



Extracting hadron potentials from the NBS wave functions: separable representation

Lu Meng (孟璐)

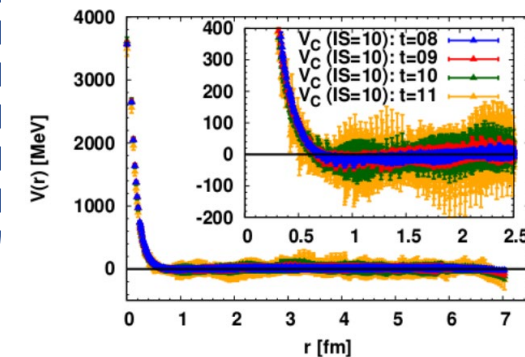
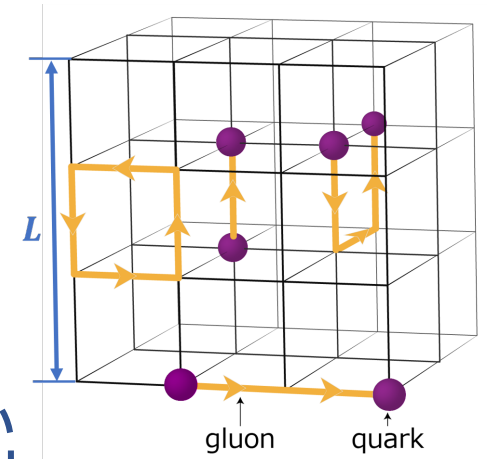
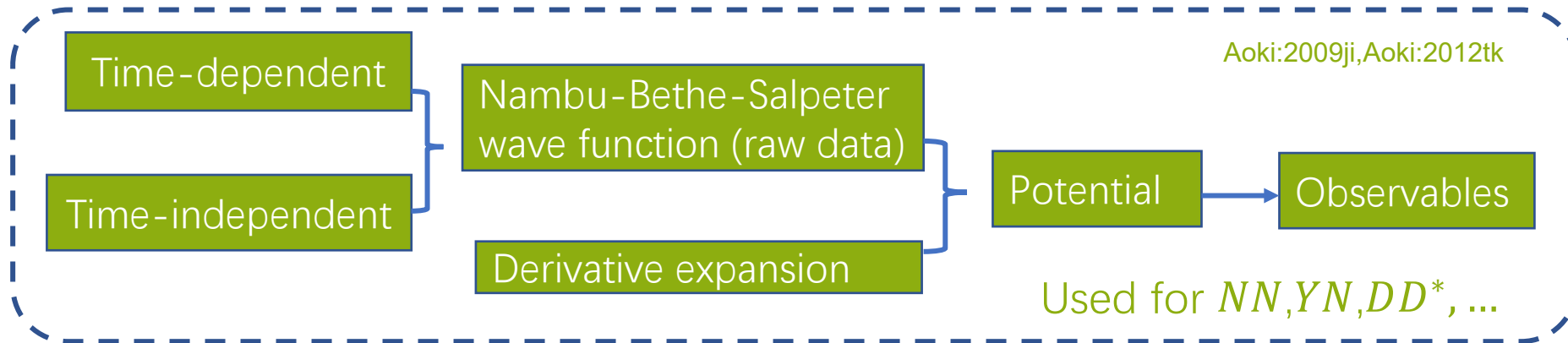
Ruhr-Universität Bochum

9th June, 2023, Genova

Based on papers in preparation
Together with Evgeny Epelbaum (RUB)

Hadron-hadron interaction from LQCD

- How to extract two-hadron interaction or observable from lattice QCD?
- Energy level method: Lüscher's formula Luscher:1990ux
 - ▶ $E^{FV} \sim \delta(E^{FV})$
- HAL QCD method or potential method Ishii:2006ec



- 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

- 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 (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
- ▶ Note: the # of wave functions is small, 2 or 3
- ▶ In general, the potential is nonlocal

- 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

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

- The general problem

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

- Time-dependent strategy without ground state saturation makes simulations with large box and small pion mass available

► $m_\pi = 146 \text{ MeV}$, $a \simeq 0.0846 \text{ fm}$, $L^4 = 96^4$, $L = 8.1 \text{ fm}$

Doi:2017zov, Lyu:2022imf, Lyu:2023xro...

Modern views of potential

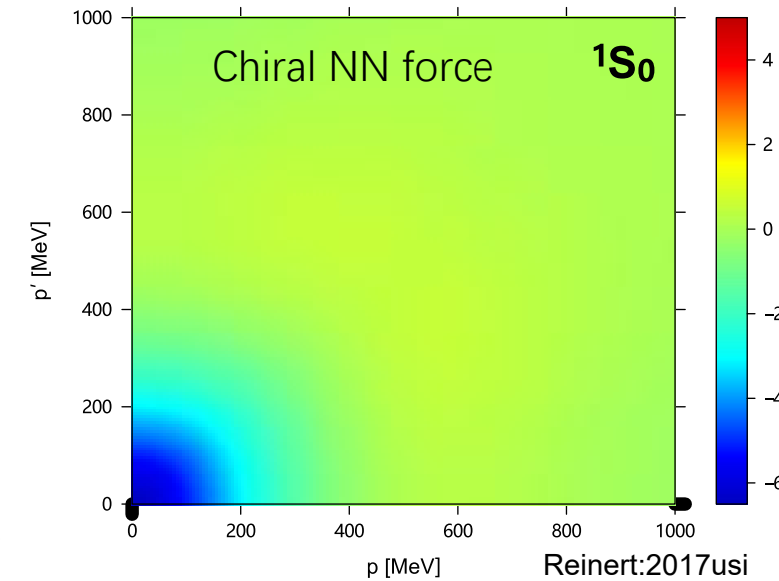
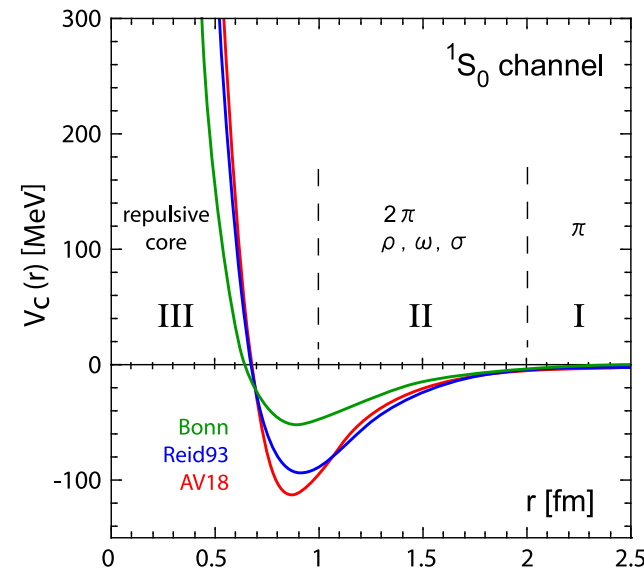
- There is no reason to rule out the nonlocal potential either in principle or phenomenologically
- Potential is not observable
 - ▶ Cannot be determined uniquely by scattering experiments
 - ▶ Observable-equivalent potentials are related by unitary trans. (UT) or field redefinition
 - ▶ UT can relate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

Bogner:2009bt

- Non-observables
 - ▶ Non-asymptotic behavior of ψ
 - ▶ Off-shell T-matrix
 - ▶ Potential

Ekstein:1960xkd

- Observables
 - ▶ Asymptotic behavior of ψ
 - ▶ Phase shift
 - ▶ On-shell T-matrix



- Inner region: $V(r, r') \neq 0$ ($r, r' < R$), outer region: $V(r, r') = 0$ ($r, r' > R$)

Aoki:2008hh

Reinert:2017usi

Interpolating operator VS potential

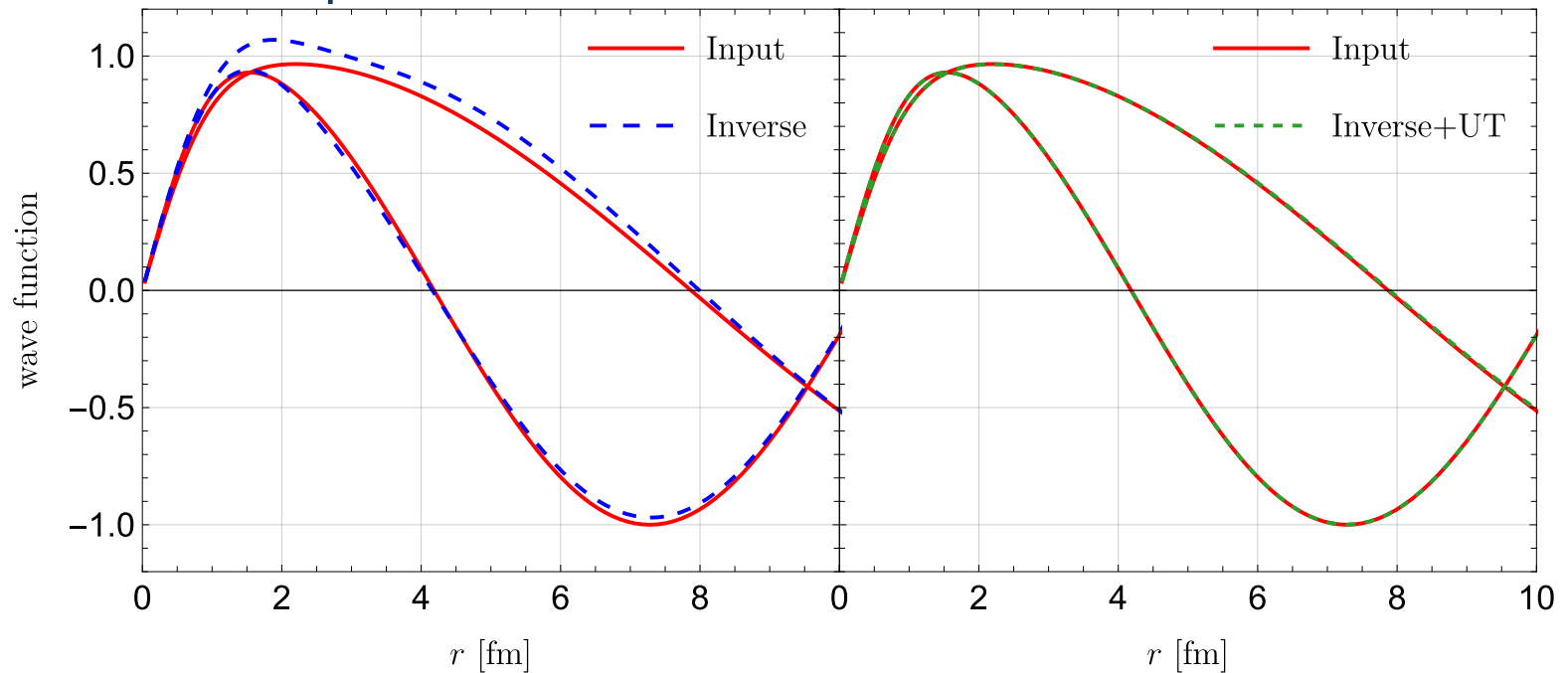
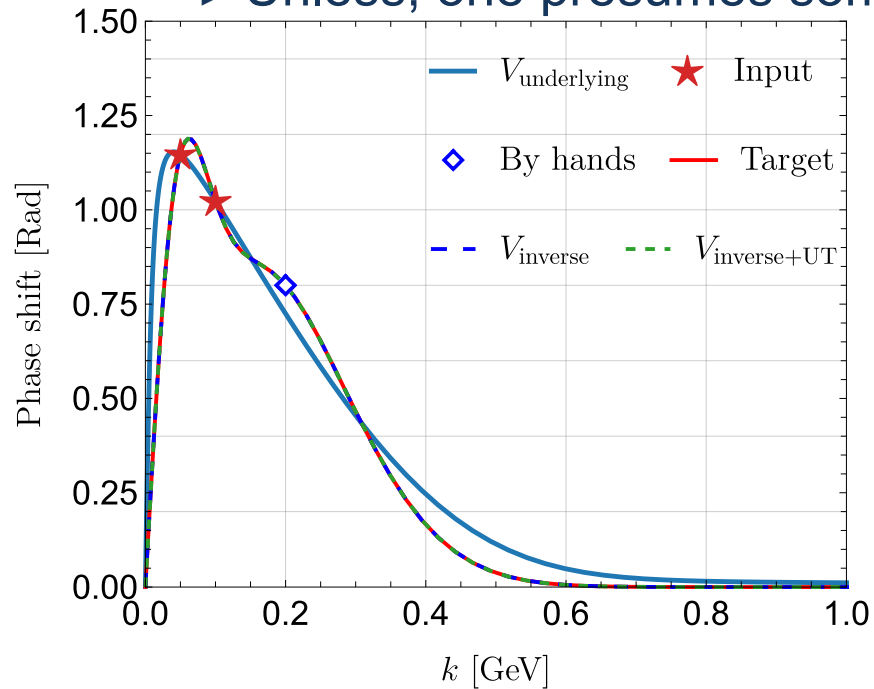
- In principle one may choose any composite operators with the same quantum numbers as the hadron to define the BS wave function
- Different operators give different BS wave functions and different hadron potentials
 - ▶ They are related by UT
 - ▶ We anticipate they lead to the same observables such 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
- From a small number of the wave functions, the potential can not be determined uniquely
 - ▶ Think it in a discrete way

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

- ▶ 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

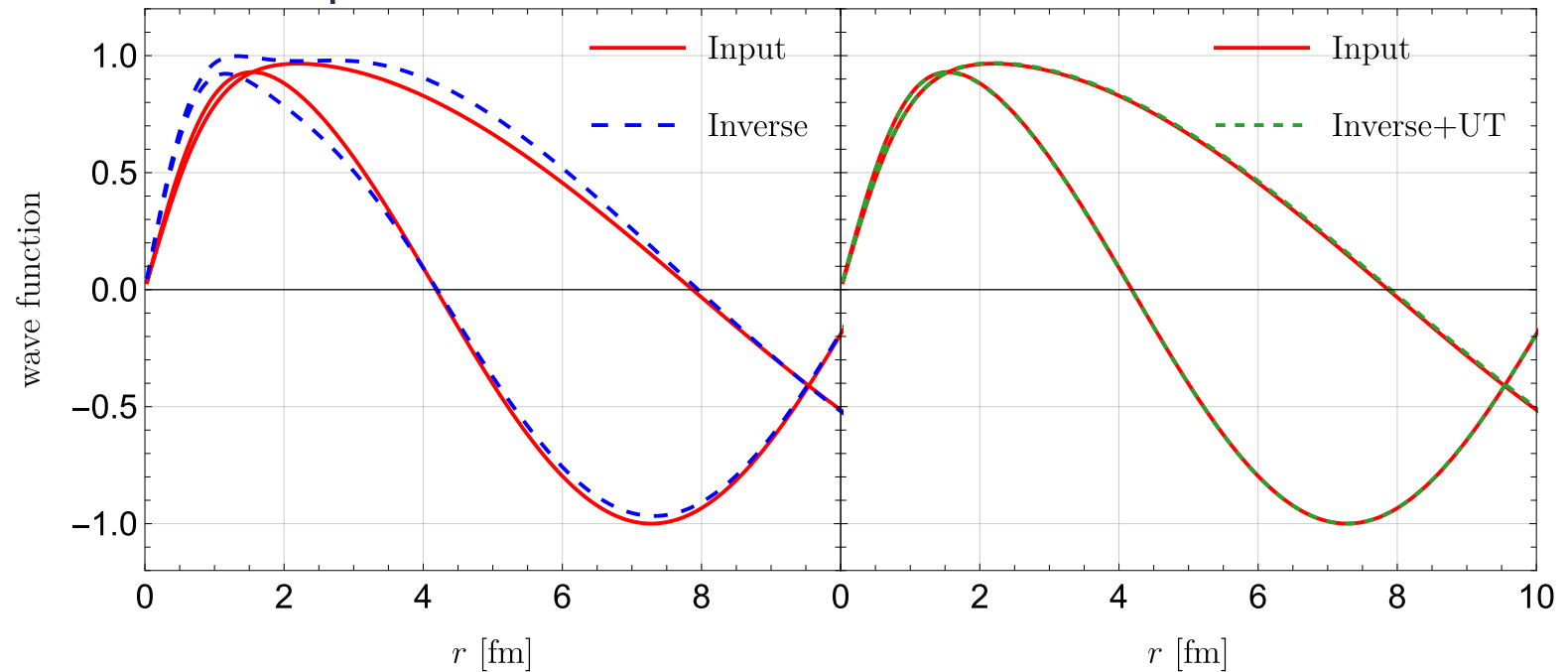
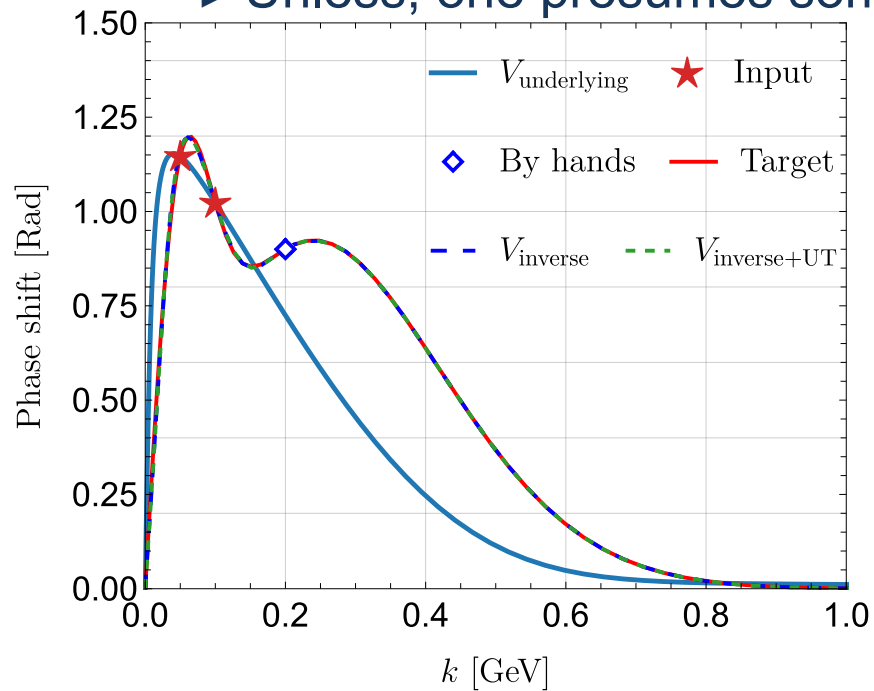
A small number of wave functions

- Using two wave functions of $V_{underlying}$ as input $\{\psi_{k_1}(r), \psi_{k_2}(r)\}$
- $\delta_{tar}(k)$ go through $\{\delta(k_1), \delta(k_2)\}$ 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 $\{\psi_{k_1}(r), \psi_{k_2}(r)\}$ Ernst:1973utx
- Conclusion:
 - ▶ A small number of wave functions cannot fix the potentials and phase shifts
 - ▶ Unless, one presumes some features of potentials



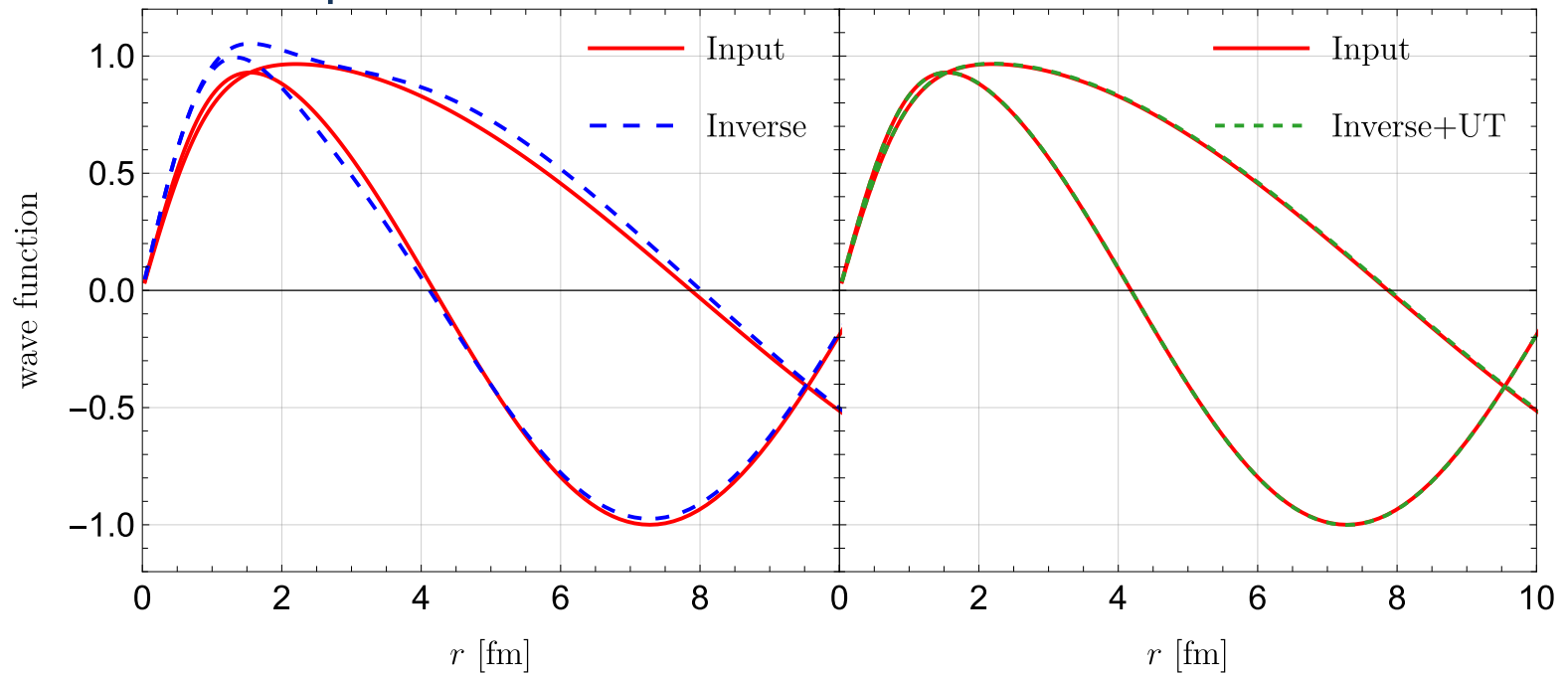
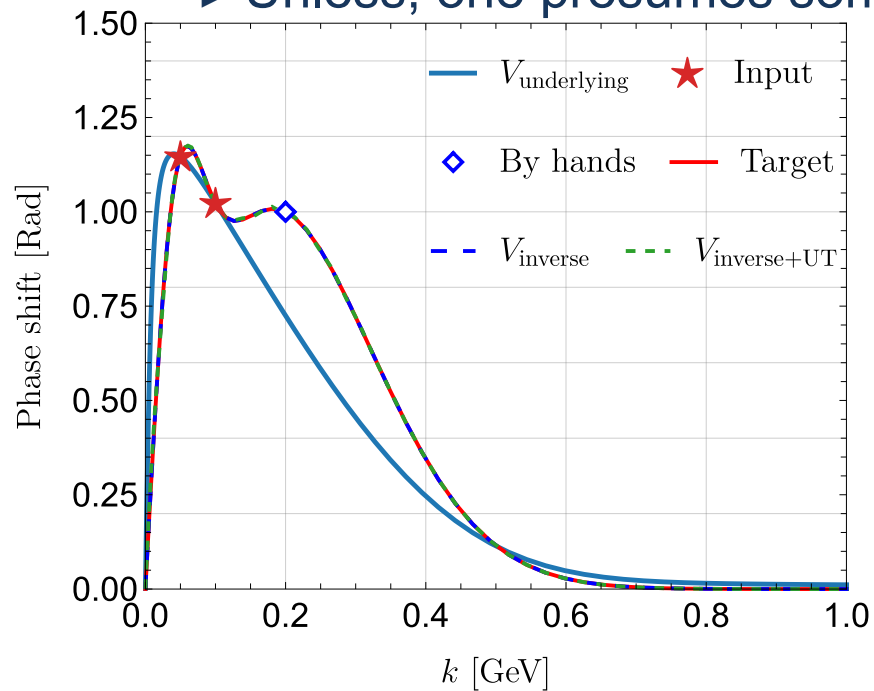
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Derivative expansion

- Derivative expansion

Aoki:2021ahj

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

- 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,

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

$$V_0 = \left[\begin{array}{c} \diagdown \\ \diagdown \\ \diagdown \end{array} \right], V_1 = \left[\begin{array}{c} \diagdown \diagdown \\ \diagdown \diagdown \\ \diagdown \diagdown \end{array} \right], V_2 = \left[\begin{array}{c} \diagdown \diagdown \diagdown \\ \diagdown \diagdown \diagdown \\ \diagdown \diagdown \diagdown \end{array} \right], \dots$$

► The band width become wider

Singular potential

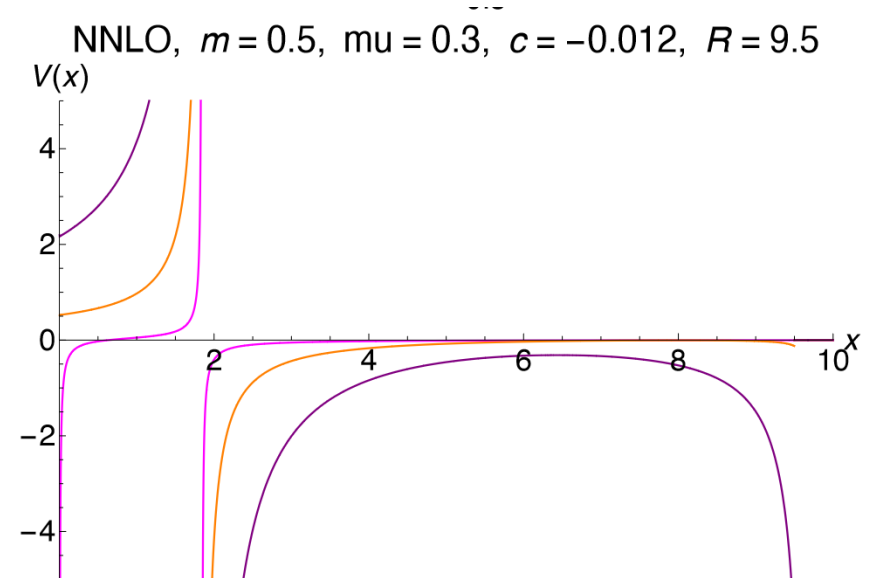
- NLO derivative expansion

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

- 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.



Separable representation

- The problem: $V|R^{(i)}\rangle = |K^{(i)}\rangle$

- Separable representation I: $V = \sum_{ij} C_{ij}|K^{(i)}\rangle\langle R^{(j)}|$, $C_{im}\langle R^{(m)}|R^{(j)}\rangle = \delta_{ij}$
 - ▶ Bad performance

Aoki:2009ji

- Separable representation II, Ernst-Shakin-Thaler (EST) method

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

Ernst:1973zzb,Haidenbauer:1984dz

- ▶ In the outer region: $K^{(i)}(r) = \left(\frac{d^2}{dr^2} + k_i^2\right)\psi_{k_i}(r) = 0$

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

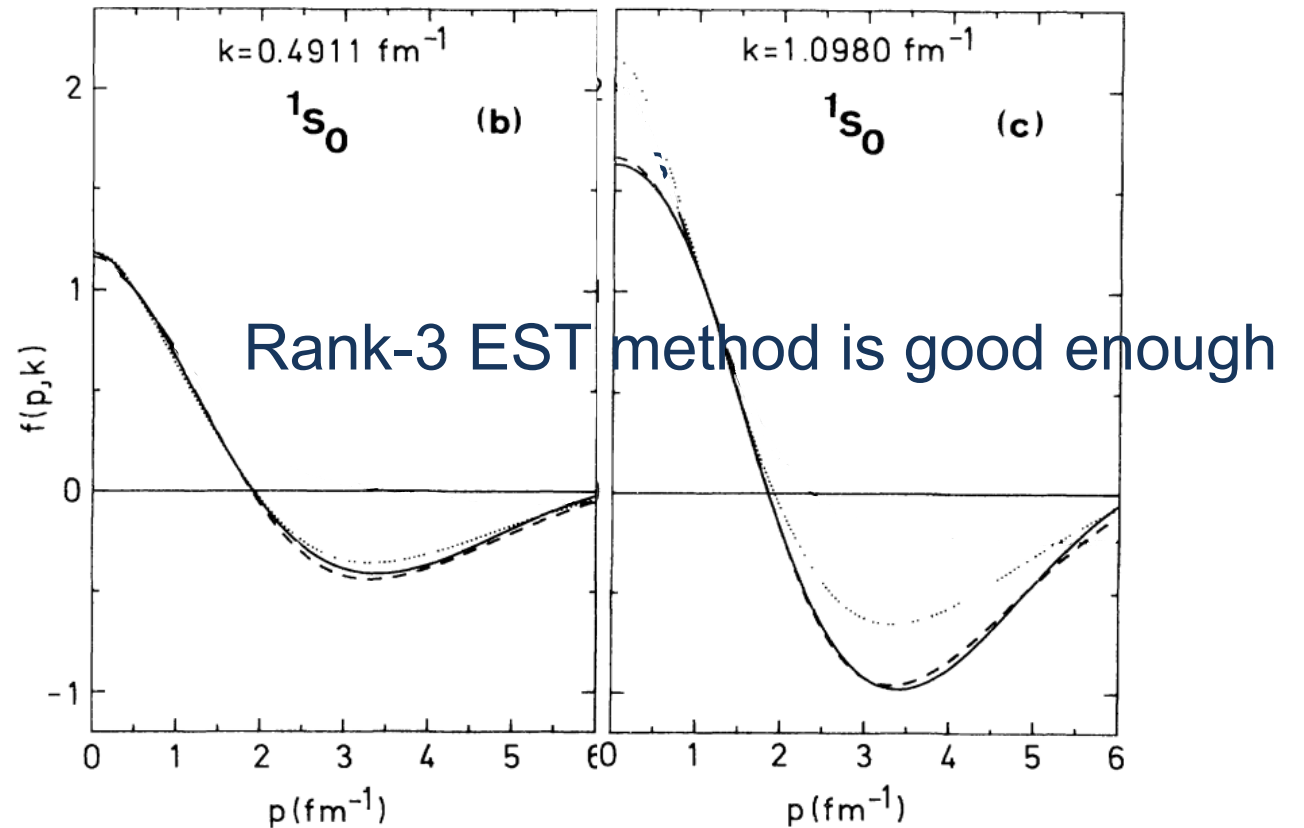
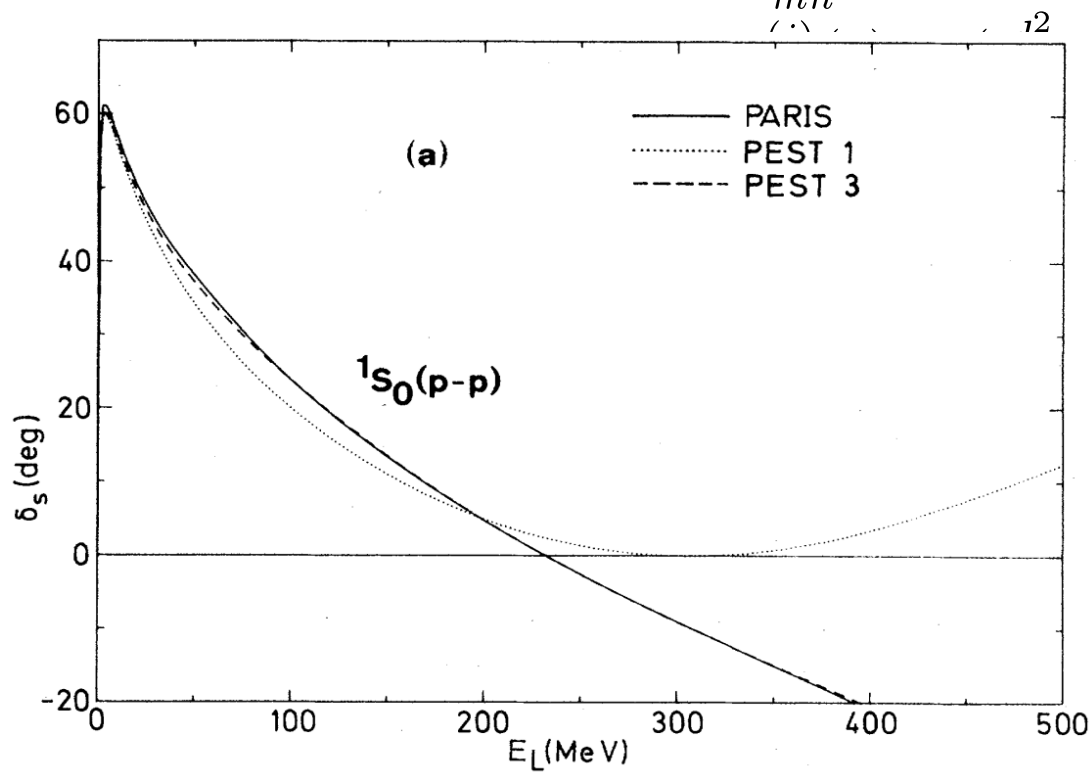
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Two underlying potentials

- Separable potential Aoki:2021ahj

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

- LO chiral nuclear force Reinert:2017usi

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

- ▶ 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

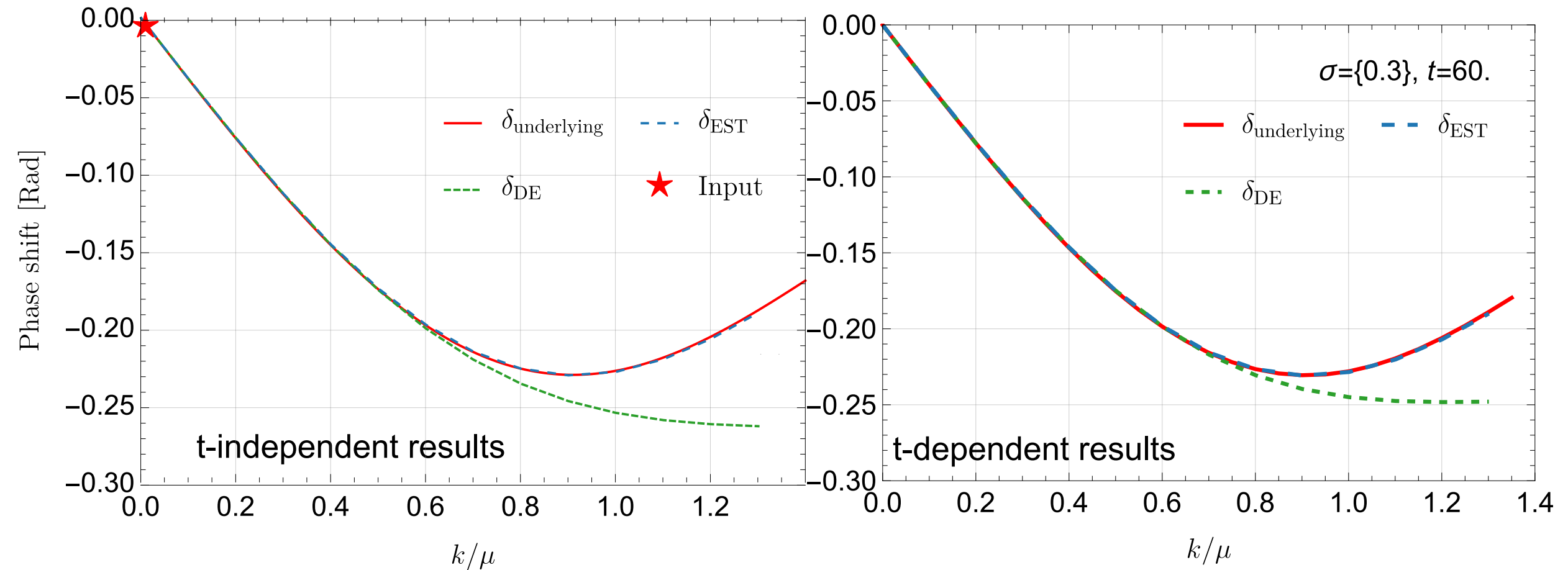
$$\tilde{R}(t=0, x) = \frac{\sigma^2 e^{-\sigma x}}{4\pi}$$

- ▶ 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

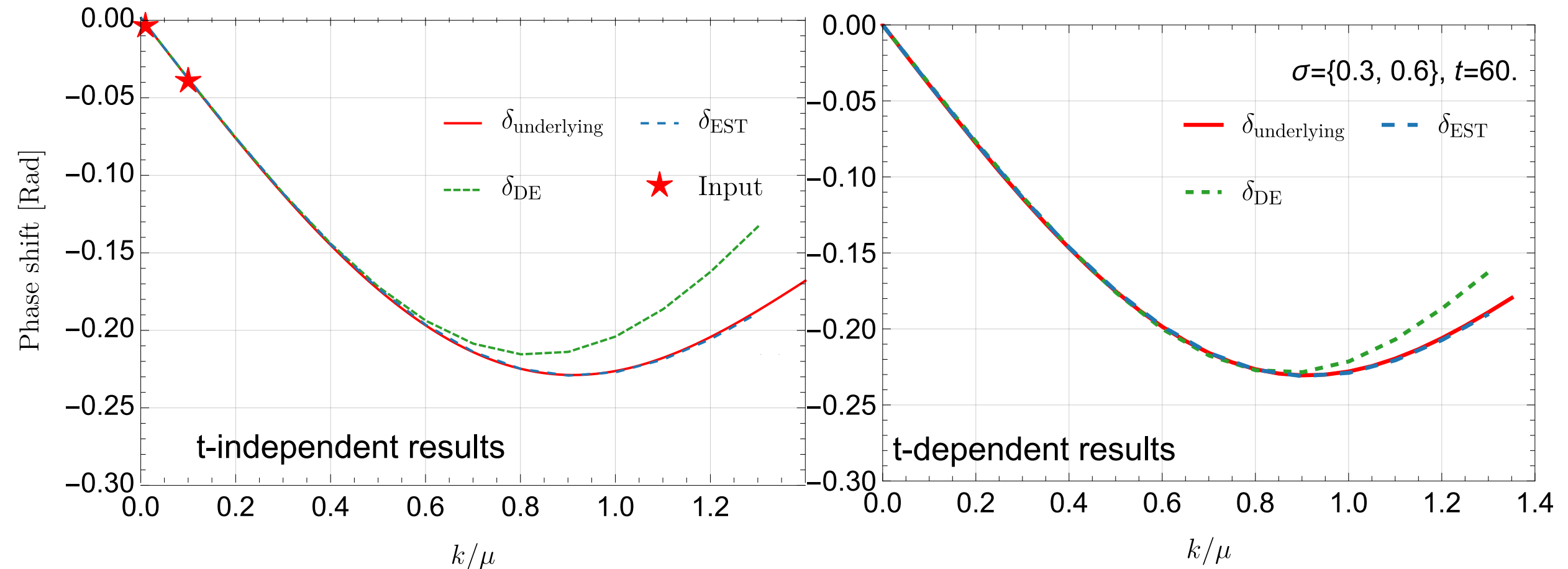
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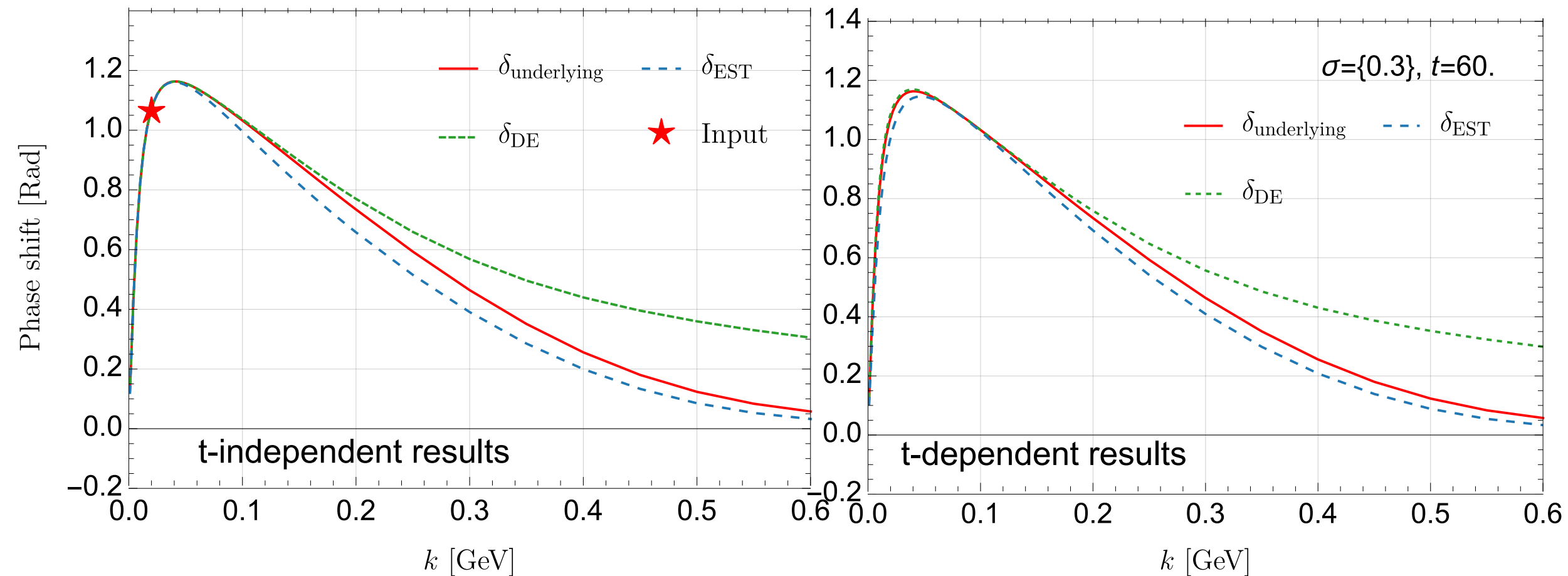


Physical interaction

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

$$V_{ctc}(\mathbf{p}, \mathbf{p}') = C e^{-\frac{p^2 + p'^2}{\Lambda^2}},$$

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

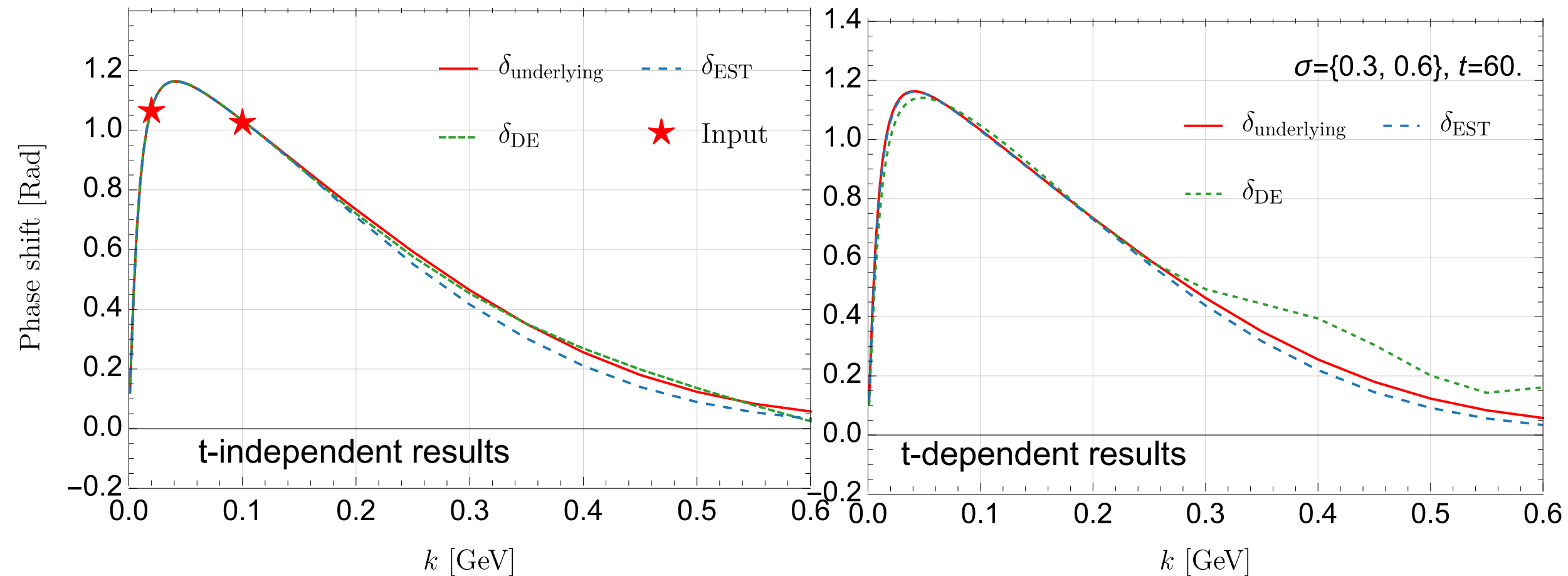


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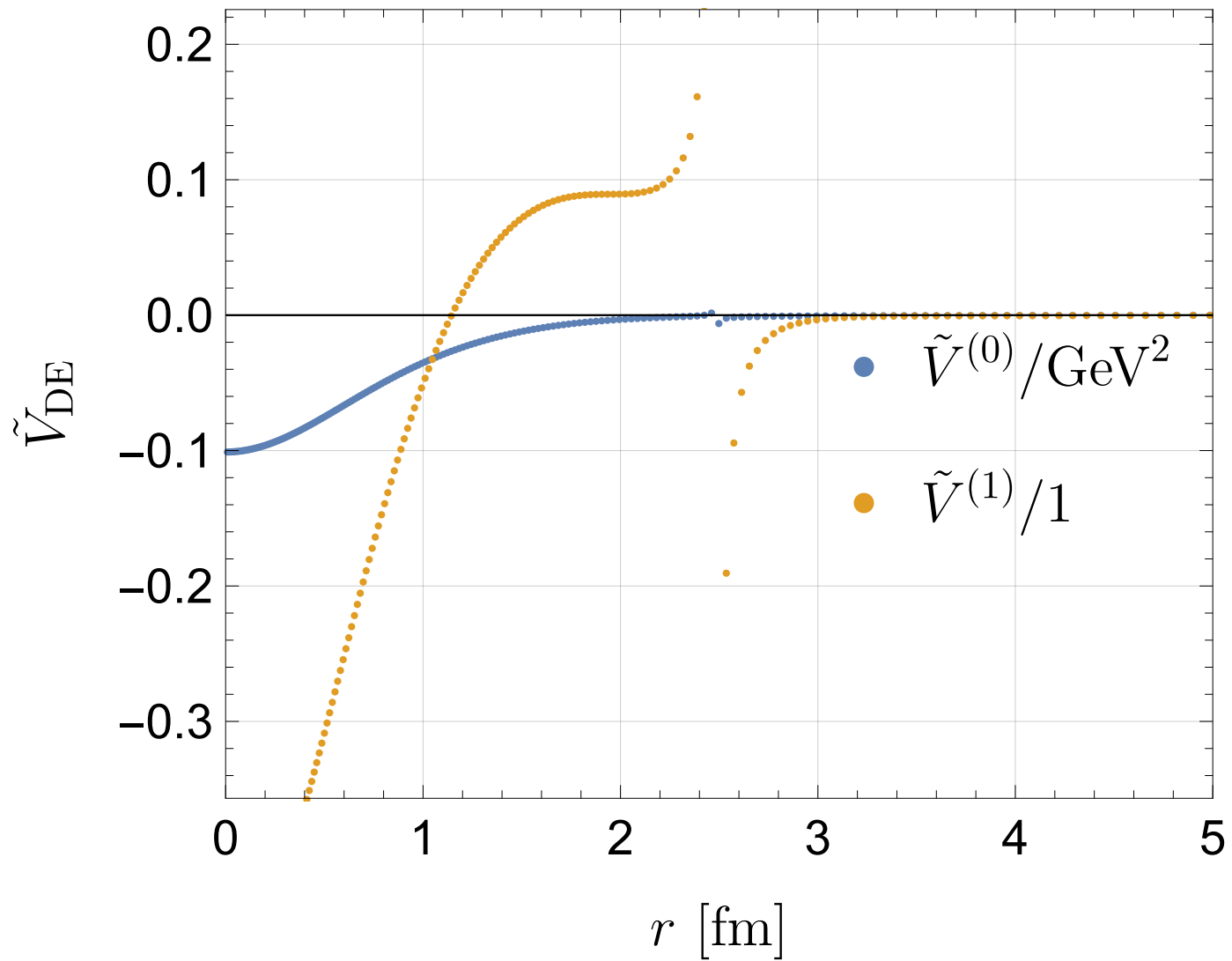
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Singularity in potential

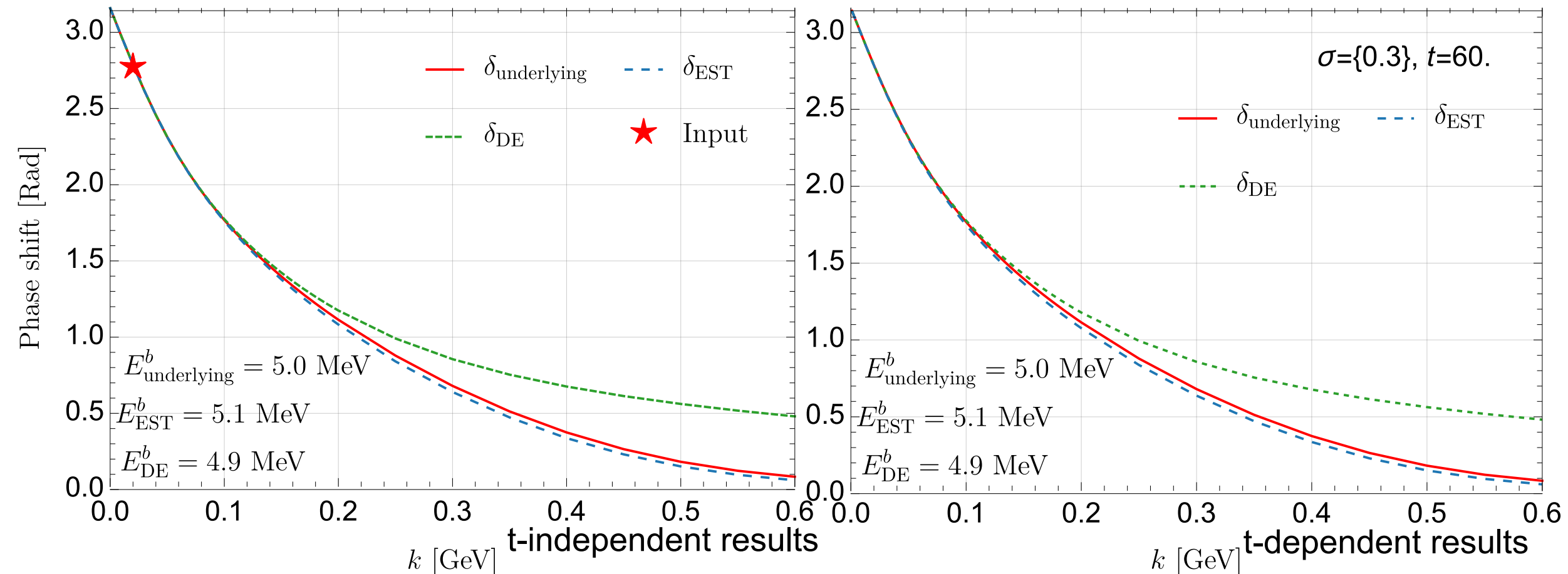


Bound state

- 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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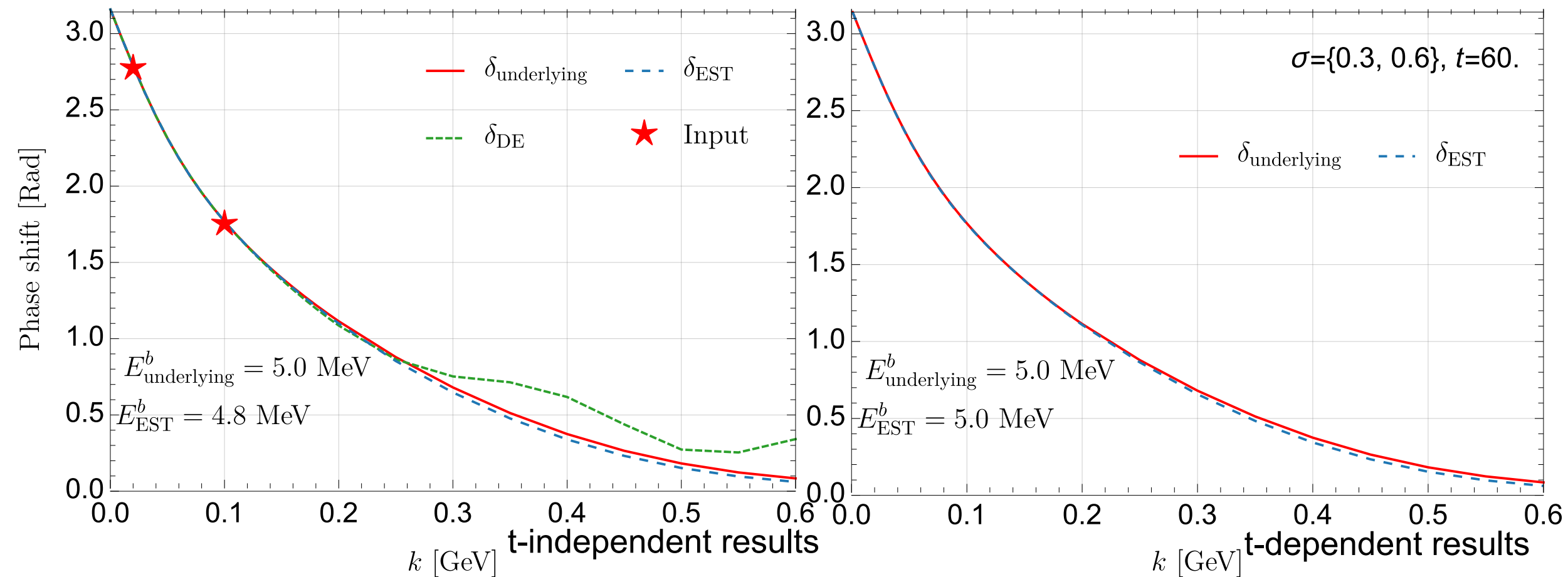


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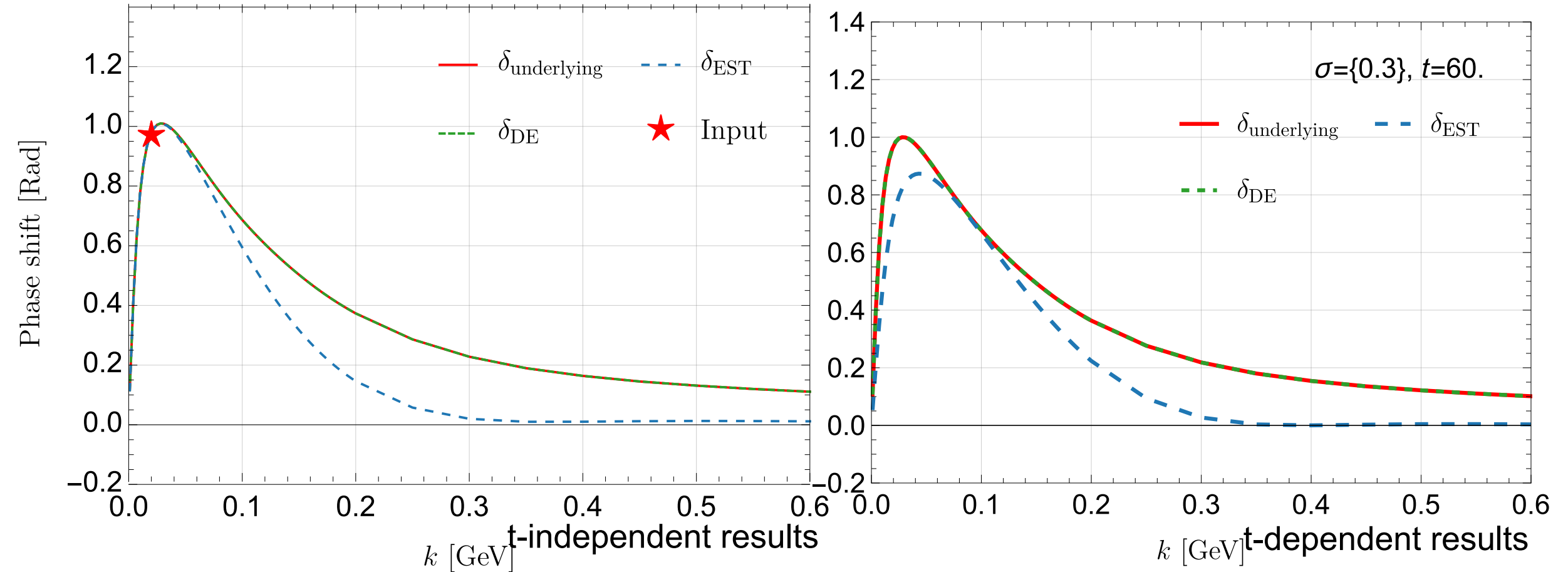


Local interaction

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

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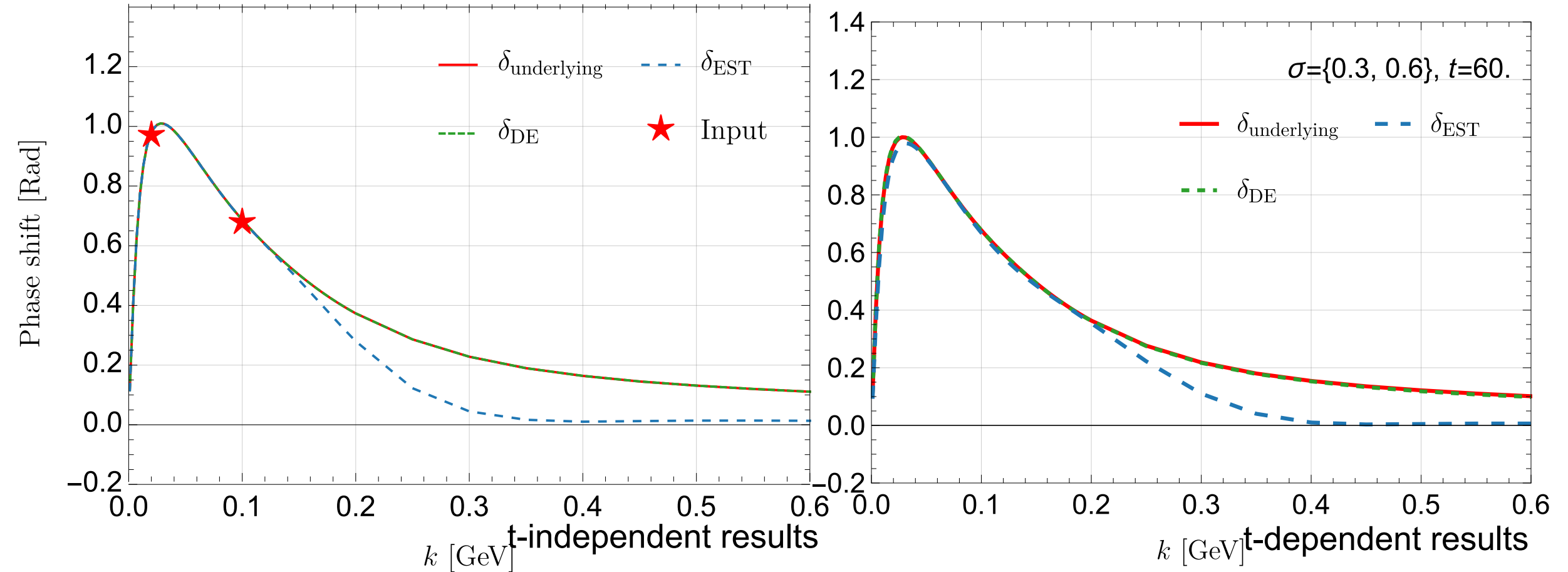


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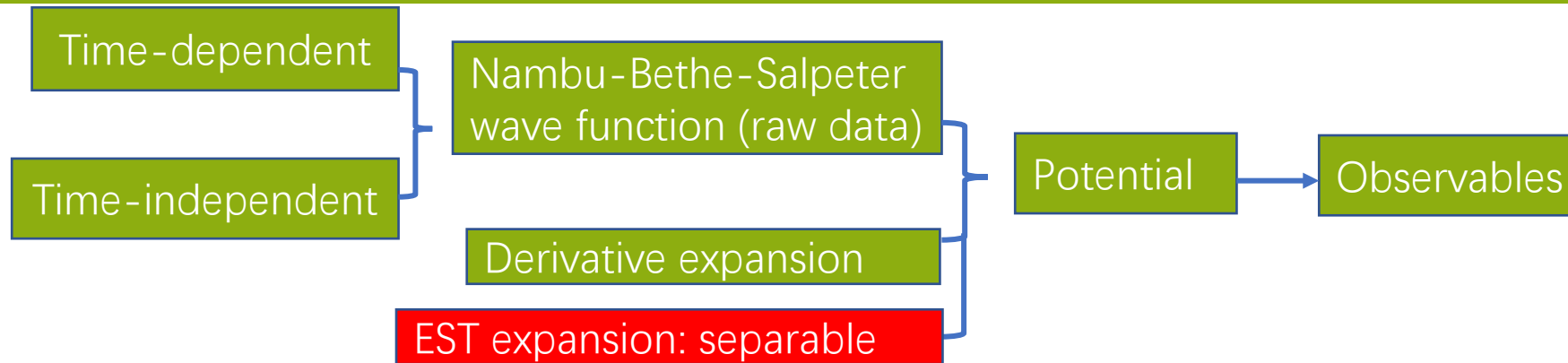
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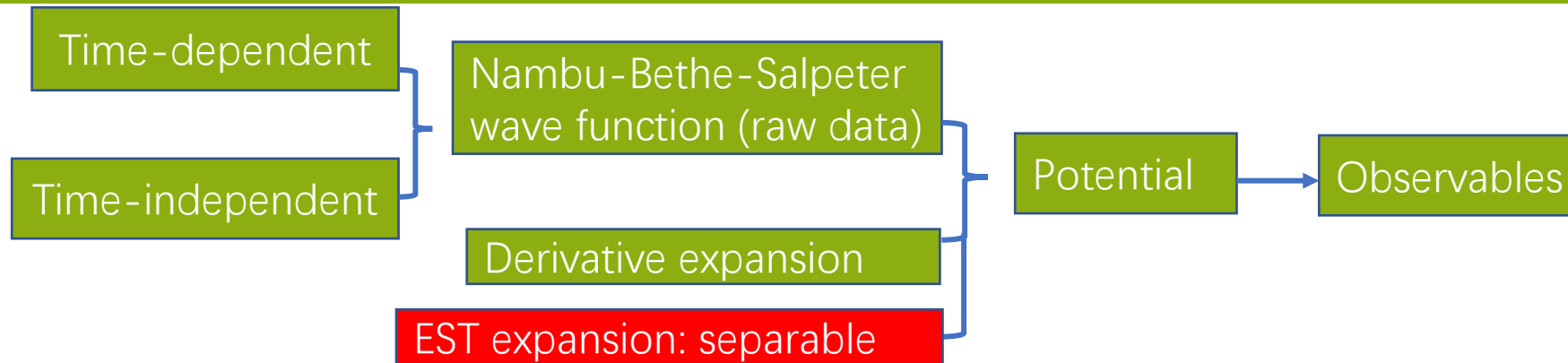


Summary



- 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 to refit 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

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Thanks for your attention!

Backup

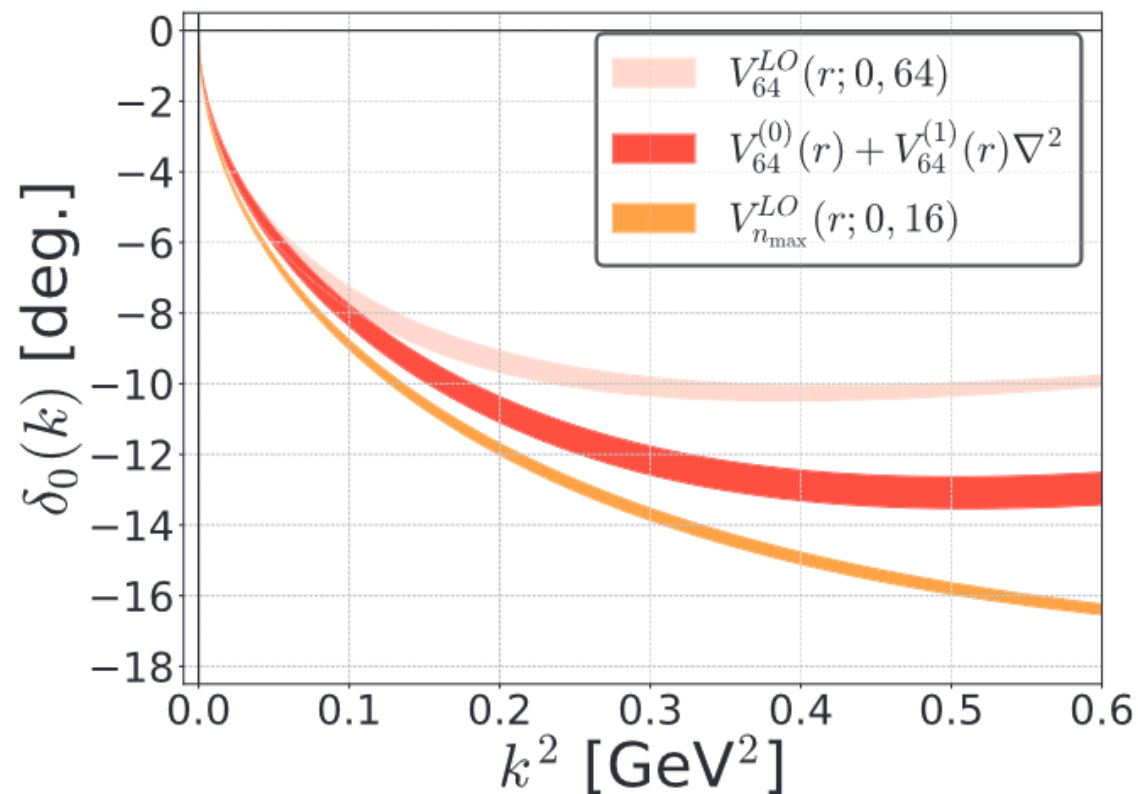


Fig. 5. The phase shifts of the S-wave $I = 2$ $\pi\pi$ scattering from the potential in the point-sink scheme (LO: orange) and the smeared-sink scheme (LO: pink, NLO: red) as a function of k^2 .

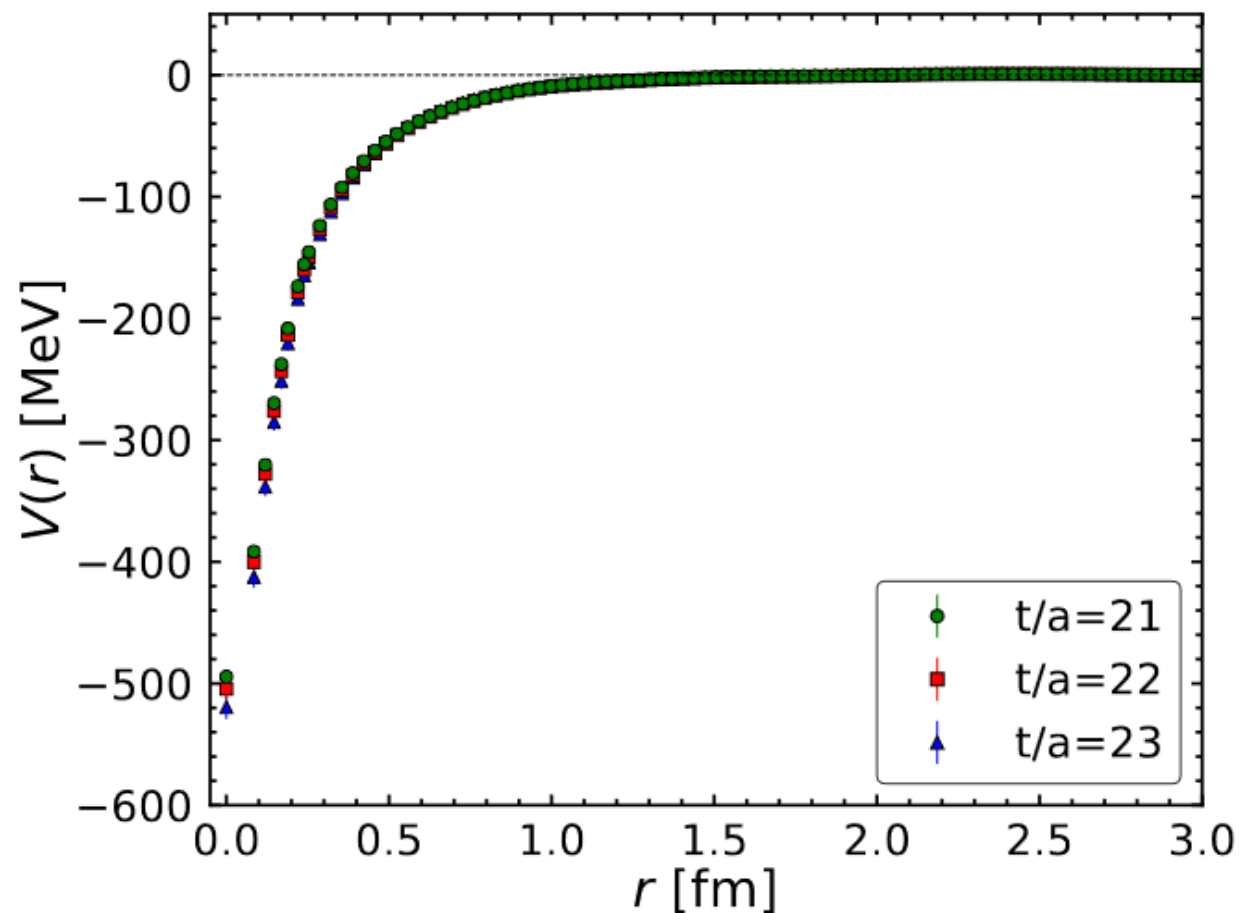
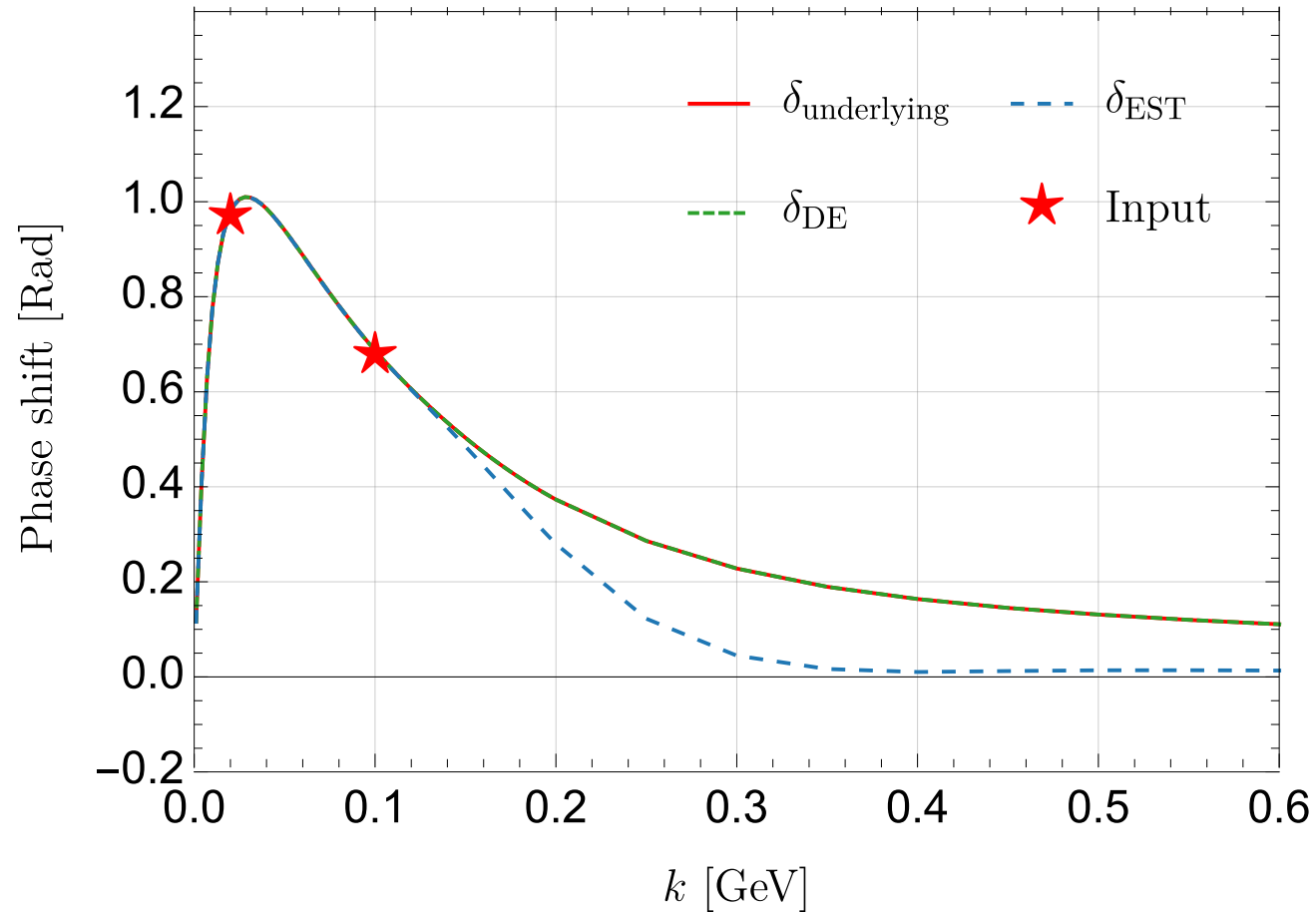


FIG. 2. The D^*D potential $V(r)$ in the $I = 0$ and S -wave channel at Euclidean time $t/a = 21$ (green circles), 22 (red squares), and 23 (blue triangles).

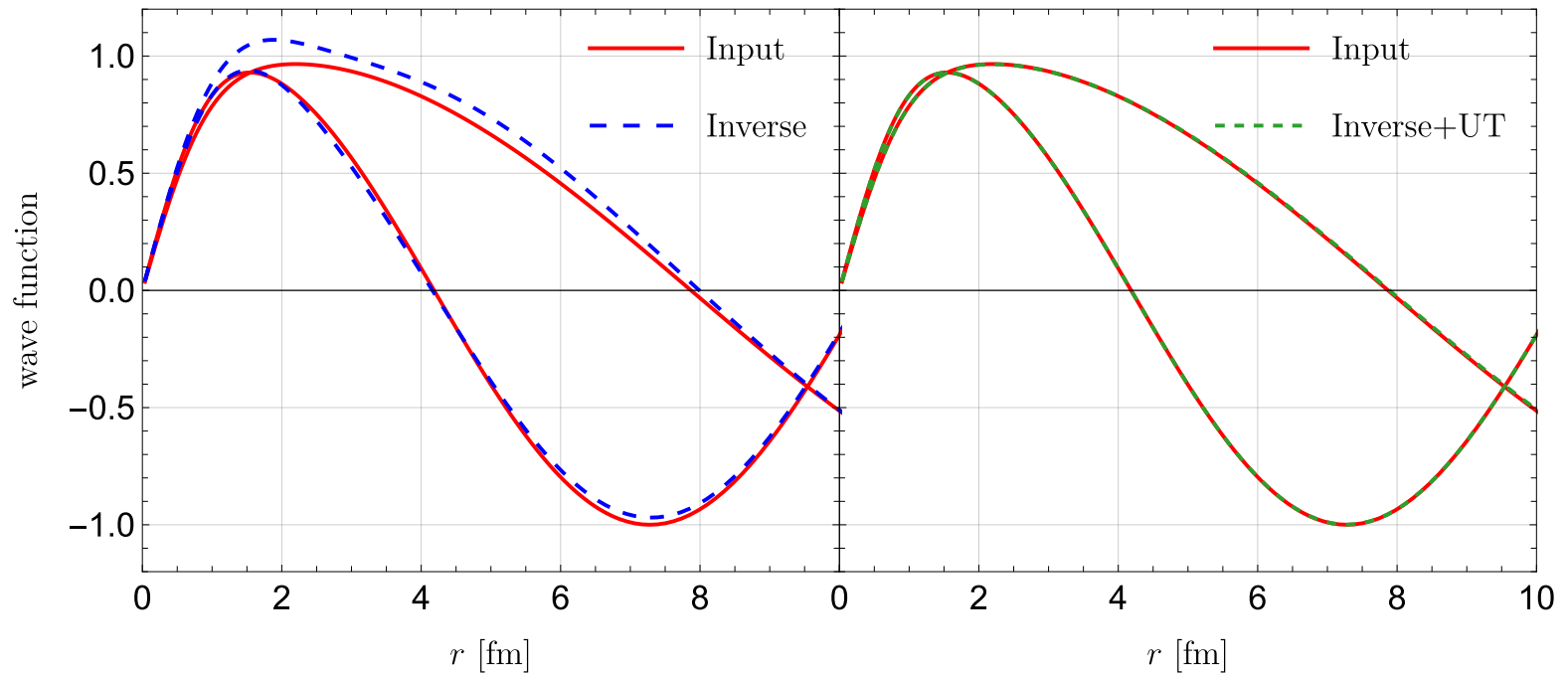
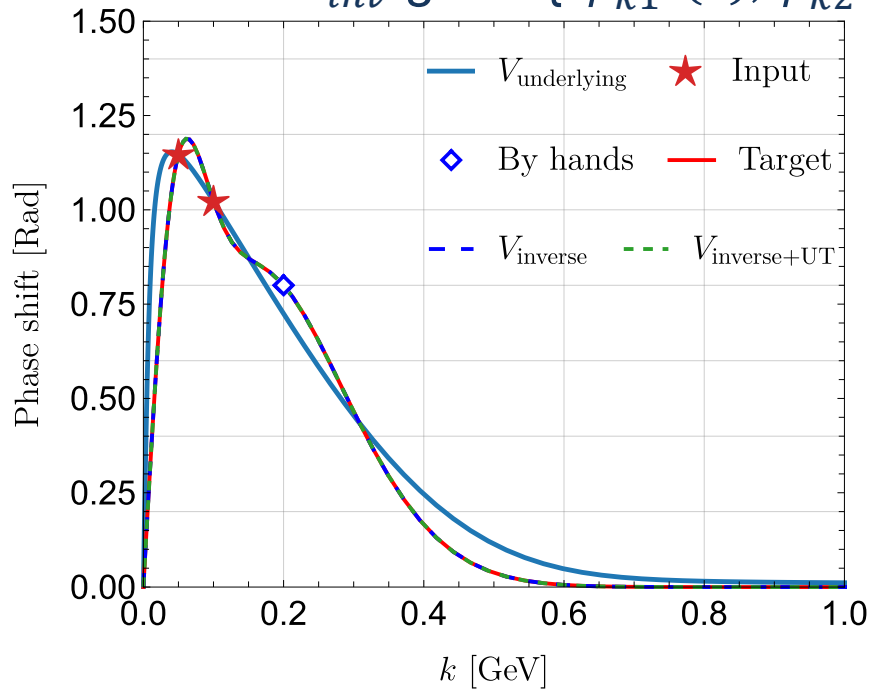
- Extracting potential from NBS is not an expansion of small quantities
- It is more like an interpolating and extrapolating
- Self-consistency test also makes sense



A small number of wave functions

1. Underlying potential $V_{underlying}$ give its phase shift $\delta(k)$
2. Using two wave functions as input $\{\psi_{k_1}(r), \psi_{k_2}(r)\}$ 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
5. The V_{inv} gives $\{\psi_{k_1}^{inv}(r), \psi_{k_2}^{inv}(r)\}$ different with $\{\psi_{k_1}(r), \psi_{k_2}(r)\}$

Tabakin:1969mr



A small number of wave functions

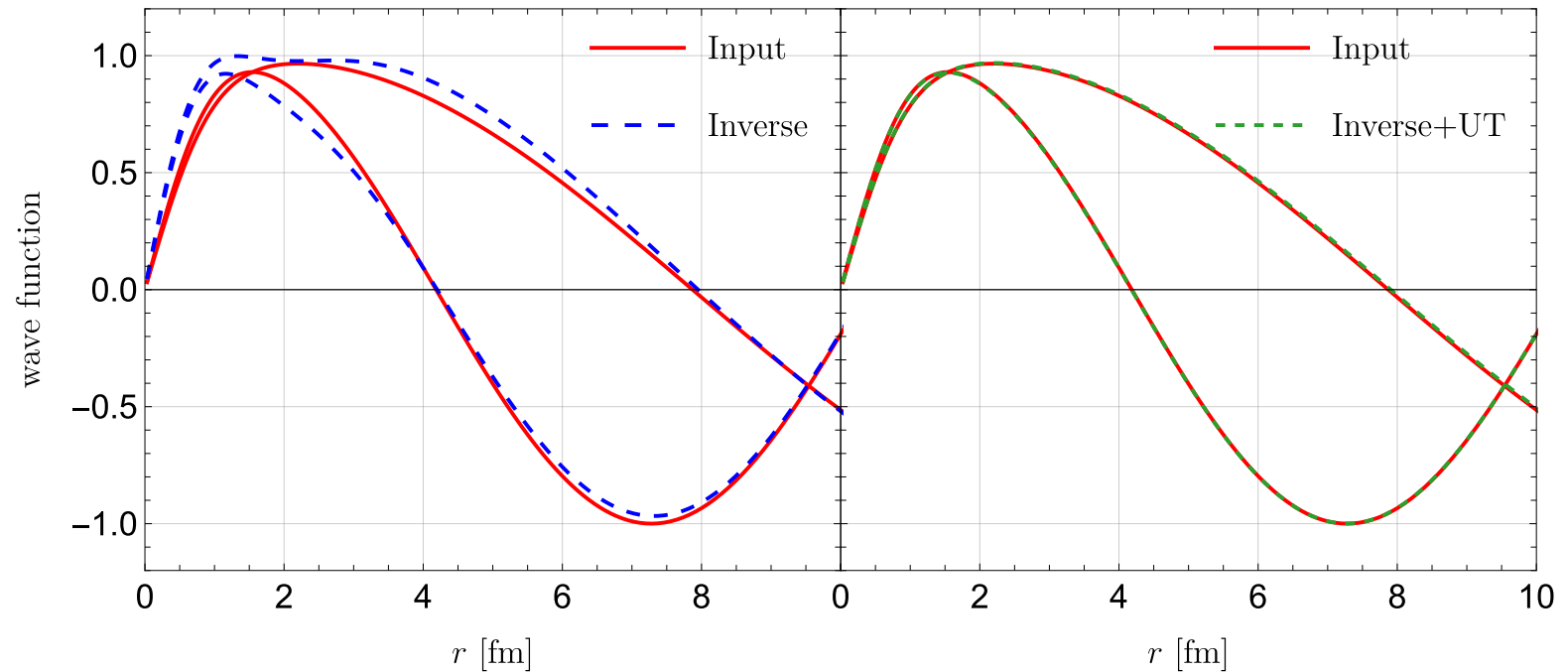
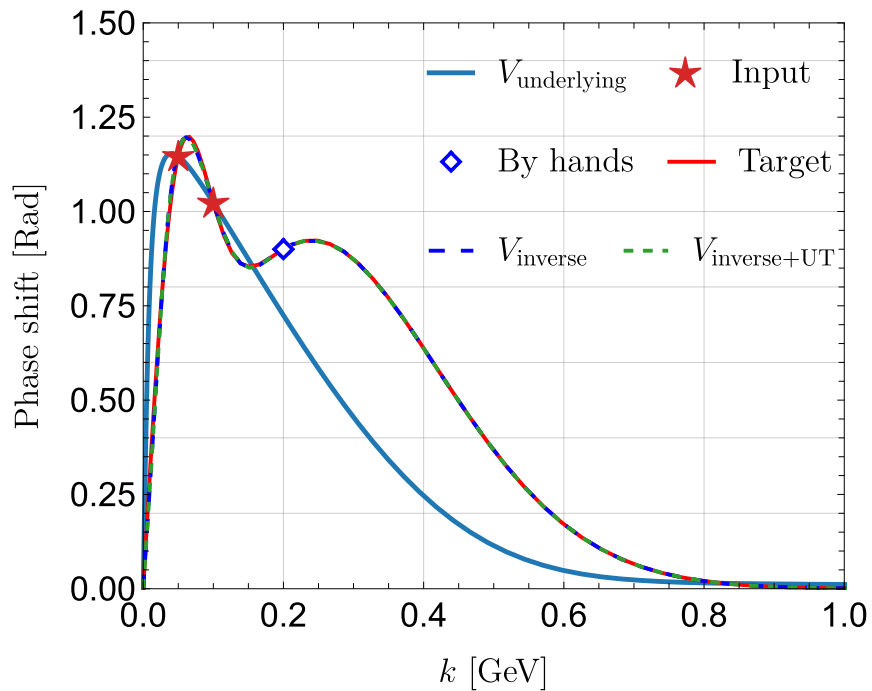
6. Construct an unitary trans. (UT): $U|\psi_{k_i}^{inv}\rangle = |\psi_{k_i}\rangle$

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 $\{\psi_{k_1}(r), \psi_{k_2}(r)\}$

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



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

