中国科学院理论物理研究所
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RUHR UNIVERSITÄT BOCHUM RUB

Extracting hadron potentials from the NBS wave functions: separable representation

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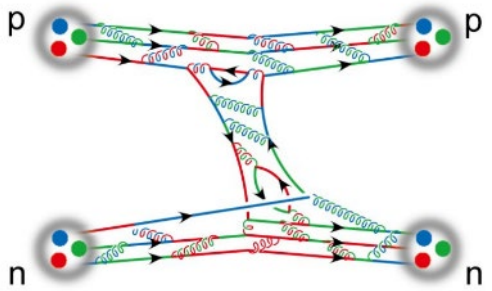
Based on papers in preparation

Together with Evgeny Epelbaum (RUB)

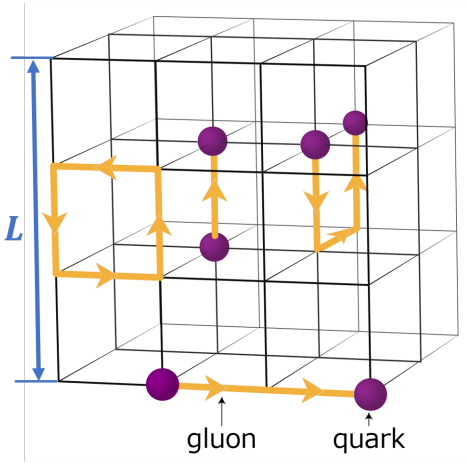
Hadron-hadron interaction from LQCD

- QCD is the fundamental theory of the strong interaction

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



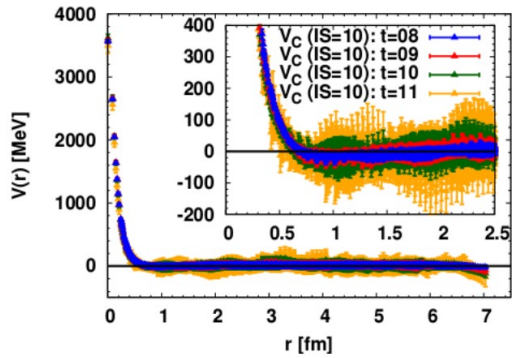
- How to extract two-hadron interaction or observable from lattice QCD?



- Energy level method: Lüscher's formula Luscher:1990ux
  - ▶ $E^{FV} \sim \delta(E^{FV})$

- HALQCD method or potential method Ishii:2006ec, Aoki:2009ji,Aoki:2012tk

Nambu-Bethe-Salpeter wave function (raw data) → Potential → Observables



  - ▶ Neither the wave functions in the interacting range nor the potential are the observables
  - ▶ Often criticized for **uncontrolled systematics**

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	$M_\pi \approx 800$ 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
3			

● Without bound NN (or inconclusive)

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

❑ 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/

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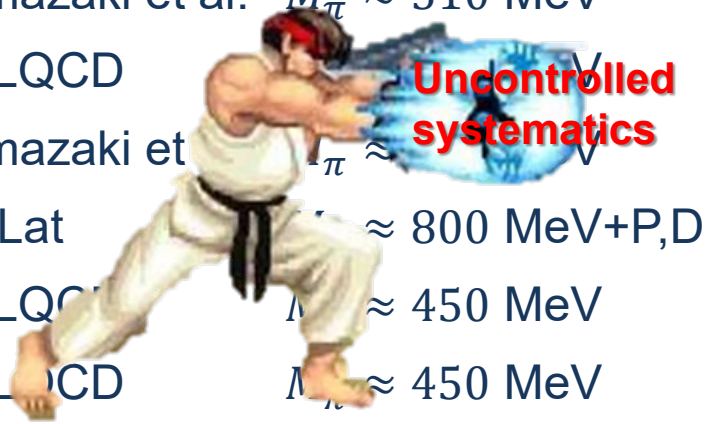

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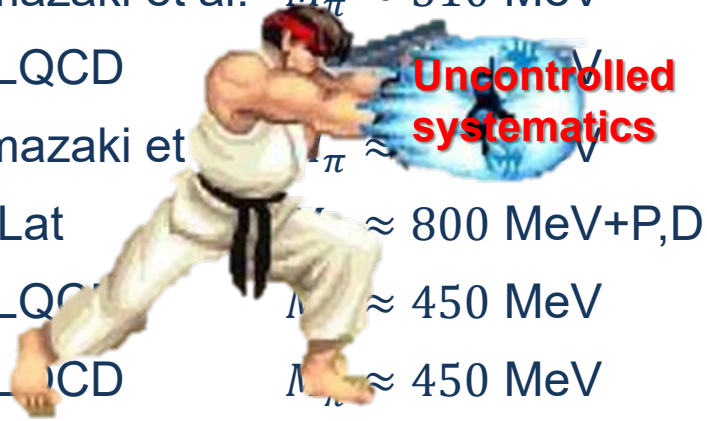

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Significance of the HALQCD method
To improve the understanding of the systematics of HALQCD

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

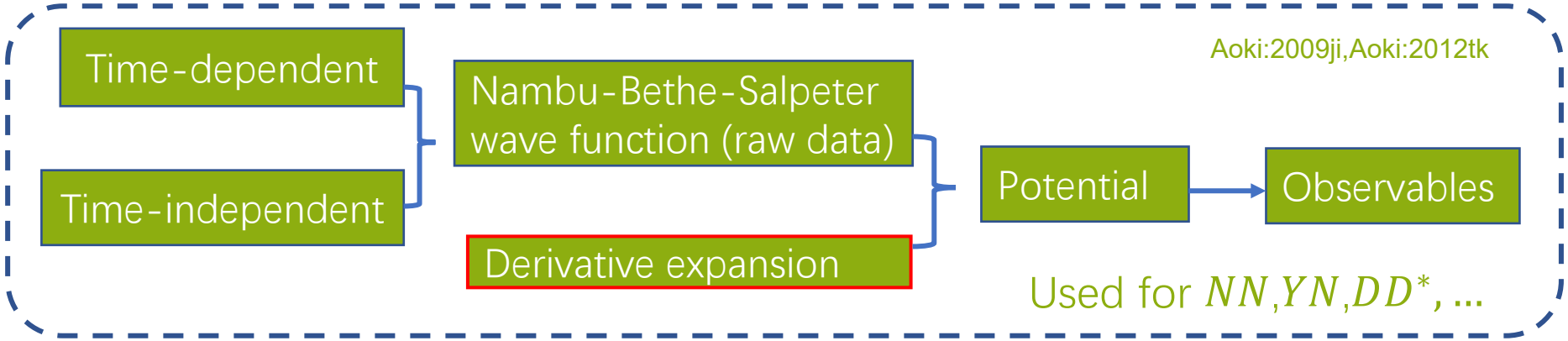
HALQCD method

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
- 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

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

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

Time-independent HAL QCD

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

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

  - ▶ 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**

- 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 $\boldsymbol{\delta(k_i)}$** 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 expansive to get the ground state saturation
- Time-dependent Schrödinger-type equation

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

- The general problem

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

- 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…

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

Modern views of potential

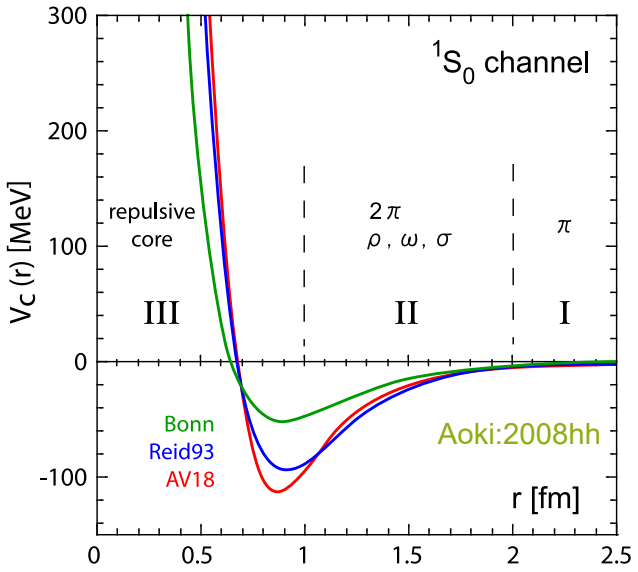
Modern views of potential

- There is no reason to rule out the nonlocal potential either in principle or phenomenologically
- Potential is not observable

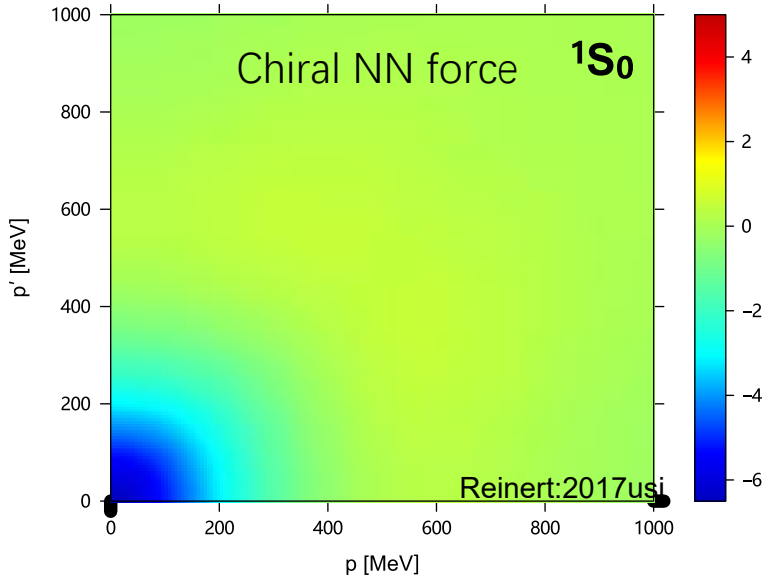
Bogner:2009bt

  - ▶ Cannot be determined uniquely by scattering experiments
  - ▶ Observable-equivalent potentials are related by unitary trans. (UT) or field redefinition
  - ▶ UT can relate local potentials to nonlocal potentials

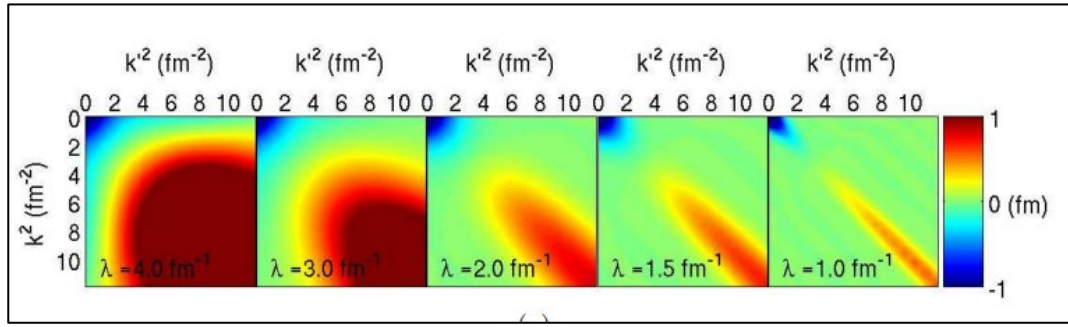
Ekstein:1960xkd



Local NN force



Nonlocal NN force



SRG evolution

- $V_{low,k}$ and Similarity renormalization group (SRG)

Modern views of potential

- Non-observables
  - ▶ Non-asymptotic behavior of ψ, e.g. the deuteron D-state probability

    Amghar:1995av
  - ▶ Off-shell T-matrix
  - ▶ Potential
- Observables
  - ▶ Asymptotic behavior of ψ
  - ▶ Phase shift
  - ▶ On-shell T-matrix

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 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

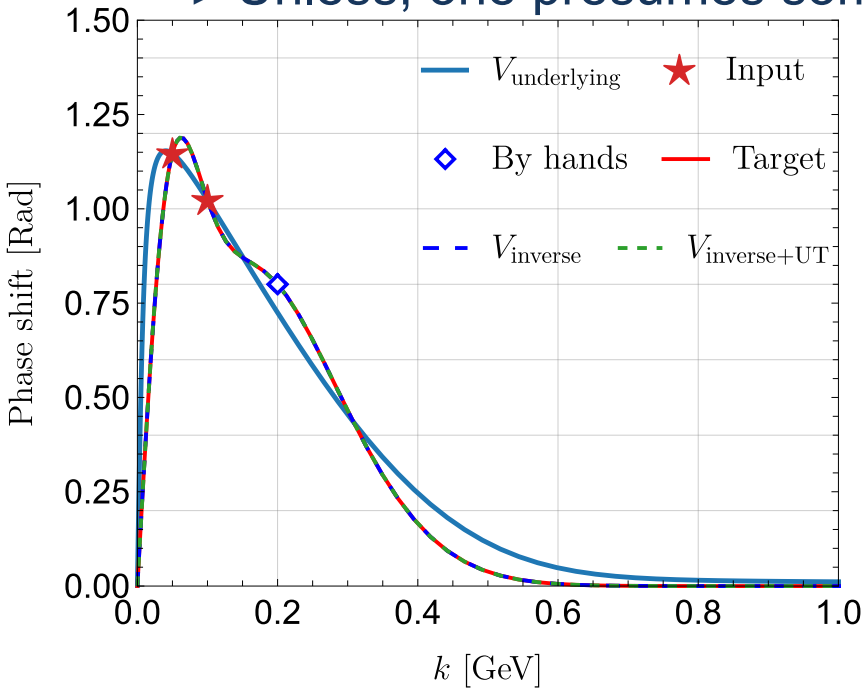
- From a small number of the wave functions, the potential can not be determined uniquely
  - ▶ Think it in a discrete way

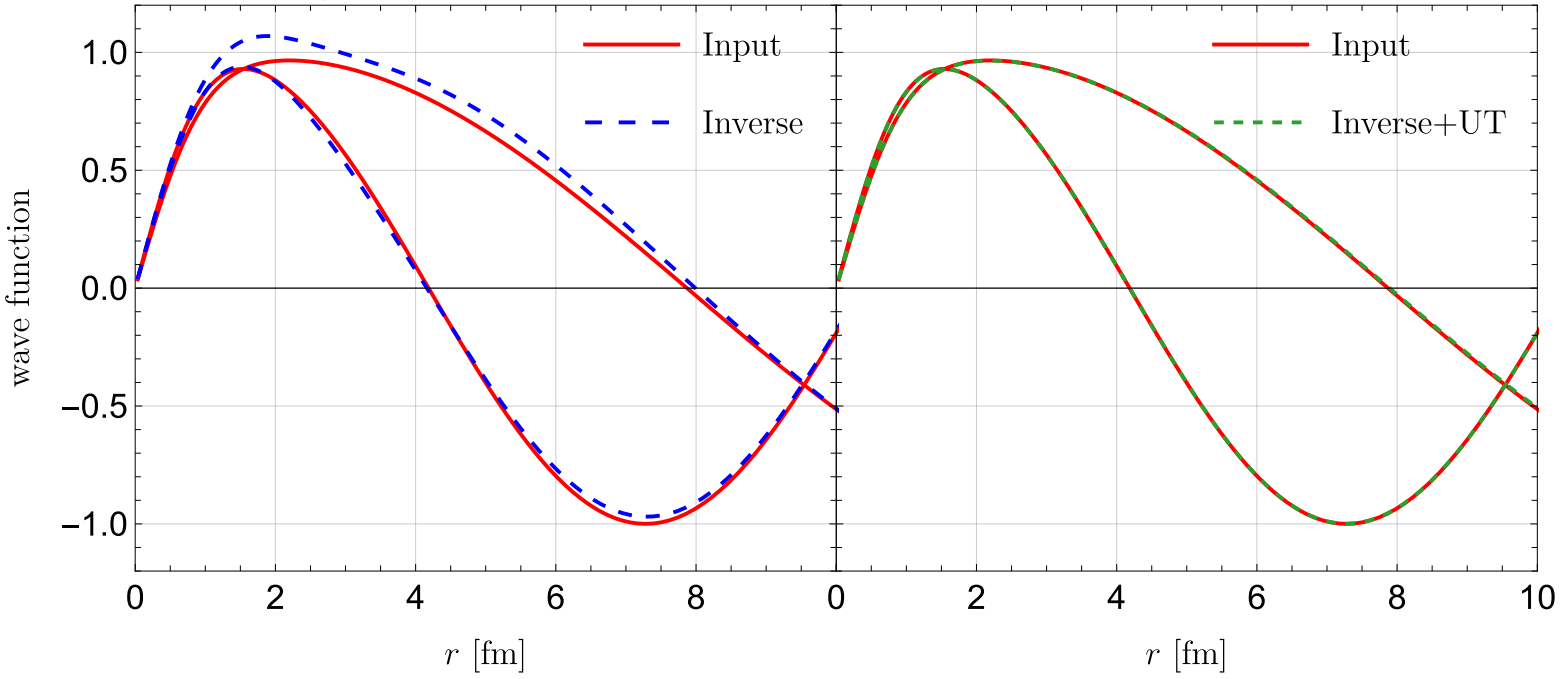
$$\int dr' V(r,r') R^{(i)}(r) = K^{(i)}(r) \Rightarrow \mathbb{V}_{N\times N} R^{(i)}_{N\times 1} = K^{(i)}_{N\times 1}$$

  - ▶ 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

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





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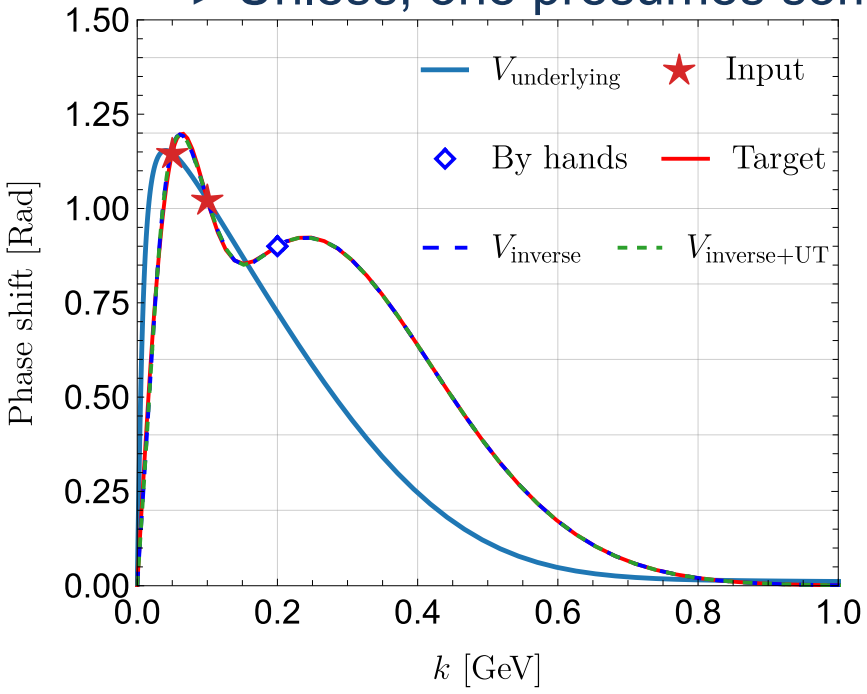

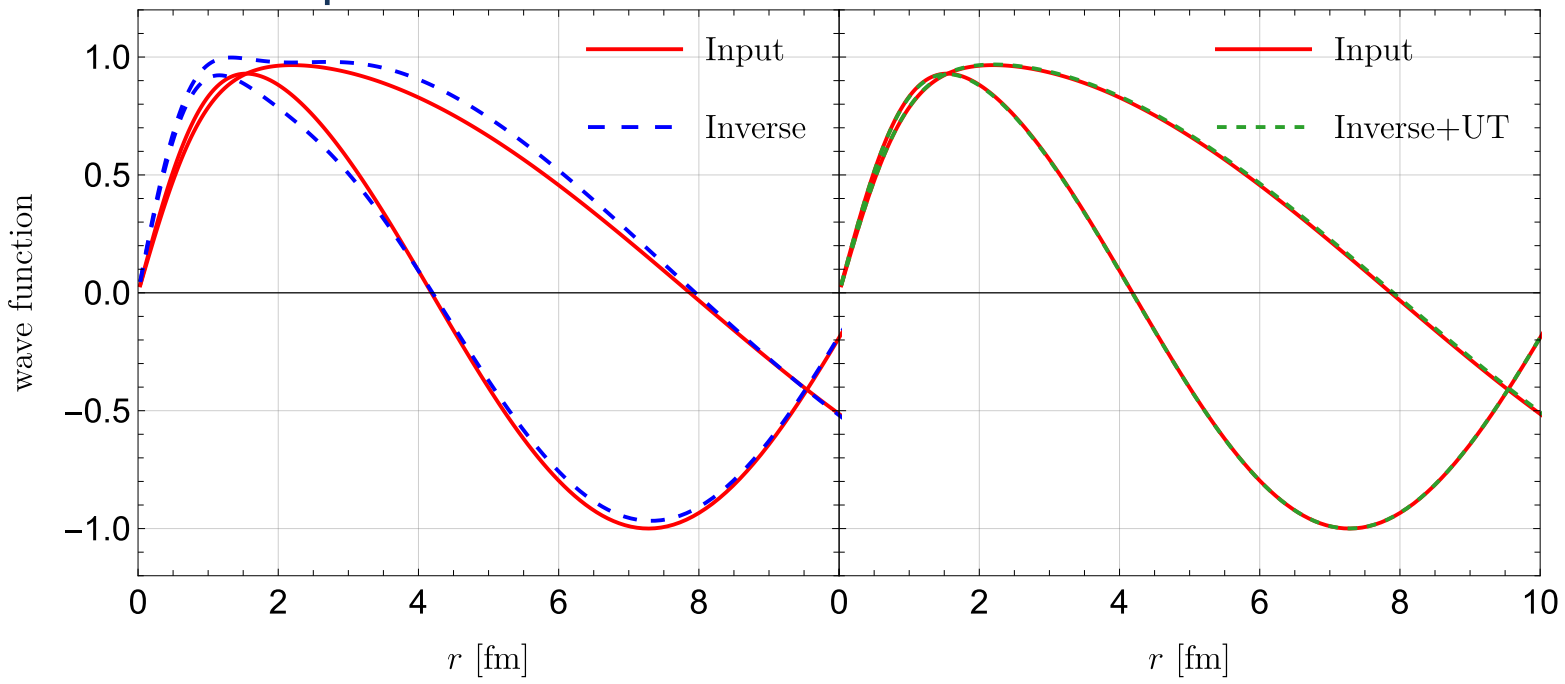

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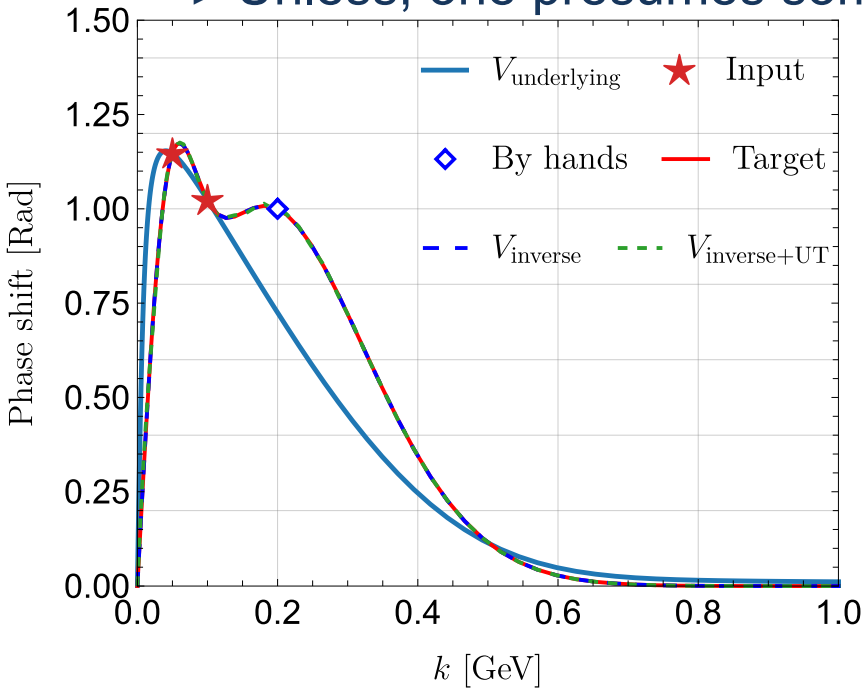
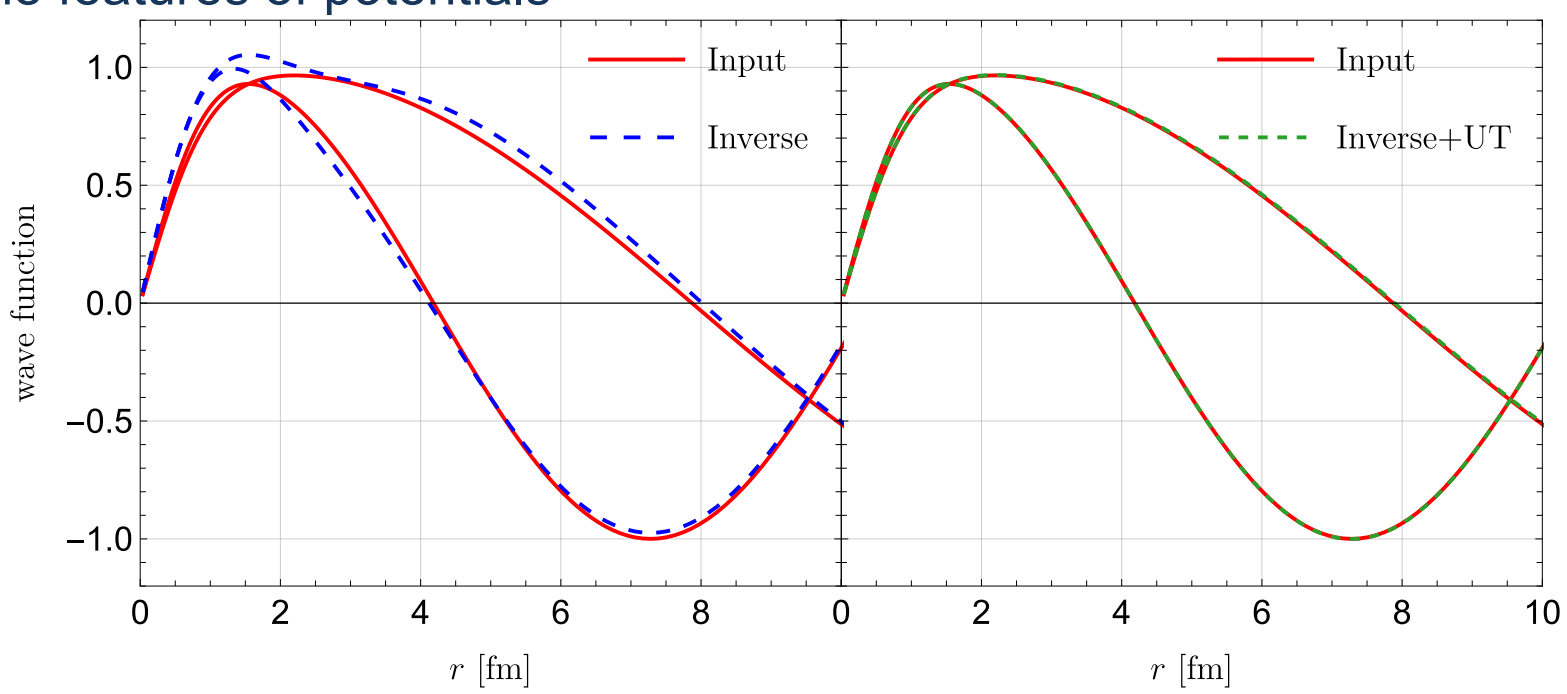




Derivative expansion VS EST expansion

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

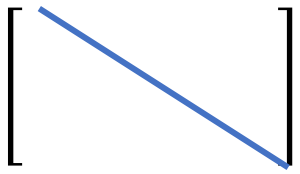
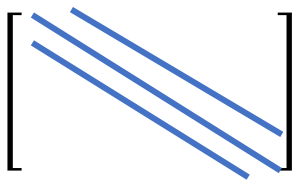
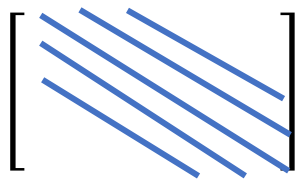
$$V_0(r)R^{(1)}(\vec{r}) = K^{(1)}(\vec{r}) \Rightarrow V_0(r) = \frac{K^{(1)}(\vec{r})}{R^{(1)}(\vec{r})}$$

- 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,

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

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

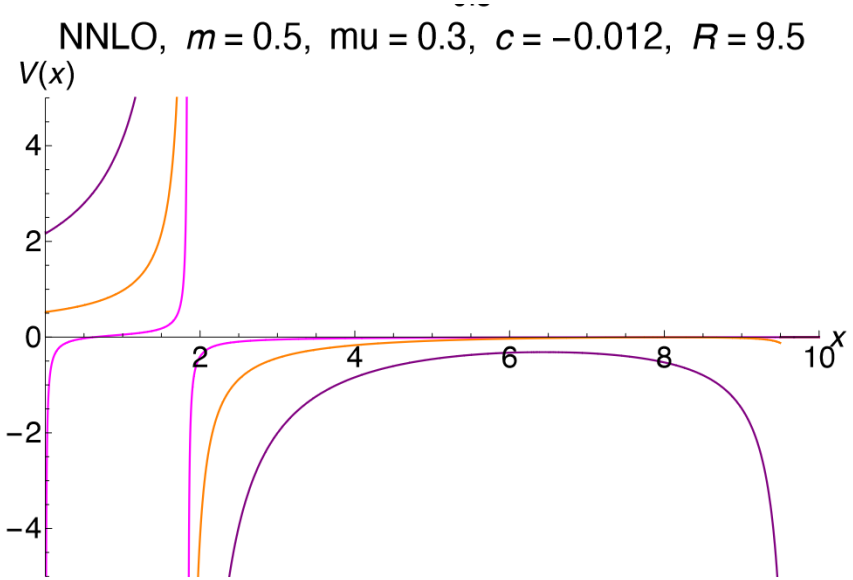
  - ▶ The band width become wider

Singular potential

- NLO derivative expansion

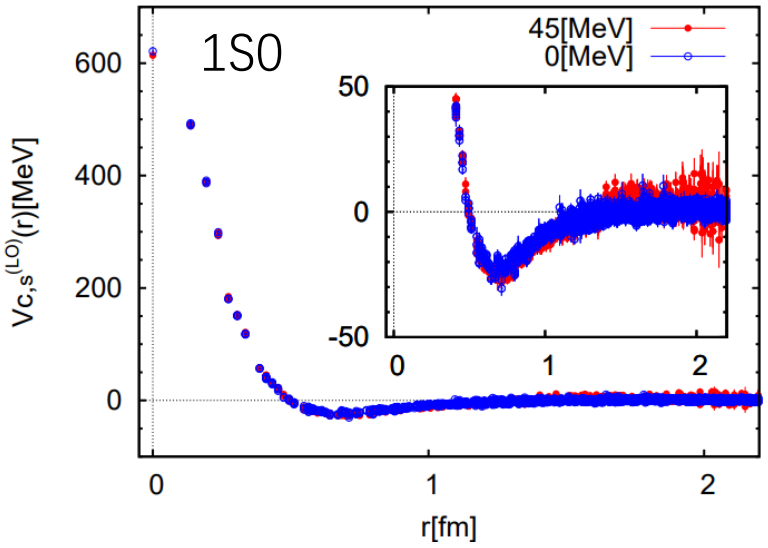
$$\begin{pmatrix} R^{(1)}(r) & \frac{d^2}{dr^2}R^{(1)}(r) \\ R^{(2)}(r) & \frac{d^2}{dr^2}R^{(2)}(r) \end{pmatrix} \begin{pmatrix} V_0(r) \\ V_1(r) \end{pmatrix} = \begin{pmatrix} K^{(1)}(r) \\ K^{(1)}(r) \end{pmatrix}$$

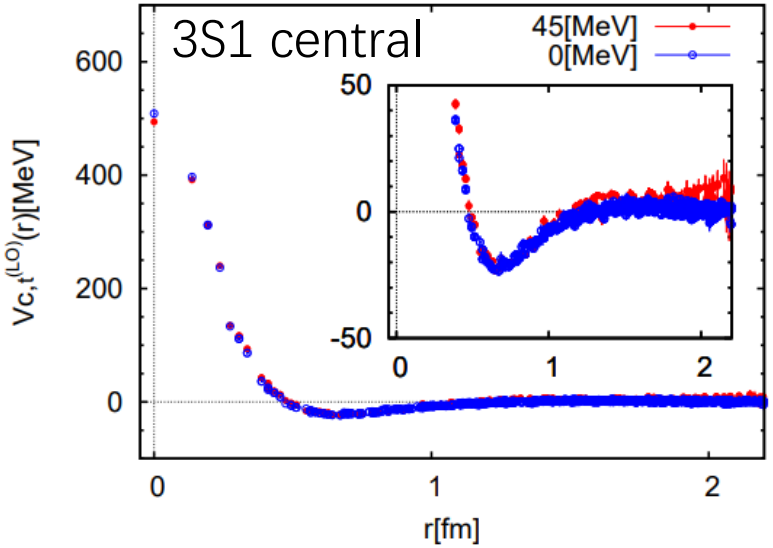
- The potential become singular at the zero of det of the coefficients matrix
- A example from toy model Aoki:2021ahj
  - ▶ In simulation, it is challenging to handle the singularity
  - ▶ Wave functions are obtained at discrete point.

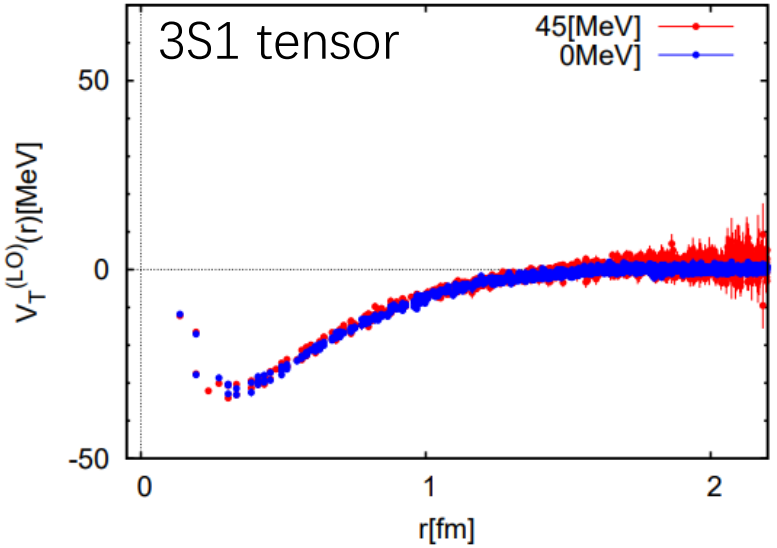


Locality of the potential

- 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







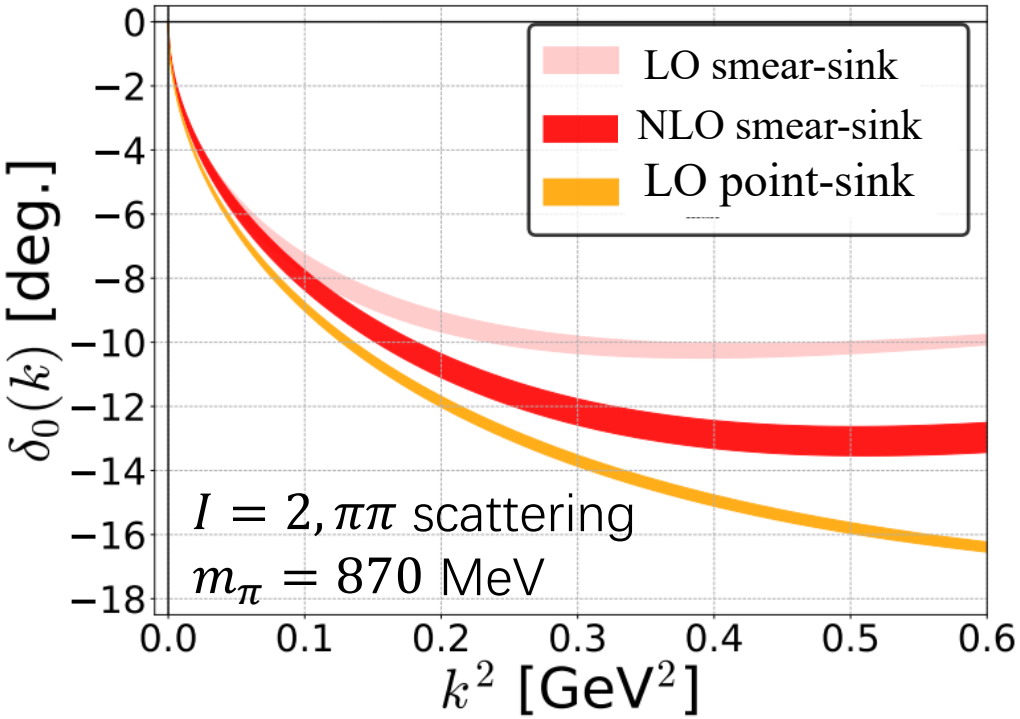
- Point-sink scheme used by HAL QCD group
  - ▶ Very local “underlying” potential, fast convergence of the DE

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: $V|R^{(i)}\rangle = |K^{(i)}\rangle$
- Separable representation I: Aoki:2009ji

$$V = \sum_{ij} C_{ij} |K^{(i)}\rangle\langle R^{(j)}|, \quad C_{im}\langle R^{(m)}|R^{(j)}\rangle = \delta_{ij}$$

  - ▶ Bad performance
  - ▶ In the outer region: $K^{(i)}(r) = (\frac{d^2}{dr^2} + k_i^2)\psi_{k_i}(r) = 0\,, \;\; R^{(i)}(r) = \psi_{k_i}(r) \neq 0$
- Separable representation II, Ernst-Shakin-Thaler (EST) method

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

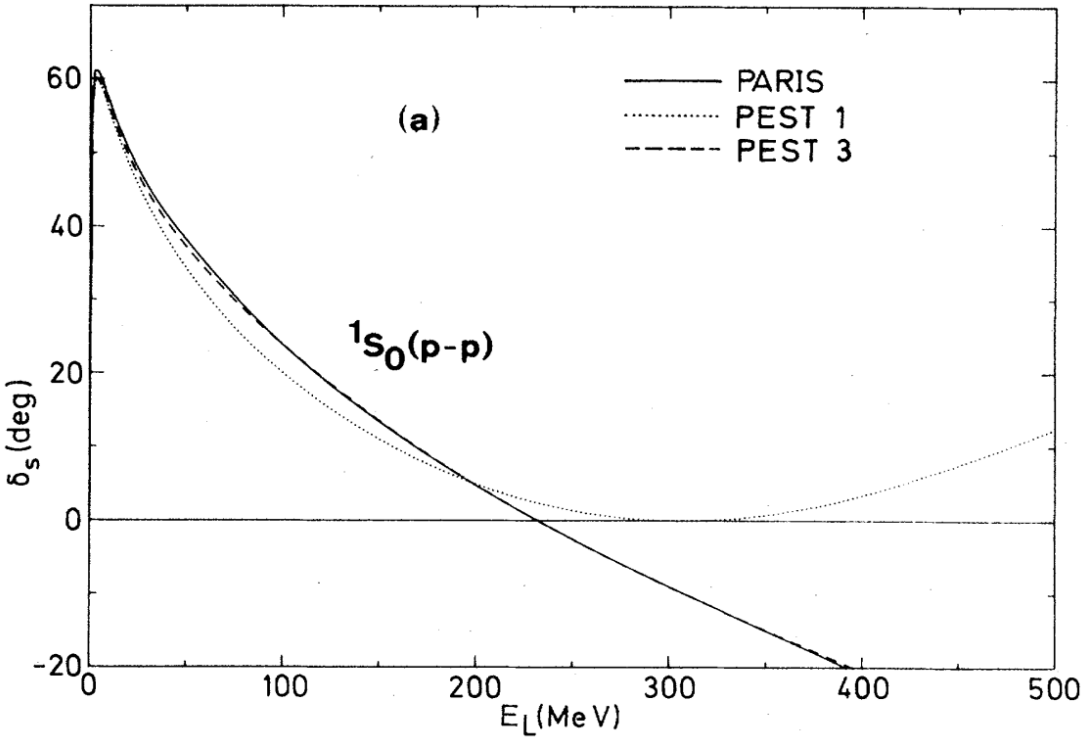
  - ▶ In the outer region: $K^{(i)}(r) = 0$

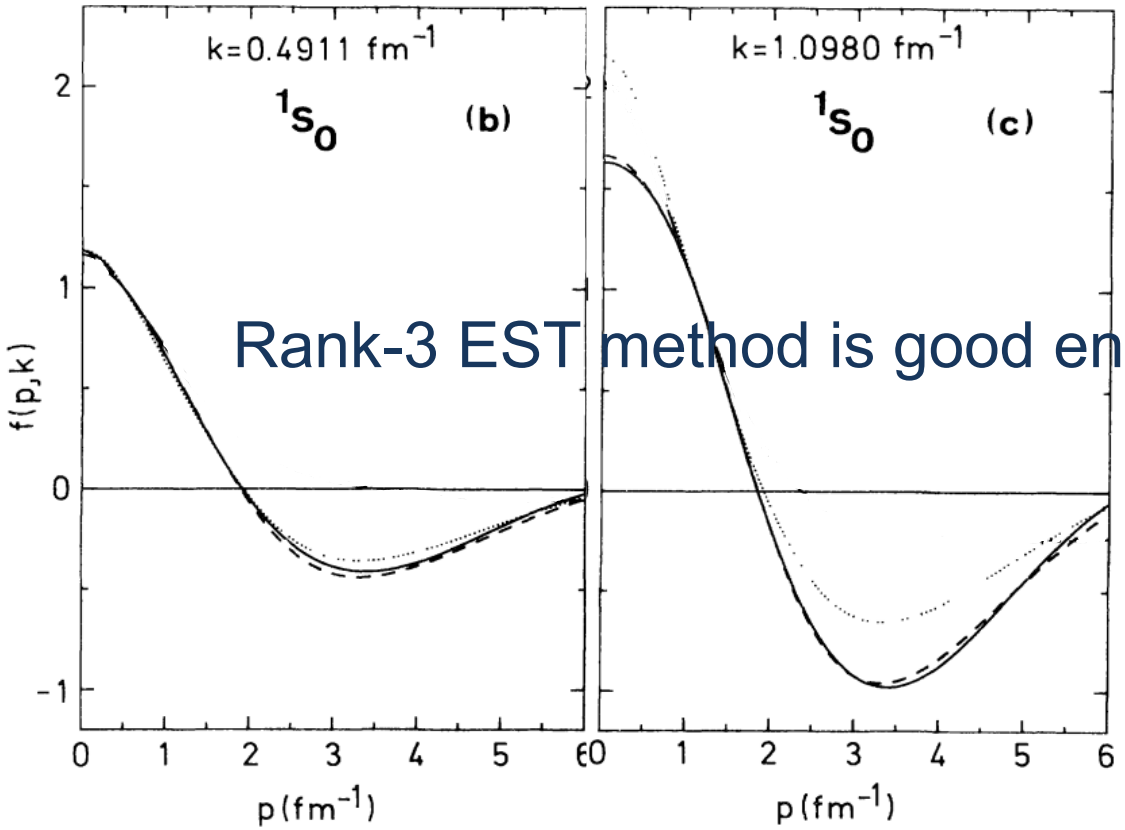
Ernst:1973zzb,Haidenbauer:1984dz

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

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

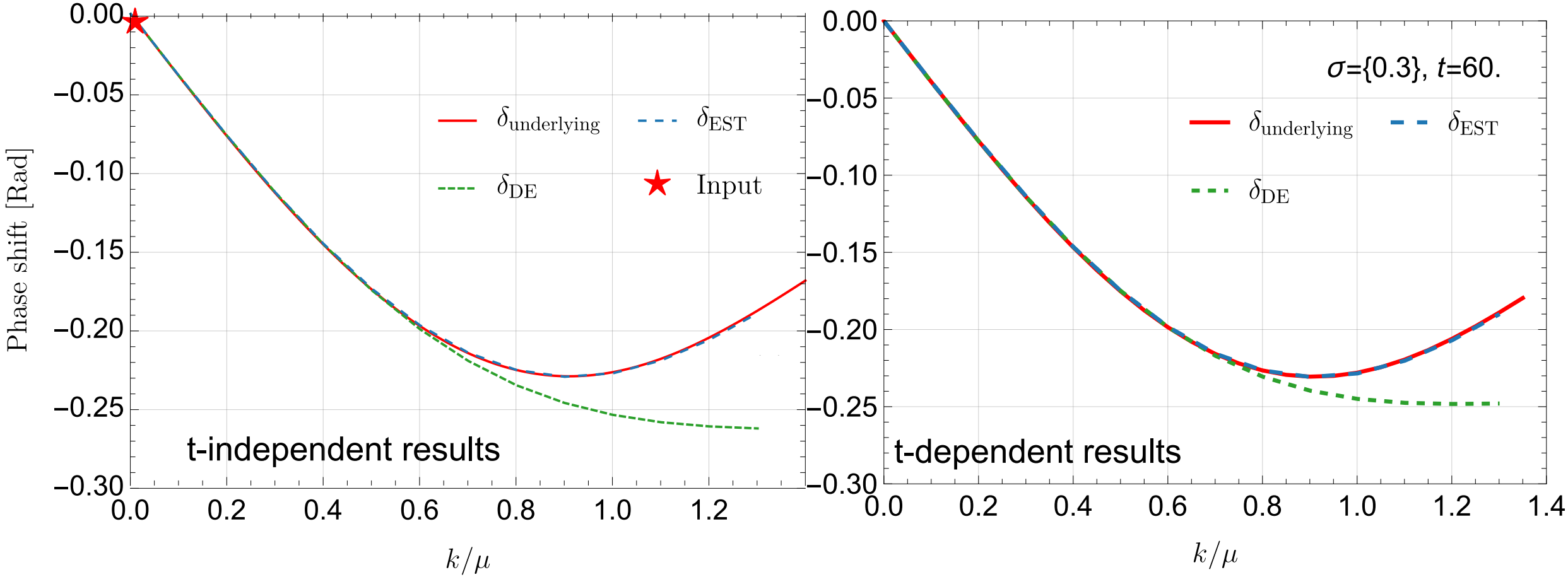
$$\tilde{R}(t=0,x) = \frac{\sigma^2 e^{-\sigma x}}{4\pi}$$

  - ▶ 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

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



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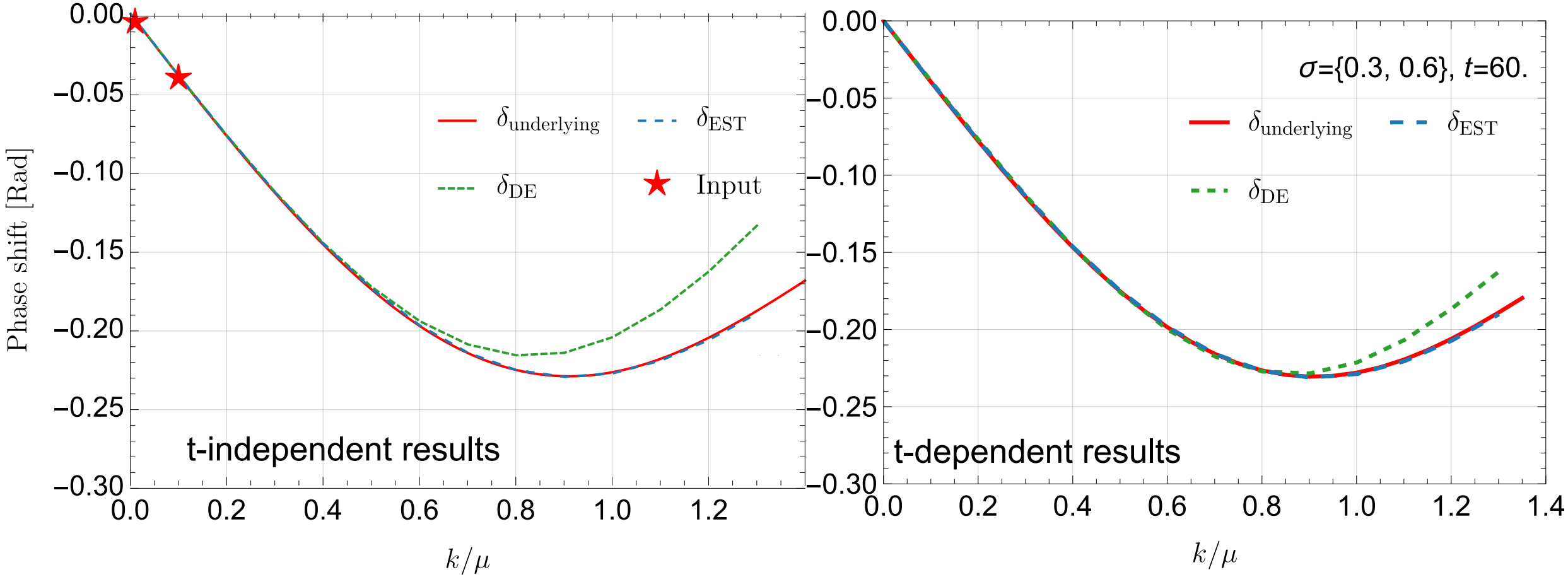

Physical interaction

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

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

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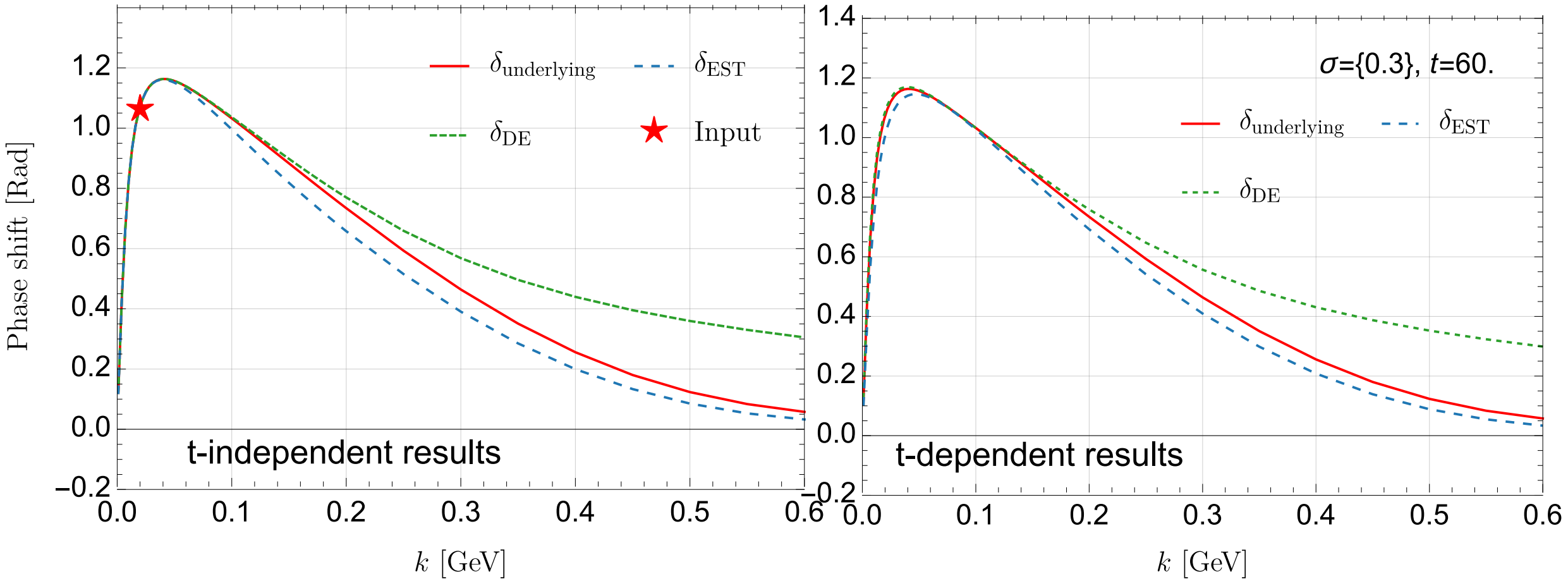

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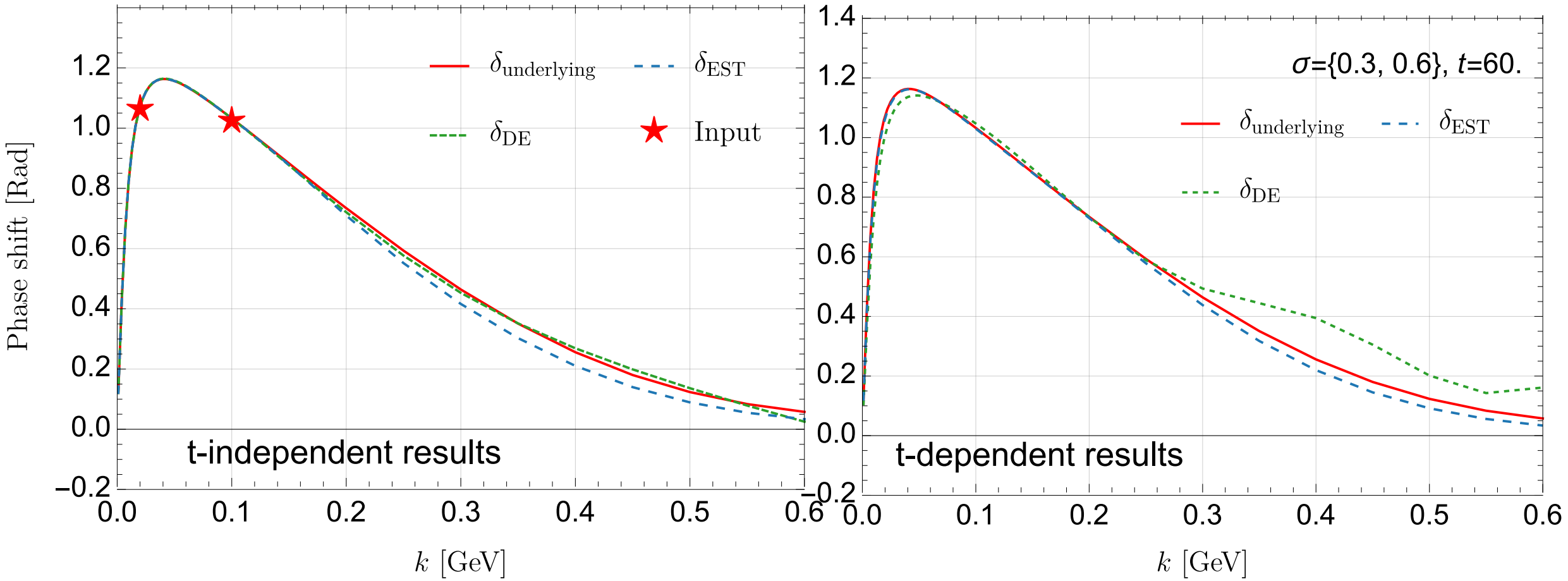
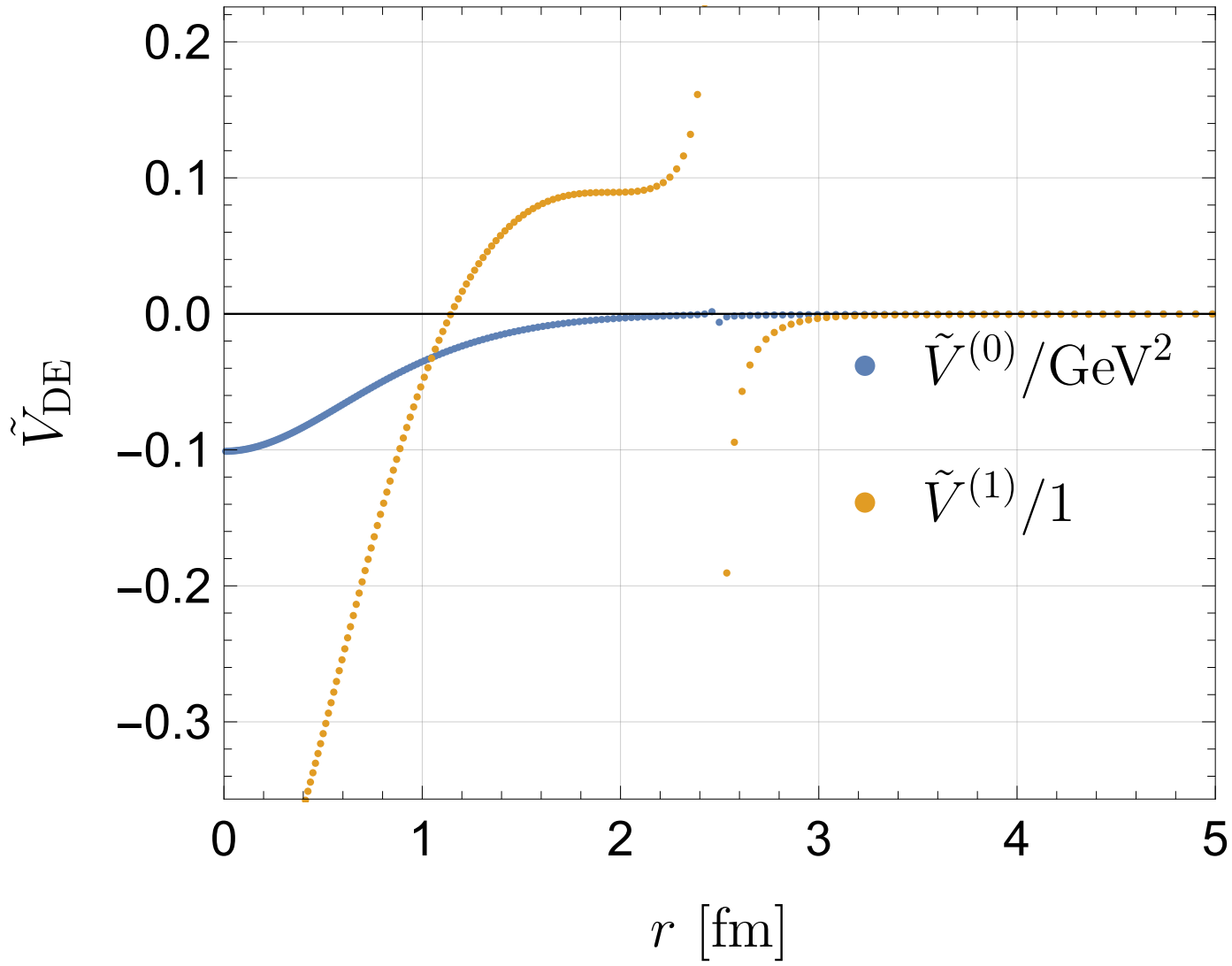


Singularity in potential



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

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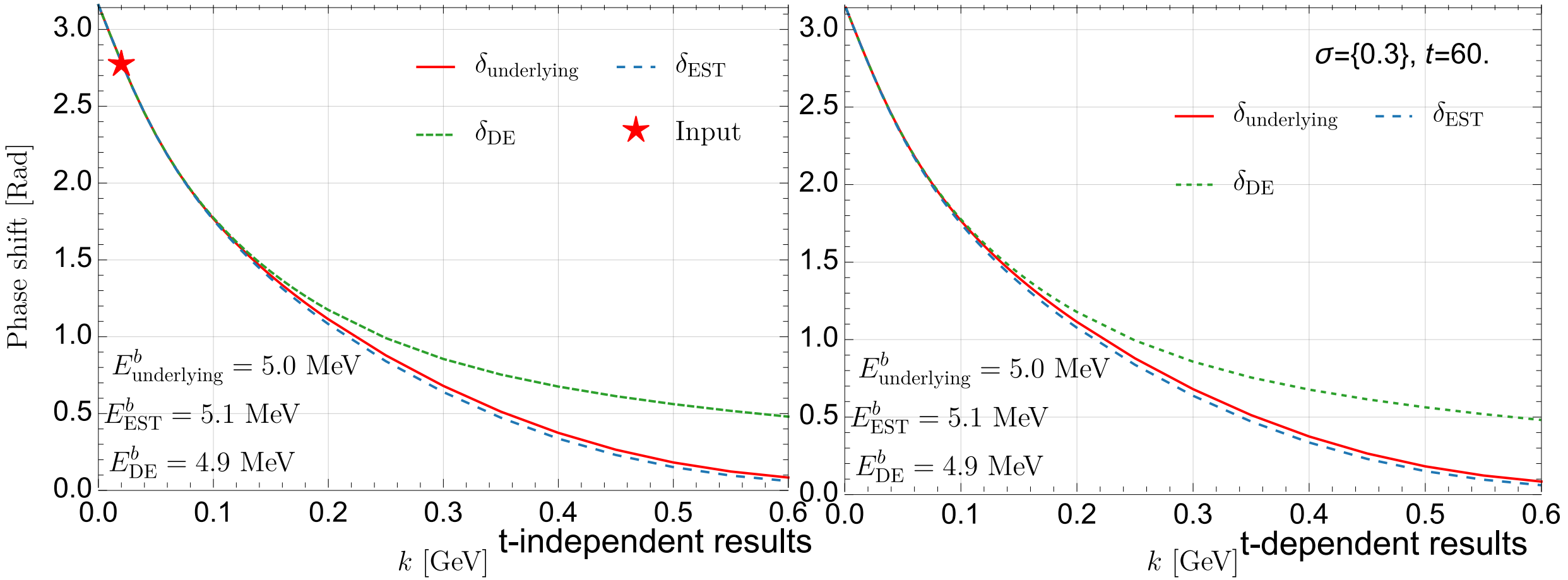

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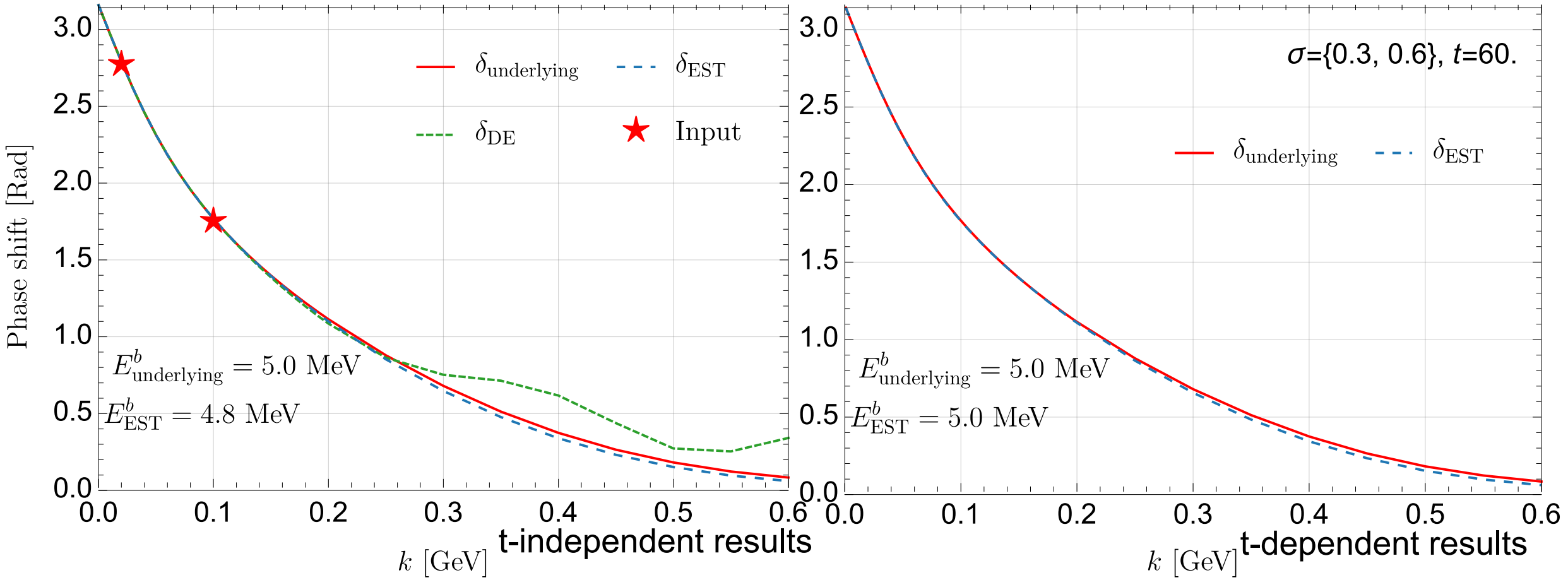

Local interaction

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

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

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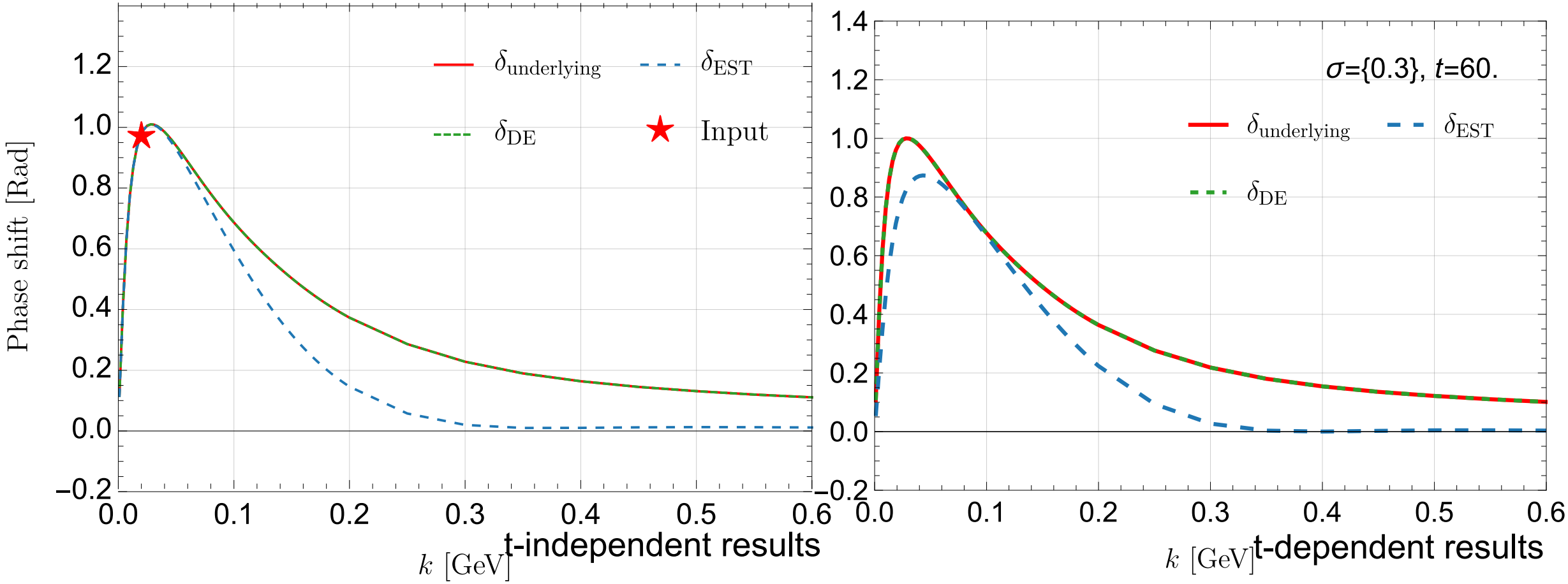

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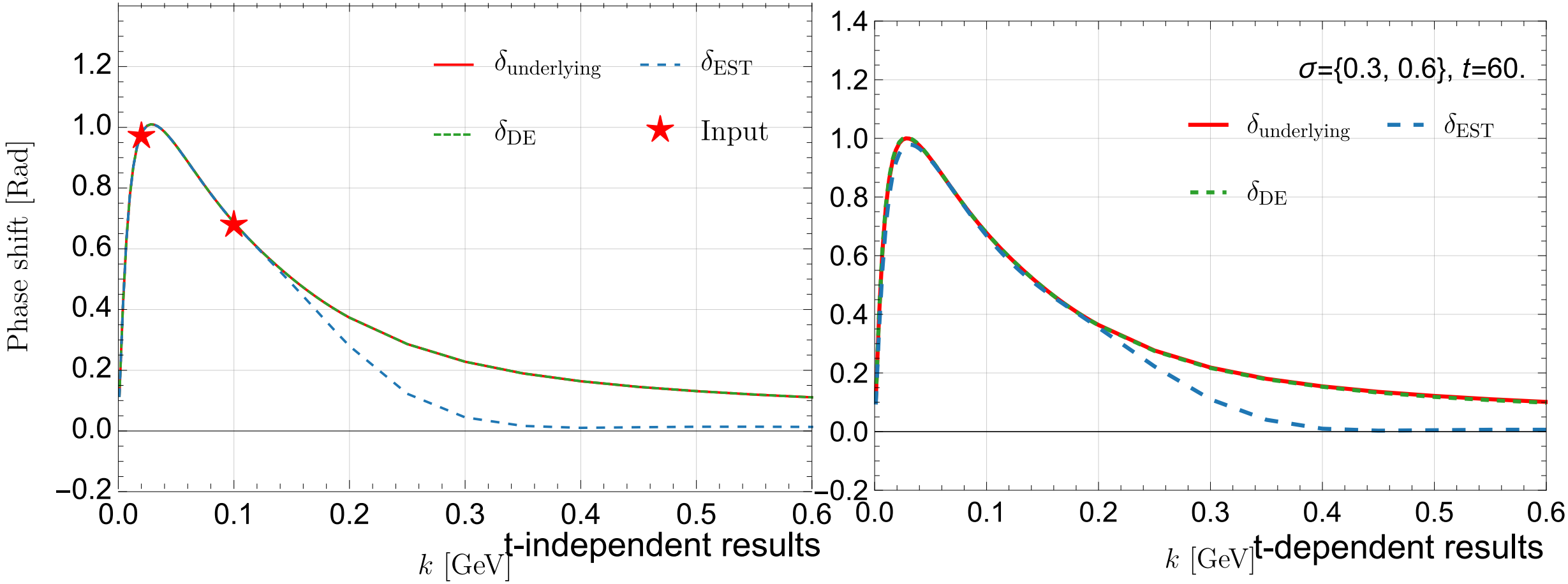
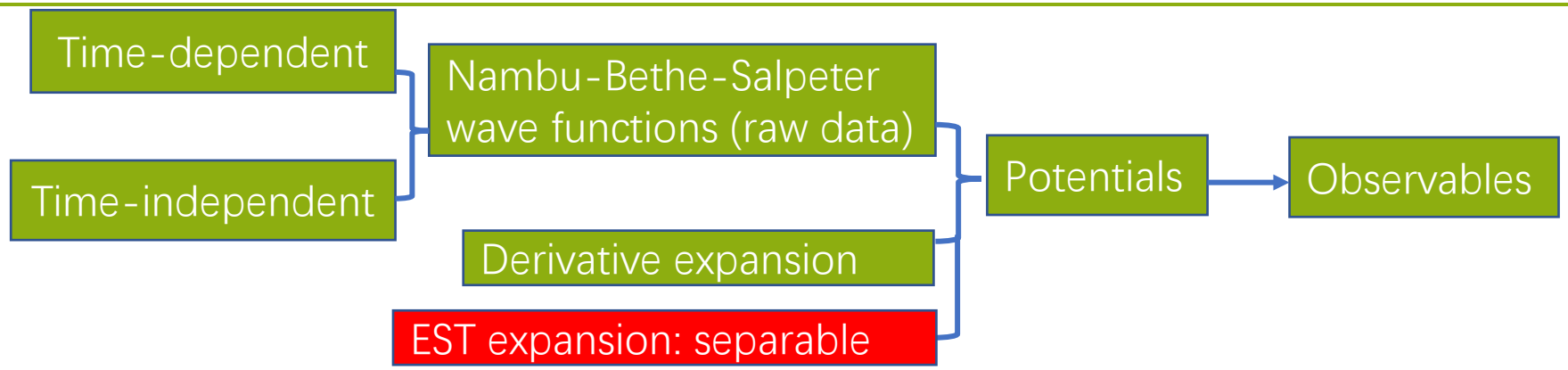


Summary



- 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
  - ▶ 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

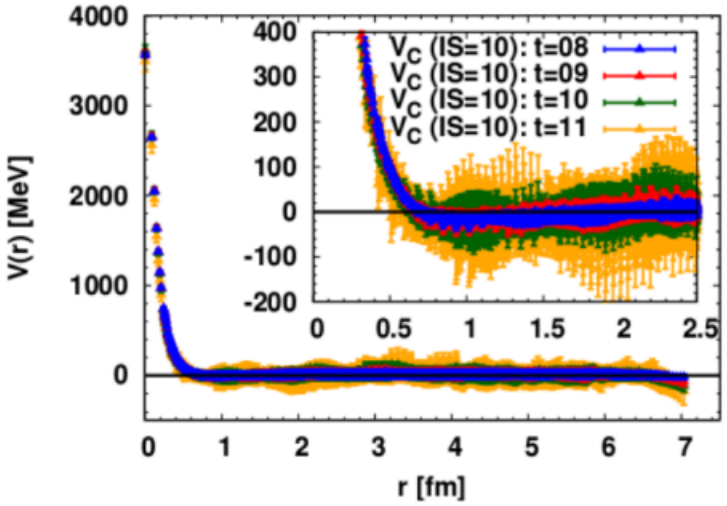
Highlight of HALQCD results: NN interaction

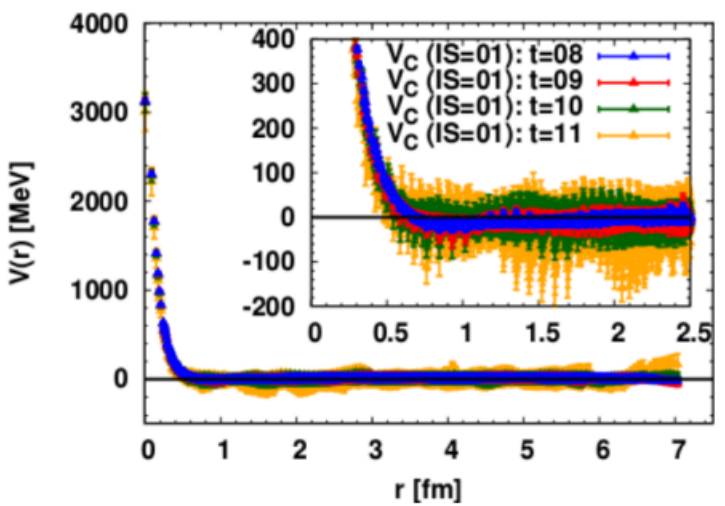
- lattice Setting: $m_\pi = 146$ MeV, $m_K = 525$ MeV, $a = 0.0846$fm, $L = 8.1$fm, 96^4

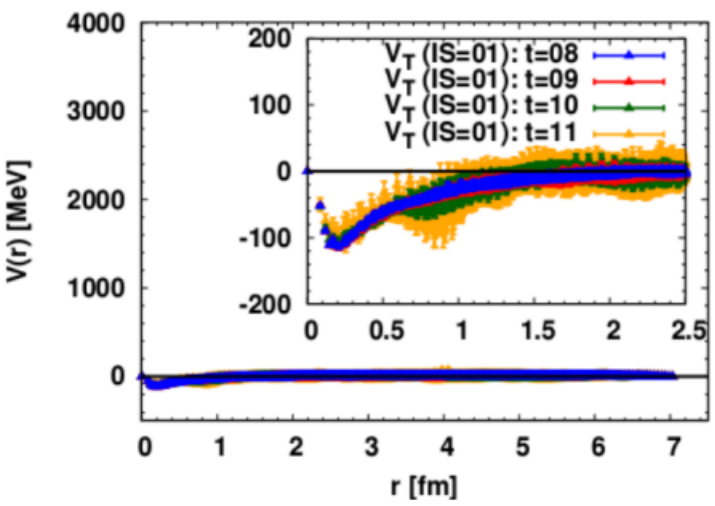
  $\Rightarrow$ Almost physical pion mass, very large box size, the finite volume effect is neglected

  $\Rightarrow$ 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

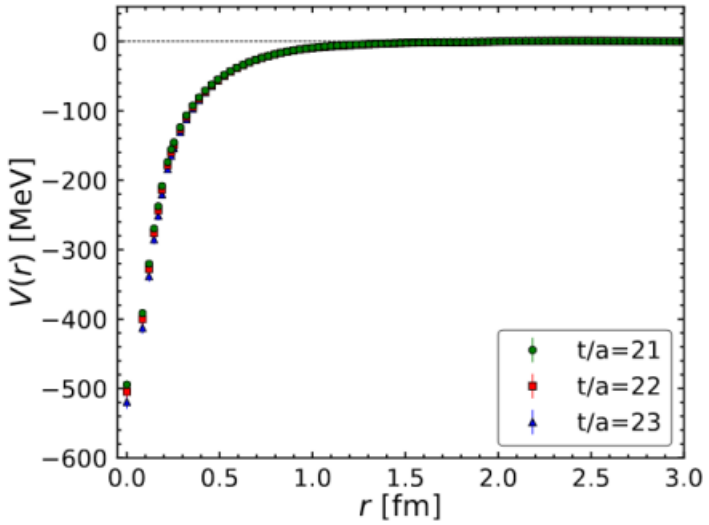
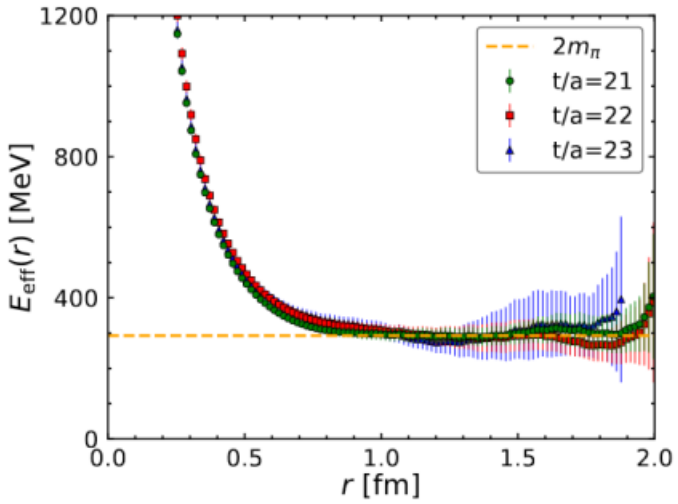


FIG. 2. The D^*D potential $V(r)$ in the $I = 0$ and S-wave channel at Euclidean time $t/a = 21$ (green circles), 22 (red squares), and 23 (blue triangles).



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

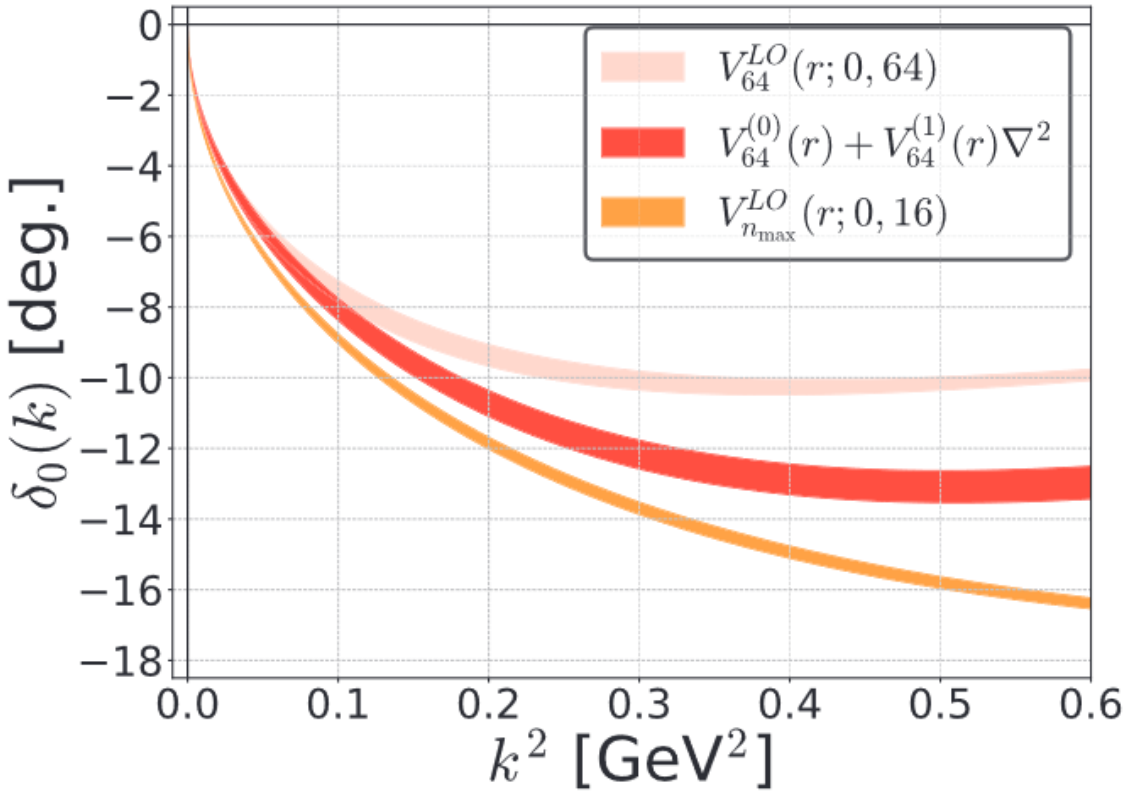


Fig. 5. The phase shifts of the S-wave $I = 2$ $\pi\pi$ scattering from the potential in the point-sink scheme (LO: orange) and the smeared-sink scheme (LO: pink, NLO: red) as a function of k^2.

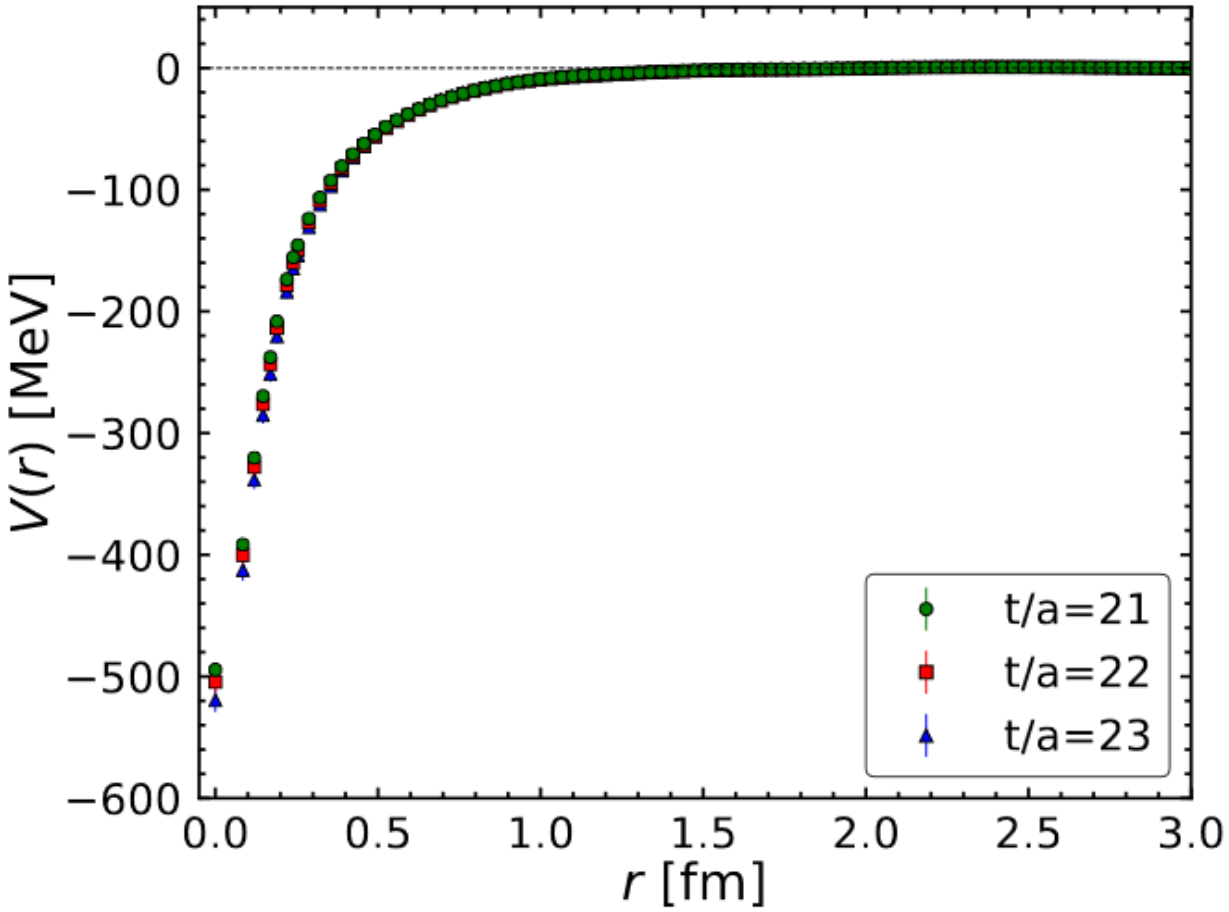
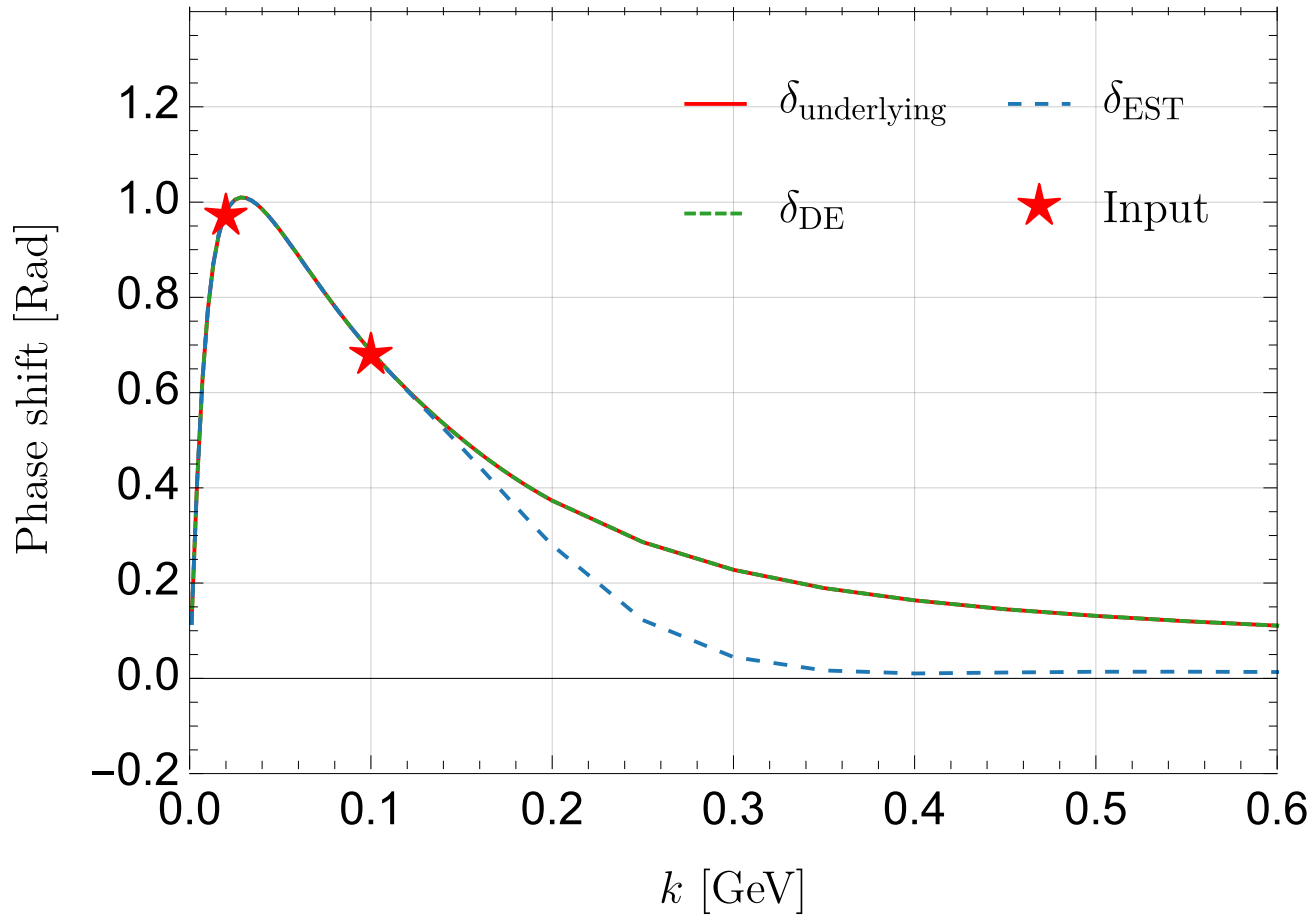


FIG. 2. The D^*D potential $V(r)$ in the $I = 0$ and S-wave channel at Euclidean time $t/a = 21$ (green circles), 22 (red squares), and 23 (blue triangles).

- 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

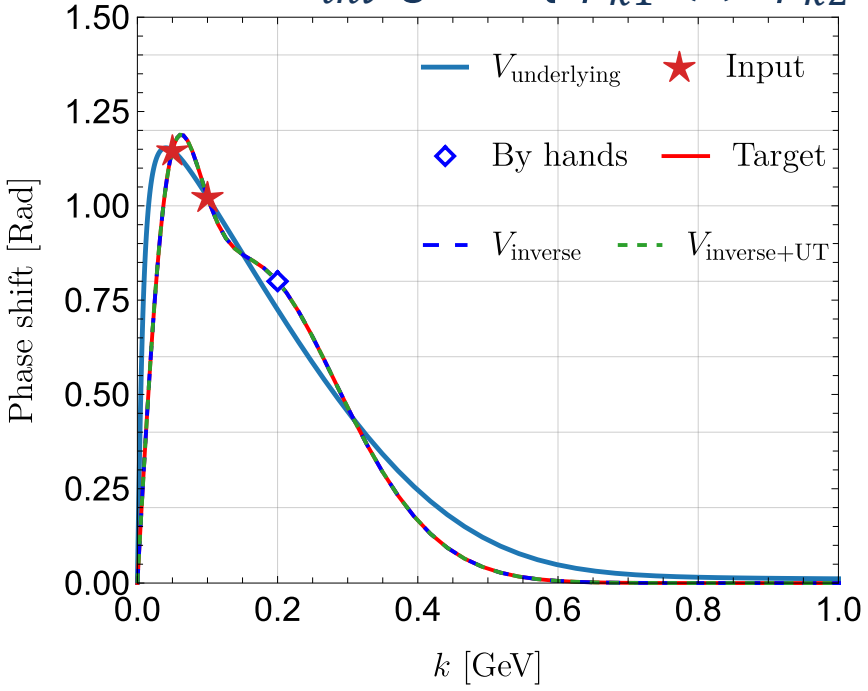


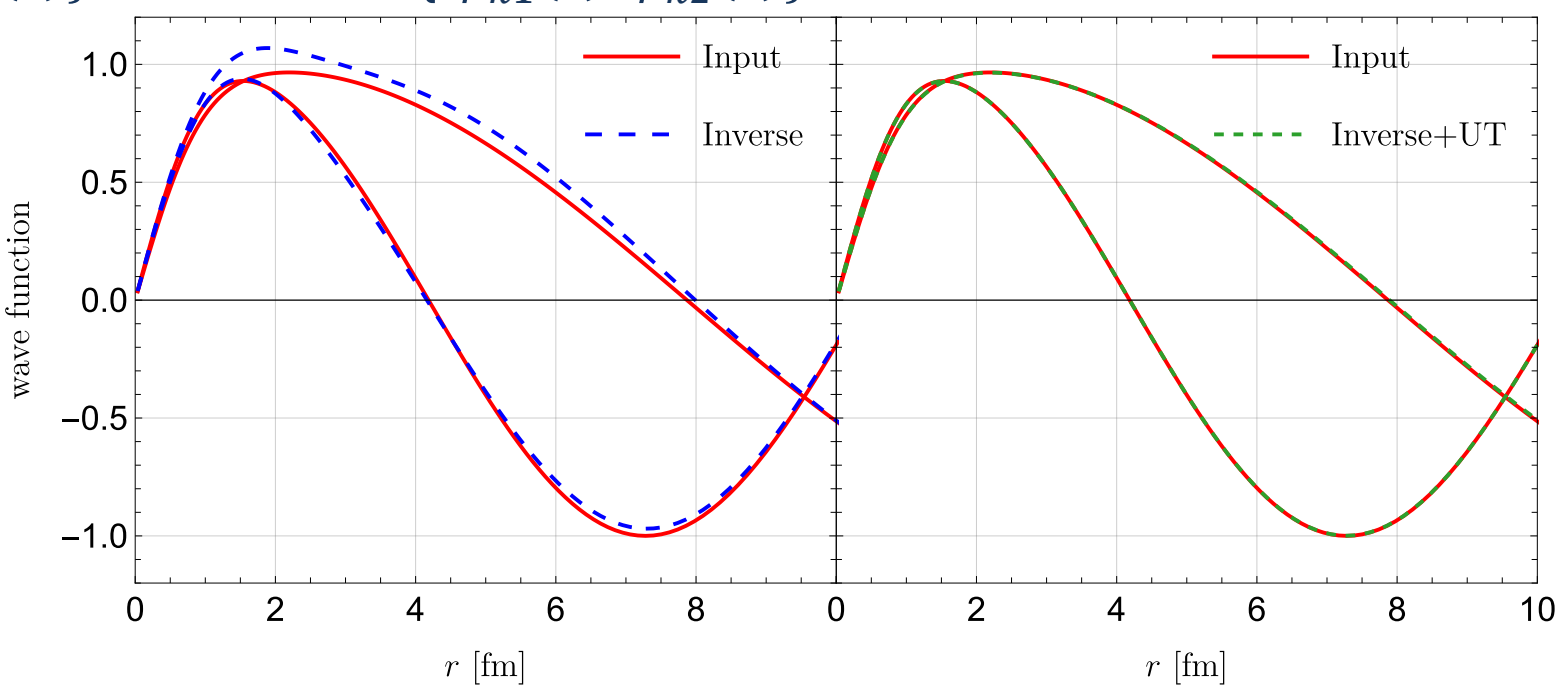
A small number of wave functions

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

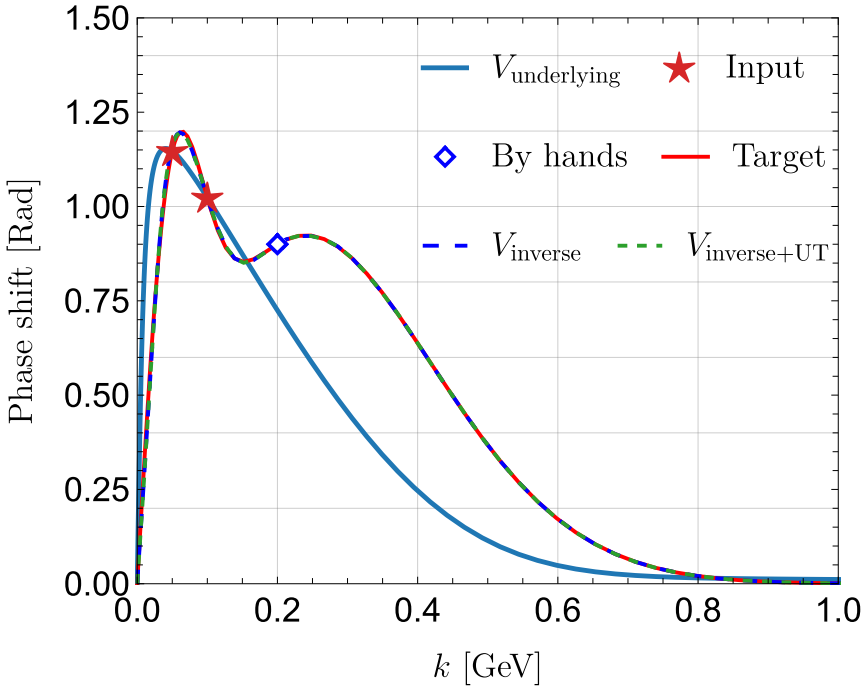
6. Construct an unitary trans. (UT): $U\left|\psi_{\mathrm{k}_i}^{inv}\right\rangle = \left|\psi_{k_i}\right\rangle$

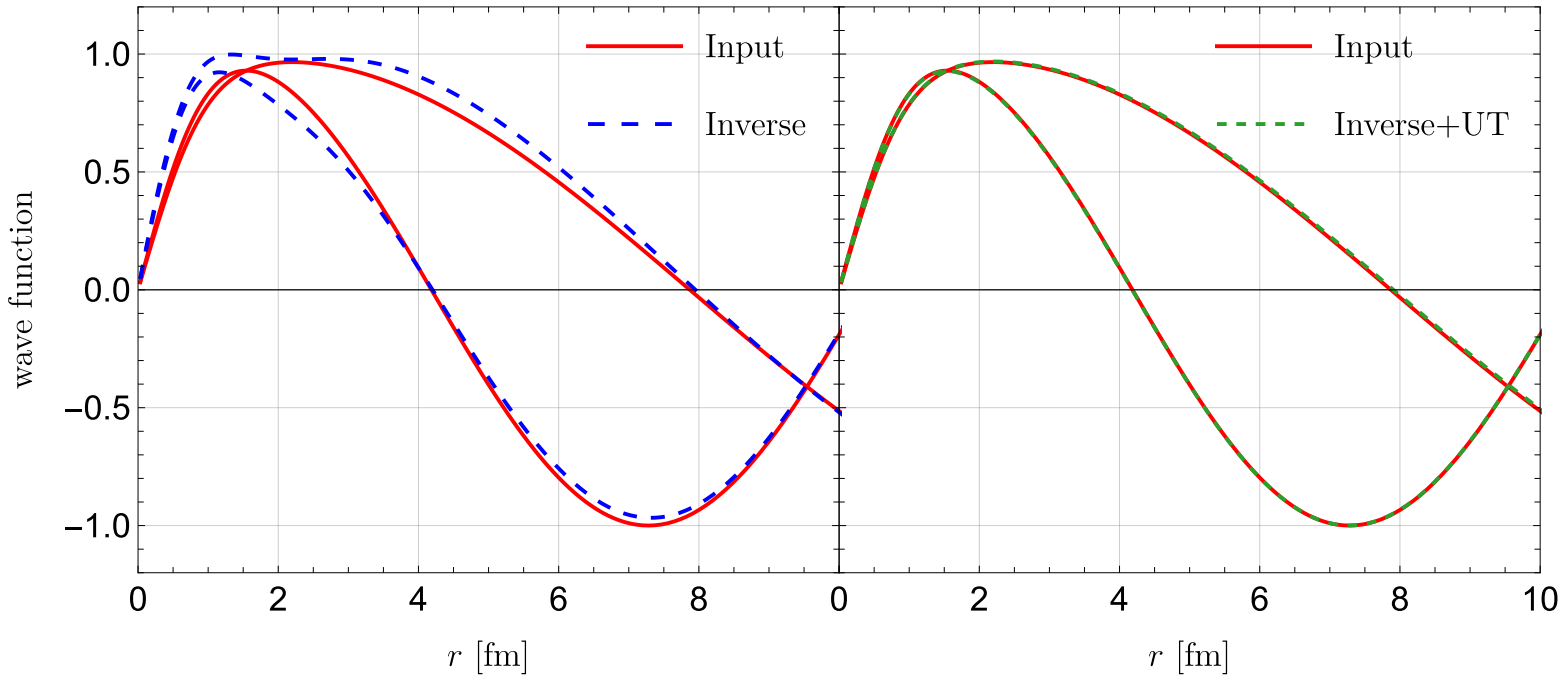
Ernst:1973utx

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

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

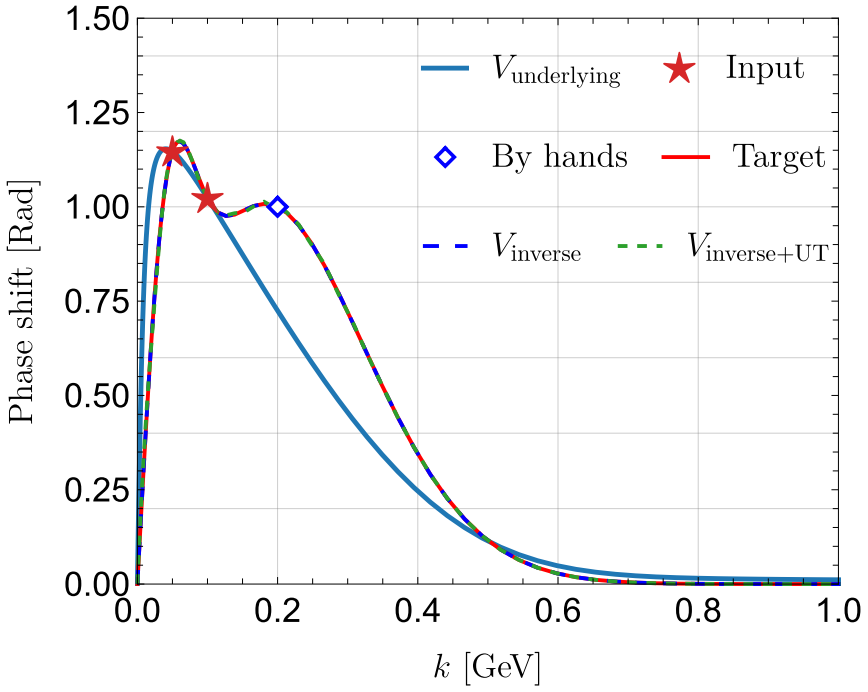
$$V^{inv+UT} = UV^{inv}U^{\dagger} + UH_0U^{\dagger} - H_0$$

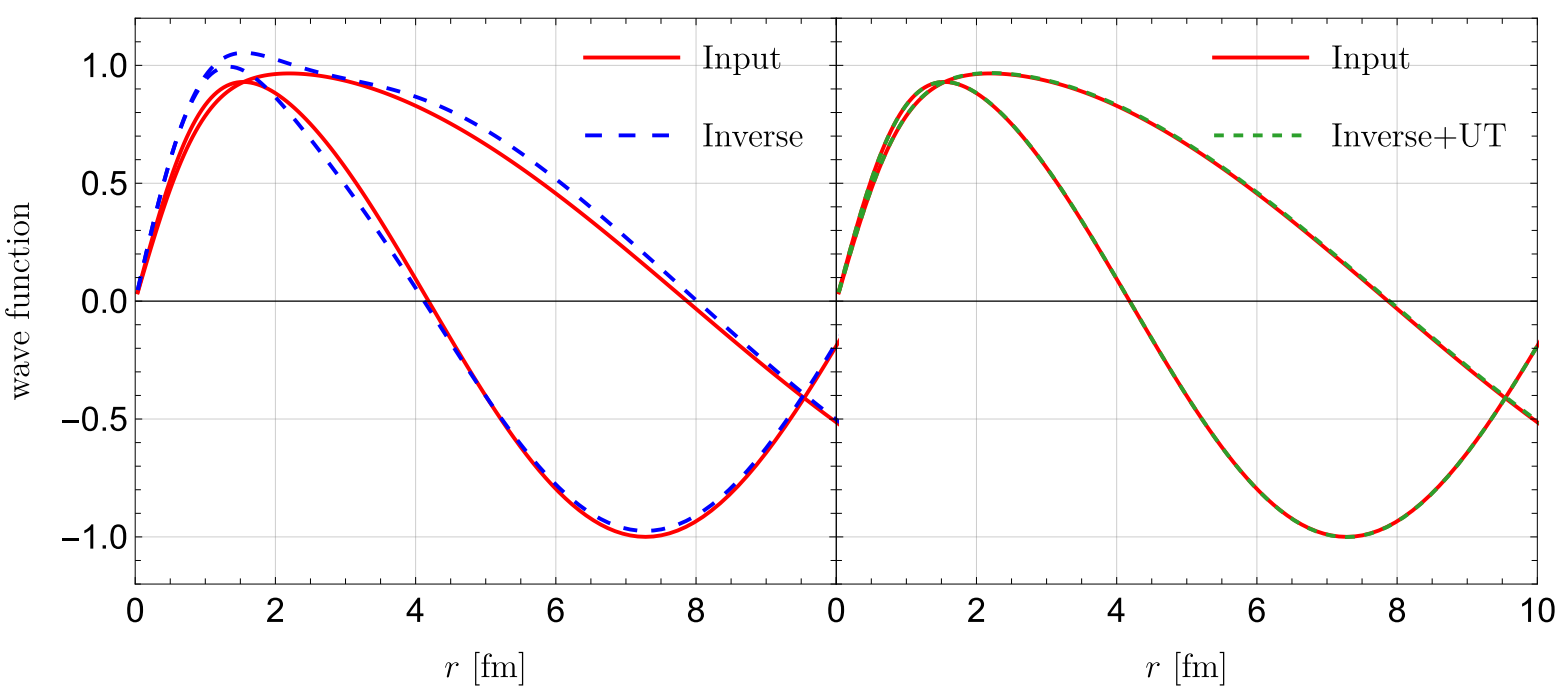


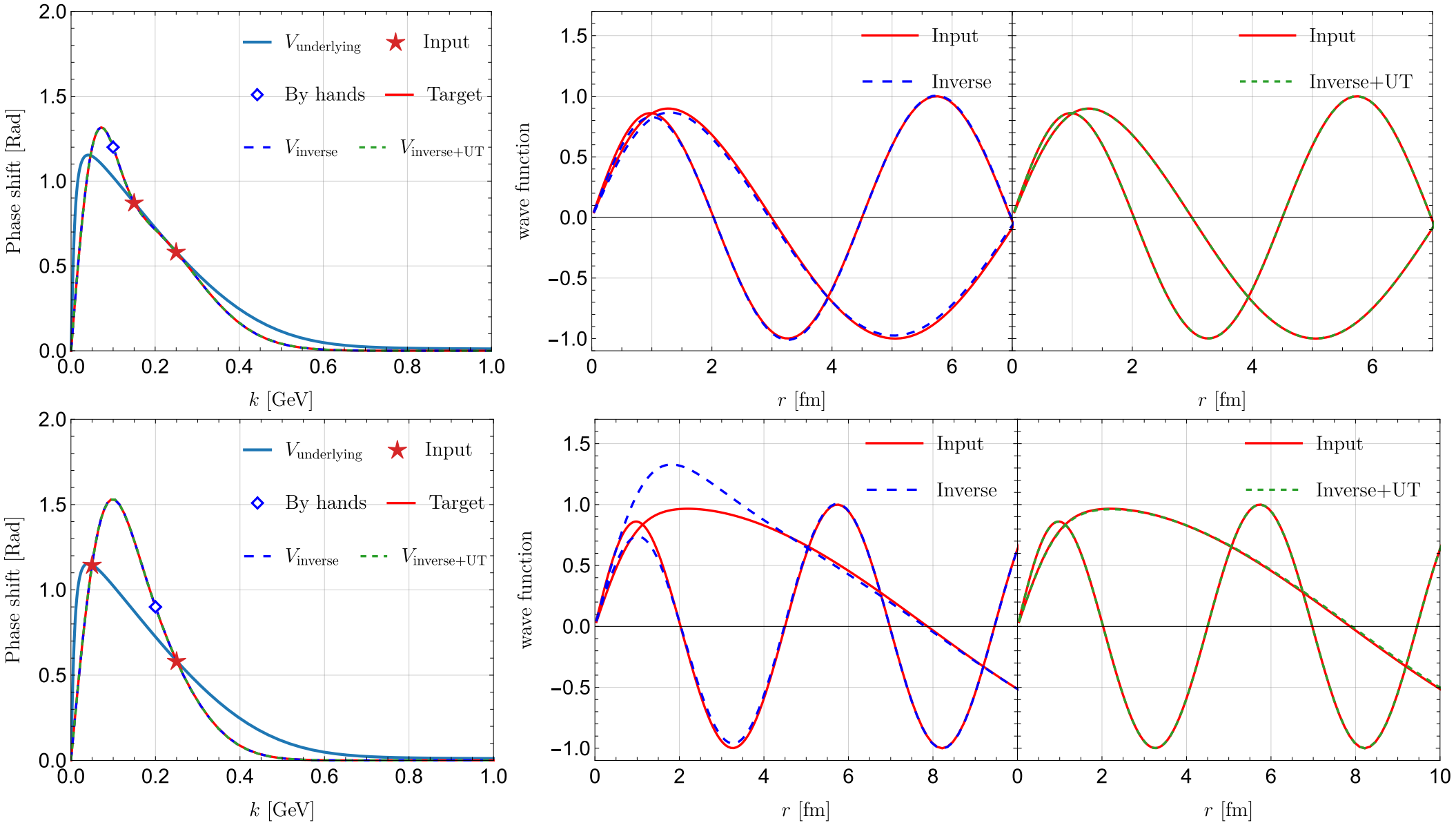


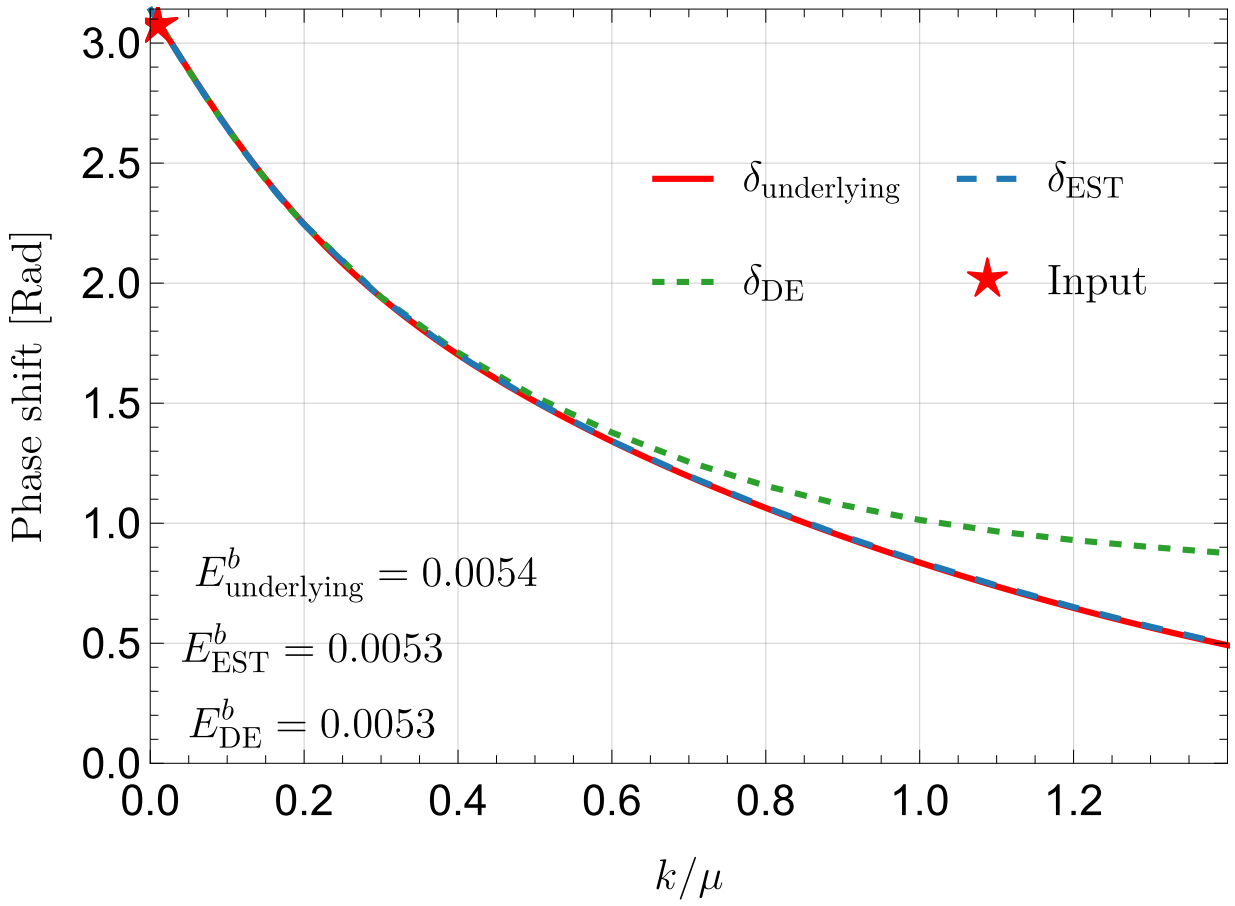
A small number of wave functions

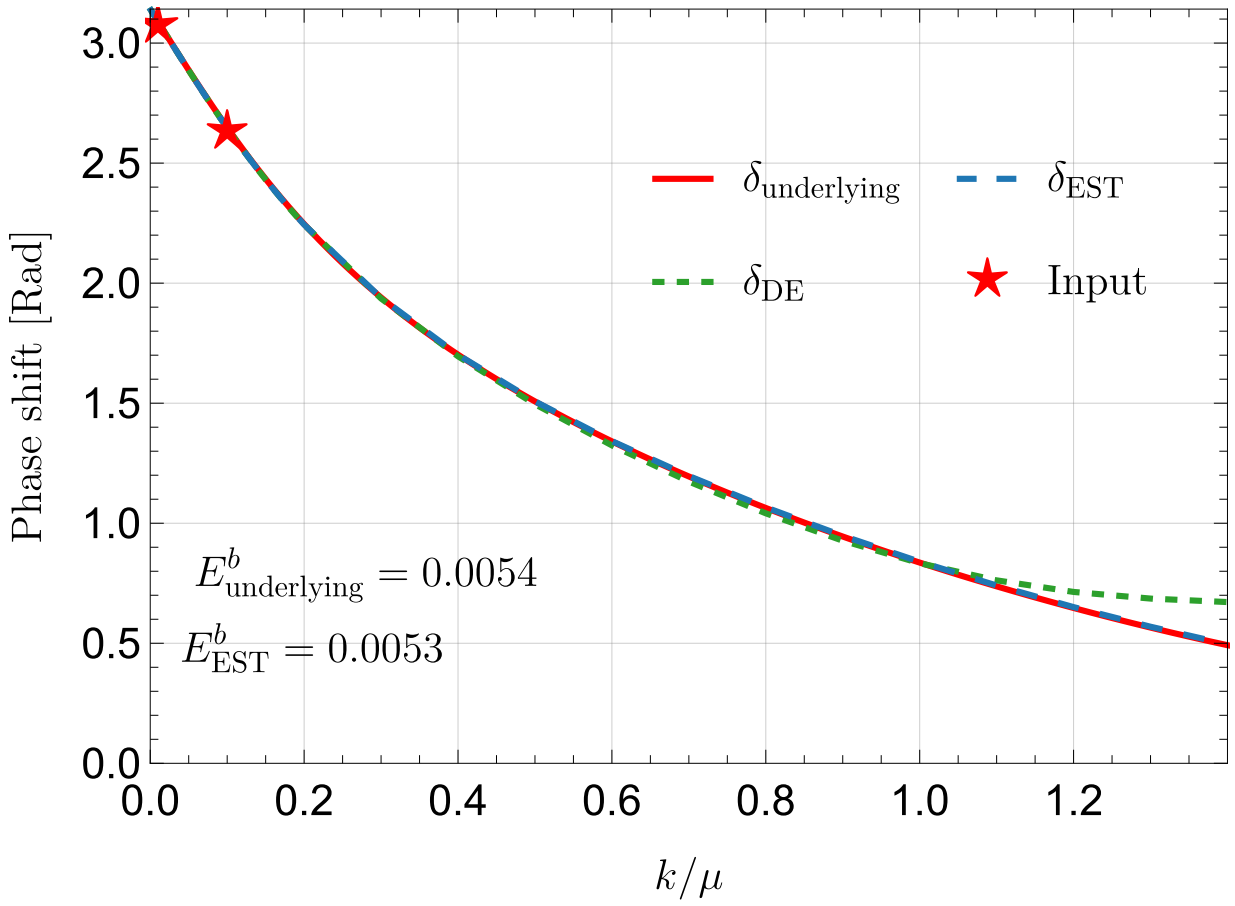
- A small number of wave functions cannot fix the potential and phase shift
- Unless, you presume some features of potentials
  - ▶ Derivative expansion: the nonlocality of potential is small
  - ▶ EST: separable






$V_{\text{underlying}}$
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
$E^b_{\text{underlying}} = 0.0054$
$E^b_{\text{EST}} = 0.0053$
$E^b_{\text{DE}} = 0.0053$


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
Phase shift [Rad]
k/μ
$\delta_{\rm underlying}$
$\delta_{\rm EST}$
$\delta_{\rm DE}$
Input
$E^b_{\rm underlying} = 0.0054$
$E^b_{\rm EST} = 0.0053$