



# 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

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

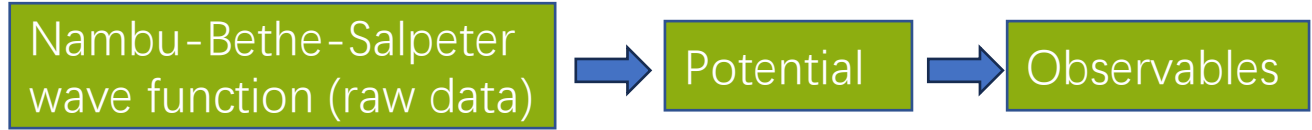
- How to extract two-hadron interaction or observable from lattice QCD?

- Energy level method: Lüscher's formula [Luscher:1990ux](#)

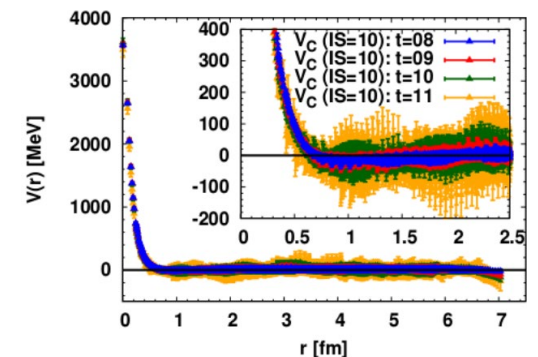
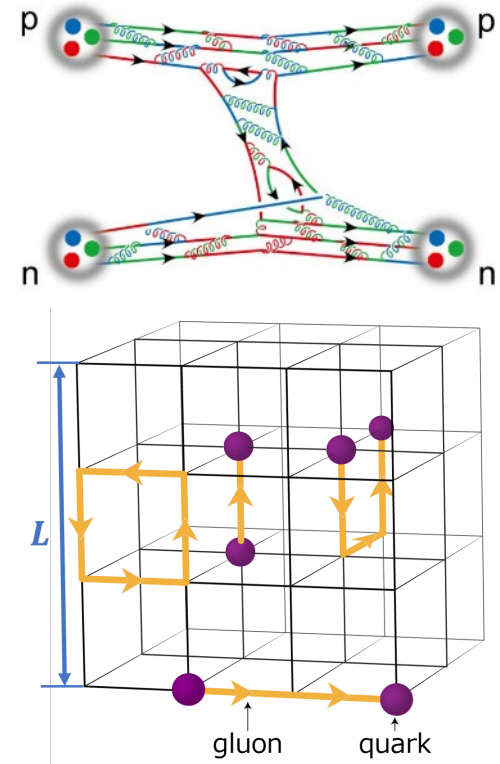
▶  $E^{FV} \sim \delta(E^{FV})$

- HALQCD method or potential method

[Ishii:2006ec](#), [Aoki:2009ji](#), [Aoki:2012tk](#)



- ▶ 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

## ● 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

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

2012 HALQCD  $M_\pi \approx 710$  MeV

2012 HALQCD  $M_\pi \approx 469 - 1171$  MeV

3

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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**Uncontrolled systematics**

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/>

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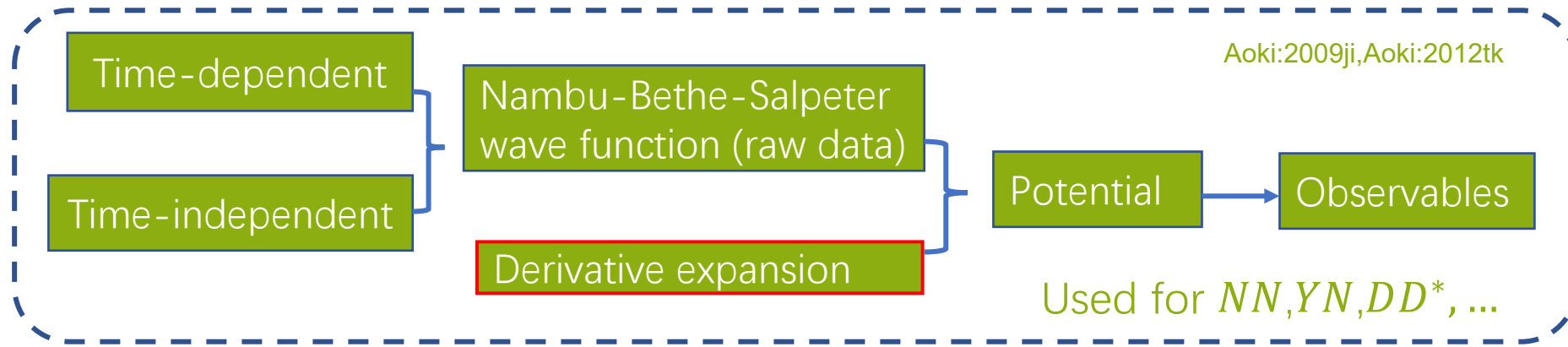
# HALQCD method

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

- 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

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

- ▶  $T(p; k)$  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:  $\psi_{k_i}(\vec{x}) \Rightarrow V$

- 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  $\delta(k_i)$**  from the  $\psi_{k_i}(\vec{x})$ ?

- $\psi_{k_i}$  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

►  $m_\pi = 146$  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**

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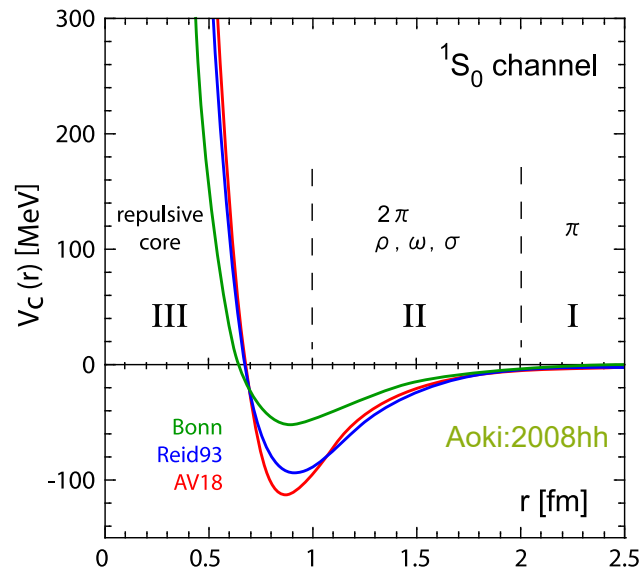
# Modern views of potential

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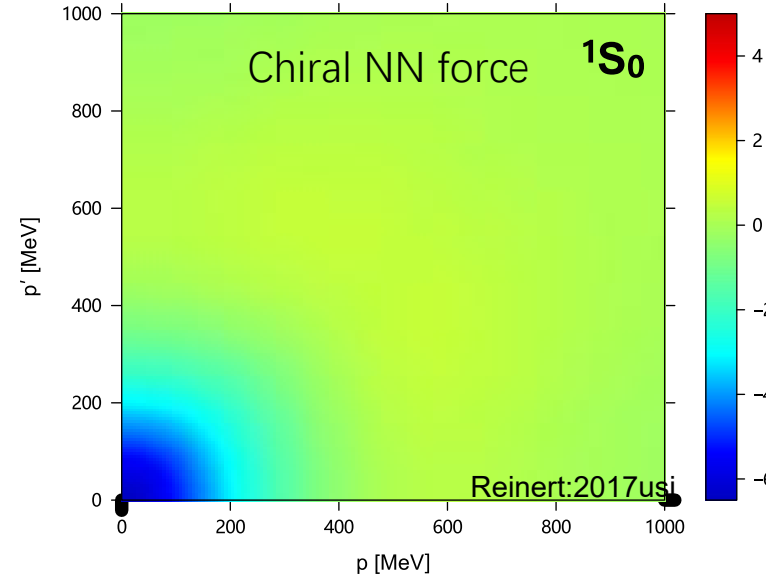
- There is no reason to rule out the nonlocal potential either in principle or phenomenologically
- Potential is not observable
  - ▶ Cannot be determined uniquely by scattering experiments
  - ▶ Observable-equivalent potentials are related by unitary trans. (UT) or field redefinition
  - ▶ UT can relate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

Bogner:2009bt

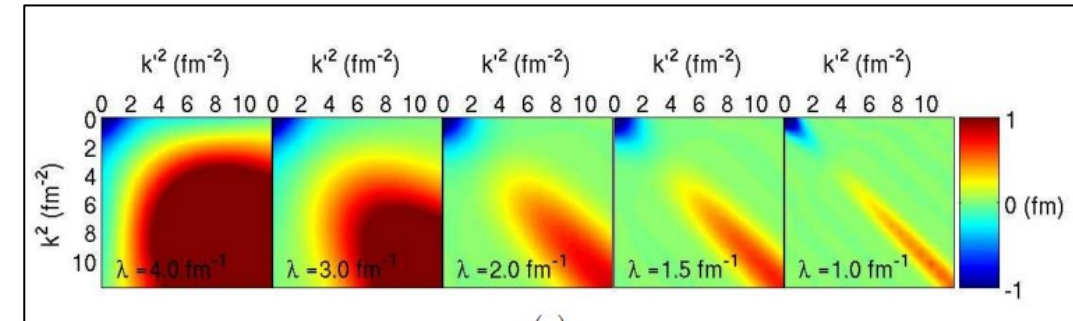
Ekstein:1960xkd



Local NN force



Nonlocal NN force



SRG evolution

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

- Non-observables

- ▶ Non-asymptotic behavior of  $\psi$ , e.g. the deuteron D-state probability

Amghar:1995av

- ▶ Off-shell T-matrix

- ▶ Potential

- Observables

- ▶ Asymptotic behavior of  $\psi$

- ▶ Phase shift

- ▶ On-shell T-matrix

# Interpolating operator VS potential

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- 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  $\delta$  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

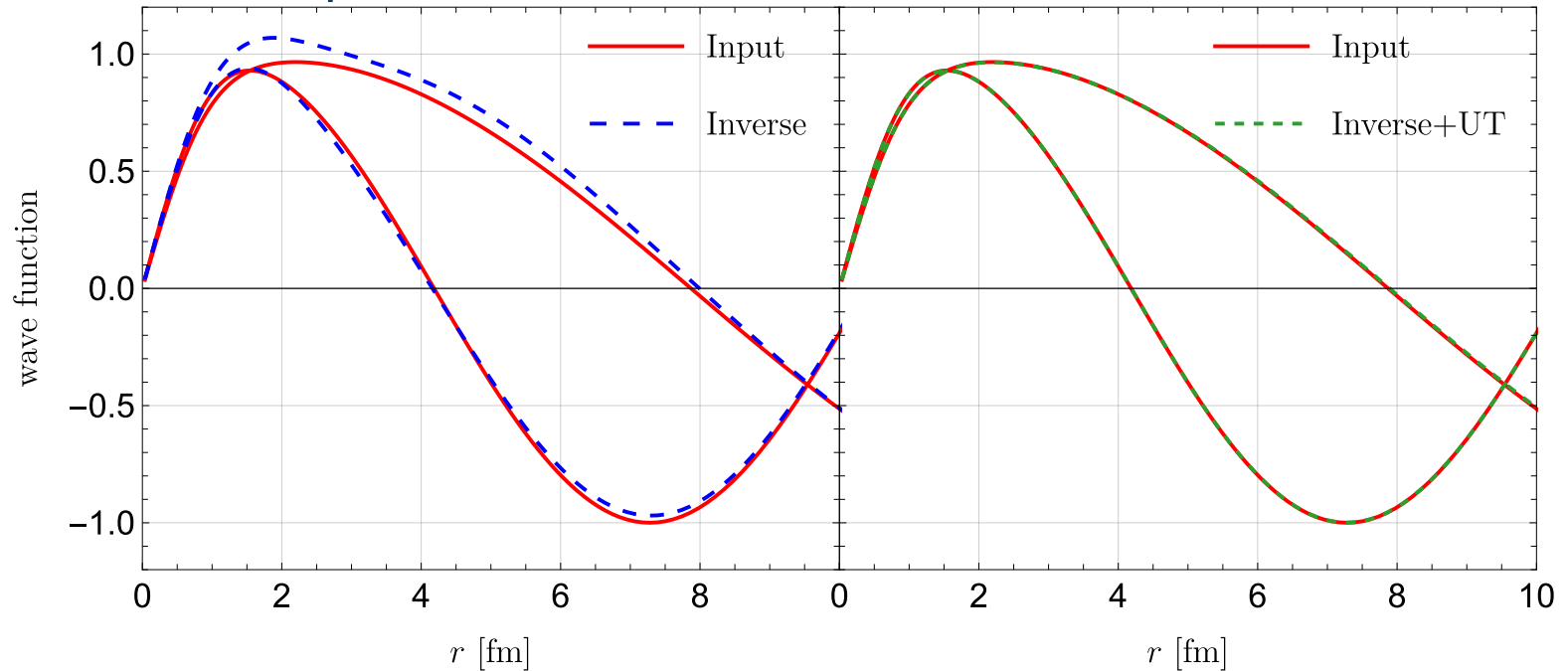
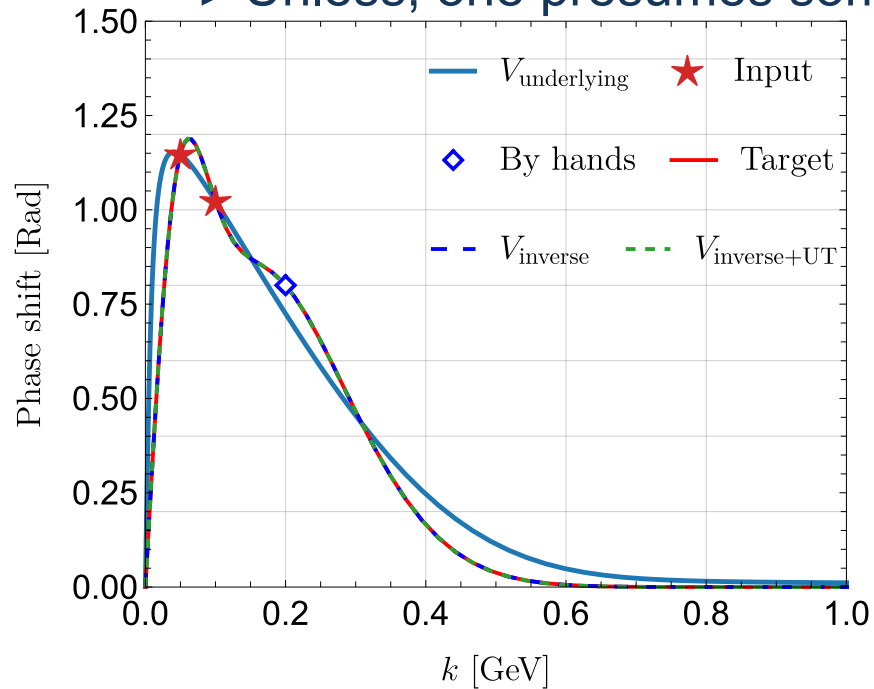
- From a small number of the wave functions, the potential can not be determined uniquely
  - ▶ Think it in a discrete way

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

- ▶ 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

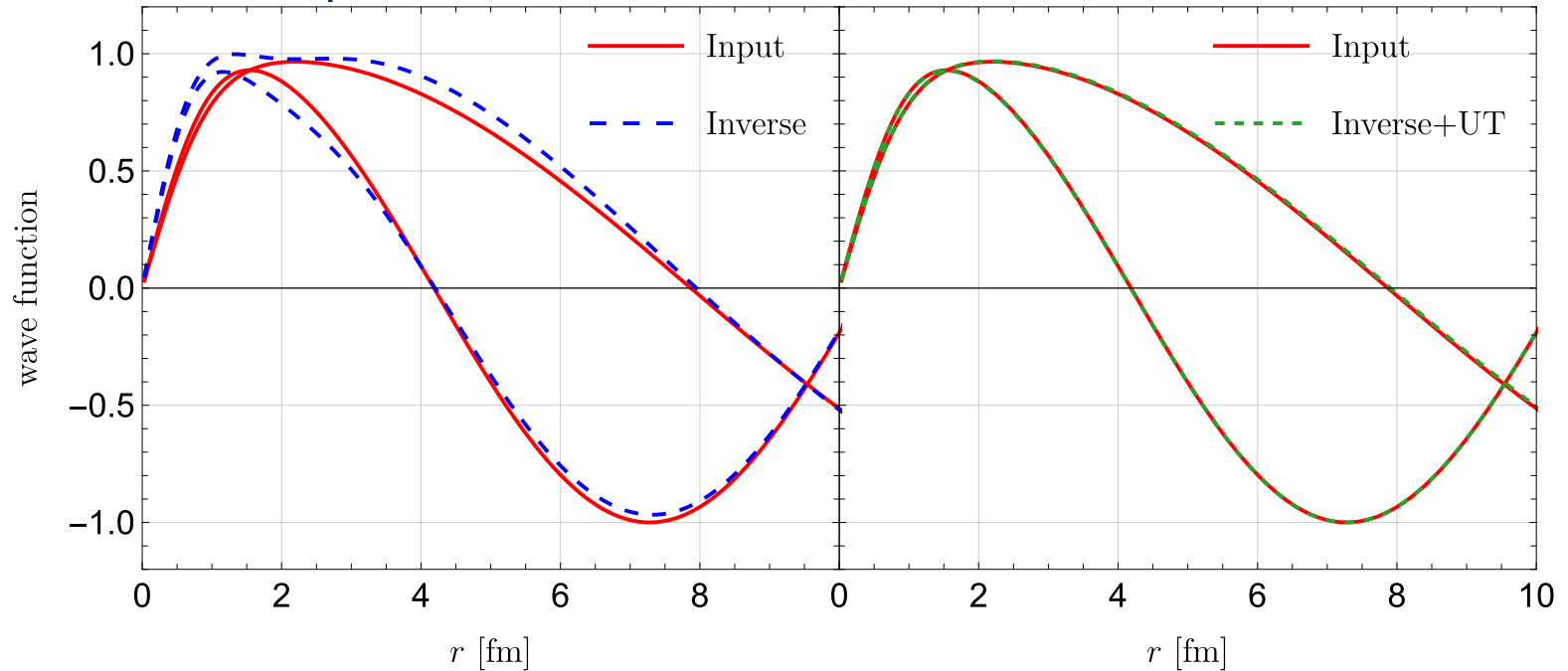
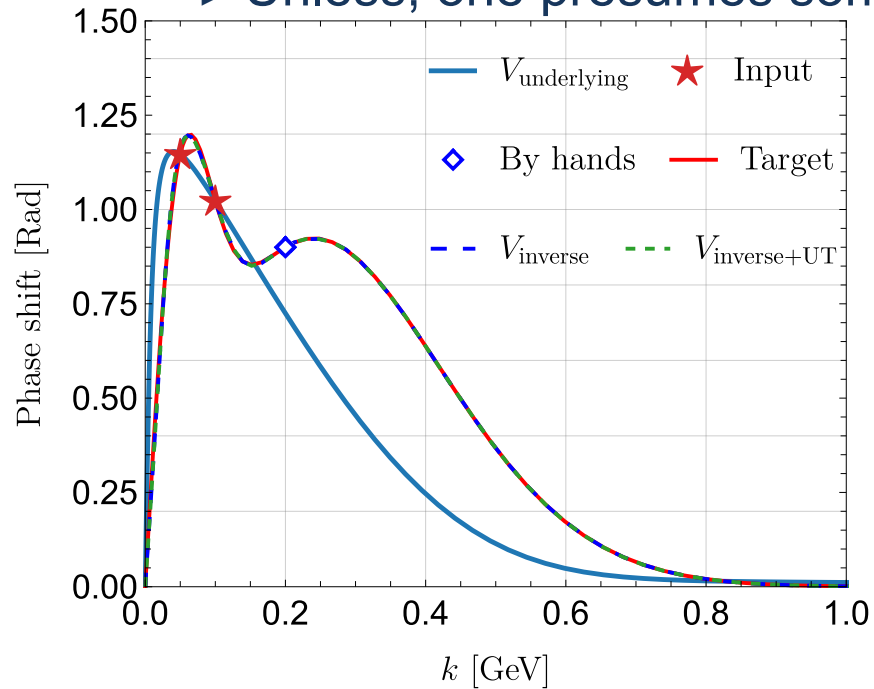
# A small number of wave functions

- 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



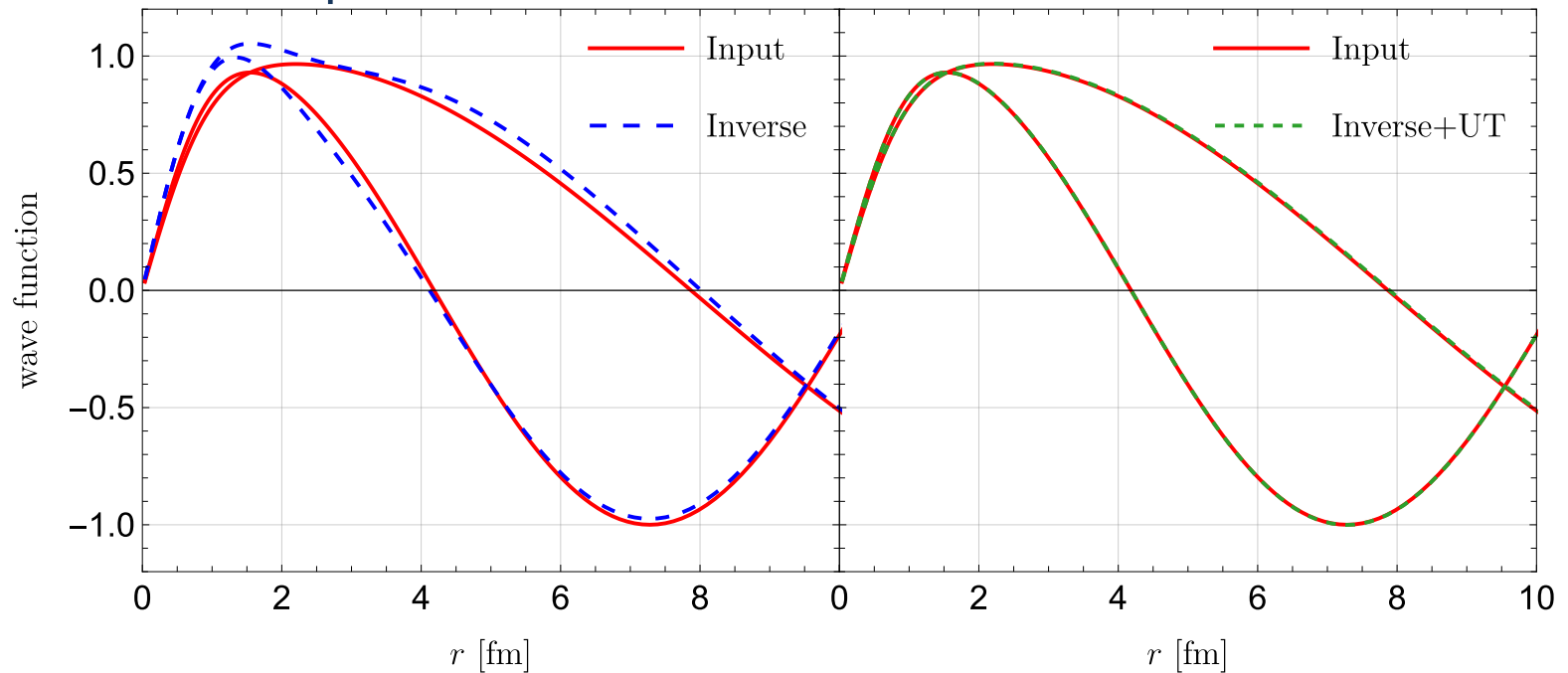
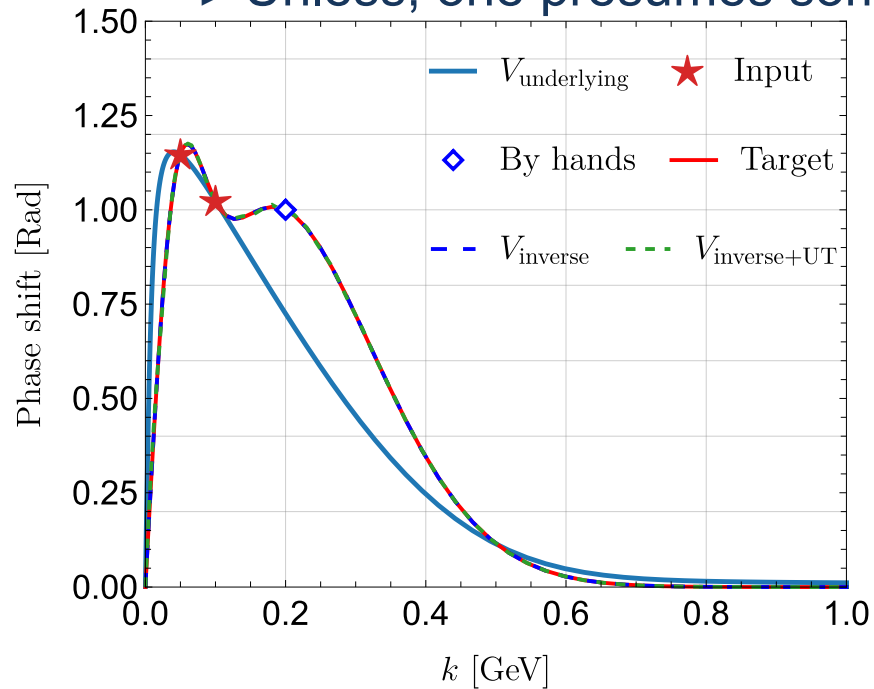
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# Derivative expansion VS EST expansion

# Derivative expansion

- Derivative expansion

Aoki:2021ahj

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

- 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

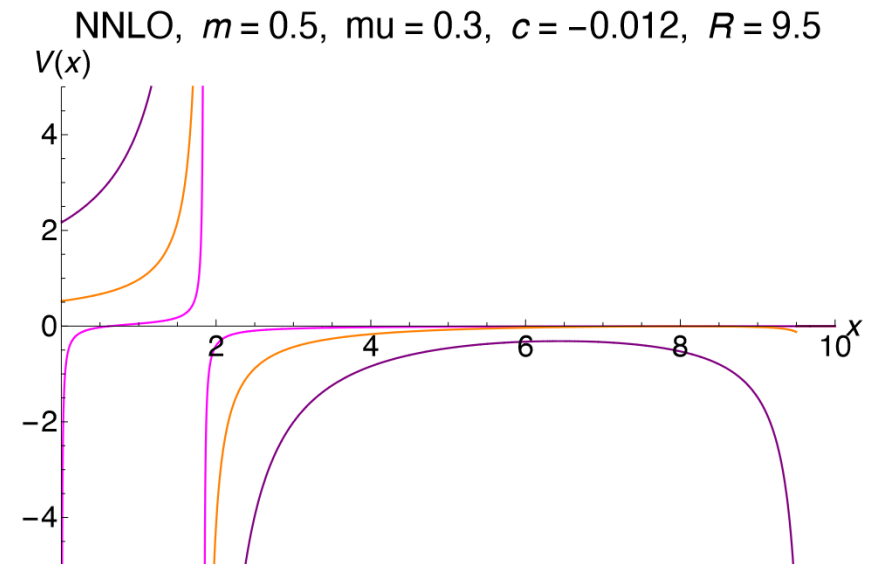
- NLO derivative expansion

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

- The potential become singular at the zero of det of the coefficients matrix

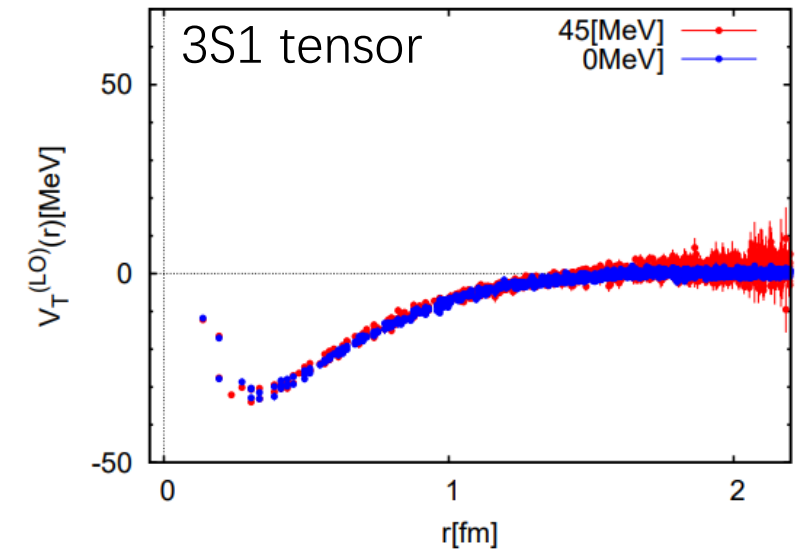
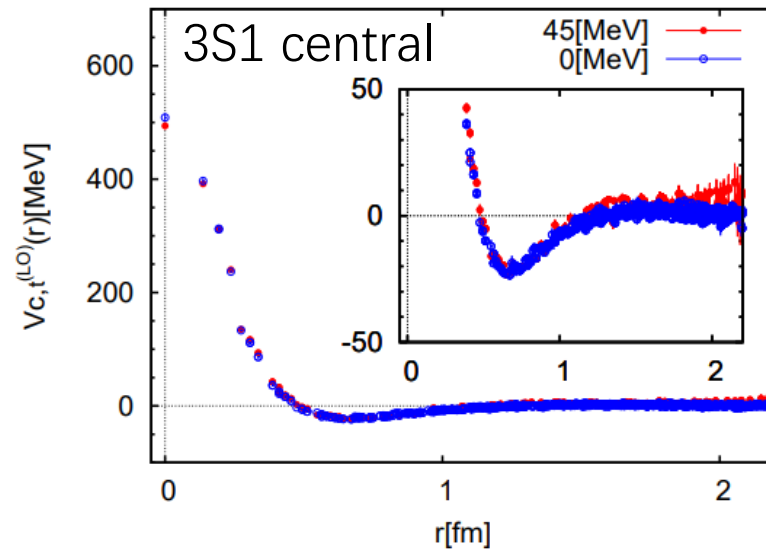
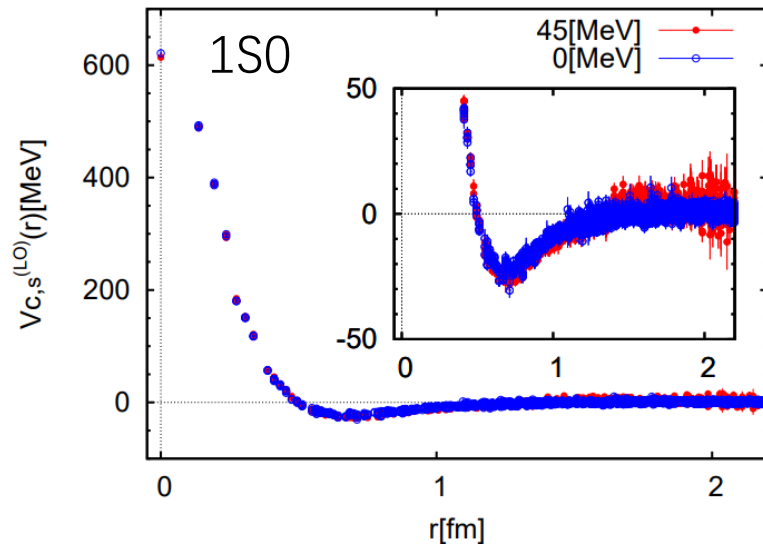
- A example from toy model [Aoki:2021ahj](#)

- ▶ In simulation, it is challenging to handle the singularity
- ▶ Wave functions are obtained at discrete point.



# Locality of the potential

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



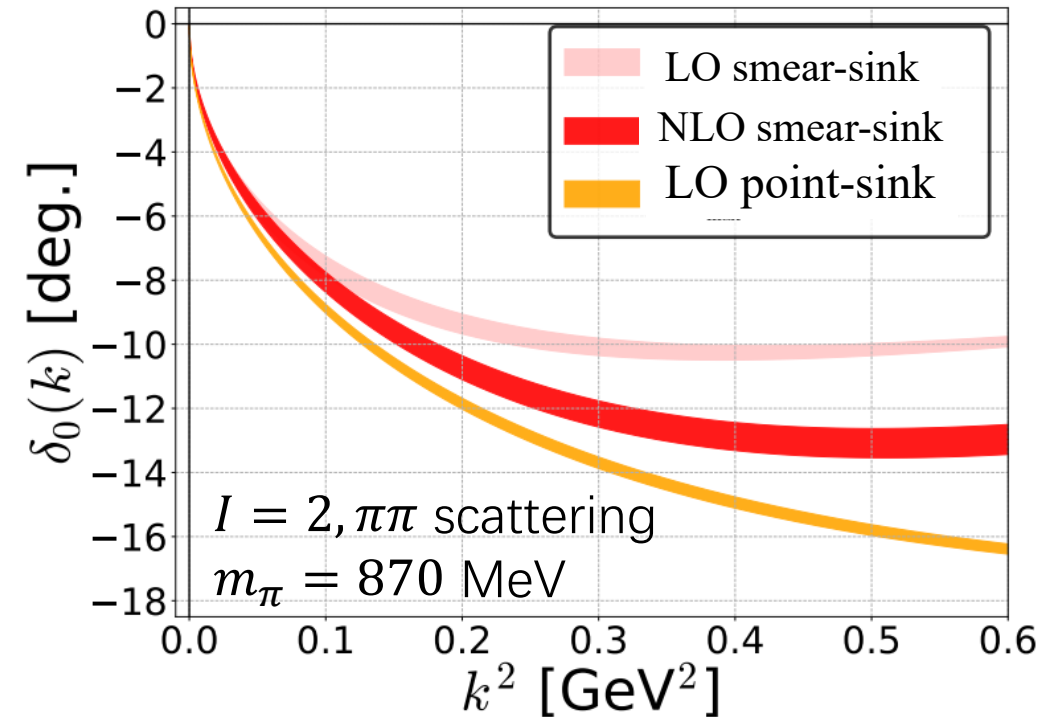
- Point-sink scheme used by HAL QCD group
  - ▶ Very local “underlying” potential, fast convergence of the DE

*By experiences*

[Murano:2011nz](#), [HALQCD:2017xsa](#), [Kurth:2013tua](#)

- 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:

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

Aoki:2009ji

▶ 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

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

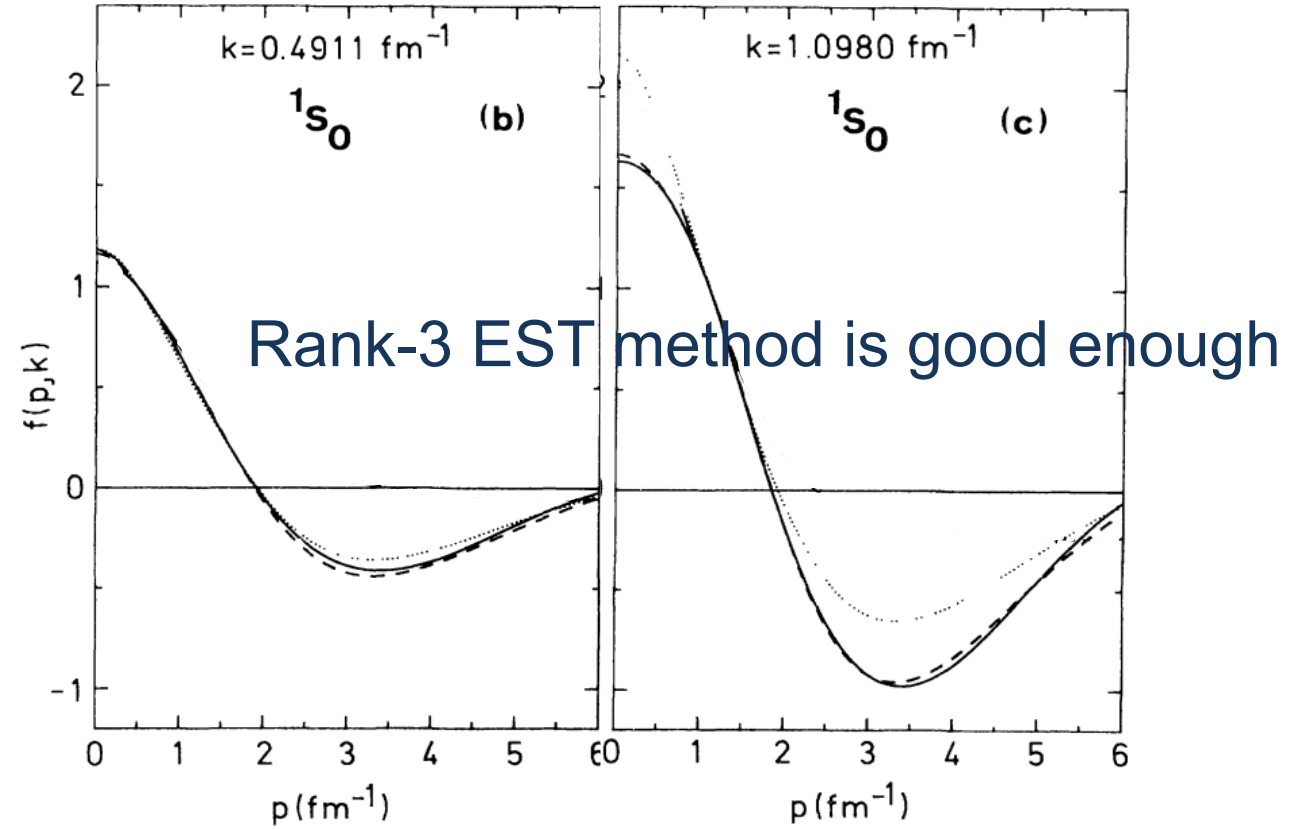
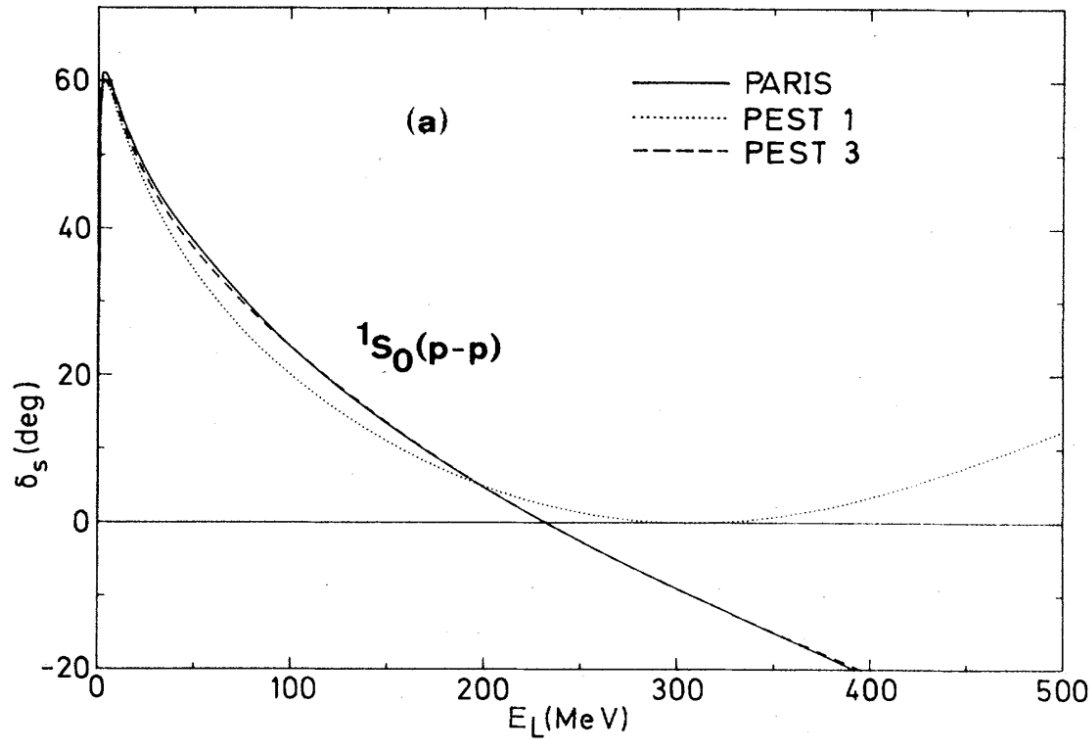
▶ In the outer region:  $K^{(i)}(r) = 0$

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



Ernst:1973zzb,Haidenbauer:1984dz

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# Numerical comparisons

# 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

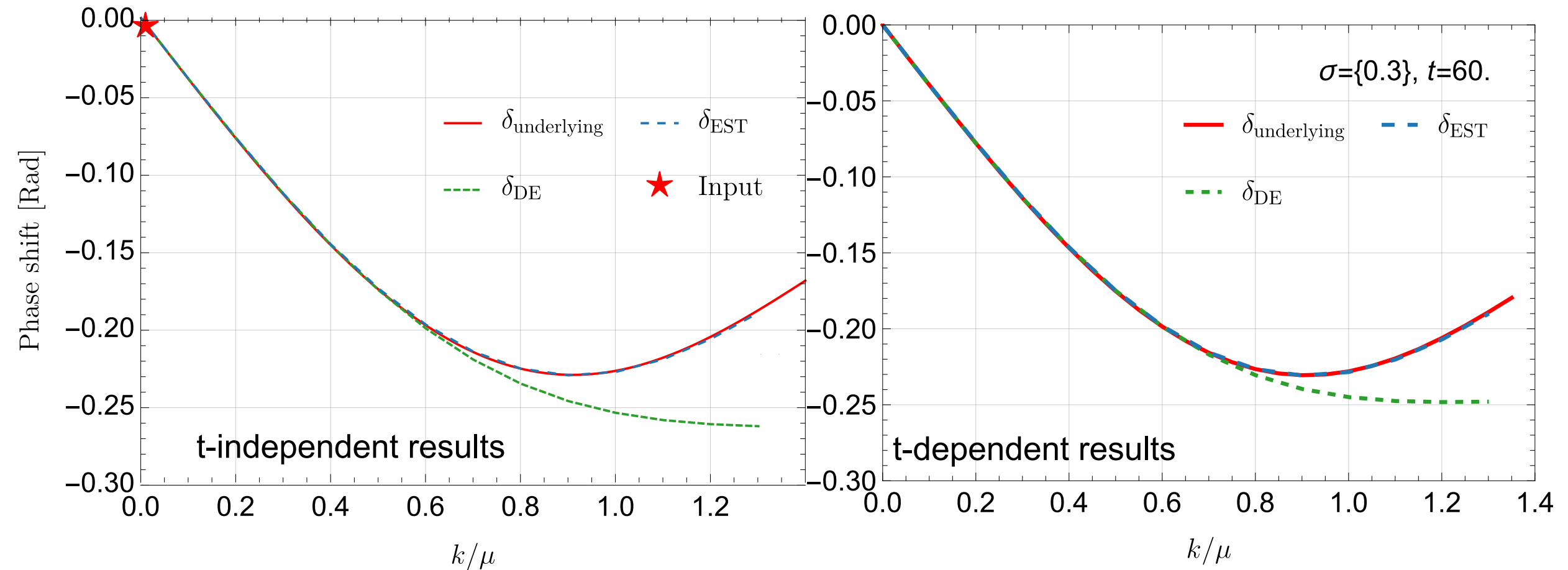
$$\tilde{R}(t=0, x) = \frac{\sigma^2 e^{-\sigma x}}{4\pi}$$

- ▶ 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

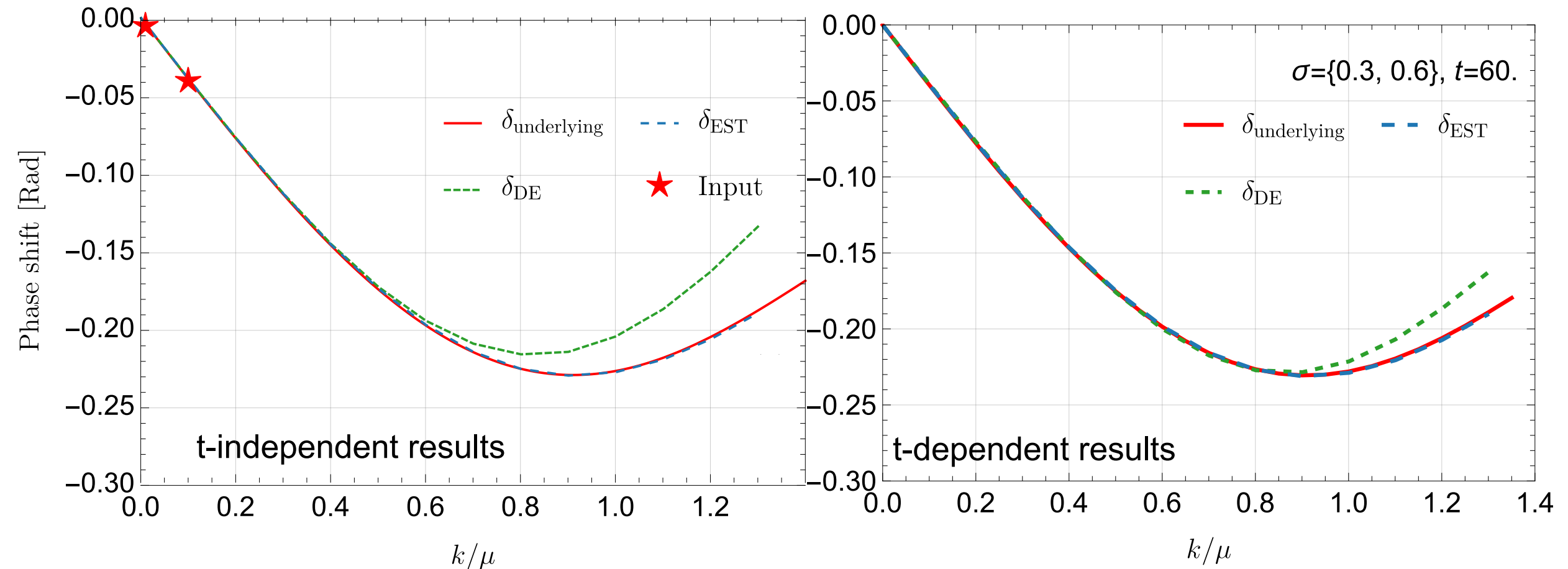
$$V(\mathbf{r}, \mathbf{r}') = \omega \frac{e^{-\mu r}}{r} \frac{e^{-\mu r'}}{r'}$$



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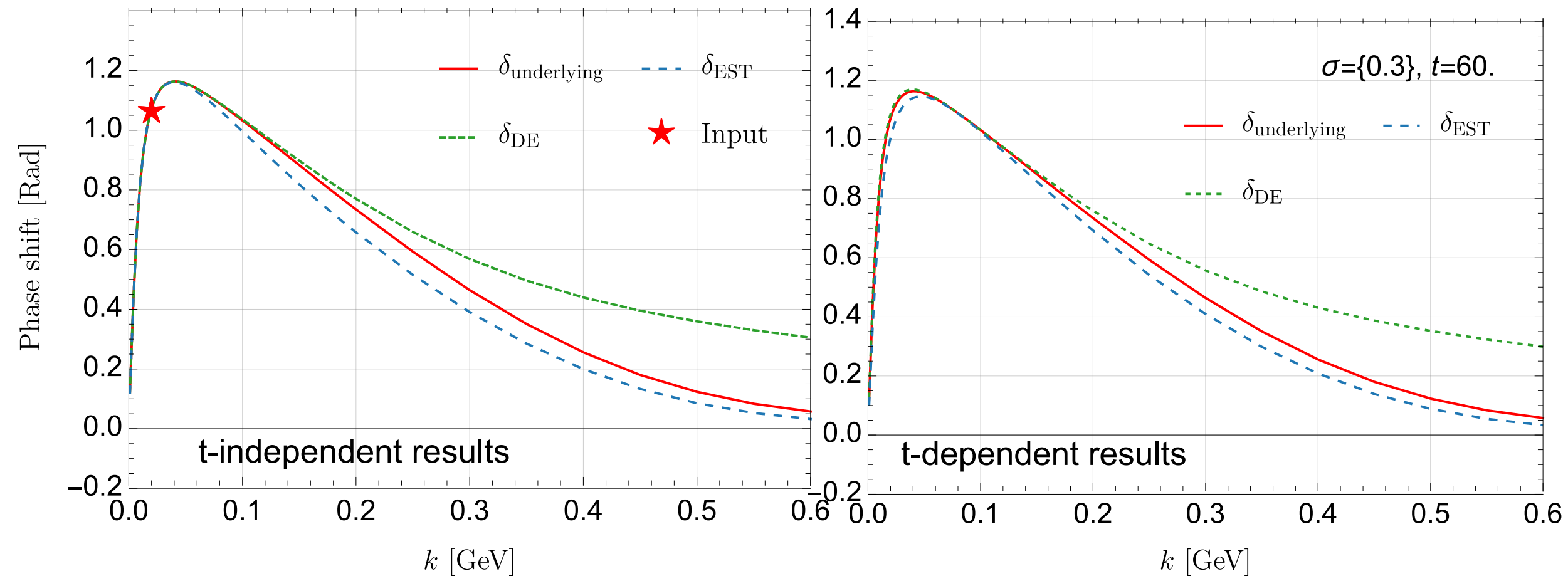


# Physical interaction

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

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

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

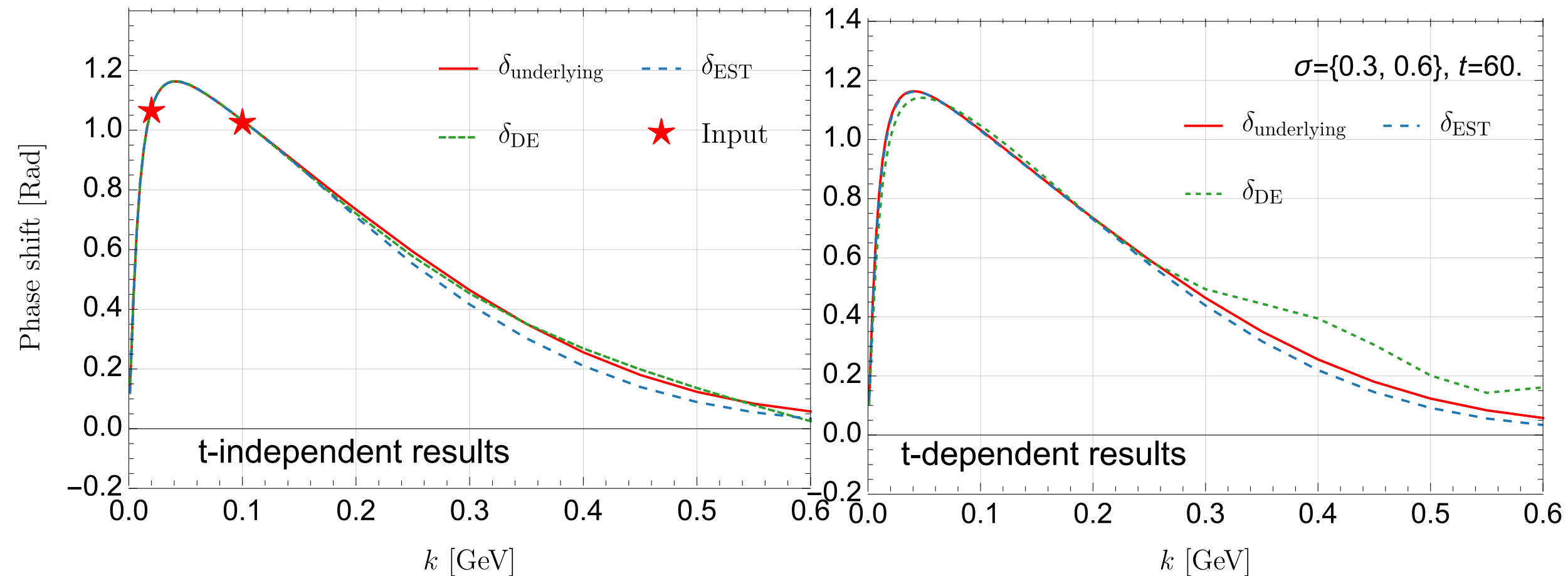


# Physical interaction

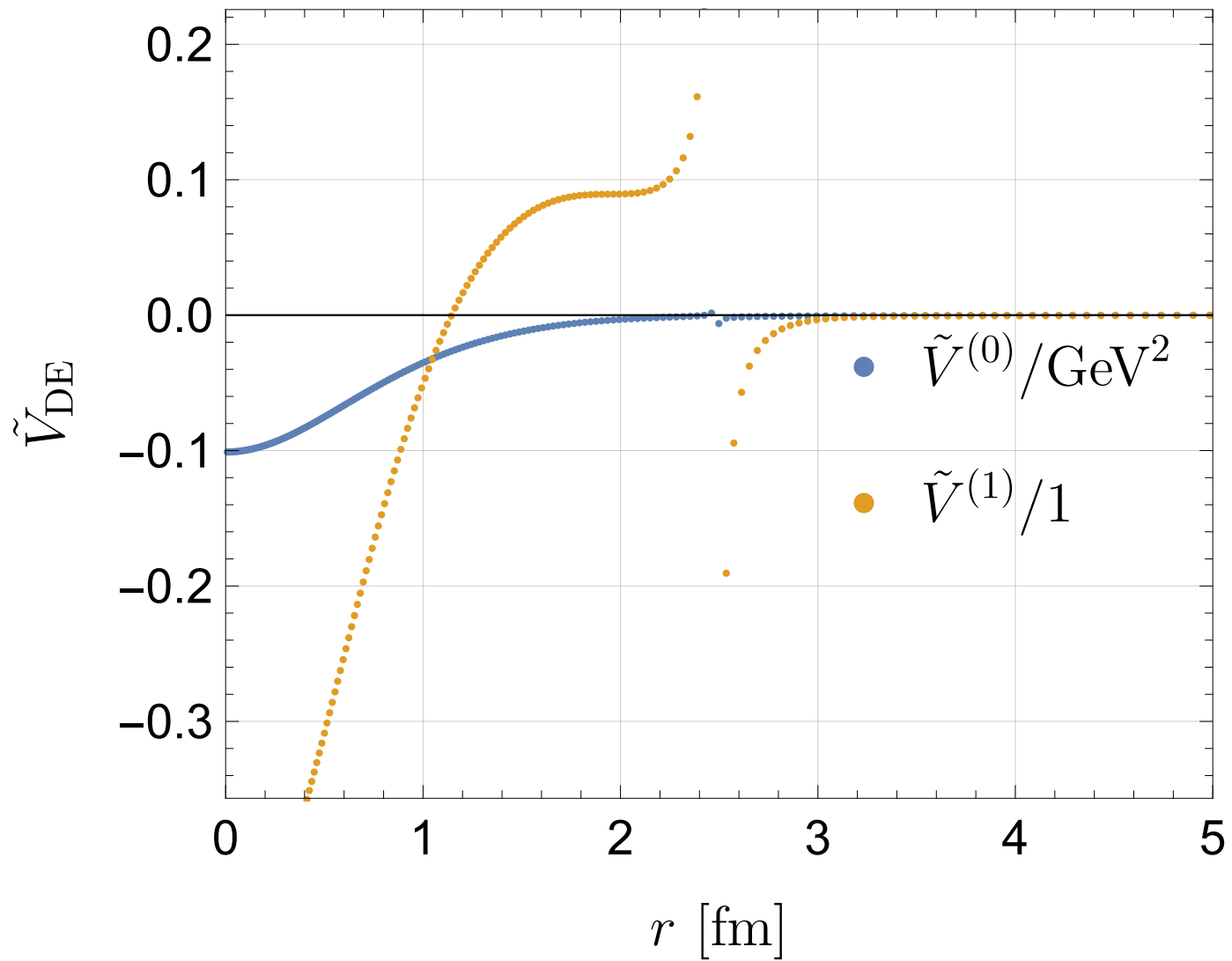
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- In t-dependent methods, singular potential

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



# Singularity in potential

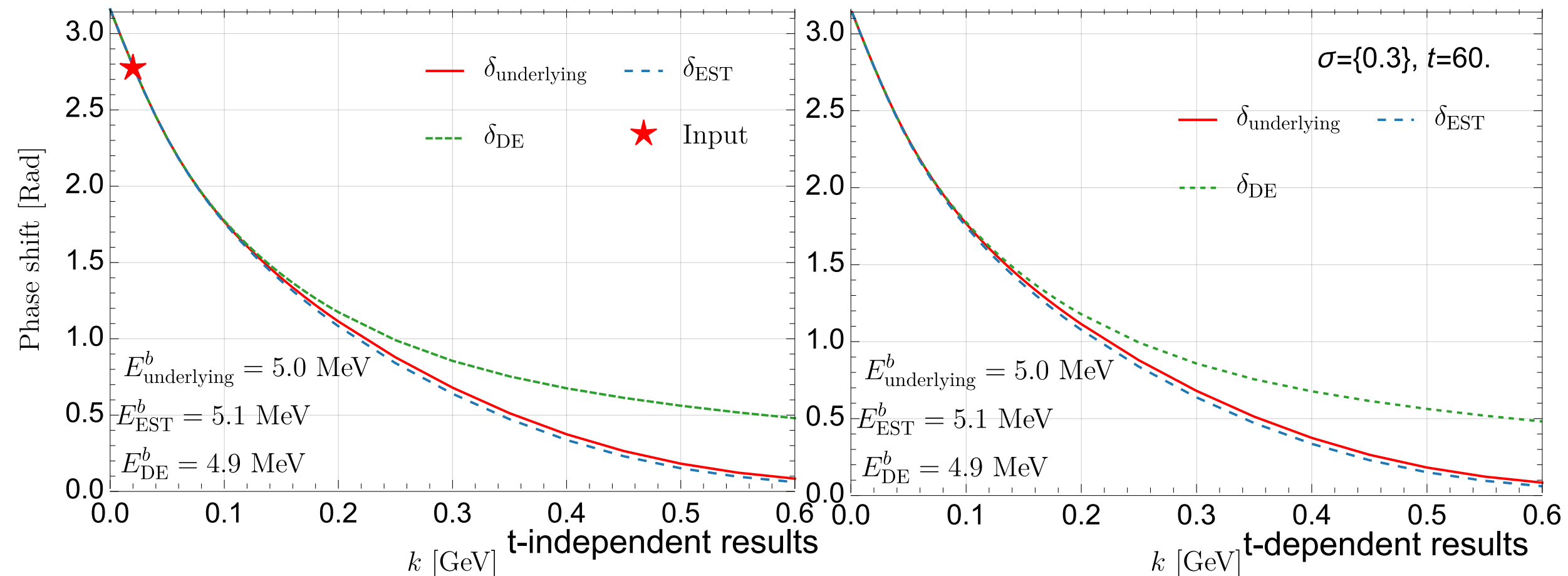


# Bound state

- 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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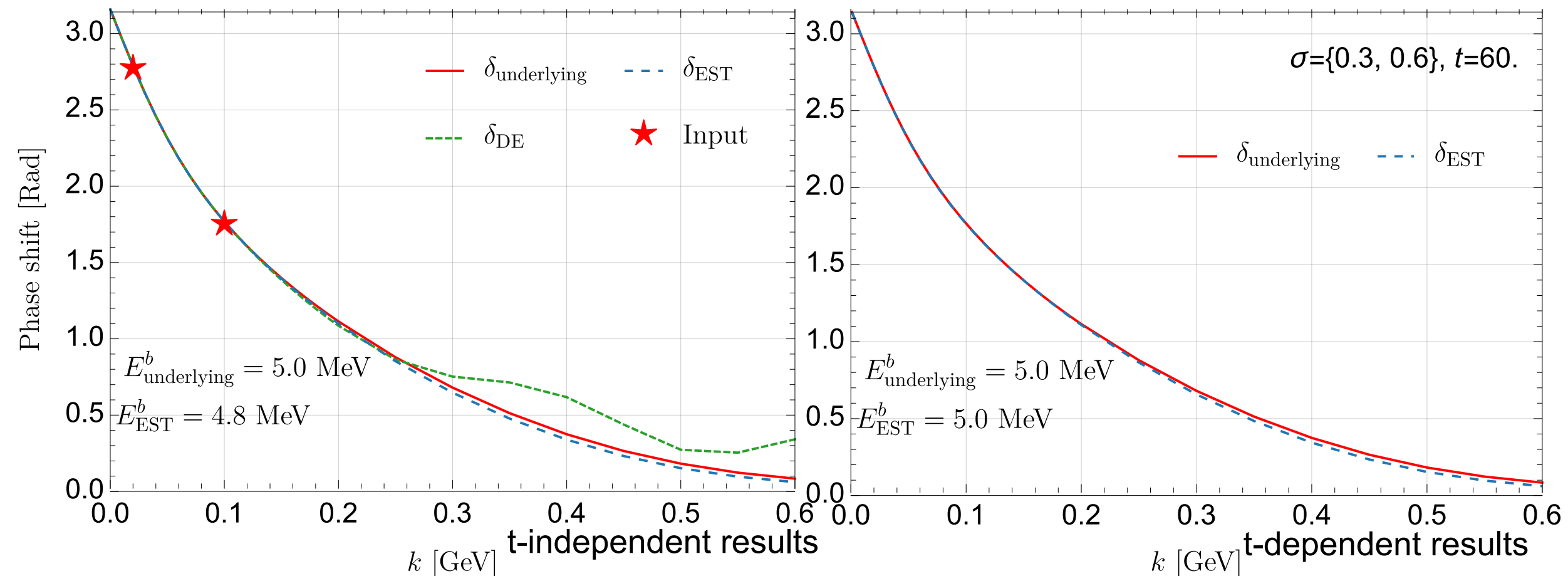


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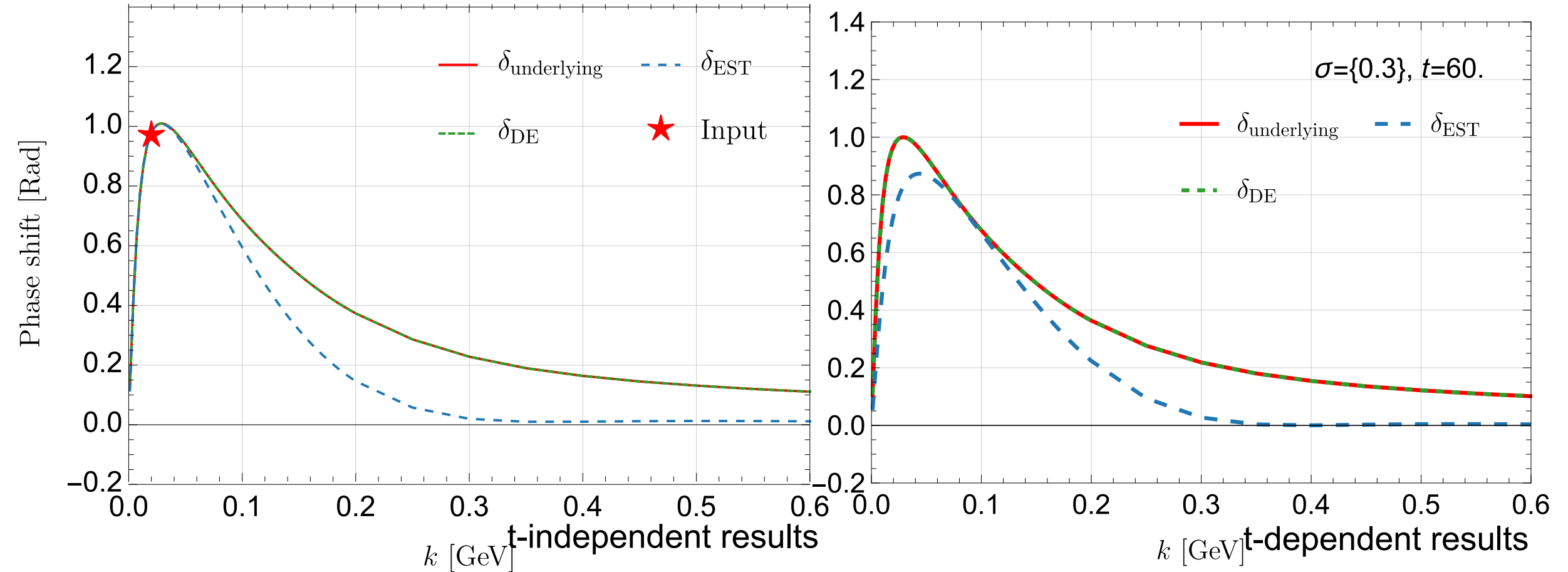


# Local interaction

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

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

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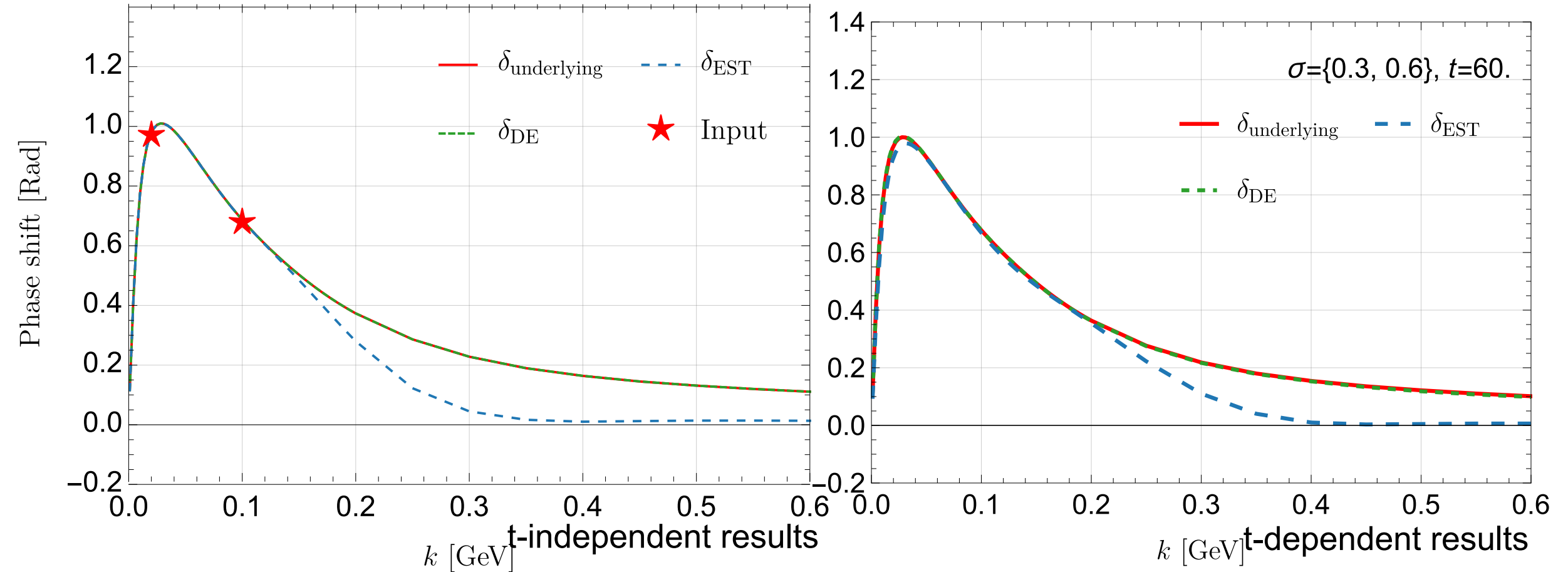


# Local interaction

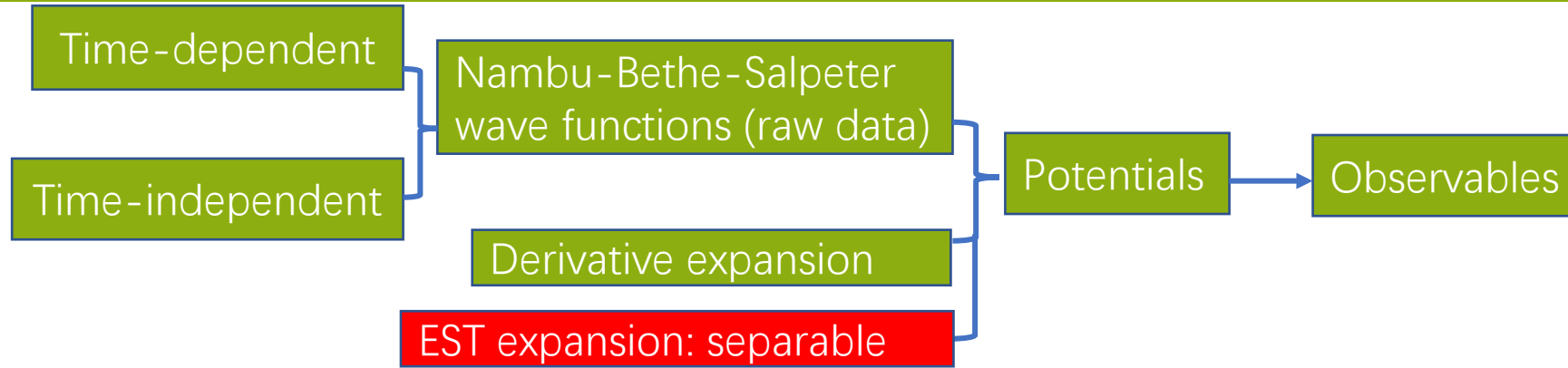
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# Summary



- 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!

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# Backup

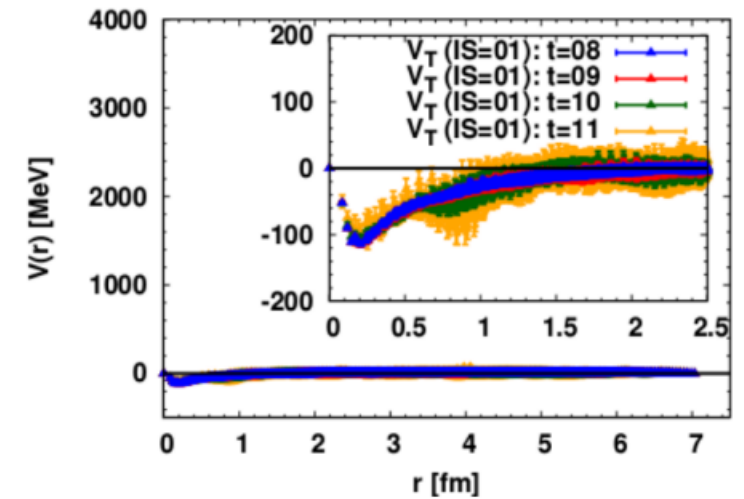
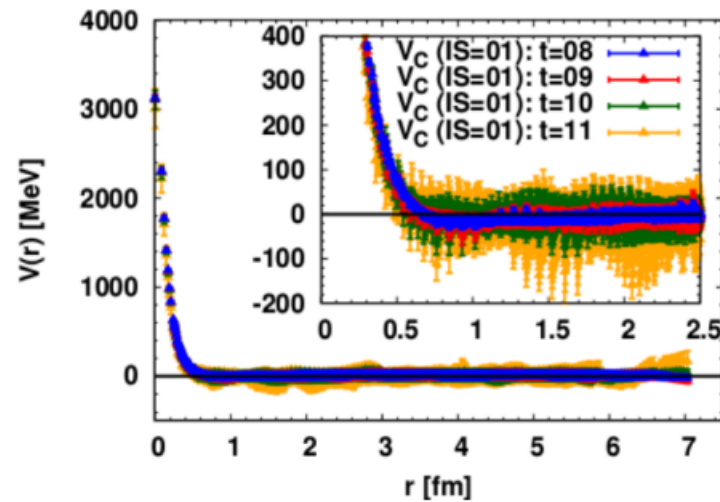
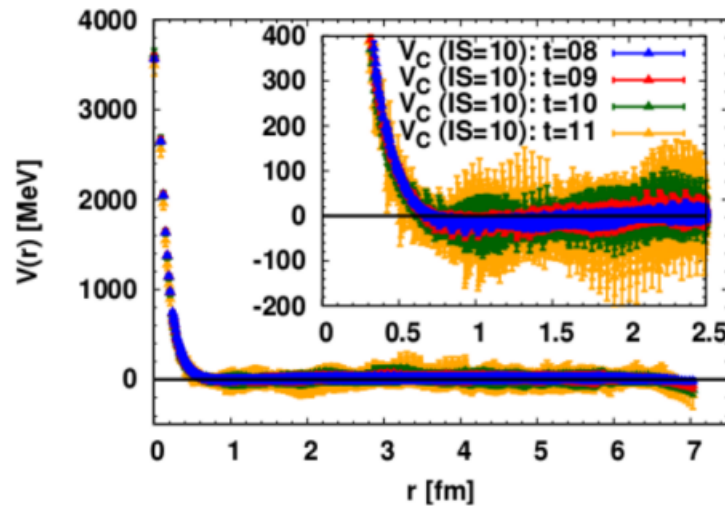
# Highlight of HALQCD results: NN interaction

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

⇒ Almost physical pion mass, very large box size, the finite volume effect is neglected

⇒ 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,  $96^4$
- $D^*D$ ,  $\phi N$  interaction...

Lyu:2022imf,Lyu:2023xro

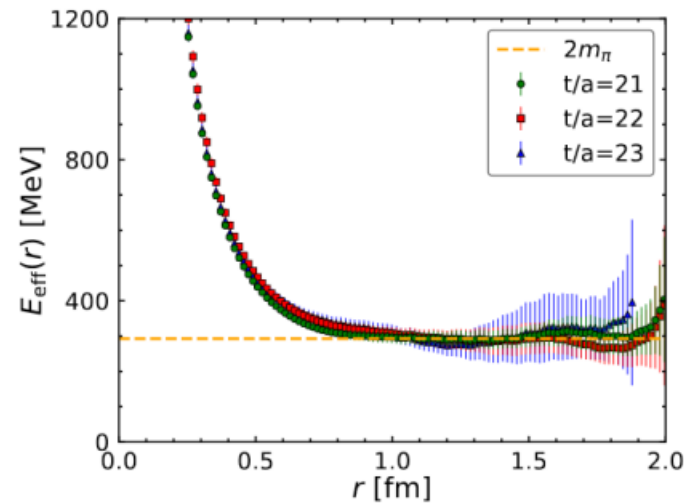
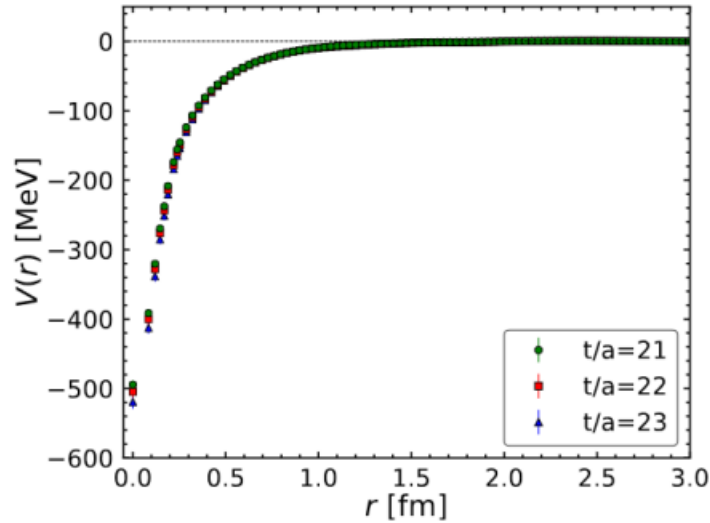


FIG. 2. The  $D^*D$  potential  $V(r)$  in the  $I = 0$  and  $S$ -wave channel at Euclidean time  $t/a = 21$  (green circles), 22 (red squares), and 23 (blue triangles).

Fitting the potential with:

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

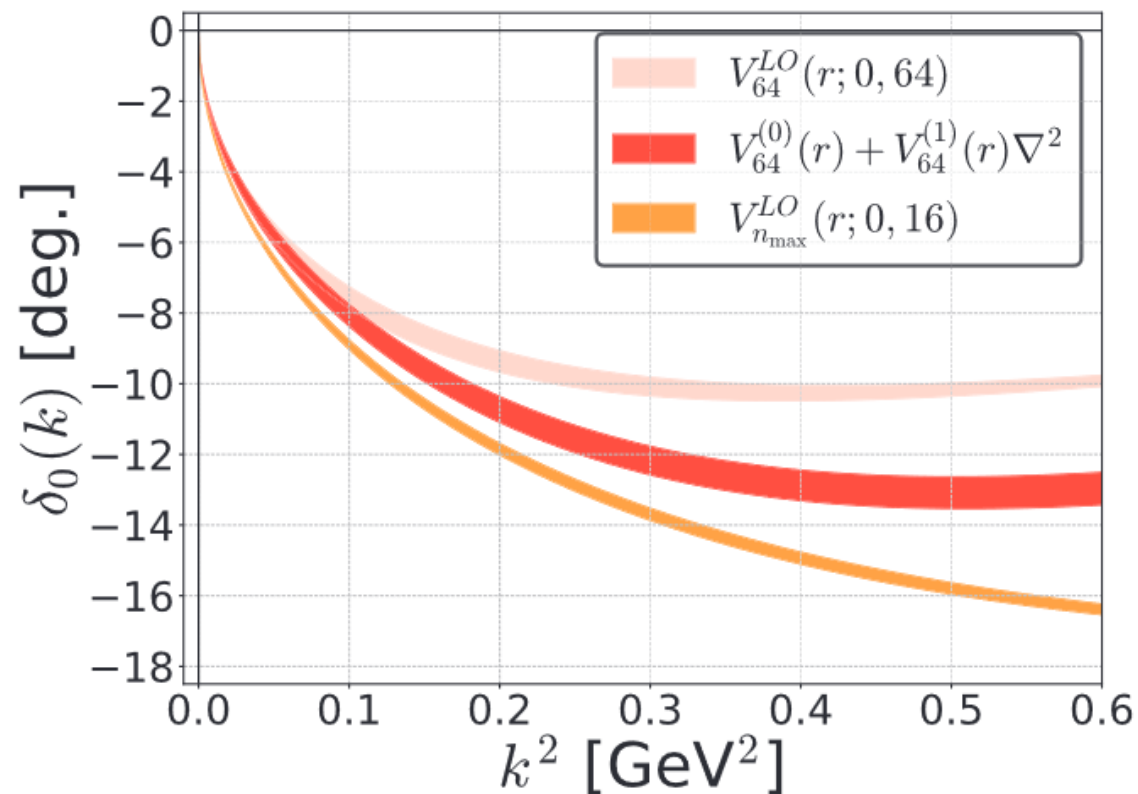
once  $a_3$  is determined

define

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

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

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



**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  $k^2$ .

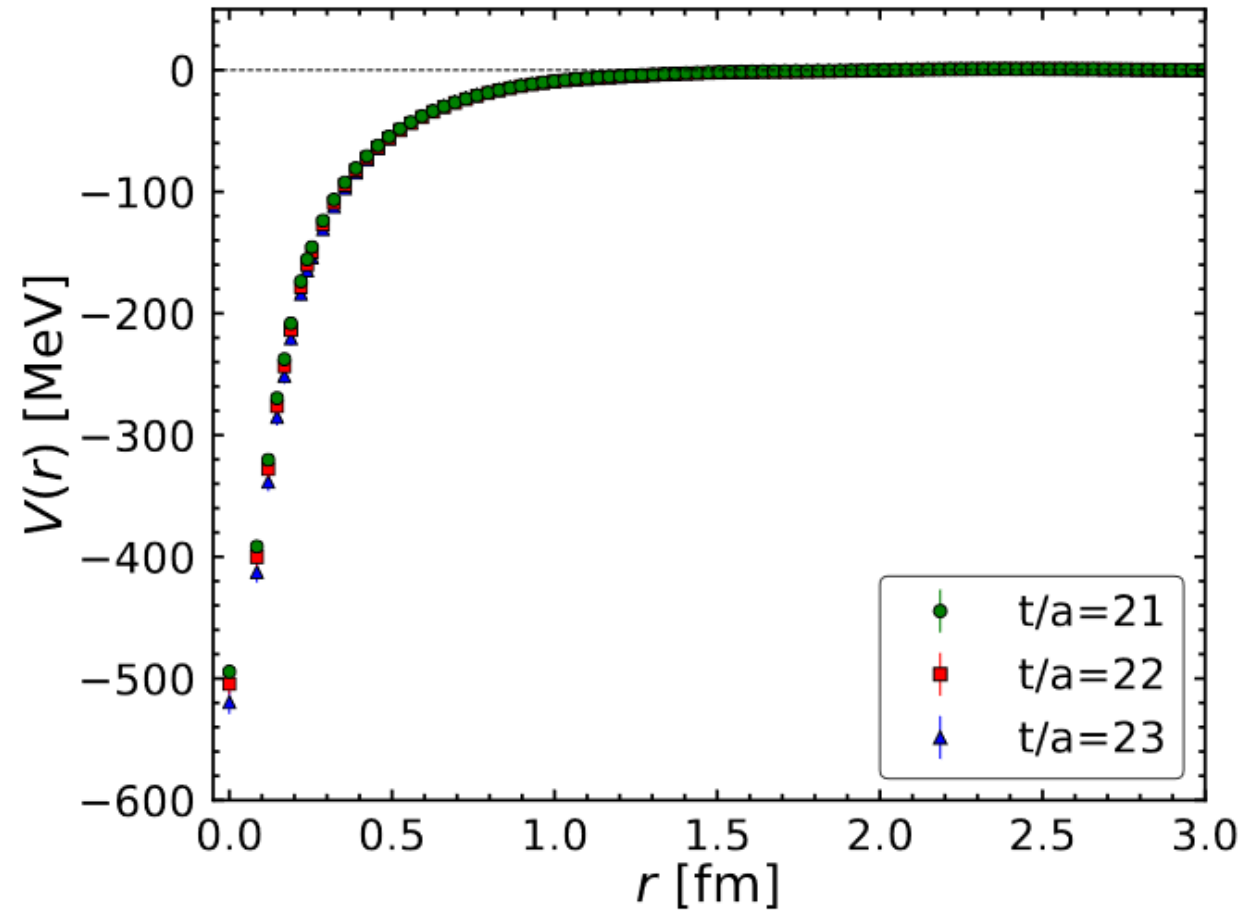
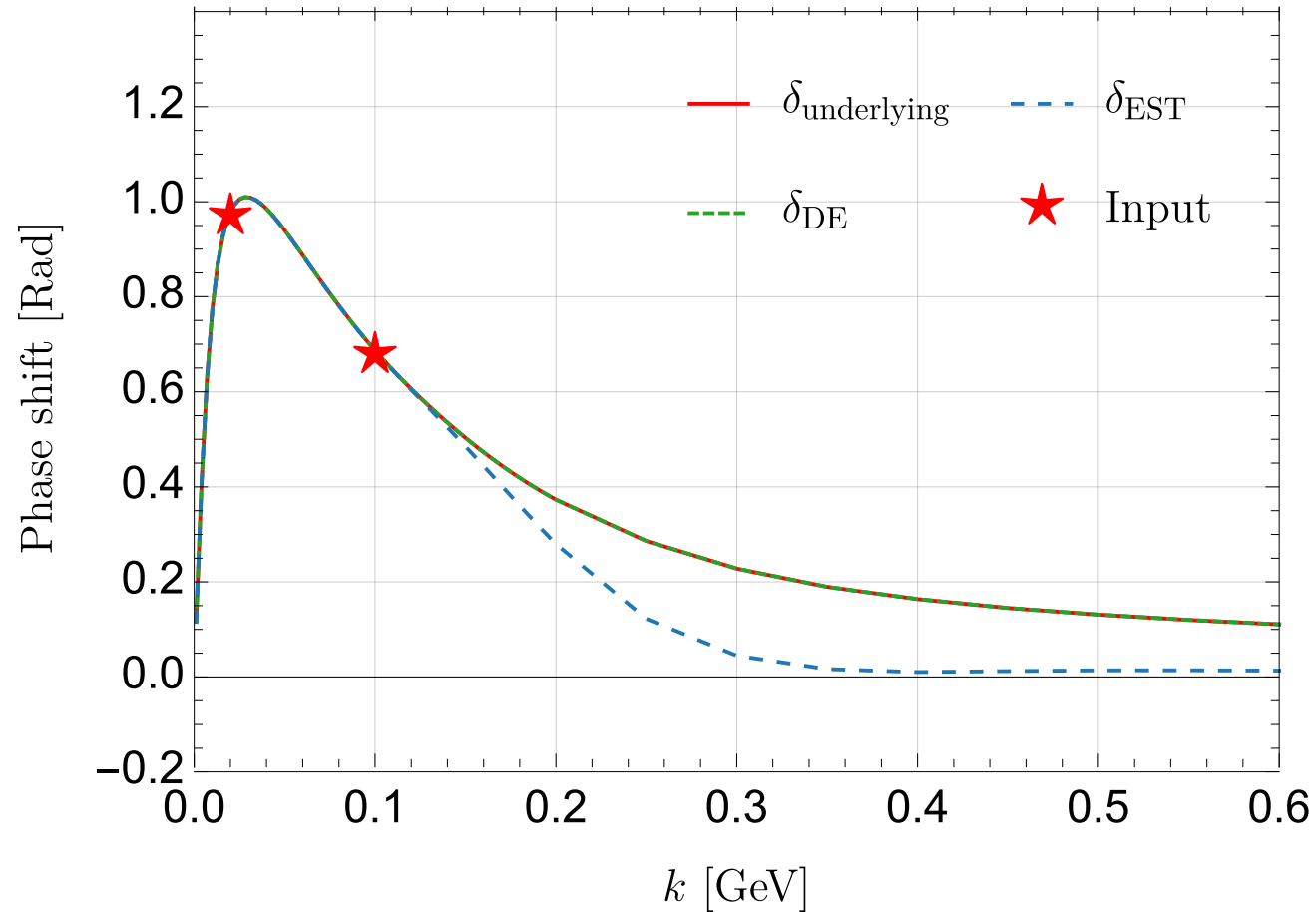


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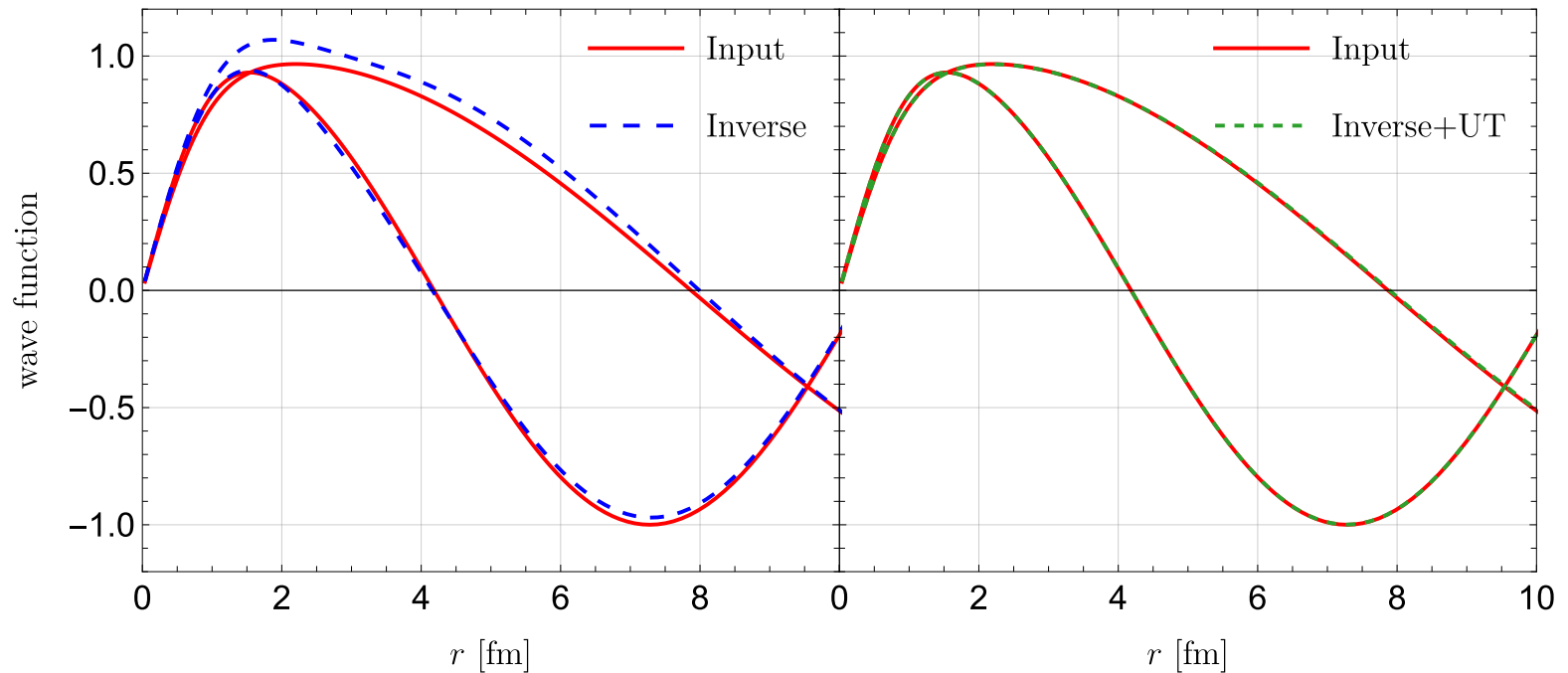
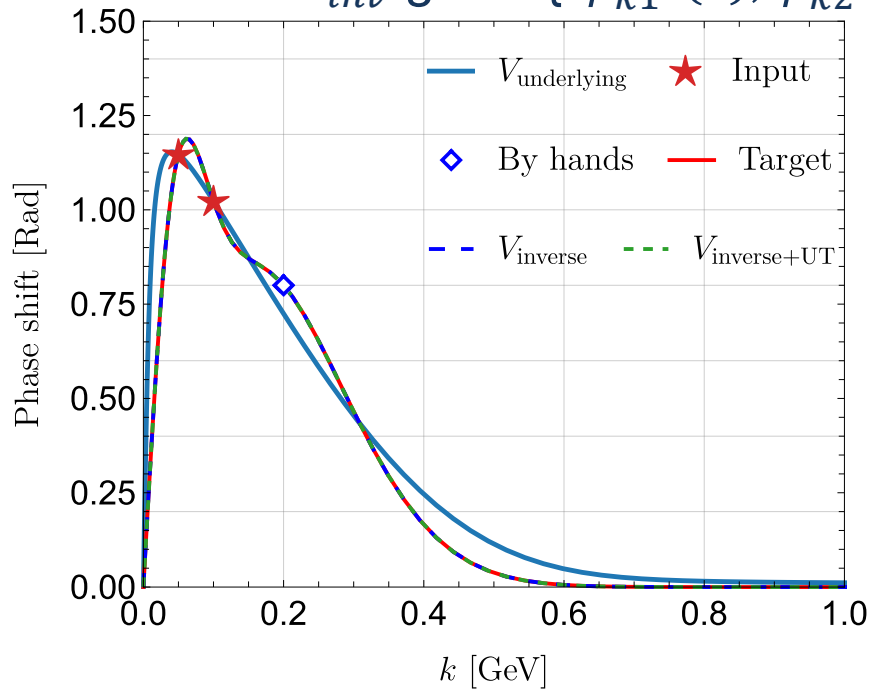
- Extracting potential from NBS is not an expansion of small quantities
- It is more like an interpolating and extrapolating
- Self-consistency test also makes sense



# 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

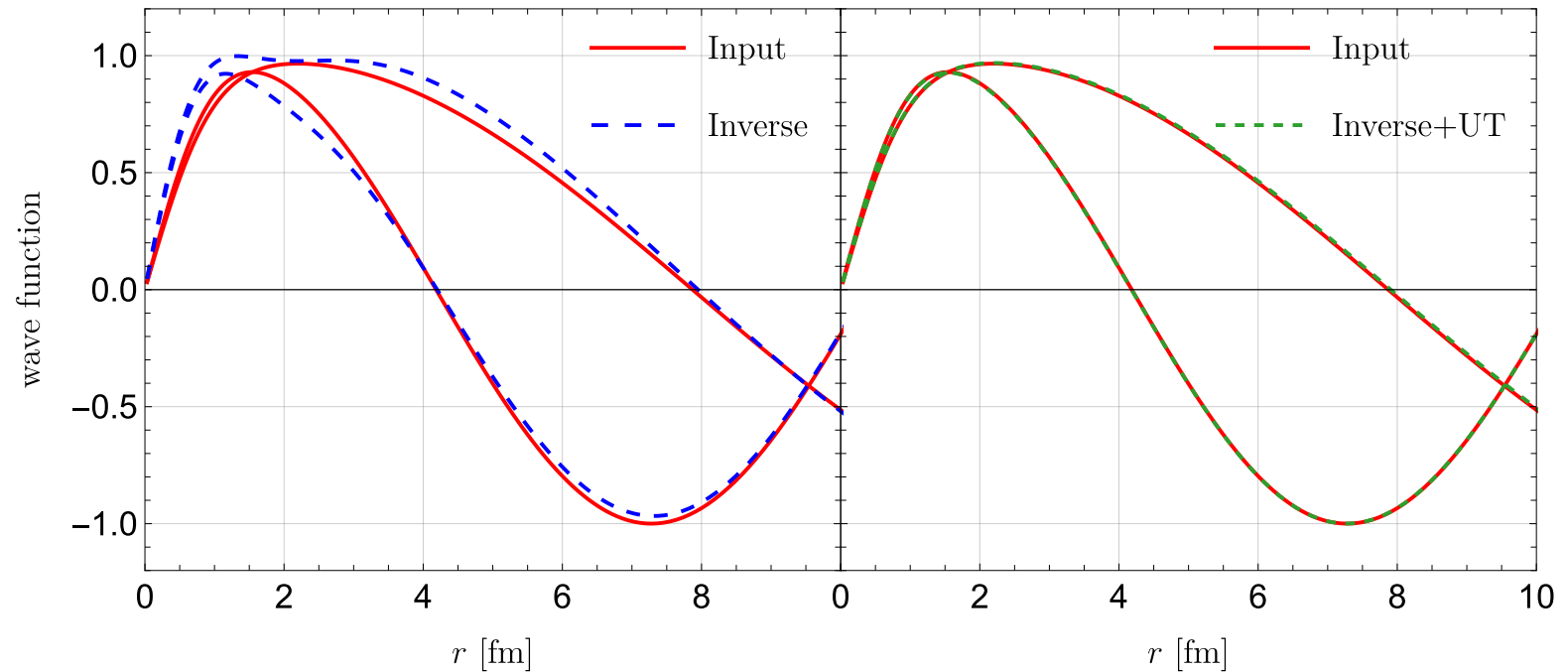
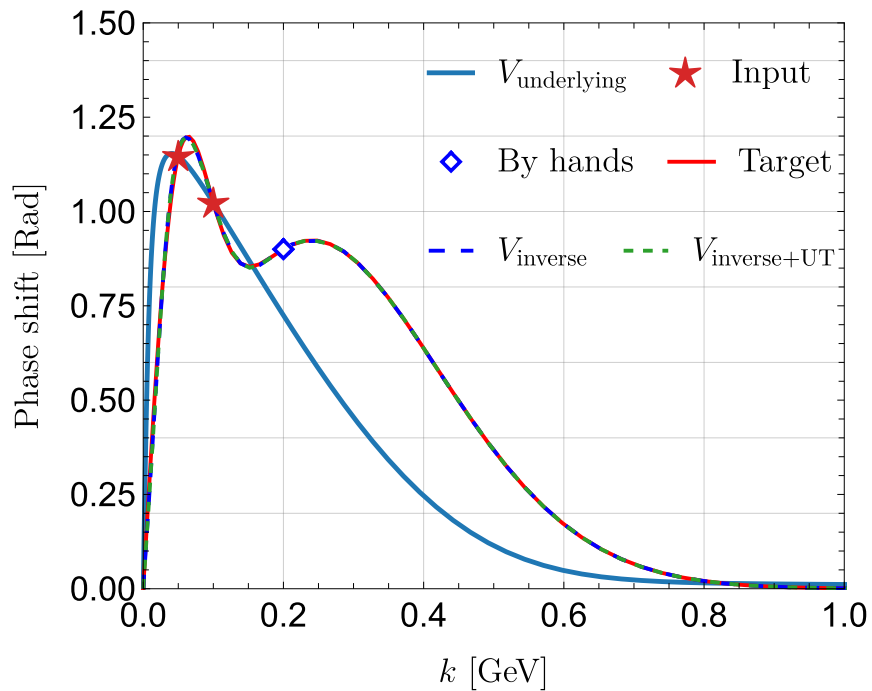
6. Construct an unitary trans. (UT):  $U|\psi_{k_i}^{inv}\rangle = |\psi_{k_i}\rangle$

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

