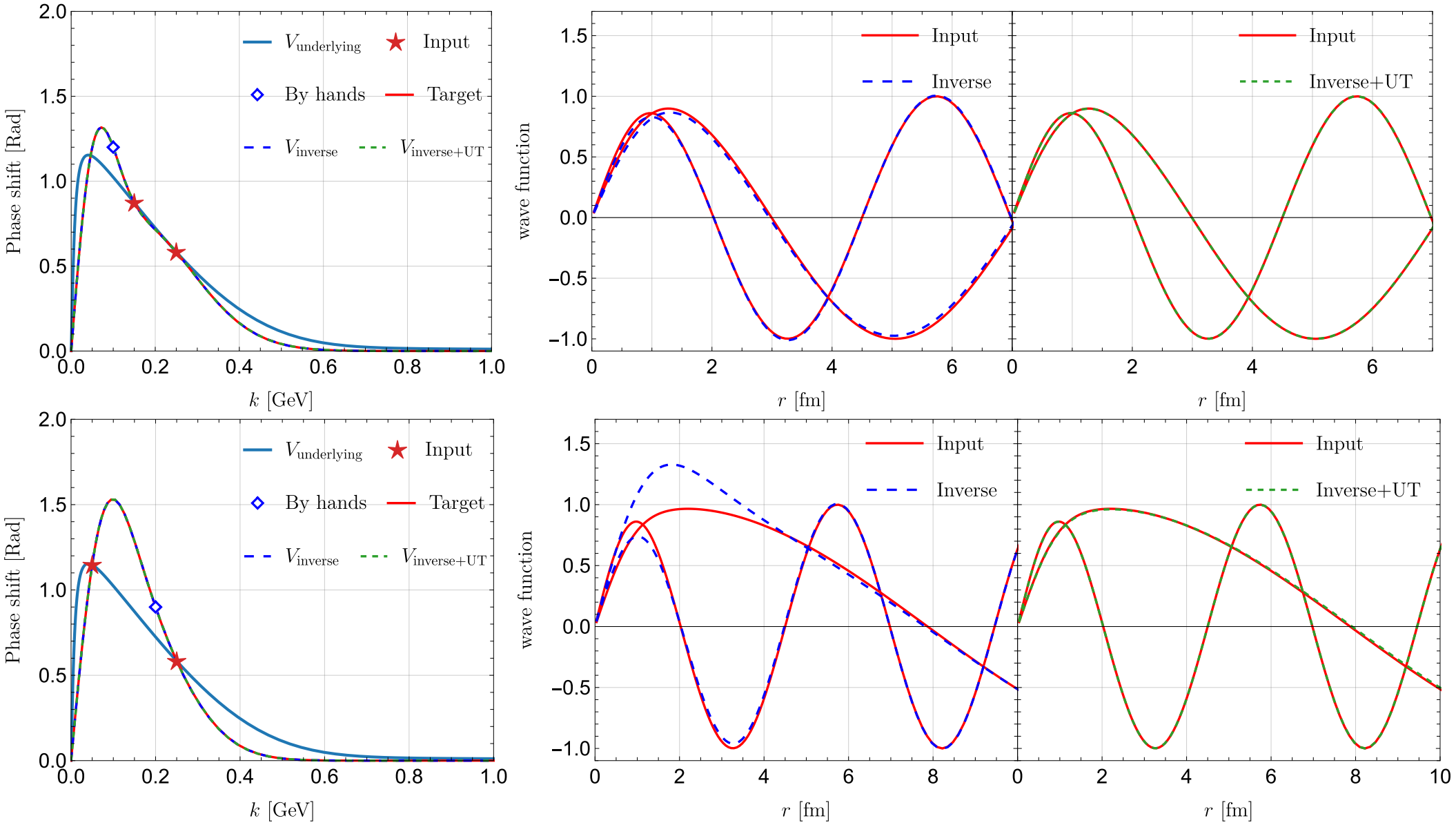


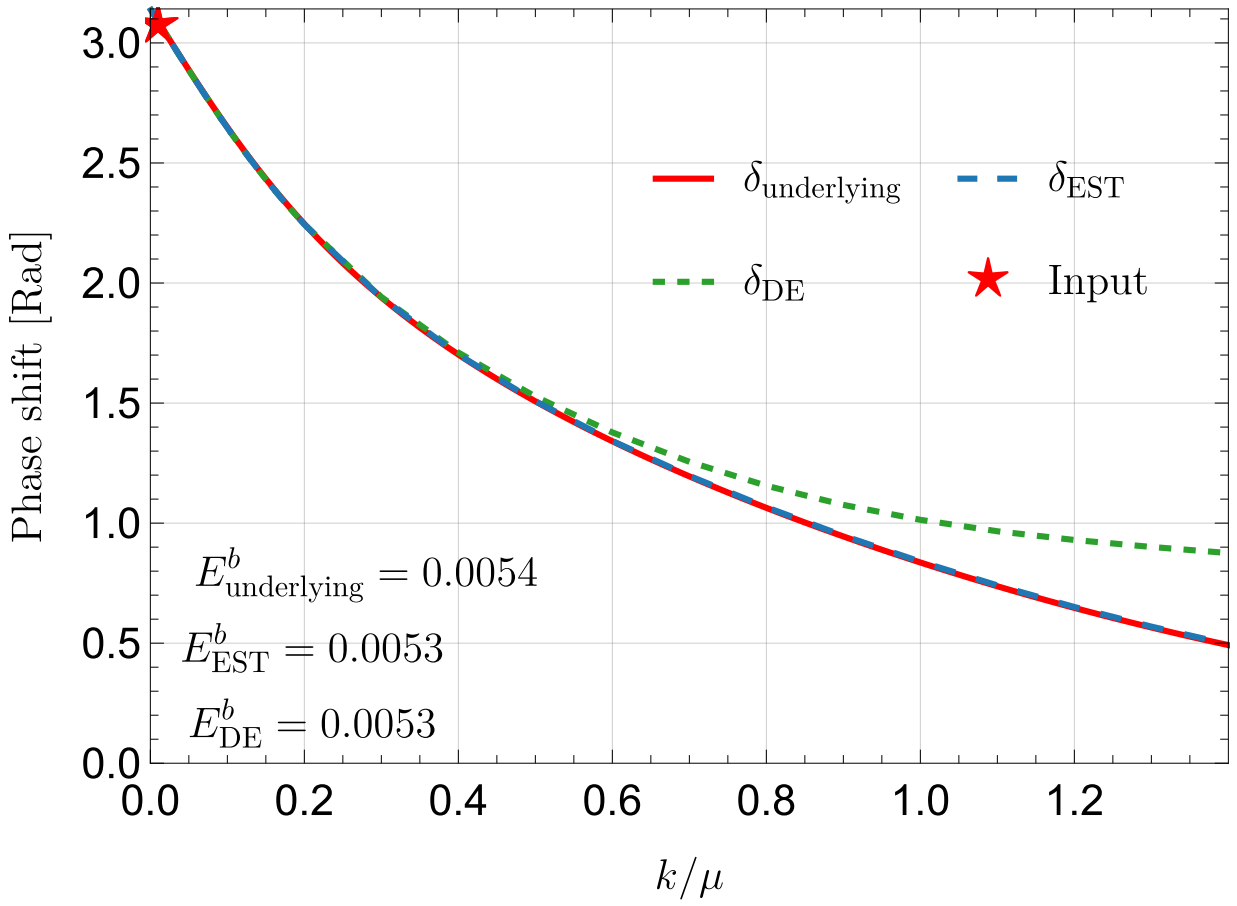
A small number of wave functions

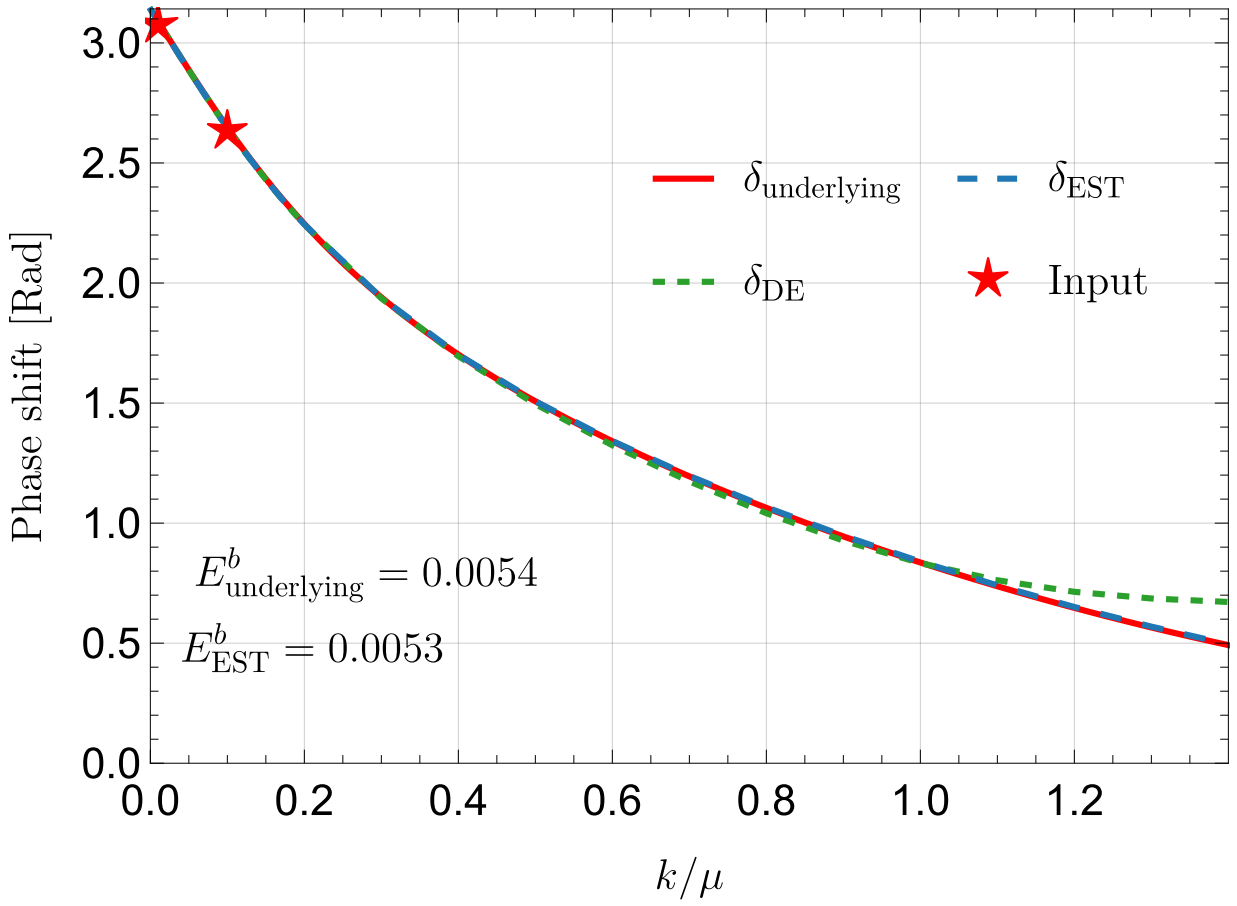
- A small number of wave functions cannot fix the potential and phase shift
- Unless, you presume some features of potentials
  - ▶ Derivative expansion: the nonlocality of potential is small
  - ▶ EST: separable






$V_{\text{underlying}}$
Input
By hands
Target
V_{inverse}
$V_{\text{inverse+UT}}$
Phase shift [Rad]
k [GeV]
wave function
Input
Inverse
Inverse+UT
r [fm]


Phase shift [Rad]
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
k/μ
$\delta_{\text{underlying}}$
δ_{EST}
δ_{DE}
Input
$E^b_{\text{underlying}} = 0.0054$
$E^b_{\text{EST}} = 0.0053$
$E^b_{\text{DE}} = 0.0053$


Phase shift [Rad]
3.0
2.5
2.0
1.5
1.0
0.5
0.0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
k/μ
$\delta_{\text{underlying}}$
δ_{EST}
δ_{DE}
Input
$E^b_{\text{underlying}} = 0.0054$
$E^b_{\text{EST}} = 0.0053$

A small number of wave functions

- Using two wave functions of $V_{underlying}$ as input $\{\psi_{k1}(r), \psi_{k2}(r)\}$
- $\delta_{tar}(k)$ go thorough $\{\delta(k_1), \delta(k_2)\}$ and the third phase shift $\delta_{by-hand}(k_3)$ assigned by hand
- Find a potential $V_{inverse}$ permit $\delta_{tar}(k)$ Tabakin:1969mr
- Find a unitary transformation give the correct wave functions $\{\psi_{k1}(r), \psi_{k2}(r)\}$ Ernst:1973utx
- Conclusion:
  - ▶A small number of wave functions cannot fix the potentials and phase shifts
  - ▶Unless, one presumes some features of potentials