

Systematics of the HAL QCD Potential at Low Energies in Lattice QCD

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Abstract

The $\Xi\Xi$ interaction in the 1S_0 channel is studied to examine the convergence of the derivative expansion of the non-local HAL QCD potential at the next-to-next-to-leading order (N²LO). We find that (i) the leading order potential from the N²LO analysis gives the scattering phase shifts accurately at low energies, (ii) the full N²LO potential gives only small correction to the phase shifts even at higher energies below the inelastic threshold, and (iii) the potential determined from the wall quark source at the leading order analysis agrees with the one at the N²LO analysis except at short distances, and thus gives correct phase shifts at low energies. We also study the possible systematic uncertainties in the HAL QCD potential such as the inelastic state contaminations and the finite volume artifact for the potential and find that they are well under control.

I. INTRODUCTION

In lattice QCD, two methods have been proposed so far to study the baryon-baryon interactions. One is the direct method [1–3], where the energy spectrum on finite volume(s) is extracted from the temporal correlation of two baryons and is converted to the scattering phase shift and/or the binding energy in the infinite volume through the Lüscher’s finite volume formula [4, 5]. The other is the HAL QCD method [6–9], where the potential between baryons is first derived from the spatial correlations of two baryons, and it is used to calculate the observables through the Schrödinger-type equation in the infinite volume.

While both methods are supposed to give the same results in principle, previous numerical studies for two-nucleon (NN) systems show clear discrepancy: The direct method indicates that both dineutron (1S_0) and deuteron (3S_1) are bound for heavy pion masses ($m_\pi \geq 300$ MeV), while the HAL QCD method does not provide such bound states in both channels for heavy pion masses. This discrepancy was recently resolved in the series of papers [10–13], where it was demonstrated that the temporal correlation function in the direct method easily picks up fake plateaux due to high contamination of the elastic scattering states. This is inherent and inevitable in the naive plateau fitting for multi-baryon systems in lattice QCD. Such uncontrolled systematic errors in all the previous results with the direct method have been revealed explicitly by the “normality (sanity) check” based on the Lüscher’s finite volume formula as well as the analytic properties of the S -matrix [11–13].

The advantage of the time-dependent HAL QCD method [8] over the direct method is that the former is free from the ground state saturation problem, since the energy-independent potential controls both ground state and the elastic excited states simultaneously [8]. In practice, however, there appear systematic uncertainties associated with the truncation of the derivative expansion for the non-local potential. Therefore, the main purpose of the present paper is to study the convergence of the derivative expansion, as well as other sources of systematic uncertainties such as the inelastic state contaminations and the distortion of the interaction under finite volume. We consider the $\Xi\Xi$ system in the 1S_0 channel and perform the (2+1)-flavor lattice QCD calculation at $m_\pi = 0.51$ GeV and $m_K = 0.62$ GeV. Because of the large quark masses, the statistical errors in this case become relatively small, so that one can focus on the detailed analysis of the systematic errors. Also, this channel and the NN system in the 1S_0 channel belong to the same multiplet in the flavor SU(3)

limit.

This paper is organized as follows. In Sec. II, we review the time-dependent HAL QCD method. In Sec. III, we present the lattice QCD results for the $\Xi\Xi$ interaction in the 1S_0 channel at the next-to-next-to-leading order (N²LO) in the derivative expansion. The systematic errors associated with the inelastic state contaminations and the distortion in the finite volume are also examined. In Sec. IV, we calculate the scattering phase shifts in this channel, and check the convergence of the derivative expansion in the HAL QCD method. In Sec. V, we demonstrate the self-consistency between the phase shifts obtained from the HAL QCD potential and those obtained from the energy spectra obtained from the HAL QCD potential combined with the Lüscher's formula. Sec. VI is devoted to the conclusion. In Appendix A, we discuss the relation between the energy-independent non-local potential and the energy-dependent local one.

II. FORMALISM

The key quantity in the HAL QCD method [6–9] is the Nambu-Bethe-Salpeter (NBS) wave function, defined by

$$\psi^W(\vec{r}) = \langle 0|T\{B(\vec{x} + \vec{r}, 0)B(\vec{x}, 0)\}|2B, W\rangle, \quad (1)$$

where $|0\rangle$ is the vacuum state of QCD, $|2B, W\rangle$ is the QCD eigenstate for two baryons with eigenenergy W , and $B(\vec{x}, t)$ is a single baryon operator with spin indices omitted for simplicity. We then define a non-local and energy-independent potential $U(\vec{r}, \vec{r}')$ so as to satisfy

$$(E_k - H_0)\psi^W(\vec{r}) = \int d\vec{r}' U(\vec{r}, \vec{r}')\psi^W(\vec{r}') \quad (2)$$

below inelastic threshold, $W < W_{\text{th}} = 2m_B + m_\pi$, with m_B the baryon mass, m_π the pion mass, and $W = 2\sqrt{m_B^2 + k^2}$. Here we define $E_k = k^2/(2\mu)$ and $H_0 = -\nabla^2/(2\mu)$ with a reduced mass $\mu = m_B/2$.

To extract the NBS wave function in lattice QCD, we start with the two-baryon correlation function,

$$C_{2B}(\vec{r}, t - t_0) = \langle 0|T\{B(\vec{x} + \vec{r}, t)B(\vec{x}, t)\overline{\mathcal{J}}_{2B}(t_0)\}|0\rangle, \quad (3)$$

where $\overline{\mathcal{J}}_{2B}(t_0)$ is a source operator for two-baryon. By inserting the complete set, we obtain

$$C_{2B}(\vec{r}, t - t_0) = \langle 0|T\{B(\vec{x} + \vec{r}, t)B(\vec{x}, t)\} \sum_n |2B, W_n\rangle \langle 2B, W_n| \overline{\mathcal{J}}_{2B}(t_0)|0\rangle + \dots$$

$$= \sum_n A_n \psi^{W_n}(\vec{r}) e^{-W_n(t-t_0)} + \dots, \quad (4)$$

where W_n is the n -th energy eigenvalue, $A_n \equiv \langle 2B, W_n | \overline{\mathcal{J}}_{2B}(0) | 0 \rangle$ corresponds to the overlap with each elastic eigenstate, and the ellipses represent the inelastic contributions. In principle, one can extract $A_0 \psi^{W_0}(\vec{r})$ for the lowest energy W_0 from the large t behavior of $C_{2B}(\vec{r}, t)$.

In practice, however, since $C_{2B}(\vec{r}, t)$ becomes too noisy at large t , we need to employ the time-dependent HAL QCD method [8]. Let us define the ratio of correlation functions, which we call the R -correlator, as

$$R(\vec{r}, t) \equiv \frac{C_{2B}(\vec{r}, t)}{\{C_B(t)\}^2} = \sum_n A'_n \psi^{W_n}(\vec{r}) e^{-\Delta W_n t} + \mathcal{O}(e^{-\Delta W_{\text{th}} t}) \quad (5)$$

with $\Delta W_n = W_n - 2m_B$, $\Delta W_{\text{th}} = W_{\text{th}} - 2m_B$ and $A'_n = A_n/\mathcal{C}^2$, where $C_B(t)$ and \mathcal{C} are a single baryon correlation function and the corresponding overlap factor, respectively. They are given by

$$C_B(t - t_0) = \sum_{\vec{x}} \langle 0 | T \{ B(\vec{x}, t) \overline{\mathcal{J}}_B(t_0) \} | 0 \rangle = \mathcal{C} \cdot e^{-m_B(t-t_0)} + \dots, \quad (6)$$

where $\overline{\mathcal{J}}_B(t_0)$ is a single baryon source operator and ellipses represent the inelastic states contributions.

Since the non-local potential $U(\vec{r}, \vec{r}')$ is defined to be energy-independent [7], all elastic scattering states below the threshold share the same $U(\vec{r}, \vec{r}')$. Therefore, Eq. (2) leads to

$$\left[-H_0 - \frac{\partial}{\partial t} + \frac{1}{4m_B} \frac{\partial^2}{\partial t^2} \right] R(\vec{r}, t) = \int d\vec{r}' U(\vec{r}, \vec{r}') R(\vec{r}', t), \quad (7)$$

where $\mathcal{O}(e^{-\Delta W_{\text{th}} t})$ contributions are neglected. Note that the ground state saturation is no more required in this time-dependent HAL QCD method. Instead, the required condition is that $R(\vec{r}, t)$ is saturated by the contributions from elastic states (“the elastic state saturation”), which can be achieved by a moderate value of t ($\sim \mathcal{O}(\Lambda_{\text{QCD}}^{-1})$).¹ This is the fundamental difference between the HAL QCD method and the direct method.

In actual calculations, it is useful to introduce the derivative expansion of the non-local potential as $U(\vec{r}, \vec{r}') = \sum_n V_n(\vec{r}) \nabla^n \delta(\vec{r} - \vec{r}')$. For the two-baryon system in the spin-singlet channel, the leading order (LO) analysis implies

$$U(\vec{r}, \vec{r}') = V_0^{\text{LO}}(r) \delta(\vec{r} - \vec{r}'), \quad (8)$$

¹ There is a possibility that the inelastic contributions cancel partially between the numerator and the denominator of $R(\vec{r}, t)$, so that the elastic state saturation in $R(\vec{r}, t)$ may appear for smaller t than those in $C_{2B}(\vec{r}, t)$ and $C_B(t)$.

which leads to

$$V_0^{\text{LO}}(r) = -\frac{H_0 R(\vec{r}, t)}{R(\vec{r}, t)} - \frac{(\partial/\partial t)R(\vec{r}, t)}{R(\vec{r}, t)} + \frac{1}{4m_B} \frac{(\partial^2/\partial t^2)R(\vec{r}, t)}{R(\vec{r}, t)}. \quad (9)$$

In order to examine the convergence of the derivative expansion, we study the N²LO analysis in this paper:

$$U(\vec{r}, \vec{r}') = \{V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r)\nabla^2\}\delta(\vec{r} - \vec{r}'). \quad (10)$$

Note that the next-to-leading order (NLO) potential, the spin-orbit interaction, is absent in the spin-singlet S-wave channel. The relation between the potential from the LO analysis, $V_0^{\text{LO}}(r)$, and those from the N²LO analysis, $V_0^{\text{N}^2\text{LO}}(r)$ and $V_2^{\text{N}^2\text{LO}}(r)$ is given by

$$V_0^{\text{LO}}(r) = V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r) \frac{\nabla^2 R(\vec{r}, t)}{R(\vec{r}, t)}, \quad (11)$$

which shows that the N²LO correction in $V_0^{\text{LO}}(r)$ depends on both $V_2^{\text{N}^2\text{LO}}(r)$ and the spatial profile of the R -correlator, the latter of which depends not only on the spatial profile of the NBS wave functions $\psi^{W_n}(r)$ but also on their magnitude A'_n in the R -correlator. The potentials $V_{0,2}^{\text{N}^2\text{LO}}(r)$ are t -independent as long as the elastic state saturation is achieved and the higher order contributions in the derivative expansion can be neglected. One may also estimate the magnitude of systematic errors from the truncation of the derivative expansion and from the inelastic state contaminations by studying the t -dependence of the potentials.

III. HAL QCD POTENTIAL

A. Lattice Setup

Throughout this paper, we use 2+1 flavor QCD ensembles [14], generated by using the Iwasaki gauge action and $\mathcal{O}(a)$ -improved Wilson quark action at $a = 0.08995(40)$ fm on $40^3 \times 48$, $48^3 \times 48$ and $64^3 \times 64$ lattice volumes with heavy up/down quark masses and the physical strange quark mass, $m_\pi = 0.51$ GeV, $m_K = 0.62$ GeV, $m_N = 1.32$ GeV and $m_\Xi = 1.46$ GeV, though only the one with the largest volume is used unless otherwise stated. We employ the wall source $q^{\text{wall}}(t) = \sum_{\vec{y}} q(\vec{y}, t)$, which has been mainly used in the previous studies by the HAL QCD method, and the smeared source $q^{\text{smeared}}(\vec{x}, t) = \sum_{\vec{y}} f(|\vec{x} - \vec{y}|)q(\vec{y}, t)$ with the smearing function $f(r) \equiv \{Ae^{-Br}, 1, 0\}$ for $\{0 < r < (L-1)/2, r = 0, (L-1)/2 \leq r\}$ [14]. For the smeared source, the same \vec{x} is taken as the center of the smeared source for

volume	La [fm]	# of conf.	# of smeared sources	(A, B)	# of wall sources
$40^3 \times 48$	3.6	207	512	(0.8, 0.22)	48
$48^3 \times 48$	4.3	200	4×384	(0.8, 0.23)	4×48
$64^3 \times 64$	5.8	327	1×256	(0.8, 0.23)	4×64

TABLE I. Simulation parameters. The rotational symmetry for isotropic lattices is used to increase statistics.

all six quarks in two baryons as has been done in Ref. [14]. For both sources, the point-sink operator for each baryon (“point-sink scheme” in the HAL QCD method [15]) is exclusively employed in this study. The correlation functions are calculated by the unified contraction algorithm (UCA) [16]. A number of configurations and other parameters are summarized in Table I. Statistical errors are evaluated by the jack-knife method. For more details on the simulation setup, see Ref. [10].

In the present study, we focus on the $\Xi\Xi$ system in the 1S_0 channel: This is one of the most convenient choices to obtain the insights of NN systems, since it belongs to the same **27** representation as the NN system in the 1S_0 channel in the flavor $SU(3)$ limit but has much better signal to noise ratio than the $NN(^1S_0)$ case. We use the relativistic interpolating operators [10] for Ξ , which are given by

$$\Xi_{\alpha}^0 = \varepsilon_{abc}(s^{aT}C\gamma_5 u^b)s_{\alpha}^c, \quad \Xi_{\alpha}^{-} = \varepsilon_{abc}(s^{aT}C\gamma_5 d^b)s_{\alpha}^c, \quad (12)$$

where $C = \gamma_4\gamma_2$ is the charge conjugation matrix, α and (a, b, c) are the indices for the spinor and color, respectively.

B. The R -correlator

We first consider the behaviors of the R -correlator defined in Eq. (5). Shown in Fig. 1 are the R -correlators on the lattice with $L = 64$ at $t = 10-16$ from the wall source (Left) and the smeared source (Right). The results show strong quark-source dependence: The R -correlator from the wall source ($R^{\text{wall}}(\vec{r}, t)$) is delocalized with a weak t -dependence, while that from the smeared source ($R^{\text{smeared}}(\vec{r}, t)$) is localized and has a strong t -dependence. If the R -correlator is saturated by the ground state, its spatial profile should be independent of the source and its temporal profile should be simply dictated by an overall factor, $\exp(-\Delta W_{n=0}t)$.

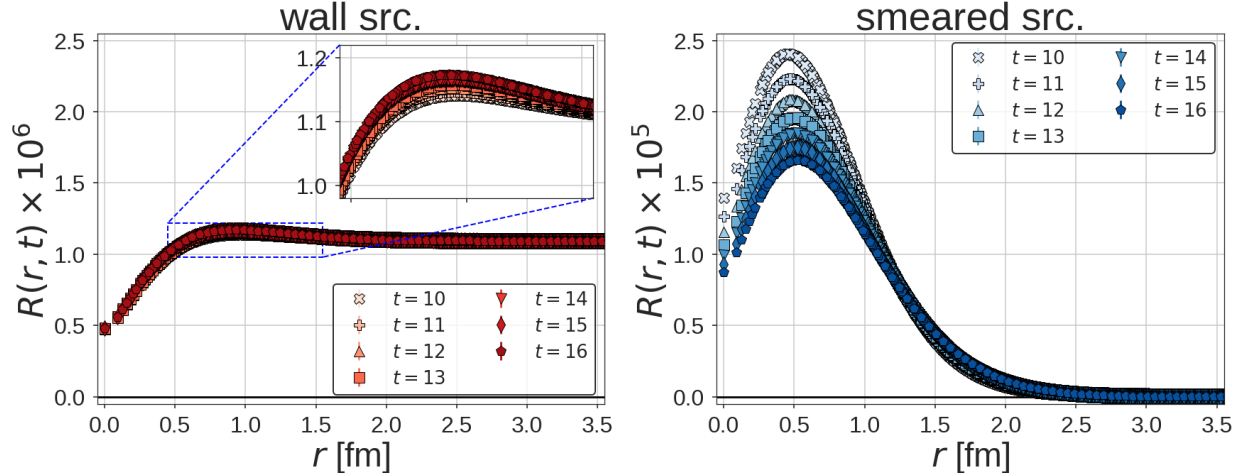


FIG. 1. The R -correlator at $t = 10 - 16$ from the wall source (Left) and the smeared source (Right).

To see more closely the t -dependence of the spatial profile of the R -correlator, we plot $R(\vec{r}, t)$ normalized to be unity at $r = 3.5$ fm for the wall source and at $r = 1.0$ fm for the smeared source in Fig. 2. The shape of the R -correlator from the wall source has a weak t -dependence, which indicates that excited state contaminations in $R^{\text{wall}}(\vec{r}, t)$ are relatively small. On the other hand, the shape of $R^{\text{smeared}}(\vec{r}, t)$ show a sizable t -dependence, which indicates that it has a substantial admixture from the excited states. Although the parameters in the smeared source are tuned to suppress inelastic states in a single-baryon correlator, the same parameters are not guaranteed to suppress the elastic states in a two-baryon correlator. Indeed, a relevant parameter, which controls contaminations from elastic states in a two-baryon system, is the relative momentum between two baryons: This has not been taken into account in all previous works in the direct method (except for [3]). See Ref. [13] for more detailed studies on this point.

C. HAL QCD potential at the leading order

Let us now study the potential in the HAL QCD method at the leading order, $V_0^{\text{LO}}(r)$. Fig. 3 shows the one for $\Xi\Xi(^1S_0)$ and its breakups (H_0 , $\partial/\partial t$ and $\partial^2/\partial t^2$ terms in Eq. (9)) on $L = 64$ at $t = 13$ from the wall source (Left) and the smeared source (Right). For the wall source, the H_0 term is dominant with sizable contributions from the $\partial/\partial t$ term, while the $\partial^2/\partial t^2$ term is negligible. The $\partial/\partial t$ term is not constant as a function of r , which indicates that there exist small but non-negligible contributions from the excited states in $R^{\text{wall}}(\vec{r}, t)$.

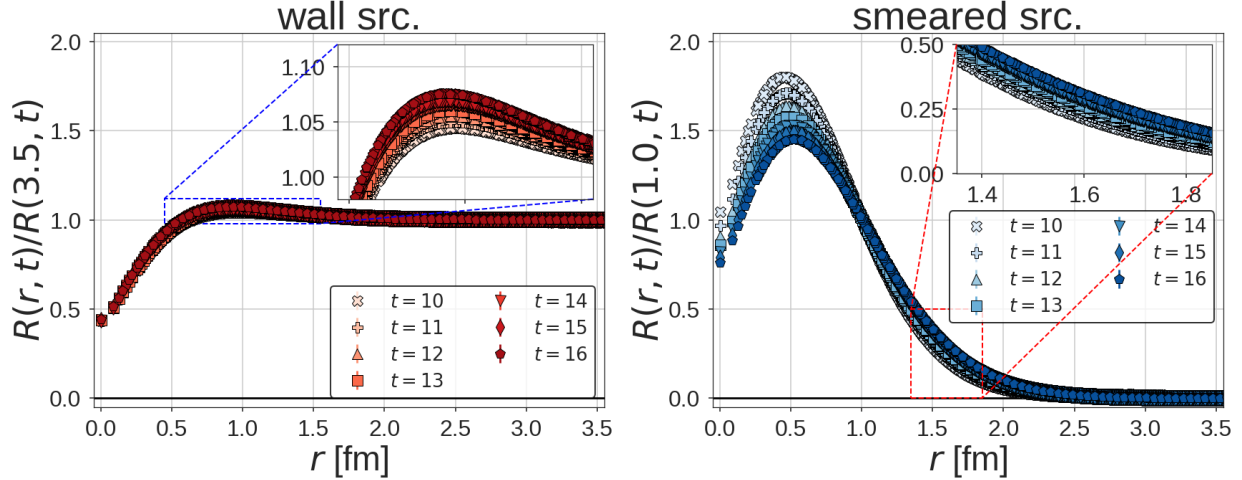


FIG. 2. The normalized R -correlator at $t = 10 - 16$ from the wall source (Left) and the smeared source (Right).

For the smeared source, on the other hand, all terms are important. In particular, the $\partial/\partial t$ term (green triangles) shows substantial r -dependence indicating large contributions from the excited states in the smeared source. However, such dependence is cancelled by the H_0 term (blue squares) and is further corrected by the $\partial^2/\partial t^2$ term (black diamonds). The final results (red circles) with the smeared source and the wall source show qualitatively similar behaviors, i.e., the repulsive core at the short distance and the attractive pocket at the intermediate distance. This illustrates that the time-dependent HAL QCD method works well for extracting the $\Xi\Xi$ potential irrespective of the source structures.

Shown in Fig. 4 is a comparison among the LO potentials ($V_0^{\text{LO}}(r)$) for different t in each source. For the wall source, the potentials at $t = 10 - 16$ are consistent with each other within statistical errors, while those from the smeared source show the detectable t -dependence. Shown in Fig. 5 is a comparison of $V_0^{\text{LO}}(r)$ between two sources at $t = 10, 12, 14, 16$. As t increases, the LO potential from the smeared source gradually converges to that from the wall source. The relatively large t -dependence of the potentials from the smeared source as well as the remaining small discrepancy of potentials between two sources even at $t = 16$ indicate that the N^2LO analysis in the derivative expansion is necessary to understand the data from the smeared source. This is a natural consequence of the fact that the N^2LO contributions in $V_0^{\text{LO}}(r)$, $\nabla^2 R(\vec{r}, t)/R(\vec{r}, t)$ ($\propto H_0$ term) in Eq. (11), is much more significant in the smeared source than the wall source as shown in Fig. 3.

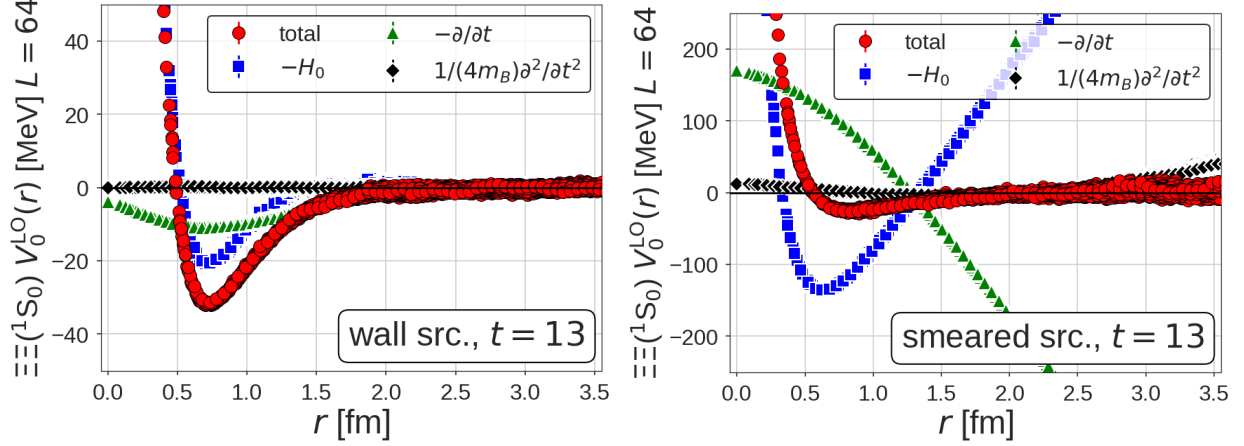


FIG. 3. The potential at the leading order analysis, $V_0^{\text{LO}}(r)$, (red circles) for the wall source (Left) and the smeared source (Right) at $t = 13$. The blue squares, green triangles and black diamonds denote 1st, 2nd and 3rd terms in Eq. (9), respectively.

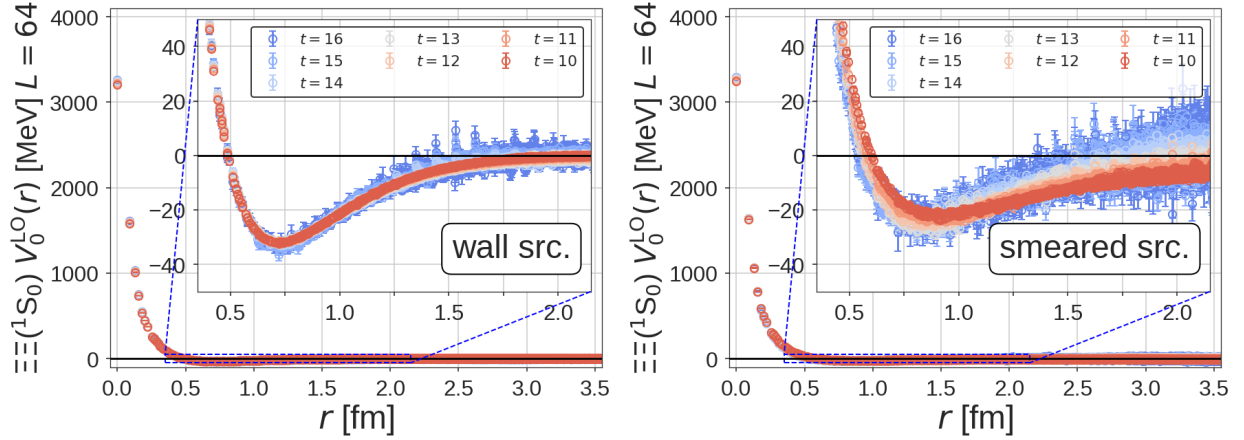


FIG. 4. The potential at the leading order analysis, $V_0^{\text{LO}}(r)$, for the wall source (Left) and the smeared source (Right) at $t = 10 - 16$.

D. HAL QCD potential at the next-to-next-to-leading order

We next apply the N^2LO analysis in the derivative expansion to R -correlators for both sources. The potential at the LO analysis, $V_0^{\text{LO}}(r)$, and those at the N^2LO analysis, $V_0^{\text{N}^2\text{LO}}(r)$, $V_2^{\text{N}^2\text{LO}}(r)$, satisfy the linear equations given by

$$\{V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r)\nabla^2\}R^{\text{source}}(\vec{r}, t) = V_0^{\text{LO}(\text{source})}(r)R^{\text{source}}(\vec{r}, t), \quad (13)$$

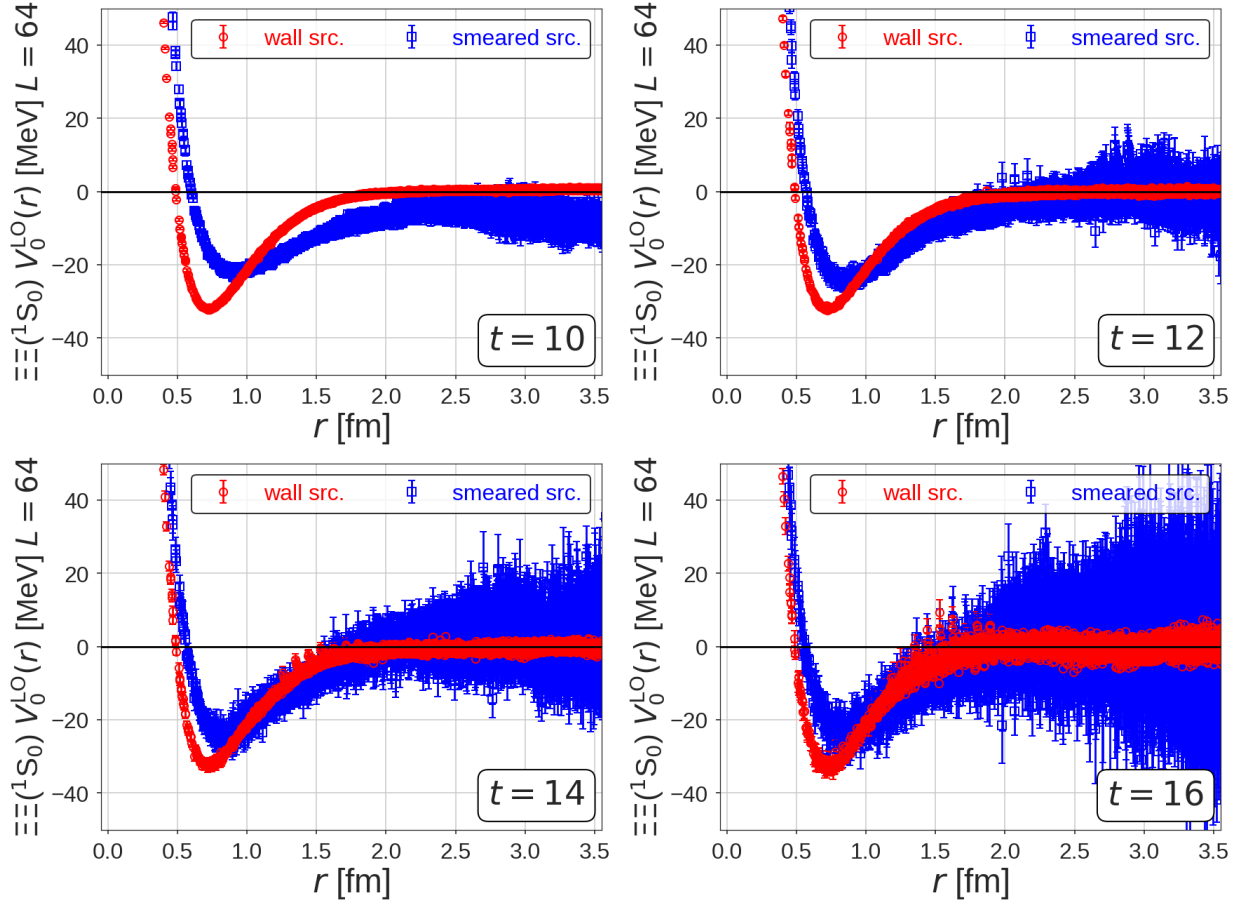


FIG. 5. A comparison of the potential at the leading order analysis, $V_0^{\text{LO}}(r)$, between the wall source (red circles) and the smeared source (blue squares) at $t = 10, 12, 14, 16$.

where source = wall or smear. To extract $V_{0,2}^{\text{N}^2\text{LO}}(r)$, we first consider the relation obtained from Eq. (13),

$$V_0^{\text{LO}(\text{wall})}(r) - V_0^{\text{LO}(\text{smear})}(r) = D \times V_2^{\text{N}^2\text{LO}}(r), \quad (14)$$

with $D \equiv \nabla^2 R^{\text{wall}}(\vec{r}, t)/R^{\text{wall}}(\vec{r}, t) - \nabla^2 R^{\text{smear}}(\vec{r}, t)/R^{\text{smear}}(\vec{r}, t)$. We extract $V_2^{\text{N}^2\text{LO}}(r)$ by fitting Eq. (14) with an ansatz $V_2^{\text{N}^2\text{LO}}(r) = b_1 e^{-b_2(r-b_3)^2} + b_4 e^{-b_5(r-b_6)^2}$ at each t . Then the result can be combined with Eq. (11) to obtain $V_0^{\text{N}^2\text{LO}}(r)$.

Fig. 6 shows the $V_0^{\text{N}^2\text{LO}}(r)$ together with the $V_0^{\text{LO}(\text{wall})}(r)$ (Left), and the $V_2^{\text{N}^2\text{LO}}(r)$ (Right) on $L = 64$ at $t = 13$. We multiply $V_2^{\text{N}^2\text{LO}}(r)$ by m_π^2 to make its mass dimension +1 for a comparison to $V_0(r)$'s. We find that $V_0^{\text{N}^2\text{LO}}(r)$ agrees well with the $V_0^{\text{LO}(\text{wall})}(r)$ except at short distances. We also find that $V_2^{\text{N}^2\text{LO}}(r)$ is localized within the range of 1 fm, which is much shorter than the range of $V_0^{\text{LO}(\text{wall}), \text{N}^2\text{LO}}(r)$. We note here that the negative sign

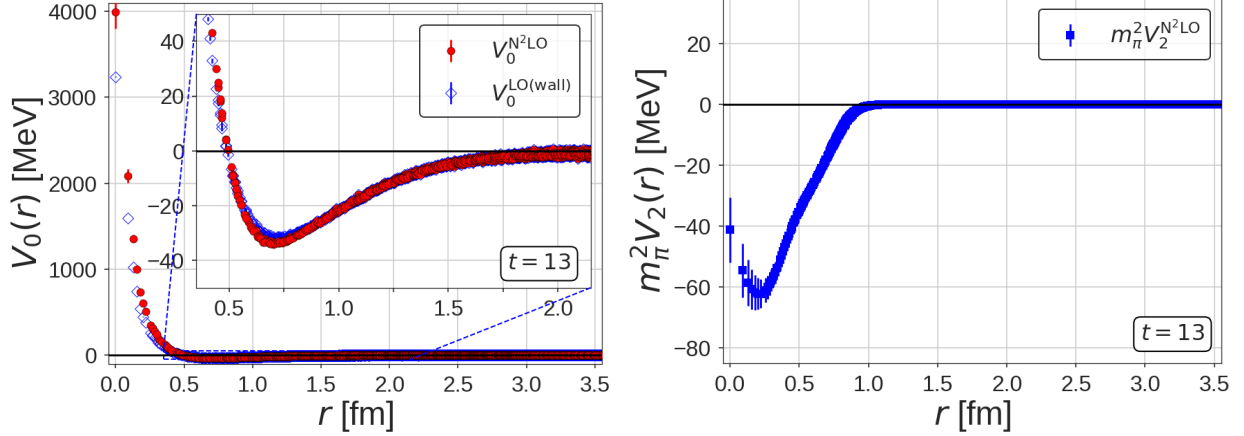


FIG. 6. (Left) The LO potential at the N²LO analysis, $V_0^{\text{N}^2\text{LO}}(r)$ (red circles), together with the potential at the LO analysis for the wall source, $V_0^{\text{LO(wall)}}(r)$ (blue diamonds) at $t = 13$. (Right) The N²LO potential at the N²LO analysis, $V_2^{\text{N}^2\text{LO}}(r)$, multiplied by m_π^2 .

of $V_2^{\text{N}^2\text{LO}}(r)$ does not necessarily implies attraction, since the N²LO potential is given by $V_2^{\text{N}^2\text{LO}}(r)\nabla^2$.

As already mentioned, $\nabla^2 R(\vec{r}, t)/R(\vec{r}, t)$ from the smeared source is much larger than that of the wall source (see Fig. 3). Intuitively, this is because $R^{\text{smeared}}(r, t)$ ($R^{\text{wall}}(r, t)$) contains larger (smaller) contributions from excited states and thus is more (less) sensitive to higher order terms in the derivative expansion of the potential. Therefore, the N²LO analysis is mandatory for the smeared source, while the LO analysis for the wall source leads to the potential which is almost identical to $V_0^{\text{N}^2\text{LO}}(r)$.

Shown in Fig. 7 are the t -dependence of $V_{0,2}^{\text{N}^2\text{LO}}(r)$ in the range of $t = 13 - 16$. Since appreciable t -dependence is not seen within the error bars, the N⁴LO contribution is expected to be small.

E. Effect of the Inelastic states

Fig. 8 (Left) compares the effective mass of a single Ξ for two sources. The smeared source is tuned to have a large overlap with the ground state of a single baryon, so that the corresponding effective mass shows a plateau at an earlier time than the case of the wall source. Eventually, the plateaux for the single Ξ from two different sources converge at $t \gtrsim 16$. Shown in Fig. 8 (Right) is the $\Xi\Xi$ potential at the LO analysis for the wall

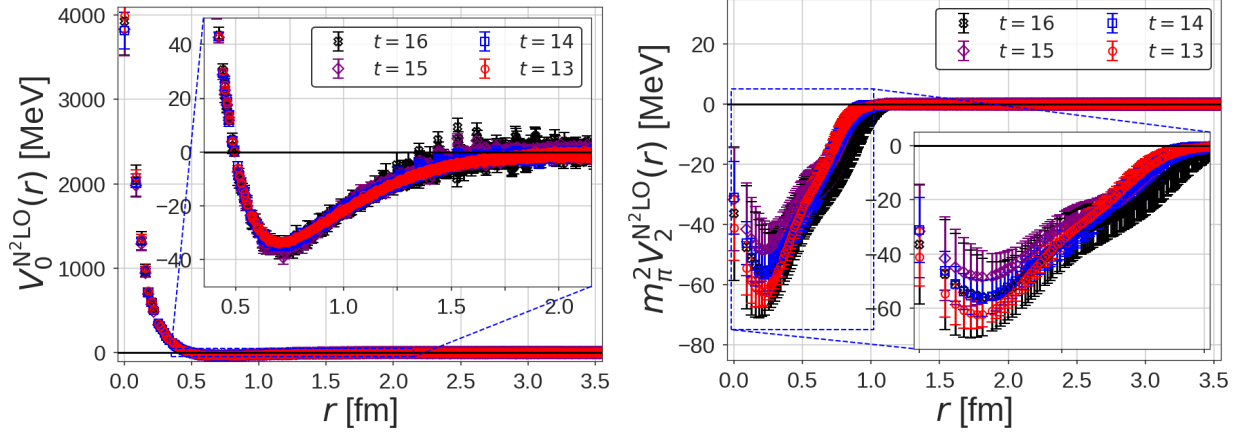


FIG. 7. The LO (Left) and N^2 LO (Right) potentials at the N^2 LO analysis in the range of $t = 13$ – 16 .

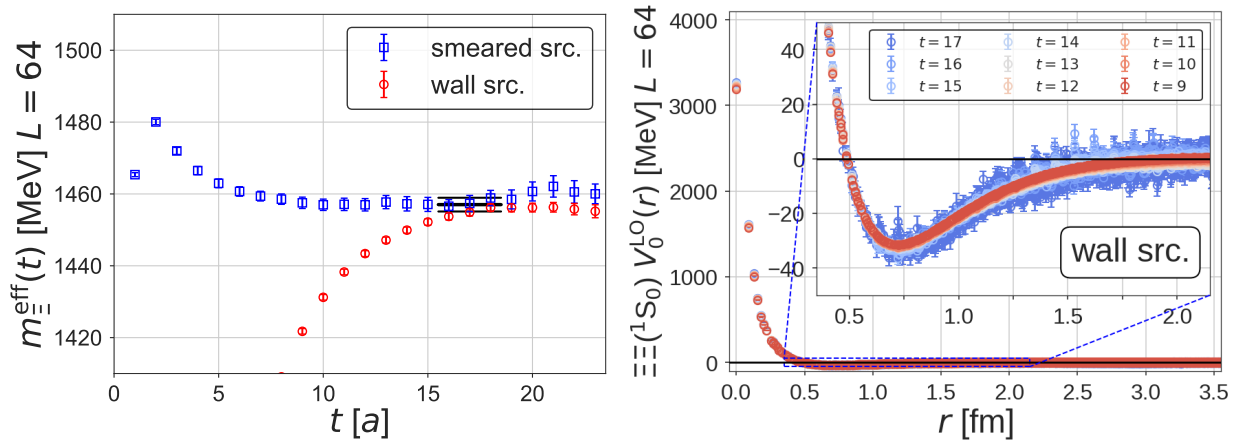


FIG. 8. (Left) The effective mass of a single baryon Ξ for the wall source (red circles) and the smeared source (blue squares). (Right) The potential at the LO analysis, $V_0^{LO}(r)$, for the wall source at $t = 9$ – 17 .

source in the range of $t = 9$ – 17 . Unlike the case of the single Ξ , the resultant potential is stable for t much less than 16, suggesting that the systematic error originating from the inelastic contributions of the single-baryon cancels largely between the numerator and the denominator of the R -correlator for the wall source.

F. Effect of the finite volume

In Fig. 9, we show the volume dependence of the potential at the LO analysis for the wall source at $t = 13$ with $L = 40, 48$ and 64 . All the potentials are consistent with each other

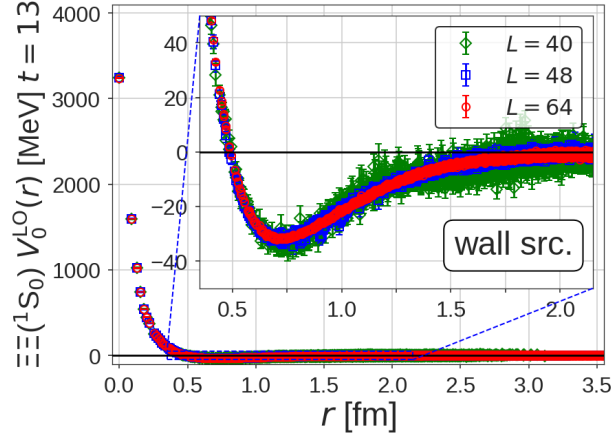


FIG. 9. The potential at the LO analysis, $V_0^{\text{LO}}(r)$, for the wall source on $L = 40, 48$ and 64 at $t = 13$.

within statistical errors. This indicates that the artifact due to finite volume is negligible for the potential, mainly because the potential is short ranged.

IV. SCATTERING PHASE SHIFTS

In the previous section, we examine systematic uncertainties on the HAL QCD potential. In this section, we examine how these systematic uncertainties affect the physical observables such as the scattering phase shifts, in particular the effect of the derivative expansion. To calculate the scattering phase shifts, $\delta_0(k)$, we first fit the potentials by a sum of Gaussians, $V_0^{\text{LO(wall),N}^2\text{LO}}(r) = \sum_{n=1,3,5,7} a_n e^{-a_n + 1r^2}$ and $V_m^{\text{N}^2\text{LO}}(r) = \sum_{n=1,4} b_n e^{-b_{n+1}(r-b_{n+2})^2}$. Resulting parameters are summarized in Table II.

In Fig. 10, we show the comparison of the scattering phase shifts from $V_0^{\text{LO(wall)}}(r)$, $V_0^{\text{N}^2\text{LO}}(r)$ and $V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r)\nabla^2$ at $t = 13$. At low energies (Fig. 10 (Left)), the N²LO correction is found to be negligible, showing not only that the derivative expansion converges well but also that the LO analysis for the wall source is sufficiently good at low energies. The N²LO correction becomes non-negligible only at high energies as shown in Fig. 10 (Right)². We note that $(k/m_\pi)^2 = 0.5$ corresponds to the energy from the threshold as $\Delta E \equiv W - 2m_B \simeq 90$ MeV. The good convergence of the derivative expansion has been also observed for the NN systems in the 1S_0 and 3S_1 channels [17] and the $I = 2$ $\pi\pi$

² We discuss the magnitude of the N²LO correction in the potential at high energies in Appendix A.

	$V_0^{\text{LO(wall)}}(r)$	$V_0^{\text{N}^2\text{LO}}(r)$	$V_2^{\text{N}^2\text{LO}}(r)$
a_1	0.8759 ± 0.0270	1.1426 ± 0.0621	$b_1 -0.5291 \pm 0.0418$
a_2	1.2040 ± 0.0317	0.9332 ± 0.0871	$b_2 0.0757 \pm 0.0162$
a_3	0.4261 ± 0.0128	0.4245 ± 0.0397	$b_3 2.195 \pm 0.333$
a_4	0.3028 ± 0.0217	0.2358 ± 0.0382	$b_4 -0.1091 \pm 0.0194$
a_5	0.2010 ± 0.0124	0.2415 ± 0.0410	$b_5 0.2177 \pm 0.0633$
a_6	0.07373 ± 0.00364	0.07876 ± 0.00646	$b_6 7.025 \pm 0.464$
a_7	-0.02922 ± 0.00148	-0.03005 ± 0.00159	
a_8	0.008977 ± 0.000456	0.009107 ± 0.000467	

TABLE II. Summary of fitting parameters for the LO and N²LO potentials in the lattice unit at $t = 13$. The fitting range is $r \in [0, 3.5]$ fm, and χ^2/dof are 1.14, 1.01 and 0.0019 for $V_0^{\text{LO(wall)}}(r)$, $V_0^{\text{N}^2\text{LO}}(r)$ and $V_2^{\text{N}^2\text{LO}}(r)$, respectively.

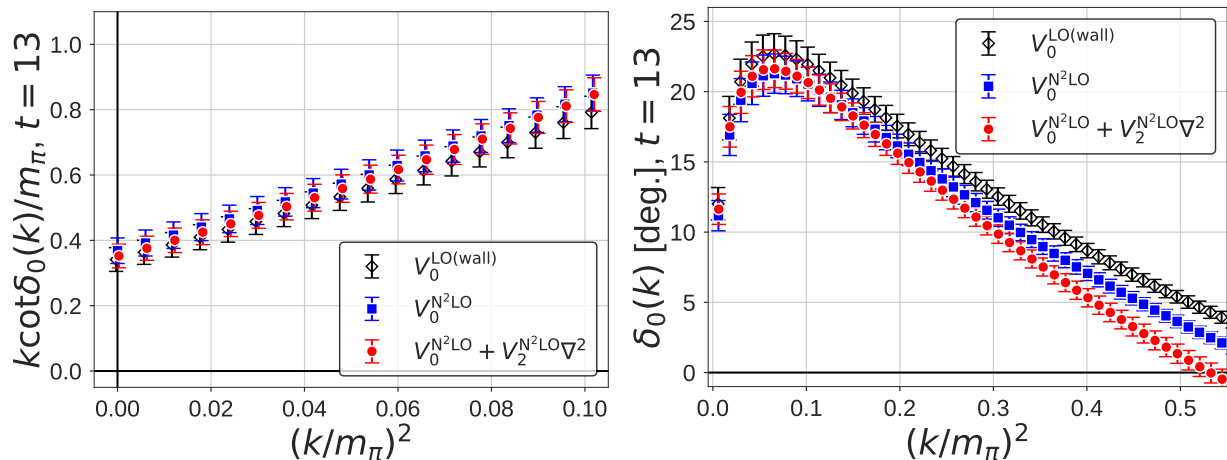


FIG. 10. The scattering phase shifts in the form of $k \cot \delta_0(k)/m_\pi$ (Left) and $\delta_0(k)$ (Right) from $V_0^{\text{LO(wall)}}(r)$ (black diamonds), $V_0^{\text{N}^2\text{LO}}(r)$ (blue squares) and $V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r)\nabla^2$ (red circles) at $t = 13$.

system [15].

The scattering length a_0 obtained through $\lim_{k \rightarrow 0} k \cot \delta_0(k) = 1/a_0$ from $V_0^{\text{LO(wall)}}(r)$, $V_0^{\text{N}^2\text{LO}}(r)$ and $V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r)\nabla^2$ at $t = 13 - 16$ is shown in Fig. 11. The result indicates that the scattering length is almost insensitive to the degrees of the approximation but has a small variation in t , which is, however, within statistical errors. We thus conclude that

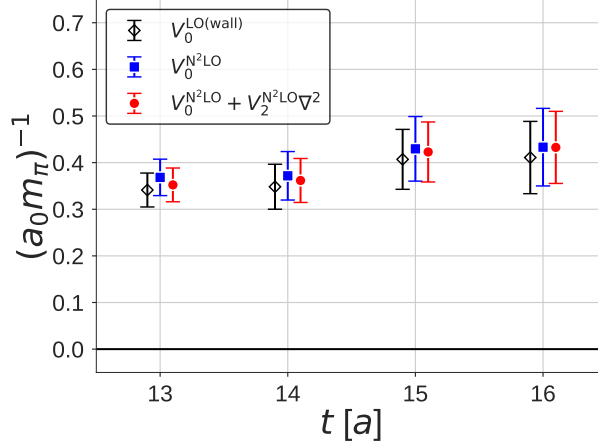


FIG. 11. The scattering length a_0 in the form of $(a_0 m_\pi)^{-1}$ from $V_0^{\text{LO(wall)}}(r)$ (black diamonds) , $V_0^{\text{N}^2\text{LO}}(r)$ (blue squares) and $V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r)\nabla^2$ (red circles) at $t = 13 - 16$.

	$V_0^{\text{LO(wall)}}(r)$	$V_0^{\text{N}^2\text{LO}}(r)$	$V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r)\nabla^2$
$(a_0 m_\pi)^{-1}$	0.341(36) $^{(+70)}_{(-0)}$	0.368(39) $^{(+65)}_{(-0)}$	0.352(36) $^{(+80)}_{(-0)}$

TABLE III. The scattering length a_0 in the form of $(a_0 m_\pi)^{-1}$ from $V_0^{\text{LO(wall)}}(r)$, $V_0^{\text{N}^2\text{LO}}(r)$ and $V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r)\nabla^2$. The central values and statistical errors (in the first parenthesis) are evaluated at $t = 13$, while the systematic errors (in the second) are estimated using the potentials at $t = 14, 15, 16$.

the systematic errors from the derivative expansion and the inelastic state contaminations are well under control for this observable. Numerical values for the scattering length are summarized in Table III, where the central value and statistical errors are evaluated at $t = 13$ and the systematic errors are estimated from the t -dependence among $t = 13 - 16$. We have checked that alternative fitting functions of the potential such as the combination of two Gaussians + (Yukawa) 2 form as employed in [18, 19] give results consistent with those from the present fitting function within errors.

V. FINITE VOLUME FORMULA AND EFFECTIVE RANGE EXPANSION

Before closing the paper, we discuss the relation among the energy spectrum, the Lüscher's finite volume formula and the effective range expansion (ERE). Once the energy shift of the two-body system on a finite volume is measured, the scattering phase shift

is obtained by the Lüscher's formula as

$$k \cot \delta_0(k) = \frac{1}{\pi L} \sum_{\vec{n} \in \mathbf{Z}^3} \frac{1}{|\vec{n}|^2 - (kL/2\pi)^2}, \quad (15)$$

where k^2 is related to the energy shift on a finite volume as $\Delta E_L = 2\sqrt{m_B^2 + k^2} - 2m_B$. For the attractive interaction, k^2 can be negative on a finite volume. Note that the poles of the S -matrix with $k \cot \delta_0(k) = -\sqrt{-k^2}$ in the infinite volume correspond to the bound states.

For the unbound two-body system, the asymptotic behavior of ΔE_L for large L reads

$$\Delta E_L \simeq -\frac{2\pi a_0}{\mu L^3} \left[1 + c_1 \frac{a_0}{L} + c_2 \left(\frac{a_0}{L} \right)^2 \right] + \mathcal{O}(L^{-6}), \quad (16)$$

with the reduced mass μ , the scattering length a_0 , $c_1 = -2.837297$, and $c_2 = 6.375183$ [4, 5].

Let us now calculate k^2 from eigenvalue spectra of the Hamiltonian³ $H = H_0 + V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r)\nabla^2$ on the finite volume ($L = 40, 48, 64$) for the A_1^+ representation of the cubic group, by employing fitted $V_0^{\text{N}^2\text{LO}}(r)$ and $V_2^{\text{N}^2\text{LO}}(r)$ at $L = 64$ in Table II. Fig. 12 (Left) shows the volume dependence of the lowest eigenvalues: The data are found to be well described by Eq. (16), which indicates that the system does not have a bound state. By fitting the data with Eq. (16), we obtain the scattering length as $(a_0 m_\pi)^{-1} = 0.402(14)$ consistent with the values in Table III, $(a_0 m_\pi)^{-1} = 0.352(36)^{(+80)}$.

As extensively discussed in Ref. [11], the ERE, $k \cot \delta_0(k) = 1/a_0 + (1/2)r_{\text{eff}}k^2 + \dots$, provides a systematic and reliable way to relate the volume dependence of ΔE_L , the scattering phase shifts and the bound state pole around $k^2 = 0$.⁴ In Fig. 12 (Right), we plot the finite volume spectra on the $(k^2, k \cot \delta_0(k))$ plane, using the lowest eigenvalues of H on $L = 40, 48, \text{ and } 64$, and the eigenvalue of the first excited state on $L = 64$. Note that the data (triangle, square and diamonds) and their errors are plotted together with the Lüscher's formula (dotted lines). The blue band corresponds to the results obtained by solving the Schrödinger equation in the infinite volume. We find that the finite volume energy spectra at $k^2 < 0$ and $k^2 > 0$ are smoothly connected around $k^2 = 0$ along with the blue band, as is expected from the analytic properties of S -matrix and the ERE. In fact, the ERE at the NLO determined from these 4 data (pink band) is consistent with the blue band at $|(k/m_\pi)^2| \lesssim 0.2$ within errors. One also observes that the positive intercept at $k^2 = 0$ ($1/a_0$) supports the conclusion from Fig. 12 (Left) that the system has no bound state.

³ Since this non-hermitian eigenvalue problem can be written as the definite generalized Hermitian eigenvalue problem, eigenvalues are all real.

⁴ It was pointed out in [11] that the singular and/or unphysical behaviors of $k \cot \delta_0(k)$ around $k^2 = 0$ arise in the direct method [1–3] due to the “fake plateau problem” [10].

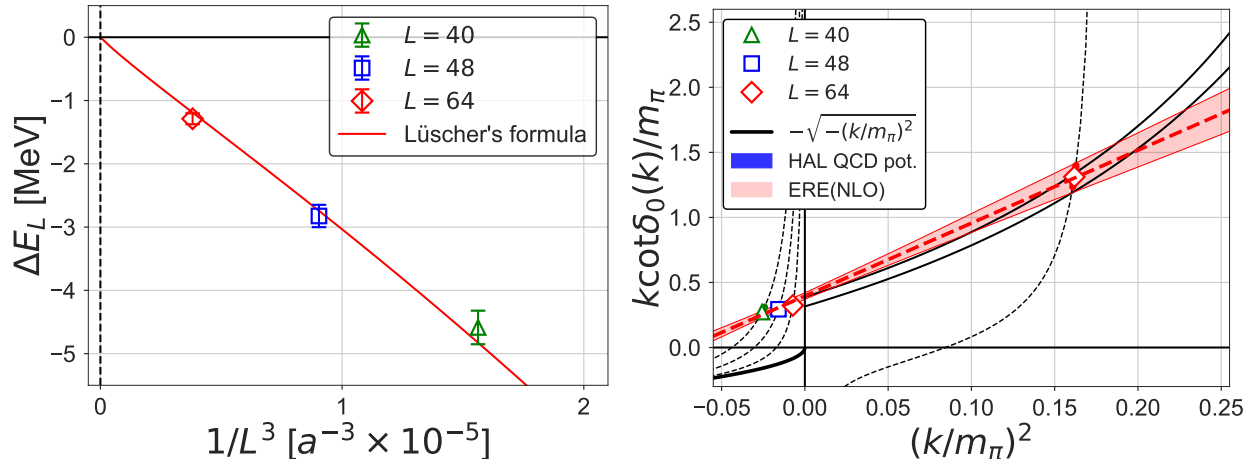


FIG. 12. (Left) The lowest eigenenergies on finite volumes from the HAL QCD potential. The red line corresponds to the fit by the asymptotic Lüscher's finite volume formula in the large L , Eq. (16). (Right) The scattering phase shifts from finite volume eigenenergies using Lüscher's finite volume formula (green triangle, blue square, red diamonds), together with those in the infinite volume from the Schrödinger equation (blue band). The black dotted lines denote the constraints by the Lüscher's finite volume formula, and the black solid line represents the bound state condition in the infinite volume. The red dashed line with the pink band corresponds to the NLO ERE analysis to the finite volume data.

VI. SUMMARY

In this paper, we have made critical investigations on the systematic uncertainties in the HAL QCD method. While the time-dependent HAL QCD method is free from the issue associated with the ground state saturation, the approximation of the energy-independent non-local potential by the derivative expansion introduces systematic uncertainties, so that it is necessary to check the errors introduced by the expansion.

We have performed the (2+1)-flavor lattice QCD calculation for the $\Xi\Xi(^1S_0)$ system at $m_\pi = 0.51$ GeV. Using the four-point correlation functions from both wall and smeared quark sources, we have established the theoretical and numerical method to determine LO and N²LO potentials in the derivative expansion. Scattering phase shifts calculated from these potentials reveal that the LO potential is sufficient to reproduce observables at low energies ($k^2/m_\pi^2 < 0.1$), while the N²LO correction becomes non-negligible but remains small even at high energies ($k^2/m_\pi^2 \simeq 0.5$), confirming the good convergence of the derivative

expansion below the inelastic threshold.

We have also found that the potential at the LO analysis for the wall source agree with the LO potential at the N²LO analysis except at short distances and can reproduce the scattering phase shifts precisely at low energies. This observation confirms the reliability of the previous HAL QCD results, which are based on the LO analysis using the wall source. Other systematic uncertainties such as the inelastic state contaminations and the finite volume effect to the potential are investigated and are found to be well under control.

After establishing the reliability of the HAL QCD potential, we have calculated the eigenvalues of the Hamiltonian in finite boxes with the potential. The volume dependence of the lowest eigenvalues is well described by $1/L$ -expansion for scattering states obtained from the Lüscher's finite volume formula. We have also discussed the relation among the energy spectrum, phase shifts and the effective range expansion.

In a forthcoming paper [13], we will perform the spectral decomposition of the correlation function based on the eigenmodes of the Hamiltonian in a finite box with the HAL QCD potential, which enables us to diagnose the origin of the fake plateaux in the direct method.

ACKNOWLEDGMENTS

We thank the authors of Ref. [14] and ILDG/JLDG [20, 21] for providing the gauge configurations. Lattice QCD codes of CPS [22], Bridge++ [23] and the modified version thereof by Dr. H. Matsufuru, cuLGT [24] and domain-decomposed quark solver [25, 26] are used in this study. The numerical calculations have been performed on BlueGene/Q and SR16000 at KEK, HA-PACS at University of Tsukuba, FX10 at the University of Tokyo and K computer at RIKEN, AICS (hp150085, hp160093). This work is supported in part by the Japanese Grant-in-Aid for Scientific Research (No. JP24740146, JP25287046, JP15K17667, JP16K05340, JP16H03978), by MEXT Strategic Program for Innovative Research (SPIRE) Field 5, by a priority issue (Elucidation of the fundamental laws and evolution of the universe) to be tackled by using Post K Computer, and by Joint Institute for Computational Fundamental Science (JICFuS).

Appendix A: Non-locality vs. Energy dependence

Here we examine the relation between the energy-independent non-local potential with the derivative expansion, $U(\vec{r}, \vec{r}') = \{V_0(r) + V_2(r)\nabla^2 + \dots\}\delta(\vec{r} - \vec{r}')$, and the energy-dependent local potential, $V^{\text{eff}}(r; E)$. For simplicity, in this appendix, we restrict ourselves to the N²LO analysis. In other words, we assume as if the non-local potential were given exactly by $U(\vec{r}, \vec{r}') = \{V_0(r) + V_2(r)\nabla^2\}\delta(\vec{r} - \vec{r}')$.

In this case, it is easy to show that the Schrödinger equation with this non-local potential, given by

$$\left[-\frac{\nabla^2}{2\mu} + V_0(r) + V_2(r)\nabla^2 \right] \psi(\vec{r}) = E\psi(\vec{r}), \quad \mu = m_B/2, \quad (\text{A1})$$

can be written in terms of the energy-dependent local potential as

$$\left[-\frac{\nabla^2}{2\mu} + V^{\text{eff}}(r; E) \right] \psi(\vec{r}) = E\psi(\vec{r}), \quad (\text{A2})$$

where

$$V^{\text{eff}}(r; E) \equiv \frac{V_0(r) - m_B E V_2(r)}{1 - m_B V_2(r)}, \quad (\text{A3})$$

which gives an exact relation between the energy-independent non-local potential and the energy-dependent local potential (within the N²LO analysis). Although both descriptions for the potential are theoretically equivalent as shown above, we stress that the HAL QCD method is based on the energy-independent non-local potential, which can be extracted from arbitrary linear combinations of the NBS wave function $\psi^W(\vec{r})$ thanks to the time dependent method, while the energy-dependent local potential requires the eigenstate saturation, which is difficult to achieve in practice, particularly for excited states. Also $V^{\text{eff}}(r; E)$ gives the correct scattering phase shift at each E (one potential per energy), while $V_0(r) + V_2(r)\nabla^2$ gives the correct scattering phase shifts (within the N²LO analysis) at all $E \leq E_{\text{th}}$ (one potential for all).

Fig. 13 shows the energy dependence of $V^{\text{eff}}(r; E)$ from $E = 10$ MeV to $E = 200$ MeV. In these figures, we use $V_0^{\text{N}^2\text{LO}}(r)$ and $V_2^{\text{N}^2\text{LO}}(r)$ obtained at $t = 13$ for $V_0(r)$ and $V_2(r)$, respectively. The energy dependent correction is small at low energies, while it is no longer negligible at higher energies. As the energy increases, the attractive pocket at an intermediate distance becomes shallower and the radius of the repulsive core becomes larger.

This result also demonstrates how the non-locality of the energy-independent potential,

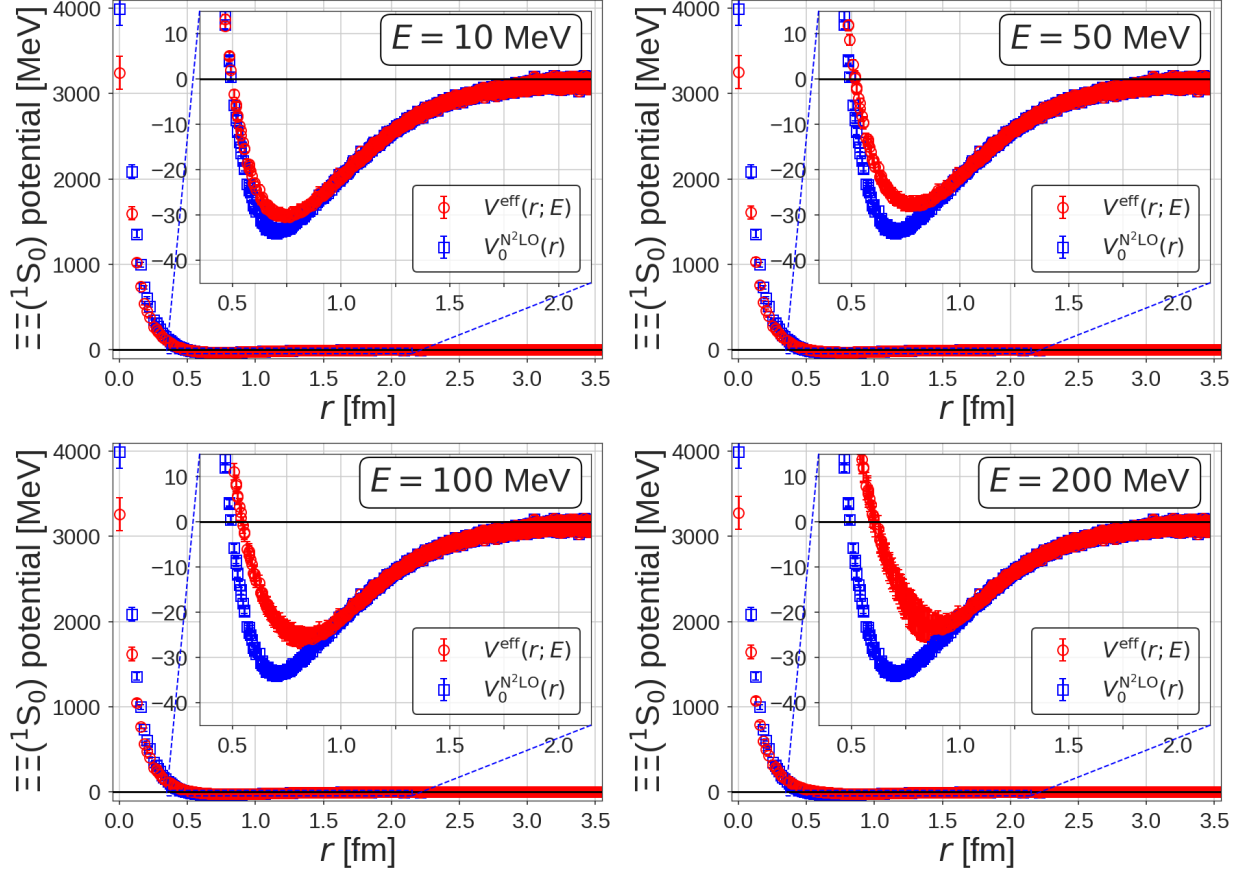


FIG. 13. The energy dependence of the effective potential, $V^{\text{eff}}(r; E)$, (red circles) compared with the LO potential at the $N^2\text{LO}$ analysis, $V_0^{N^2\text{LO}}(r)$ (blue squares) at $E = 10$ MeV (Top Left), $E = 50$ MeV (Top Right), $E = 100$ MeV (Bottom Left) and $E = 200$ MeV (Bottom Right).

$U(r, r')$, (Note that $V_0(r)$, $V_2(r), \dots$ are energy-independent by definition ⁵), is related to the energy dependence of the local potential, $V^{\text{eff}}(r; E)$.

⁵ In the literature, there appears a confusion [27] on the relation between the energy-independent non-local potential and the energy-dependent local potential. See Ref. [28], which clarifies the relation between the two in detail.

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