Theoretical and practical progresses in the HAL QCD method

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0. Introduction

Some Issues in the HAL QCD method

HAL QCD method

A powerful method to investigate hadron interactions

Strategy

NBS wave function

$$\varphi^{\vec{k}}(\vec{x})e^{-W_{\vec{k}}t} = \langle 0|N(\vec{r},t)N(\vec{r}+\vec{x},t)|NN, W_{\vec{k}}\rangle \qquad W_{\vec{k}} = 2\sqrt{\vec{k}^2 + m_N^2}$$

$$\rightarrow \sum_{lm} C_{lm} \frac{\sin(kx + \delta_l(k))}{kx} Y_{lm}(\Omega_{\vec{x}})$$

energy-independent non-local potential

$$\left(E_{\vec{k}} - H_0\right)\varphi^{\vec{k}}(\vec{x}) = \int U(\vec{x},\vec{y})\varphi^{\vec{k}}(\vec{y})d^3y, \qquad E_{\vec{k}} = \frac{\vec{k}^2}{m_N},\ H_0 = \frac{-\nabla^2}{m_N},$$

$$W_{\vec{k}} \leq W_{\rm th} = 2m_N + m_\pi$$

Derivative expansion

$$U(\vec{x},\vec{y}) = V(\vec{x},\vec{\nabla})\delta^{(3)}(\vec{x}-\vec{y})$$

$$V(\vec{x},\vec{\nabla}) = V_0(x) + V_\sigma(x)(\vec{\sigma}_1\cdot\vec{\sigma}_2) + V_T(x)S_{12} + V_{\rm LS}(x)\vec{L}\cdot\vec{S} + O(\vec{\nabla}^2)$$

Some issues

Q1. Validity of the derivative expansion ? small parameter ?

→ I. Definition of the HAL QCD potential with the derivative expansion

Q2. Is the HAL QCD potential Hermite ?

→ II. Hermitian potential from non-Hermite potential

Q3. The HAL QCD potential in the moving system ?

→ III. The HAL QCD potential from the moving system

Q4. Partial wave mixings in the cubic box ?

→ arXiv:1906.01987

Q5. Quark annihilation processes ?

→ Yutaro Akahoshi's talk in this session

I. Definition of the HAL QCD potential with the derivative expansion

$$(E_{\vec{k}} - H_0)\varphi^{\vec{k}}(\vec{x}) = \int U(\vec{x},\vec{y})\varphi^{\vec{k}}(\vec{y})d^3y, \quad \boxed{W_{\vec{k}} \leq W_{\rm th}}$$

This equation does not fix the non-local potential due to the restriction of energies. Therefore we have to fix the definition of the potential (scheme) explicitly.

We here propose a scheme to fix the potential completely using the derivative expansion.

For simplicity, let us consider the scalar particles and ignore the angular momentum dependent part of the potential.

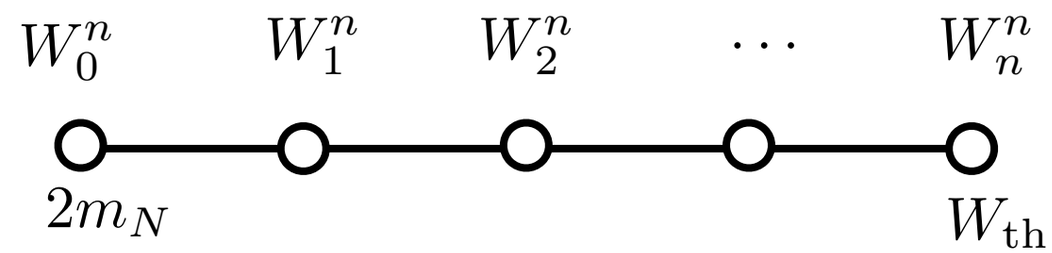
- We consider the expansion in terms of ∇^2 (but not $\mathbf{L}^2$).
- Terms with odd number of ∇ are not included. This is our scheme.
- The potential must be non-Hermitian. We can make it Hermitian as seen later.

Of course, the scheme is not unique. One may use a different one.

Definition of the potential

choice of energy

$$W_k^n := 2m_N + \frac{k}{n}(W_{\rm th} - 2m_N), \quad k = 0, 1, \cdots, n$$



approximated potential at the n-th order

$$V^{(n)}(\mathbf{x}, \nabla) := \sum_{k=0}^{n} V_k^{(n)}(\mathbf{x})(\nabla^2)^k$$

NBS wave functions at these energies

$$W_n^k = 2\sqrt{p_k^2 + m_N^2}$$

$$\sum_{k=0}^{n} V_k^{(n)}(\mathbf{x})(\nabla^2)^k \varphi_{p_k}(\mathbf{x}) = (\epsilon_{p_k} - H_0)\varphi_{p_k}(\mathbf{x})$$

$$\begin{pmatrix} \varphi_{p_0}(\mathbf{x}) & \nabla^2\varphi_{p_0}(\mathbf{x}) & \cdots & (\nabla^2)^n\varphi_{p_0}(\mathbf{x}) \\ \varphi_{p_1}(\mathbf{x}) & \nabla^2\varphi_{p_1}(\mathbf{x}) & \cdots & (\nabla^2)^n\varphi_{p_1}(\mathbf{x}) \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \varphi_{p_n}(\mathbf{x}) & \nabla^2\varphi_{p_n}(\mathbf{x}) & \cdots & (\nabla^2)^n\varphi_{p_n}(\mathbf{x}) \end{pmatrix} \begin{pmatrix} V_0^{(n)}(\mathbf{x}) \\ V_1^{(n)}(\mathbf{x}) \\ \cdot \\ \cdot \\ V_n^{(n)}(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} (\epsilon_{p_0} - H_0)\varphi_{p_0}(\mathbf{x}) \\ (\epsilon_{p_1} - H_0)\varphi_{p_1}(\mathbf{x}) \\ \cdot \\ \cdot \\ (\epsilon_{p_n} - H_0)\varphi_{p_n}(\mathbf{x}) \end{pmatrix}$$

$$V_k^{(n)}(\mathbf{x})$$

Def of potential

$$\boxed{V(\mathbf{x}, \nabla) := \lim_{n\to\infty} V^{(n)}(\mathbf{x}, \nabla) = \lim_{n\to\infty} \sum_{k=0}^{n} V_k^{(n)}(\mathbf{x})(\nabla^2)^k}$$

Demonstration

Separable potential $U(\vec{x},\vec{y}) = wv(\vec{x})v(\vec{y})$ $\quad v(\vec{x}) = e^{-\mu x}, \quad x := |\vec{x}|$

highly non-local

L=0 wave function

R: IR cut-off

$$\psi_k^0(x) = \frac{e^{i\delta(k)}}{kx}\left[\sin(kx+\delta(k)) - \sin\delta(k)e^{-\mu x}\left(1 + x\frac{\mu^2+k^2)}{2\mu}\right)\right] \qquad x \le R$$

$$= C\frac{e^{i\delta(k)}}{kx}\sin(kx+\delta_R(k)) \qquad x > R$$

phase shift $\delta_R(k)$ is exactly calculable.

phase shift

exact result from separable potential $U(\vec{x},\vec{y})$

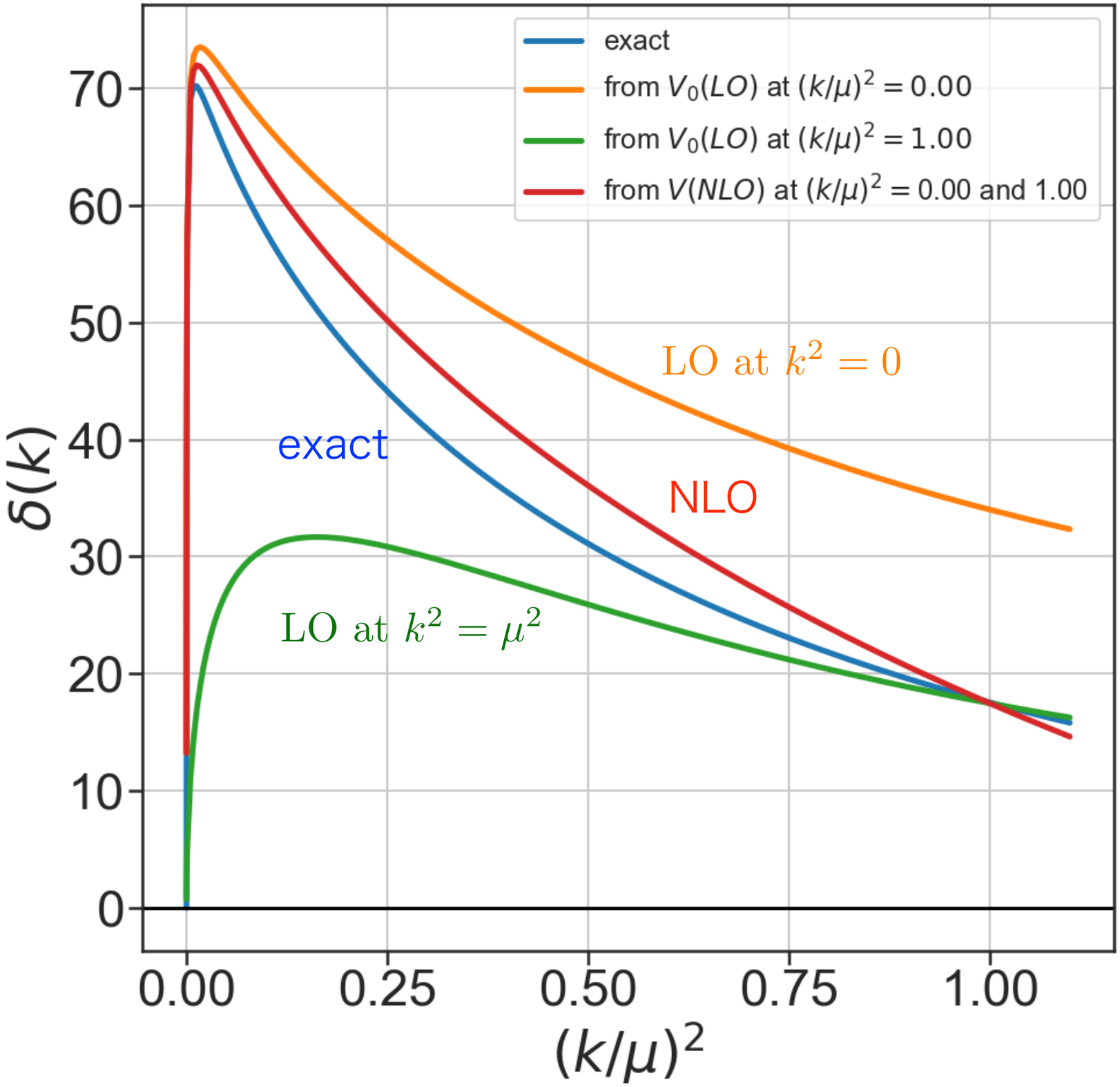
LO approximation $V_0^{\mathrm{LO}}(r)$ $\quad$ from $k^2 = 0$ or $k^2 = \mu^2$

NLO approximation $V_0^{\mathrm{NLO}}(r) + V_1^{\mathrm{NLO}}(r)\nabla^2$

$$U(\vec{x},\vec{y}) = wv(\vec{x})v(\vec{y})$$

$$v(\vec{x}) = e^{-\mu x}, \quad x := |\vec{x}|$$

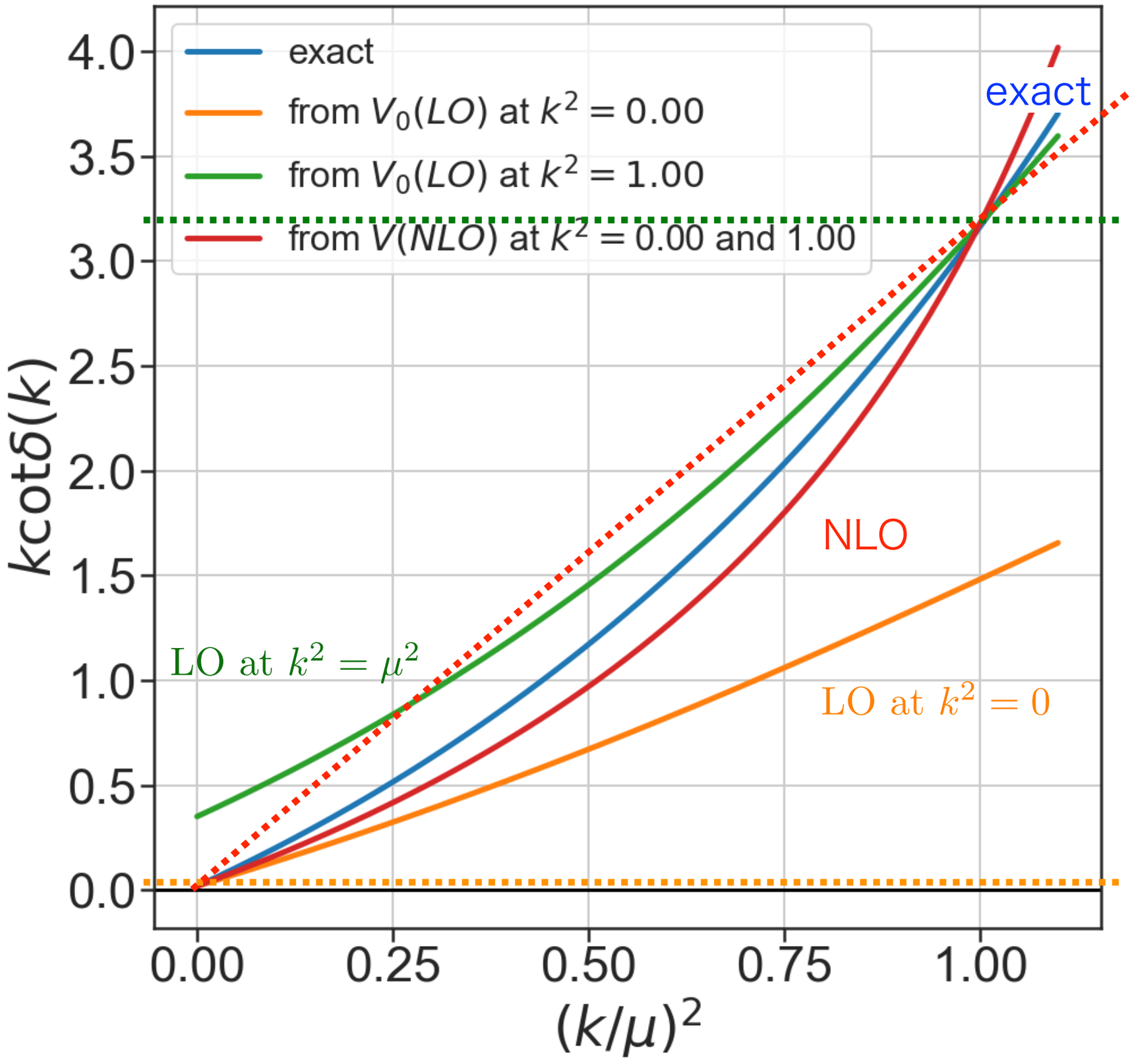
$$\omega/\mu^4 = -0.017, m/\mu = 3.30, R\mu = 2.5$$



NLO potential reproduces the exact phase shift rather well.

$k\cot(\delta_0(k))$

$\omega/\mu^4 = -0.017, m/\mu = 3.30, R\mu = 2.5$



NLO ERE

LO ERE ar $k^2 = \mu^2$

ERE =Effective Range Expansion

NLO potential is equally good to or even better than NLO ERE.

LO ERE ar $k^2 = 0$

II. Hermitian potential from non-Hermitian potential

The HAL QCD potential is non-Hermitian in general, since NBS wave functions are not orthogonal to each other.

However, we can make non-Hermitan potential Hermitian.

$$\boxed{H\psi = E\psi, E \in \mathcal{R}}$$

real eigenvalues

$$H = H_0 + U \qquad H_0 = -\frac{1}{m_N}\nabla^2,$$

$$U \ : \ \text{non-Hermitian}$$

$$\tilde{H}\phi = E\phi, \quad \tilde{H} = R^{-1}HR, \ \psi = R\phi$$

$$\boxed{\tilde{H} = H_0 + V,}$$

$$V \ : \ \text{Hermitian}$$

Lowest non-trivial case

$$U(r) = V_0(r) + V_1(r)\nabla^2 = \underbrace{V_0(r) + \nabla^i V_1(r)\nabla_i}_{\text{Hermitian}} + \underbrace{\delta V(r)\hat{r}^i\nabla_i}_{\text{non-Hermitian}}$$

$$\delta V(r) = -\frac{dV_1(r)}{dr}, \qquad \hat{r}^i := \frac{r^i}{r}$$

$$\tilde{H} = \underbrace{H_0 + \tilde{V}_0 + \nabla^i V_1 \nabla_i}_{\text{Hermitian}} + \boxed{\left\{\delta V - \frac{2}{m_N}(1 - V_1)\frac{d\log R}{dr}\right\}}\hat{r}^i\nabla_i$$

$$= 0$$

$$R(r) = \exp\left[\frac{m_N}{2}\int_{r_\infty}^{r} ds\, \frac{\delta V(s)}{1 - m_N V_1(s)}\right]$$

$$\tilde{V}_0(r) = V_0(r) - \frac{\delta V(r)}{r} - \frac{d}{dr}\frac{\delta V(r)}{2} + \frac{m_N}{4}\frac{\delta V(r)^2}{1 - m_N V_1(r)}$$

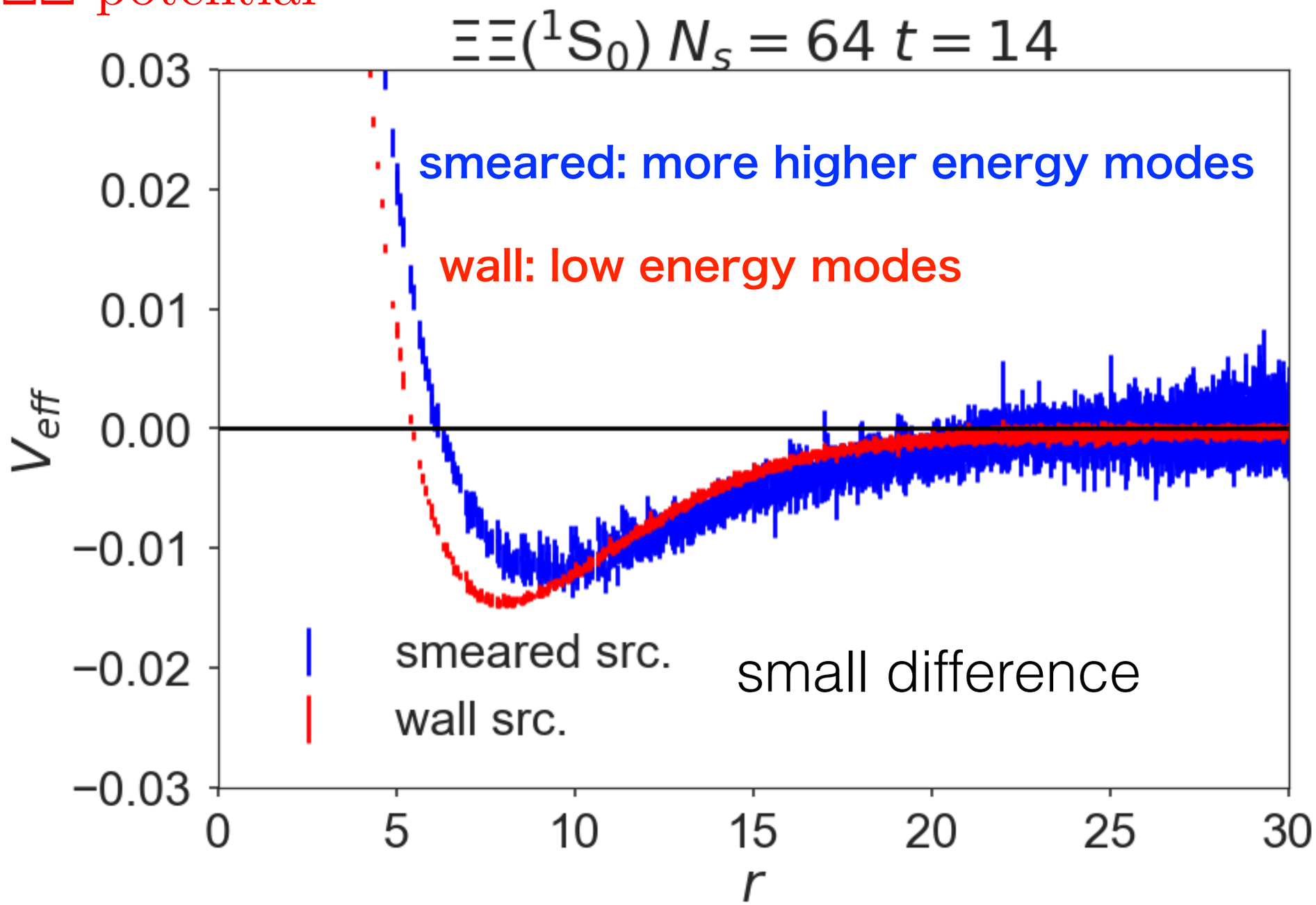
Higher orders are made Hermitian in terms of the derivative expansion.

Example of I & II

2+1 flavor QCD $a = 0.09$ fm $(a^{-1} = 2.2$ GeV$)$

$m_\pi = 0.51$ GeV, $m_N = 1.32$ GeV, $m_K = 0.62$ GeV, $m_\Xi = 1.46$ GeV

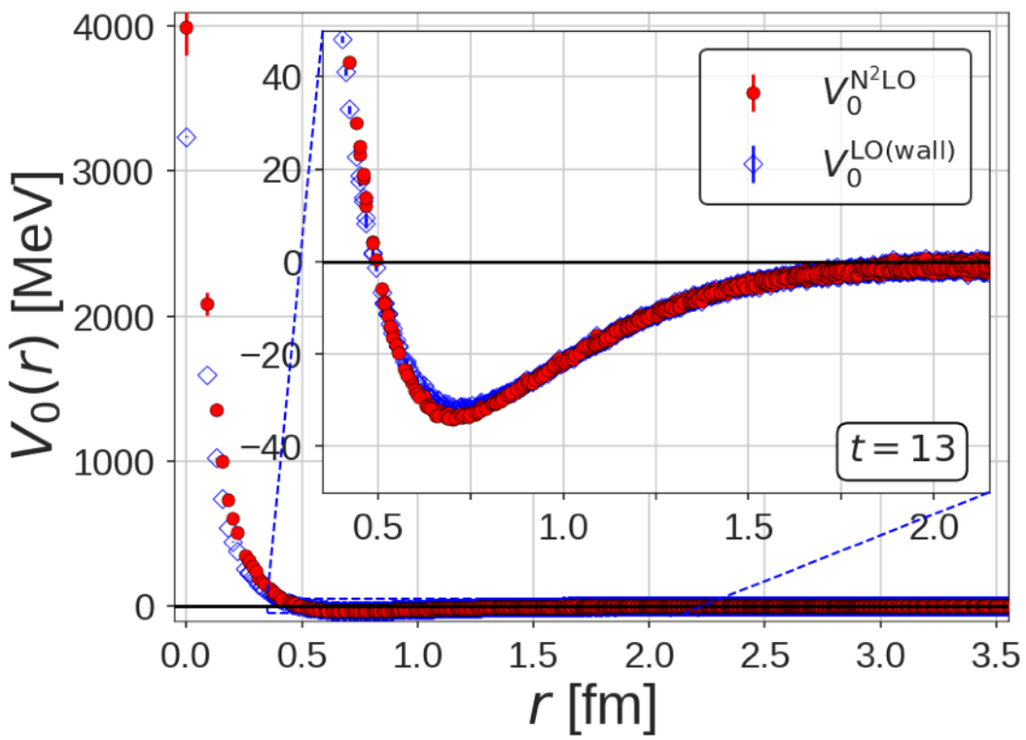
$n = 0$ $\Xi\Xi$ potential



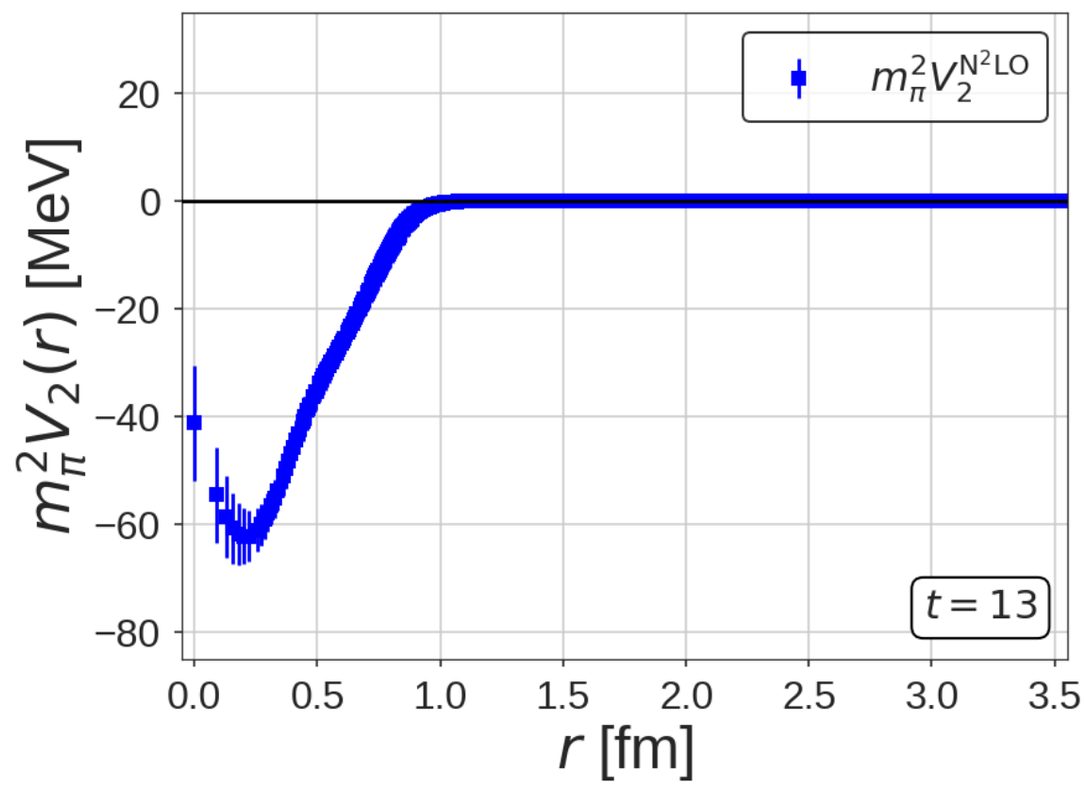
From the difference, we can determine two terms.

$$V_0(r) + V_1(r)\nabla^2$$

$V_0(r)$ **Hermite**



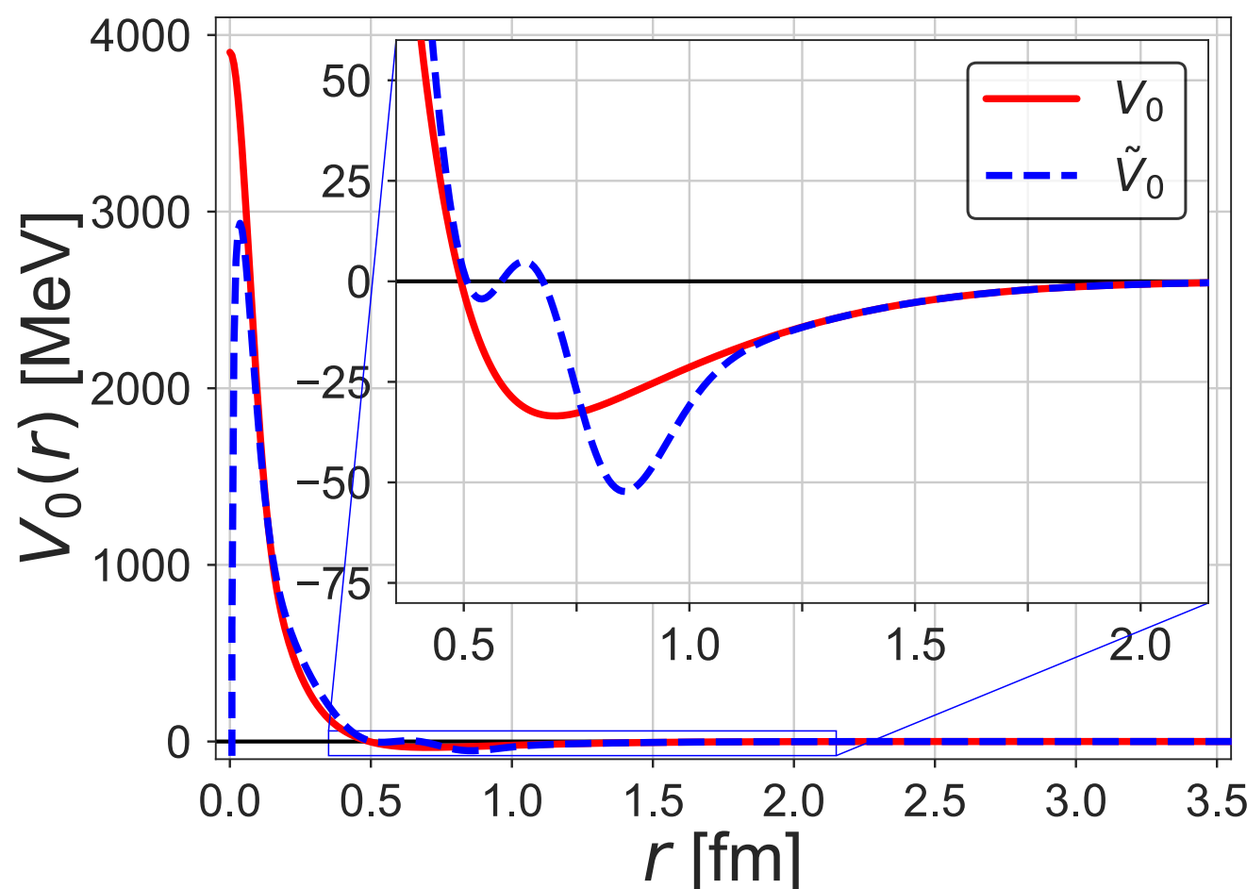
$m_\pi^2 V_1(r)$ **non-Hermite**



Hermitian

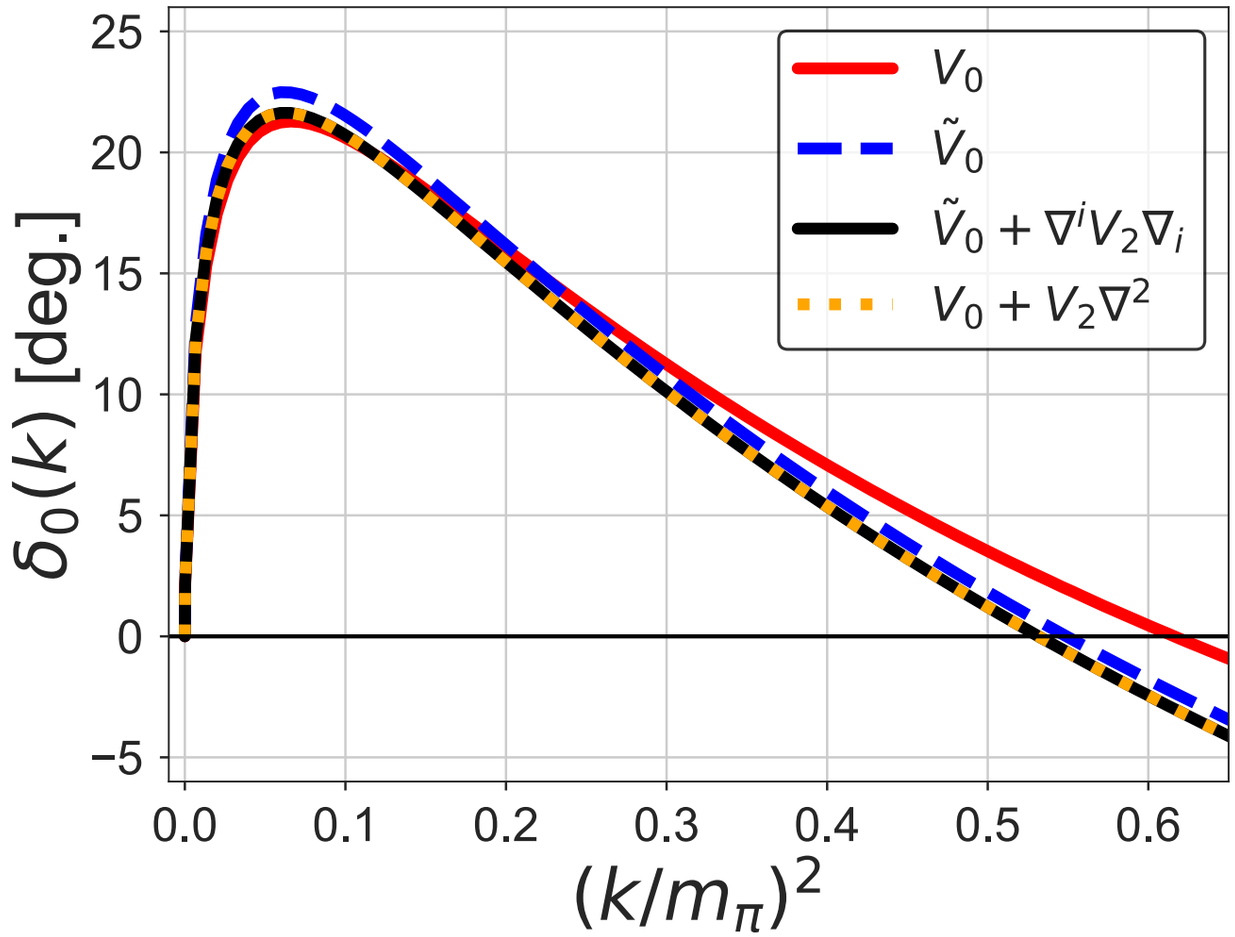
$\tilde{V}_0(r)$

$$\tilde{V}_0(r) + \nabla^i V_1(r) \nabla_i$$

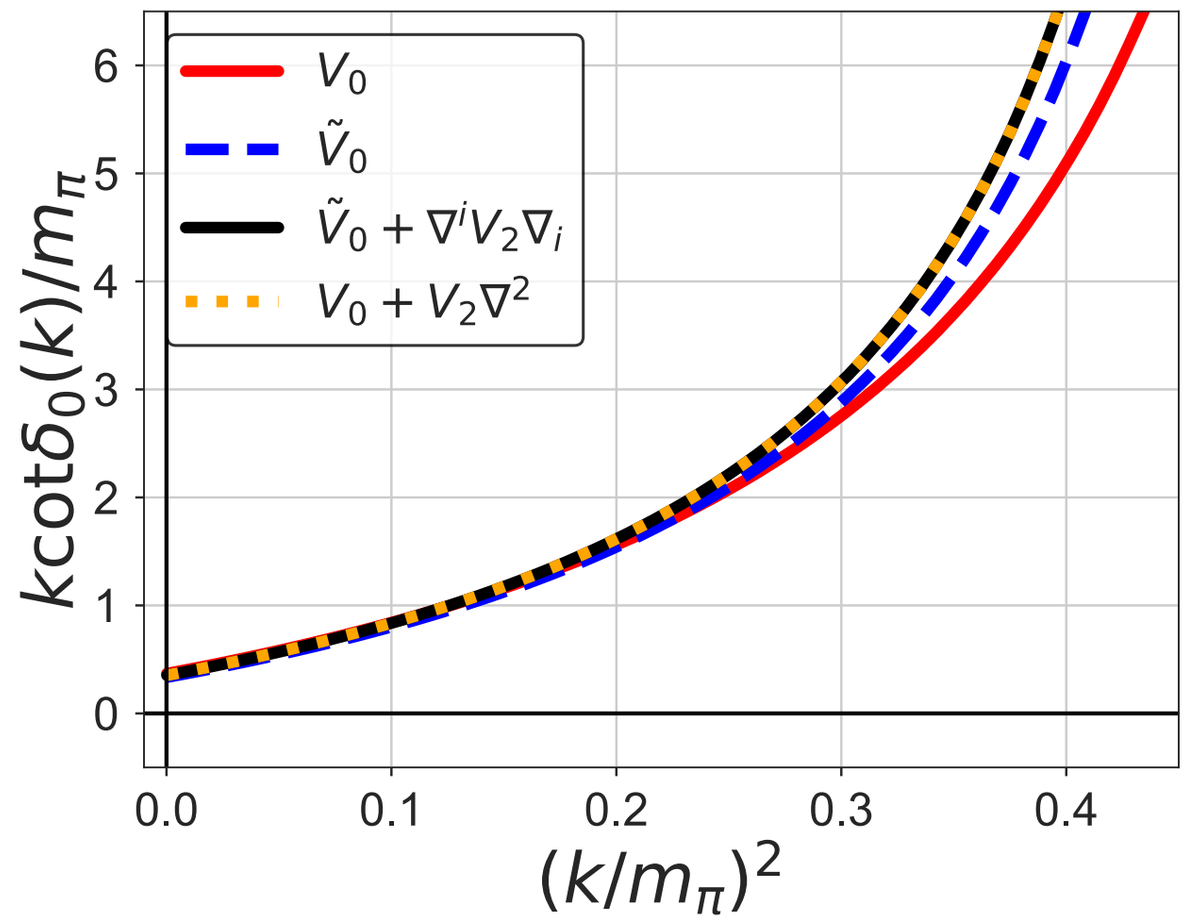


Scattering phase shift

$\delta_0(k)$



$k\cot(\delta_0(k))$



Effects of NLO contributions gradually show up as energy increases.

LO local potential after Hermitization is better than non-Hermitian one.

III. The HAL QCD potential from the moving system

Our Motivation

σ resonance from the $I = 0$ $\pi\pi$ scattering in the HAL QCD method

"vacuum" has the same quantum numbers

"vacuum" state appears in the NBS wave function in center-of-mass system

The potential describes the vacuum as the "deeply bound state" of two pions ?

Moving system no "vacuum" state in the NBS

But

$$\varphi^{\vec{k}}(\vec{x})e^{-W_{\vec{k}}t} = \langle 0|N(\vec{r},t)N(\vec{r}+\vec{x},t)|NN, W_{\vec{k}}\rangle \quad \rightarrow \sum_{lm} C_{lm} \frac{\sin(kx+\delta_l(k))}{kx} Y_{lm}(\Omega_{\vec{x}})$$

true only in the CM system

no definition of the potential directly from the boosted NBS

Generalized definition of the potential in the CM system

non-equal time NBS wave function in CM system

$$\varphi^{\vec{k}}(\vec{x}, x_4) = \left\langle 0 \left| N\left(\frac{\vec{x}}{2}, \frac{x_4}{2}\right) N\left(-\frac{\vec{x}}{2}, -\frac{x_4}{2}\right) \right| NN, W_{\vec{k}} \right\rangle$$

$$\simeq \sum_{lm} A_{lm} \frac{\sin(kx + \delta_l(k) + \pi l/2)}{kx} Y_{lm}(\Omega_{\vec{x}}) \qquad k = |\vec{k}|$$

$$\boxed{(E_k - H_0)\, \varphi^{\vec{k}}(\vec{x}, x_4) = V_{x_4}(\vec{x}, \nabla) \varphi^{\vec{k}}(\vec{x}, x_4)}$$

also in Akahoshi's talk

the HAL QCD potential in the x_4 scheme

$x_4 = 0$: equal time scheme

Can we extract the generalized potential from the boosted NBS function ?

For simplicity, we consider this problem for scalar field.

HAL QCD potential from boosted NBS wave function

$$\varphi_{p,P}(x) \quad = \quad \varphi_{p^*,P^*}(x^*),$$

Moving CM

$$V_{\gamma(x_4-iVx_{\parallel})}(\gamma(x_{\parallel}+iVx_4),x_{\perp},\nabla_{x^*})\varphi_{p,P}(x) \;=\; \frac{(\vec{p}^*)^2+\gamma^2\left(\nabla_{x_{\parallel}}+iV\partial_{x_4}\right)^2+\nabla^2_{x_{\perp}}}{m}\varphi_{p,P}(x)$$

$x_4 = 0$ (equal-time boosted NBS) is required.

$x_4 = 0$

$$V_{-i\gamma Vx_{\parallel}}(\gamma x_{\parallel},x_{\perp},\nabla_{x^*})\varphi_{p,P}(x) \;=\; \frac{(\vec{p}^*)^2+\gamma^2\left(\nabla_{x_{\parallel}}+iV\partial_{x_4}\right)^2+\nabla^2_{x_{\perp}}}{m}\varphi_{p,P}(x).$$

Each $x_{\parallel}$

potential in the $x_0^* = -\gamma x_{\parallel}$ scheme

Minkowski time from Euclidean correlates.

Time-dependent HAL QCD method can also be formulated.

Future investigations

1. Check the formula for he simple system

$$I = 2\ \pi\pi \text{ moving system}$$

2. resonance in the HAL QCD potential

$$\sigma \text{ resonance in } I = 0\ \pi\pi \text{ moving system}$$

3. extension to fermions (Baryons)

lower components mix

relativistic formulation for the “potential” ?

Our answers

Q1. Validity of the derivative expansion ? small parameter ?

➡ I. The derivative expansion is a part of the definition.

Q2. Is the HAL QCD potential Hermite ?

➡ II. The HAL QCD potential is non-Hermite, but can be made Hermitian.

Q3. The HAL QCD potential in the moving system ?

➡ III. The potential can be construed from the boosted NBS.

Q4. Partial wave mixings in the cubic box ?

➡ arXiv:1906.01987

Q5. Quark annihilation processes ?

➡ Yutaro Akahoshi's talk in this session.

IV. Partial wave decomposition in the HAL QCD method

T. Miyamoto, et al. (HAL QCD), in preparation

Lattice QCD in the finite box

Rotational symmetry $O(3, \mathbf{R})$ → **Cubic symmetry** $O(3, \mathbf{Z})$

angular momentum is conserved

partial wave decomposition is possible

a finite number of irreducible representation

different partial waves are mixed

l	rep.	basis polynomials	independent elements
0	A_1^+	1	
1	T_1^-	r_i	$i = 1, 2, 3$
2	E^+	$r_i^2 - r_j^2$	$(i, j) = (1, 2), (2, 3)$
2	T_2^+	$r_i r_j$	$i \neq j$
3	A_2^-	$r_1 r_2 r_3$	
3	T_1^-	$5r_i^3 - 3r^2 r_j$	$i = 1, 2, 3$
3	T_2^-	$r_i(r_j^2 - r_k^2)$	$(i, j, k) = (1, 2, 3), (2, 3, 1), (3, 1, 2)$
4	A_1^+	$5(r_1^4 + r_2^4 + r_3^4) - 3r^4$	
4	E^+	$7(r_i^4 - r_j^4) - 6r^2(r_i^2 - r_j^2)$	$(i, j) = (1, 2), (2, 3)$
4	T_1^+	$r_i r_j^3 - r_j r_i^3$	$i \neq j$
4	T_2^+	$7(r_i r_j^3 + r_j r_i^3) - 6r^2 r_i r_j$	$i \neq j$

$$\mathbf{0} = A_1^+,\ \mathbf{1} = T_1^-,\ \mathbf{2} = E^+ \oplus T_2^+,$$
$$\mathbf{3} = A_2^- \oplus T_1^- \oplus T_2^-,\ \mathbf{4} = A_1^+ \oplus E^+ \oplus T_1^+ \oplus T_2^+,$$

Motivation

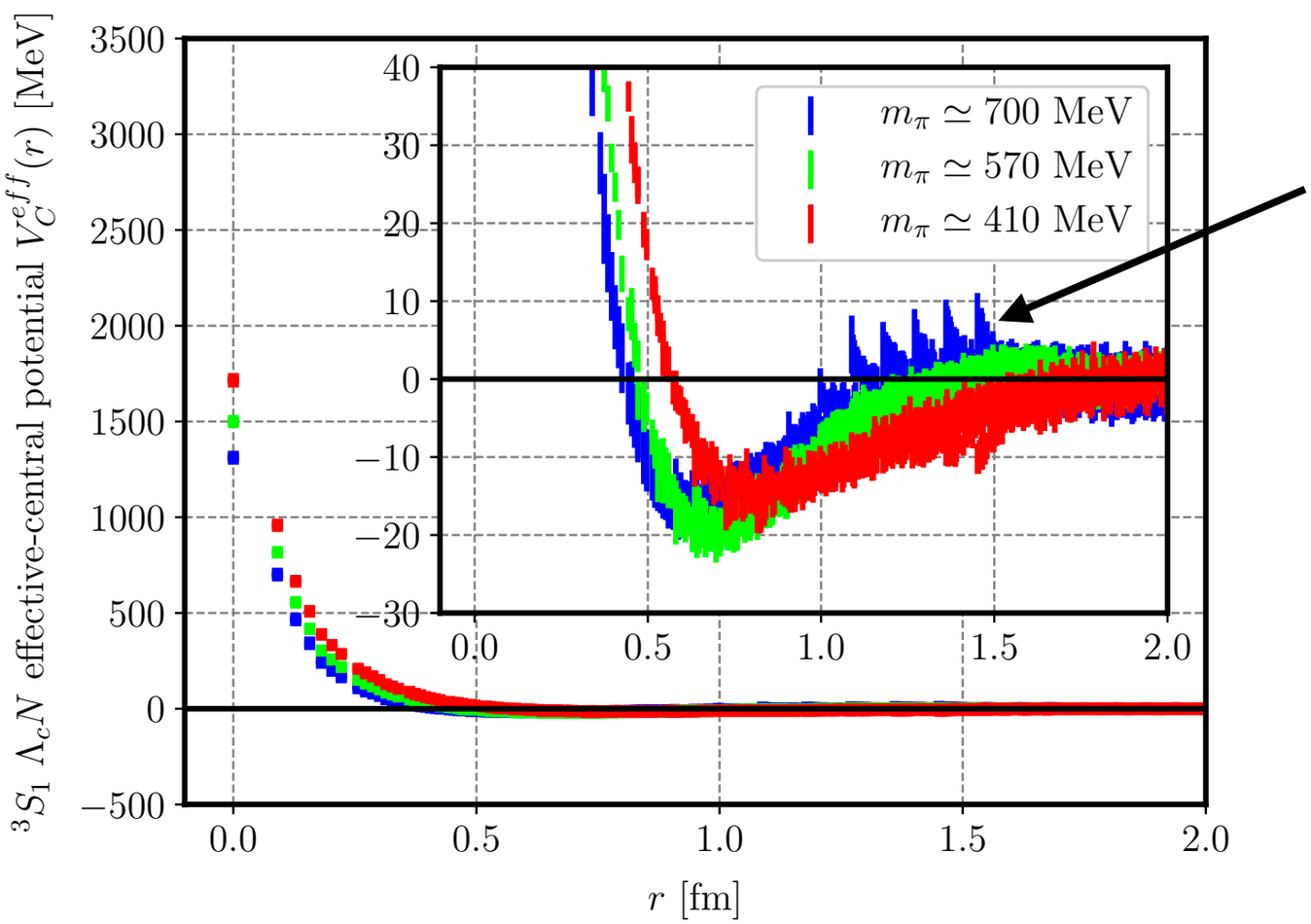
Ex. $\varphi_{\rm NBS}(\vec{x}) \longrightarrow \varphi^{L=0}_{\rm NBS}(r=|\vec{x}|)$

S-wave projection

continuous space $\varphi^{L=0}(r) = \int_s d\Omega\, Y^*_{00}(\theta,\phi)\, \varphi(\vec{x}, r=|\vec{x}|)$ spherical surface integral

discrete space $\varphi^{A_1}(\vec{x}) = \frac{1}{48} \sum_{g\in O(3,\mathbf{Z})} \varphi(g^{-1}\vec{x})$ average over cubic group

$A_1 = \mathbf{0} \oplus \mathbf{4} \oplus \mathbf{6} \oplus \cdots$



manifestation of higher (L =4,6, ..) partial waves

Can we remove these higher partial waves ?

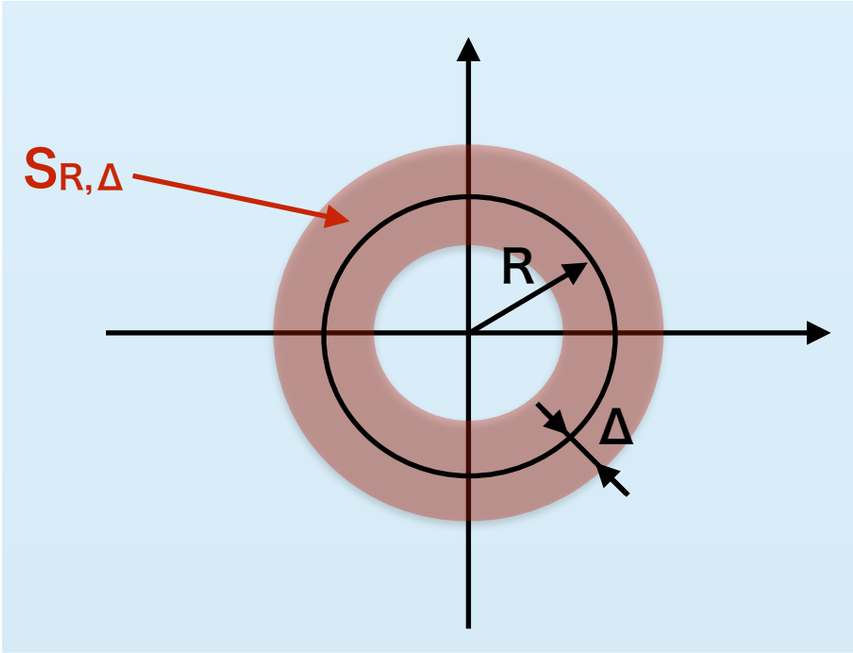
Misner's method

C. W. Misner, Class. Quantum Grav. **21** (2004) S243 - S247

setup

$$\psi(r,\theta,\phi) = \sum_{lm} g_{lm}(r) Y_{lm}(\theta,\phi) \quad \Rightarrow \quad g_{lm}(r)\ ?$$

A complete set in the shell $S_{R,\Delta} = \{\vec{x} | R-\Delta \le |\vec{x}| \le R+\Delta\}$



$$\mathcal{Y}^{R,\Delta}_{nlm}(r,\theta,\phi) := G^{R,\Delta}_n(r) Y_{lm}(\theta,\phi)$$

$$\int_{R-\Delta}^{R+\Delta} r^2 dr\, G^{R,\Delta}_n(r) G^{R,\Delta}_m(r) = \delta_{n,m}$$

Ex.

$$G^{R,\Delta}_n(r) \equiv \underbrace{P_n\left(\frac{r-R}{\Delta}\right)}_{\text{Legendre polynomial}} \frac{1}{r}\sqrt{\frac{2n+1}{2\Delta}}$$

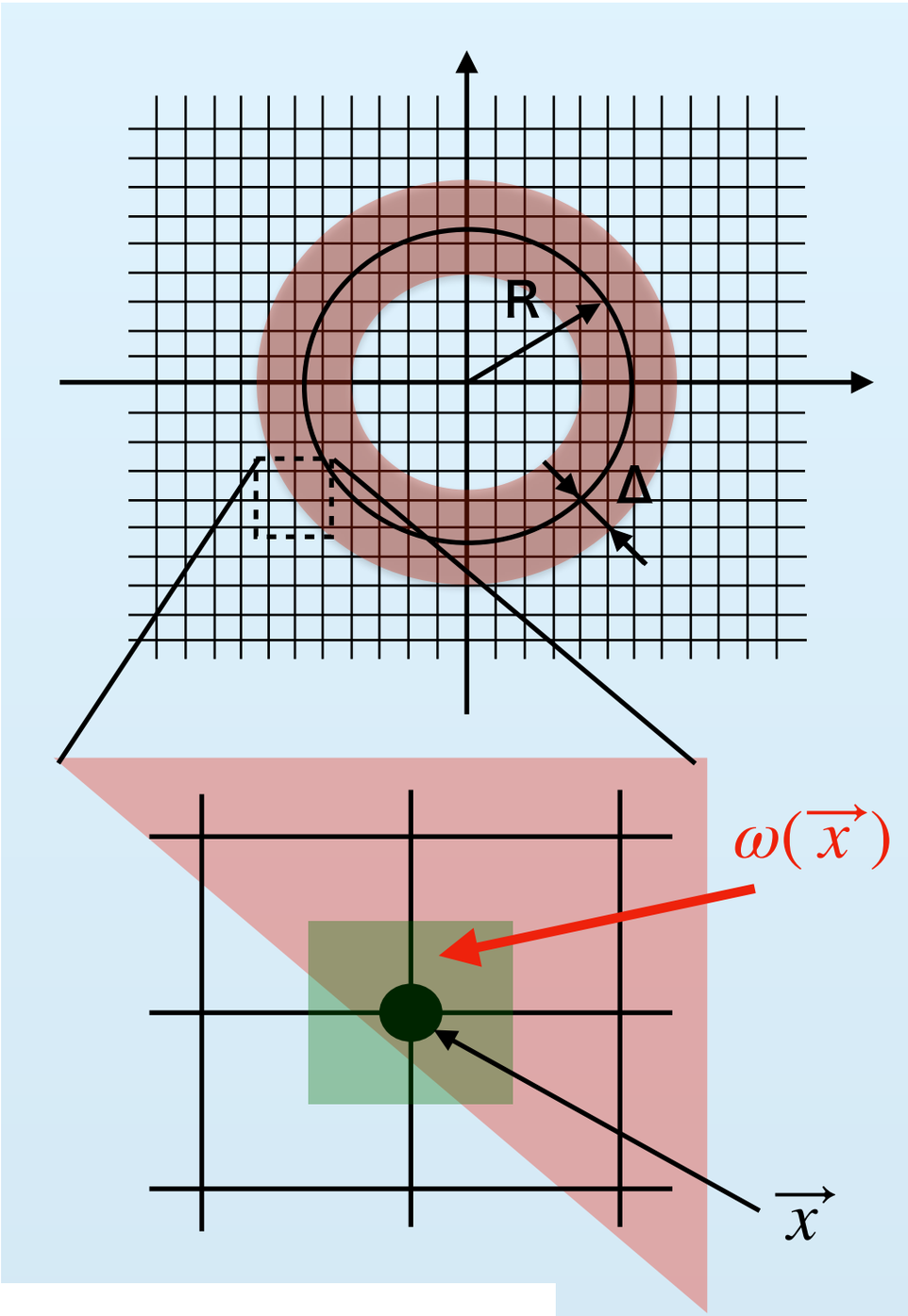
$$\psi(r,\theta,\phi) = \sum_{nlm} c_{nlm}\, \mathcal{Y}^{R,\Delta}_{nlm}(r,\theta,\phi) \quad \text{in } S_{R,\Delta} \quad \Rightarrow \quad c_{nlm} = \int_{S_{R,\Delta}} d^3r\, \overline{\mathcal{Y}^{R,\Delta}_{nlm}(r,\theta,\phi)}\, \psi(r,\theta,\phi)$$

$$\because \int_{S_{R,\Delta}} d^3r\, \overline{\mathcal{Y}^{R,\Delta}_{nlm}(\vec{r})} \mathcal{Y}^{R,\Delta}_{n'l'm'}(\vec{r}) = \delta_{nn'}\delta_{ll'}\delta_{mm'}$$

$$\Rightarrow \quad g_{lm}(R) = \sum_n c_{nlm} G^{R,\Delta}_n(R)$$

exact in continuous space

discrete space



$$\langle f|g\rangle_c \equiv \int_{\vec{x}\in S_{R,\Delta}} d^3x\, \overline{f(\vec{x})}g(\vec{x})$$

$$\langle \mathcal{Y}_A^{R,\Delta}|\mathcal{Y}_B^{R,\Delta}\rangle_c = \delta_{AB}$$

$(A,B = nlm)$

$$\langle f|g\rangle_d \equiv \sum_{\vec{x}\in S_{R,\Delta}} \omega(\vec{x})\overline{f(\vec{x})}g(\vec{x})$$

$$\langle \mathcal{Y}_A^{R,\Delta}|\mathcal{Y}_B^{R,\Delta}\rangle_d \neq \delta_{AB}$$

weight function

dual basis

$$\langle \mathcal{Y}_A^{R,\Delta}|\mathcal{Y}_B^{R,\Delta}\rangle_d = G_{AB} = G^*_{BA}$$

$$\mathcal{Y}^{R,\Delta}_{adj,A} \equiv \sum_B G^{-1}_{AB}\mathcal{Y}_B^{R,\Delta}$$

$$\langle \mathcal{Y}^{R,\Delta}_{dual,A}|\mathcal{Y}_B^{R,\Delta}\rangle_d = \delta_{AB}$$

Since a number of points in the shell is finite, we have to truncate $n \leq n_{\max}$ and $l \leq l_{\max}$ to have G^{-1}_{AB}.

This introduces an approximation !

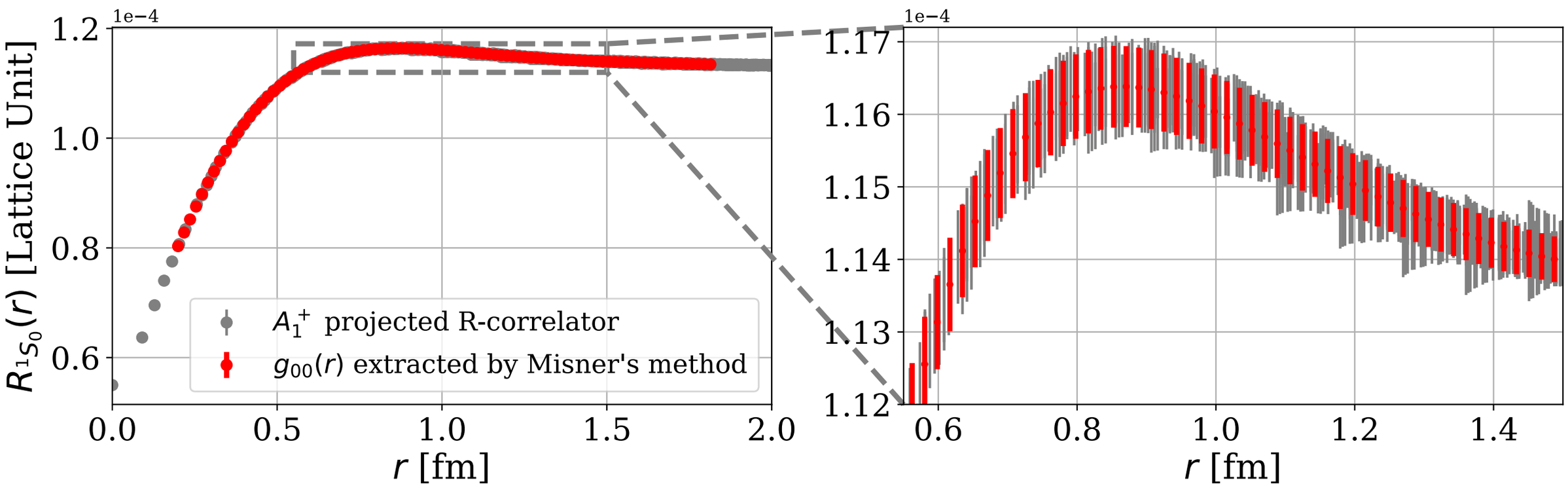
$$\left(\sum_B = \sum_{n=0}^{n_{\max}}\sum_{l=0}^{l_{\max}}\sum_{m=-l}^{l}\right)$$

A choice of Δ, $n_{\max}$ and $l_{\max}$

$G_n^{R,\Delta}$ has $O(\Delta^{n_{\max}+2})$ discretization errors → $\Delta \sim a, n_{\max} \geq 2$

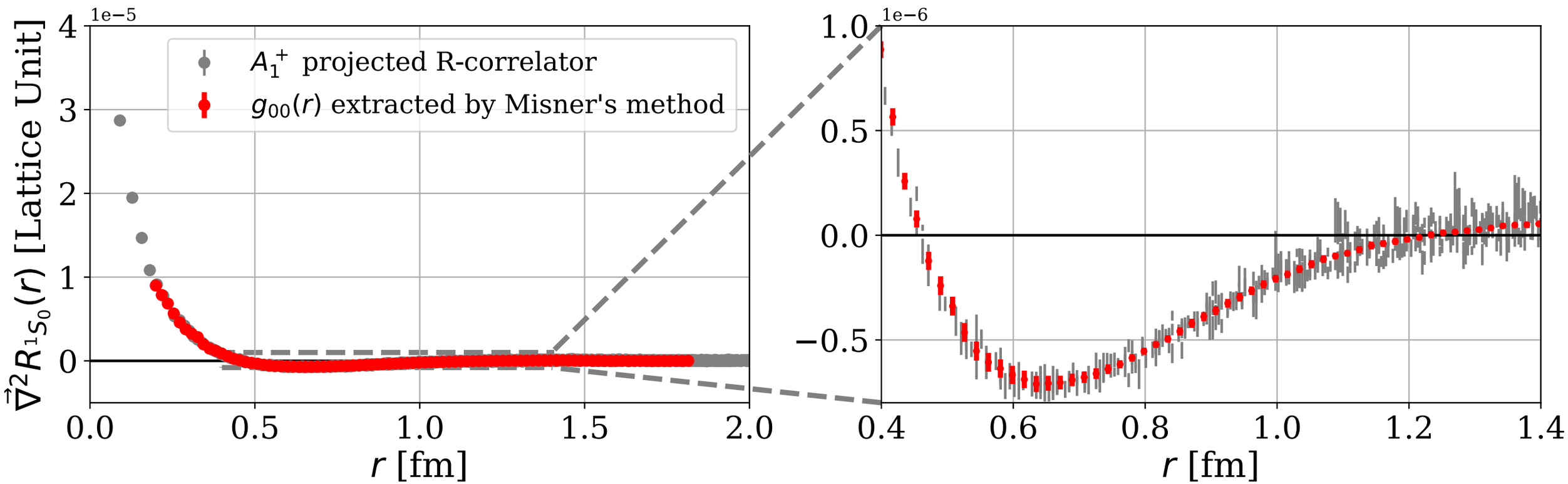
Our choice $\Delta = a, n_{\max} = 2, l_{\max} = 6$

NBS wave function



Higher L contributions seem to be removed by the Misner's method !

Laplacian term



Conventional HAL QCD

$$\vec{\nabla}^2 \varphi^{A_1}(\vec{x}) \simeq \sum_{k=1}^{3} \frac{\varphi^{A_1}(\vec{x}+a\vec{k}) + \varphi^{A_1}(\vec{x}-a\vec{k}) - 2\varphi^{A_1}(\vec{x})}{a^2}$$

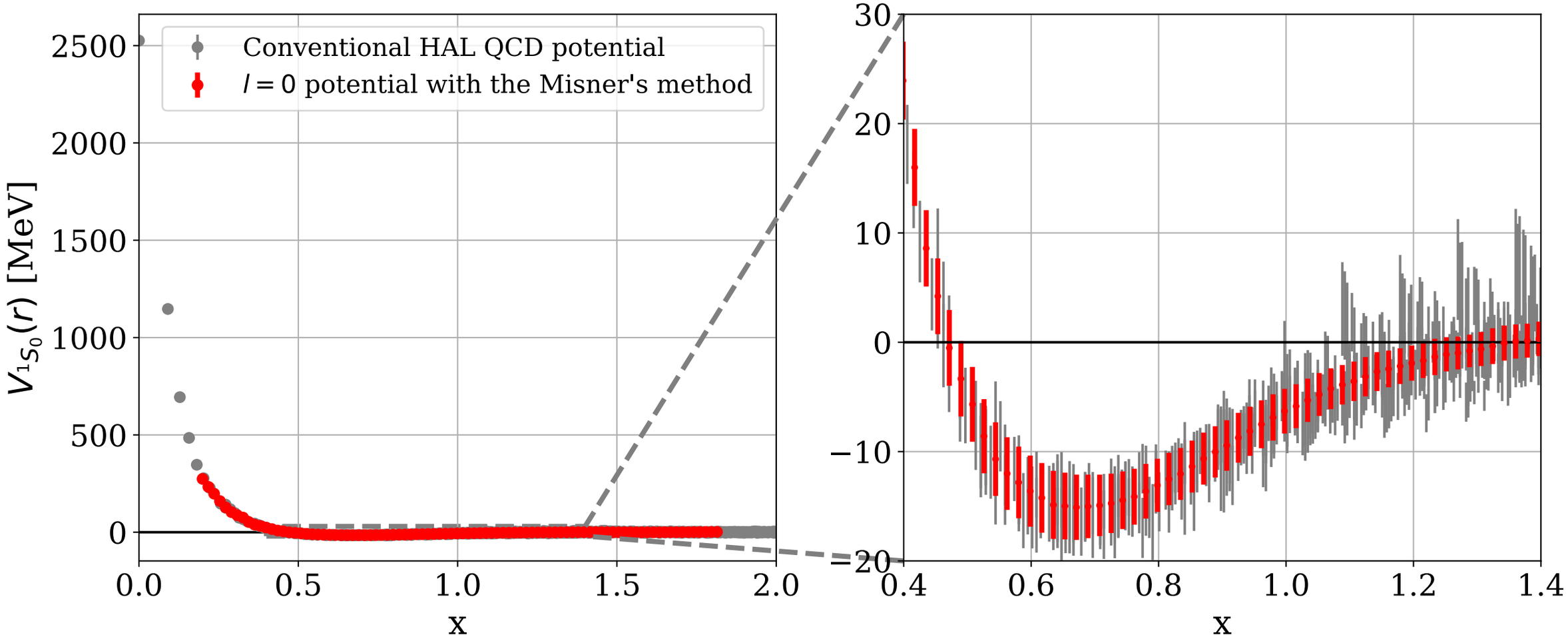
Misner's method

$$\vec{\nabla}^2 g_{lm}(r) = \sum_{n=0}^{n_{\max}} c_{nlm}^{R,\Delta} \frac{1}{r} \frac{\partial^2}{\partial r^2} \left[r G_n^{R,\Delta}(r) \right]$$

analytic derivative

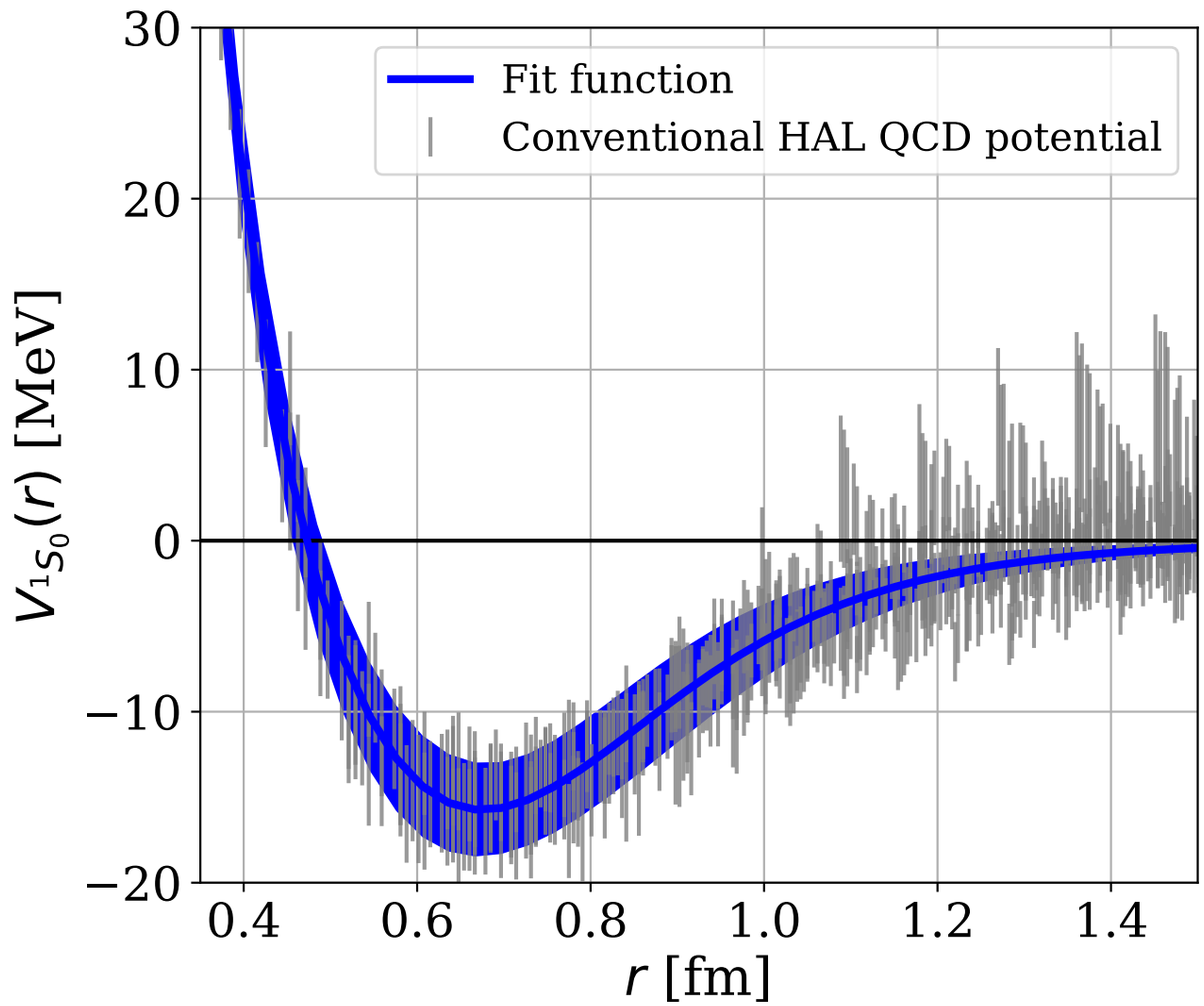
The finite difference approximation enhances higher partial wave contributions.

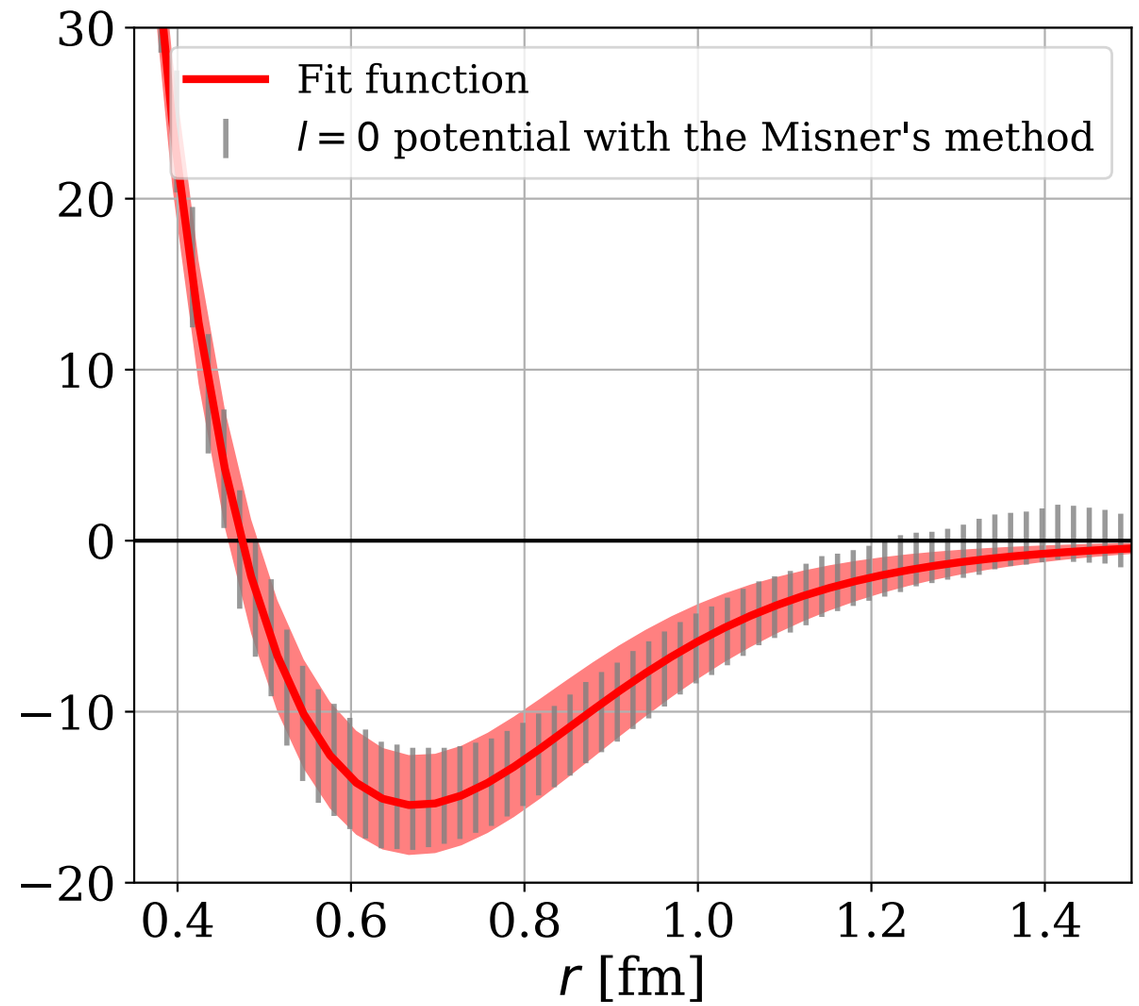
Potential



The Misner's method can remove large fluctuations caused by the contamination from higher partial waves to the S=0 component.

Fits

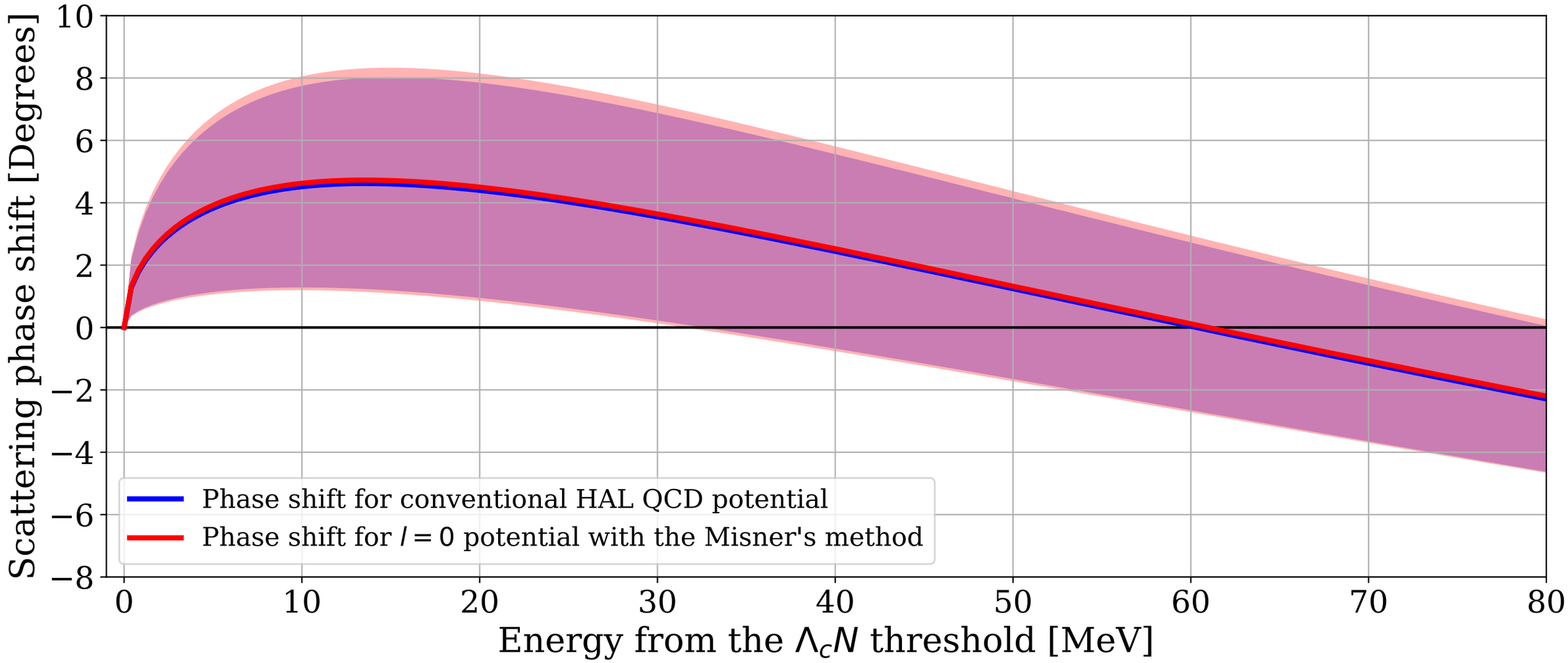




Fit to the conventional HAL QCD data $\simeq$ **The Misner's method**

Statistical errors of the fit to the conventional HAL QCD data are not affected by contaminations from higher partial waves.

Scattering phase shift



Almost identical between the conventional result and the Misner's method.

No improvement of statistical errors,
but we have more confidence on validity of our results !