

Finite volume analysis on systematics of the derivative expansion in HAL QCD method

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We study the convergence of the derivative expansion in HAL QCD method from the finite volume analysis. Employing the (2+1)-flavor lattice QCD data obtained at nearly physical light quark masses (m_π, m_K) \simeq (146, 525) MeV and the physical charm quark mass, we study two representative systems, $\Omega\Omega$ and $\Omega_{ccc}\Omega_{ccc}$ in the 1S_0 channel, where both systems were found to have a shallow bound state in our previous studies. The HAL QCD potentials are determined at the leading-order in the derivative expansion, from which finite-volume eigenmodes are obtained. Utilizing the eigenmode projection, we find that the correlation functions are dominated by the ground state (first excited state) in the case of $\Omega\Omega$ ($\Omega_{ccc}\Omega_{ccc}$). In both $\Omega\Omega$ and $\Omega_{ccc}\Omega_{ccc}$, the spectra obtained from eigenmode-projected temporal correlators are found to be consistent with those from the HAL QCD potential for both the ground and first excited state. These results show that the derivative expansion is well converged in these systems, and also provide a first explicit evidence that the HAL QCD method enables us to reliably extract the binding energy of the ground state even from the correlator dominated by excited scattering states.

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1. Introduction

The determination of hadron interactions is one of the most active areas in lattice QCD these days. Currently, there are two major theoretical methods, Lüscher's finite volume method [1] and HAL QCD method [2–4]. The former first determines a finite volume spectrum from a temporal correlation function, and converts the spectrum to a scattering phase shift at that energy through Lüscher's formula. The latter calculates an energy-independent non-local potential from a tempo-spatial correlation function, and binding energies and phase shifts are obtained by solving Schrödinger-type equation with the potential in the infinite volume.

While these two methods are equivalent theoretically, each method has its own pros and cons in practical calculations. In Lüscher's method, it is essential to isolate each eigenstate in the correlator, but it becomes difficult to suppress contaminations from nearby states if the energy splittings between states are small. In fact, we pointed out [5] that naive plateau identification for two-baryon systems employed in the literature (so-called “direct method”) leads to unreliable results due to the excited state contaminations. Our finding is also being confirmed by recent lattice QCD studies with Lüscher's method [6–8]. On the other hand, HAL QCD method is free from such a problem (as far as elastic states are concerned), since one can extract the signal of energy-independent potential even from excited states through its time-dependent formalism [3]. The method, however, introduces another type of systematic errors in practice, because the non-locality of the potential is usually determined order by order in the derivative expansion. In Ref. [9] we explicitly determined the potential up to next-to-next-to-leading order (N²LO) and found that the truncation error is well under control even at the leading-order (LO) at low energies.

Since the calculation of higher order terms in the derivative expansion is usually expensive, we consider an alternative method [5] in this report to study the convergence of the derivative expansion. The method essentially examines the consistency between Lüscher's finite volume method and the HAL QCD method, utilizing the finite volume eigenmodes obtained from the HAL QCD potential. Considering that the origin of systematic errors of two methods are quite independent, the observation of the consistency provides non-trivial confirmation that the systematic errors are well under control.

In this report, we study two representative systems, $\Omega\Omega$ and $\Omega_{ccc}\Omega_{ccc}$ systems in the 1S_0 channel near physical quark masses on a large volume ($La \simeq 8.1$ fm). These systems have several good characteristics for our study: (1) Heavy mass and large volume make energy splittings between finite volume eigenstates small (\sim a few MeV) (2) Absence of valence ud -quarks makes statistical fluctuations small (3) It was found that there is one shallow bound state for each system [10, 11]. In addition, it turns out that the correlator of each system serves as two representative cases, i.e., the $\Omega\Omega$ correlator is dominated by the ground state, while the $\Omega_{ccc}\Omega_{ccc}$ correlator is dominated by the first excited state. In this report, we examine whether binding energies and scattering phase shifts are reliably extracted for both cases in the HAL QCD method.

2. HAL QCD method and finite volume analysis

The key quantity in the HAL QCD method is the equal-time Nambu-Bethe-Salpeter (NBS) wave function. In the case of a BB system with $B = \Omega$ or Ω_{ccc} in this study, it is defined by

$\phi_W(\mathbf{r}) \equiv 1/Z_B \cdot \langle 0 | \hat{B}(\mathbf{r}, 0) \hat{B}(\mathbf{0}, 0) | BB, W \rangle$, where \hat{B} is an operator for a B -baryon with its wave-function renormalization constant Z_B and $|BB, W\rangle$ denotes the BB eigenstate at the total energy of $W = 2\sqrt{k^2 + m_B^2}$, and we consider the elastic region, $W < W_{\text{th}}$. Since the information of the phase shift is encoded in the asymptotic behavior ($r \equiv |\mathbf{r}| \rightarrow \infty$) of the NBS wave function, one can define energy-independent non-local potential, $U(\mathbf{r}, \mathbf{r}')$, through the Schrödinger equation, $(E_W - H_0)\phi_W(\mathbf{r}) = \int d\mathbf{r}' U(\mathbf{r}, \mathbf{r}')\phi_W(\mathbf{r}')$, where $H_0 = -\nabla^2/(2\mu)$ and $E_W = k^2/(2\mu)$ with the reduced mass $\mu = m_B/2$ [2–4].

Generally speaking, the NBS wave function at each eigenenergy can be extracted from the four-point correlator. Such a procedure, however, is exponentially difficult in practice, if one relies on the ground state (or eigenstate) saturation utilizing the temporal behavior of the correlator. The time-dependent HAL QCD method [3] overcomes this problem by exploiting the fact that the same potential governs all elastic states. Namely, we define the normalized four-point function as $R(\mathbf{r}, t) \equiv \sum_{\mathbf{x}} \langle 0 | \hat{B}(\mathbf{r} + \mathbf{x}, t) \hat{B}(\mathbf{x}, t) \overline{\mathcal{J}}(0) | 0 \rangle / e^{-2m_B t}$ and the potential can be determined by the following master formula:

$$\left(\frac{1}{4m_B} \frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} - H_0 \right) R(\mathbf{r}, t) = \int d\mathbf{r}' U(\mathbf{r}, \mathbf{r}') R(\mathbf{r}', t). \quad (1)$$

The systematic error in this equation is the contaminations from the inelastic states, which can be suppressed by taking moderately large Euclidean time, $t \gg (W_{\text{th}} - W)^{-1}$.

In practical calculation, non-locality of the potential is handled by the derivative expansion at low energies, $U(\mathbf{r}, \mathbf{r}') = \sum_n V_n(\mathbf{r}) \nabla^n \delta(\mathbf{r} - \mathbf{r}')$. For instance, the central potential $V(r)$ at the LO is given as

$$V(r) = R^{-1}(\mathbf{r}, t) \left(\frac{1}{4m_B} \frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} - H_0 \right) R(\mathbf{r}, t). \quad (2)$$

This procedure, however, introduces new systematic errors associated with the truncation in the derivative expansion. In order to quantify such systematic uncertainties, it is most desirable to calculate the higher order terms explicitly and examine the convergence. Such a study was performed up to N²LO for the $\Xi\Xi$ system in the 1S_0 channel at $m_\pi = 0.51$ GeV [9], and it was found that the truncation error is well under control even at the LO at low energies. However, the explicit computations of higher order terms require large resources, which leads us to study an alternative method in this report.

We here perform the finite volume analysis [5] as a new measure which can quantify the systematic uncertainties of the derivative expansion without requiring any additional lattice QCD simulation. In this analysis, we first consider the following Hamiltonian H in a finite box, and calculate its eigenenergies and eigenfunctions (eigenmodes),

$$H = H_0 + V(r), \quad H\psi_n = \epsilon_n\psi_n, \quad (3)$$

where $V(r)$ is the HAL QCD potential obtained at the LO in the derivative expansion, and ϵ_n is related to the relativistic energy, $W_n = 2\sqrt{\epsilon_n m_B + m_B^2}$. Obtained eigenfunctions are useful to isolate the contribution from each eigenmode in the correlator. More specifically, we utilize the eigenfunctions to construct a two-baryon sink operator optimized for each eigenstate on a finite

volume,

$$\sum_{\mathbf{r}} \psi_n^\dagger(\mathbf{r}) \left[\sum_{\mathbf{x}} \hat{B}(\mathbf{r} + \mathbf{x}, t) \hat{B}(\mathbf{x}, t) \right]. \quad (4)$$

A temporal correlator with such an optimized two-baryon sink operator can be obtained as follows,

$$R_n(t) \equiv \sum_{\mathbf{r}} \psi_n^\dagger(\mathbf{r}) R(\mathbf{r}, t), \quad (5)$$

where ψ_n serves as a projection operator to the designated eigenstate.

One can extract the finite volume energy from this temporal correlator, which value has one-to-one correspondence to the phase shift via Lüscher's formula. Note that, while the information of the HAL QCD potential is implicitly used to construct the optimized operator, the theoretical formulation is solely based on Lüscher's finite volume method. The result of the finite volume spectrum can be compared to that obtained directly from the HAL QCD potential (i.e., eigenenergies of H on a finite volume). If we observe consistency, it is non-trivial confirmation that the systematic errors in the HAL QCD potential are well under control.

3. Lattice QCD setup

Numerical data used in this study are obtained from the $(2+1)$ -flavor gauge configurations with Iwasaki gauge action at $\beta = 1.82$ and nonperturbatively $O(a)$ -improved Wilson quark action with stout smearing at nearly physical quark masses [12]. The relativistic heavy quark (RHQ) action is used for the charm quark to remove cutoff errors associated with the charm quark mass up to next-to-leading order, with RHQ parameters determined in Ref. [13]. The lattice cutoff is $a^{-1} \simeq 2.333$ GeV ($a \simeq 0.0846$ fm) and the lattice volume is $(La)^4 = (96a)^4 \simeq (8.1 \text{ fm})^4$. The hadron masses most relevant to this study are $(m_\pi, m_K, m_\Omega, m_{\Omega_{ccc}}) \simeq (146, 525, 1712, 4796)$ MeV. The NBS correlation functions for $\Omega\Omega$ and $\Omega_{ccc}\Omega_{ccc}$ systems are calculated by the unified contraction algorithm [14] with the wall-type source operator combined with the Coulomb gauge fixing. In order to reduce statistical fluctuations, forward and backward propagations are averaged, the hypercubic symmetry on the lattice (4 rotations) are utilized, and multiple measurements are performed by shifting the source position along the temporal direction. The total measurements for $\Omega\Omega$ ($\Omega_{ccc}\Omega_{ccc}$) amounts to 307200 (896). For more details, see Refs. [10, 11].

4. Results

In Fig. 1, we show the LO HAL QCD potentials $V(r)$ in the 1S_0 channel for $\Omega\Omega$ at $t/a = 17$ and $\Omega_{ccc}\Omega_{ccc}$ at $t/a = 26$, where t/a are chosen so that contaminations from inelastic excited states are suppressed in the single-baryon correlators. By solving the Schrödinger equation in the infinite volume, we find that each system forms a loosely bound state with the binding energy $B \simeq 1.6$ MeV, root-mean-square distance $\sqrt{\langle r^2 \rangle} \simeq 3.4$ fm for $\Omega\Omega$ [10], and $B \simeq 5.7$ MeV, $\sqrt{\langle r^2 \rangle} \simeq 1.1$ fm for $\Omega_{ccc}\Omega_{ccc}$ [11]. (If we consider the effect of the Coulomb repulsion, both dibaryons are located in the unitary regime [11], but we study only QCD in this report.)

Using the obtained potentials, we consider the HAL QCD Hamiltonian $H = H_0 + V$ on a finite volume and calculate eigenmodes in the A_1 representation. The lowest four eigenfunctions ψ_n with

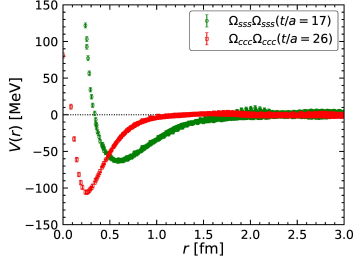


Figure 1: The LO HAL QCD potentials $V(r)$ for $\Omega\Omega(= \Omega_{SSS}\Omega_{SSS})$ (green circles) and $\Omega_{ccc}\Omega_{ccc}$ (red squares) in the 1S_0 channel.

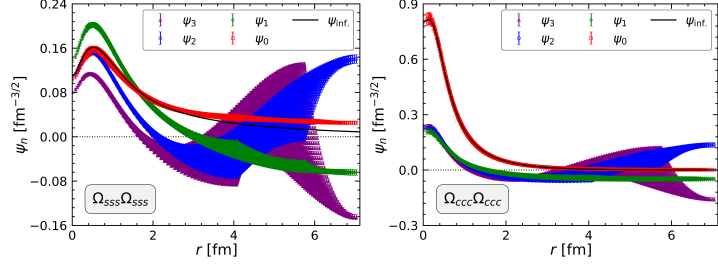


Figure 2: The lowest four eigenfunctions (colored points) in the A_1 representation of the HAL QCD Hamiltonian on a finite volume for $\Omega\Omega(= \Omega_{SSS}\Omega_{SSS})$ (left) and $\Omega_{ccc}\Omega_{ccc}$ (right). The black solid lines denote the bound state wavefunctions in the infinite volume.

$n = 0, 1, 2$ and 3 are shown in Fig. 2, which are normalized as $\sum_{\mathbf{r}} |\psi_n(\mathbf{r})|^2 = 1$ and $\psi_n(\mathbf{0}) > 0$. Shown together are the bound state wavefunctions $\psi_{\text{inf.}}$, which are calculated in the infinite volume.

As described in Sec. 2, each eigenfunction can be used as the projection operator for the corresponding eigenstate. This enables us to decompose the correlators, $R(\mathbf{r}, t)$ and $R(t)$, as

$$\begin{aligned} R(\mathbf{r}, t) &= \sum_n a_n \psi_n(\mathbf{r}) e^{-(\Delta E_n)t}, \\ R(t) &\equiv \sum_{\mathbf{r}} R(\mathbf{r}, t) = \sum_n b_n e^{-(\Delta E_n)t}, \end{aligned} \quad (6)$$

with $\Delta E_n \equiv W_n - 2m_B$. Here, a_n and b_n represent the magnitude of contribution of the n -th state to the correlator $R(\mathbf{r}, t)$ and $R(t)$, respectively, and they can be determined by $a_n = \sum_{\mathbf{r}} \psi_n^\dagger(\mathbf{r}) R(\mathbf{r}, t) e^{(\Delta E_n)t}$, $b_n = a_n \sum_{\mathbf{r}} \psi_n(\mathbf{r})$ with ΔE_n calculated from the eigenenergies of H . In Fig. 3, we show a_n/a_0 and b_n/b_0 with $n = 0, 1, 2$ and 3 for both of $\Omega\Omega$ and $\Omega_{ccc}\Omega_{ccc}$. We find that two systems correspond to two different representative cases: the correlator of $\Omega\Omega$ is dominated by the ground state, while that of $\Omega_{ccc}\Omega_{ccc}$ is dominated by the first excited state. One can intuitively understand the origin of this observation. In the case of $\Omega\Omega$, the ground state wavefunction is long-ranged in r , and thus the lattice source operator constructed by the wall source is expected to couple the ground state strongly. On the other hand, the ground state wavefunction of $\Omega_{ccc}\Omega_{ccc}$ is much more short-ranged, and the coupling between the lattice source operator and the ground state is expected to be suppressed.

In order to examine the systematic uncertainties of the derivative expansion, we construct the optimized two-baryon sink operator utilizing the eigenfunctions (Eq. (4)), and calculate the eigenmode-projected temporal correlator, $R_n(t)$ (Eq. (5)). In Fig. 4, we show the effective energies $\Delta E_n^{\text{eff}}(t)$ obtained from $R_n(t)$ with $n = 0$ (the ground state) and $n = 1$ (the first excited state) for both $\Omega\Omega$ and $\Omega_{ccc}\Omega_{ccc}$. Shown together are the corresponding ΔE_n calculated directly from the HAL QCD Hamiltonian H .

In both cases of $\Omega\Omega$ and $\Omega_{ccc}\Omega_{ccc}$, we find that the effective energies $\Delta E_n^{\text{eff}}(t)$ are stable in terms of t , which values are consistent with ΔE_n for both of the ground state ($n = 0$) and the first excited state ($n = 1$). This establishes the consistency between Lüscher's finite volume method and the HAL QCD method, indicating that systematic errors associated with the truncation of the derivative expansion are well under control. In fact, if such artifacts were to be large, eigenfunctions

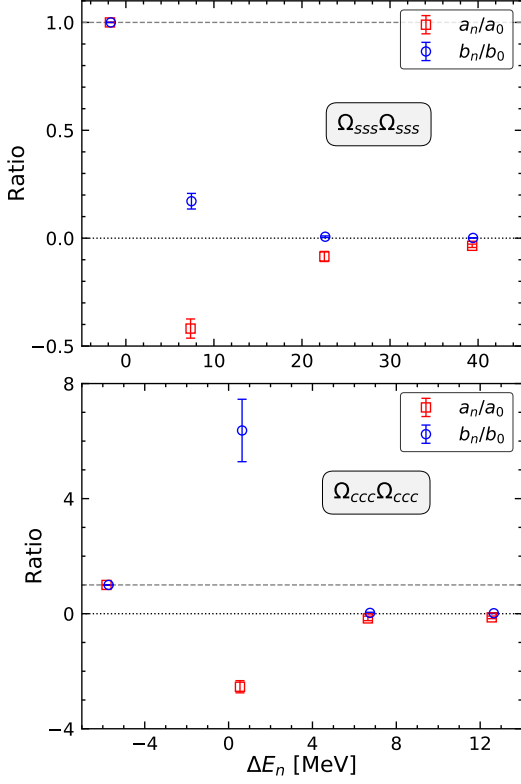


Figure 3: The ratio a_n/a_0 (red squares) and b_n/b_0 (blue circles) for lowest four states ($n = 0, 1, 2, 3$) as a function of ΔE_n for $\Omega\Omega(= \Omega_{SSS}\Omega_{SSS})$ (upper) and $\Omega_{ccc}\Omega_{ccc}$ (lower).

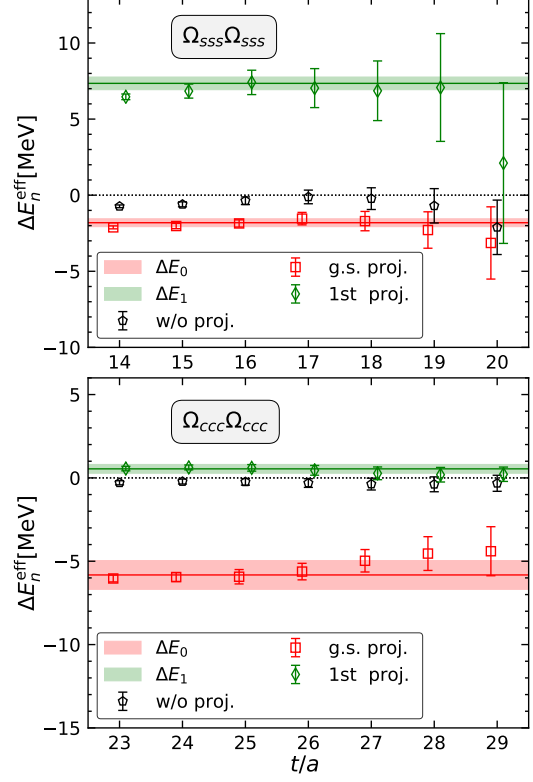


Figure 4: The effective energies $\Delta E_n^{\text{eff}}(t)$ from the projected temporal correlators $R_n(t)$ for the ground state ($n = 0$, red squares) and the first excited state ($n = 1$, green diamonds) for $\Omega\Omega$ (upper) and $\Omega_{ccc}\Omega_{ccc}$ (lower). The red (green) bands show ΔE_0 (ΔE_1) obtained from the HAL QCD Hamiltonian H . The black pentagons represent the effective energies from the temporal correlators without projection.

$\psi_n(r)$ would be so different from the n -th eigenstate of the system that the effective energies from $R_n(t)$ would be distorted and do not agree with those from H . Our observation also confirms that the HAL QCD method can make reliable predictions regardless whether a correlator is dominated by the ground state or (first) excited state.

This is in sharp contrast to the naive extraction of finite volume energies from the temporal correlators. To demonstrate this point, we show in Fig. 4 the effective energies from the temporal correlators without any sophisticated projection, i.e., $R(t) = \sum_{\mathbf{r}} R(\mathbf{r}, t)$. Such effective energies have been customary employed in the “direct method” to calculate the ground state spectrum for two-baryon systems. We find that effective energies show stable plateau-like structures, which values, however, significantly deviate from the correct values of the ground states. In particular, the effective energy of $\Omega_{ccc}\Omega_{ccc}$ is very close to the value of the first excited state, reflecting the fact that the $\Omega_{ccc}\Omega_{ccc}$ correlator is dominated by the first excited state. The calculations based on such pseudo-plateaux, of course, lead to unreliable predictions.

5. Conclusions

We studied the convergence of the derivative expansion in the HAL QCD potential. As good representative systems, we considered $\Omega\Omega$ and $\Omega_{ccc}\Omega_{ccc}$ in the 1S_0 channel, each of which has a shallow bound state. The lattice calculations were performed in (2+1)-flavor QCD with nearly physical light quark masses $(m_\pi, m_K) \simeq (146, 525)$ MeV and the physical charm quark mass.

The HAL QCD potentials were determined at the leading-order in the derivative expansion. The corresponding finite-volume eigenmodes were obtained, from which the eigenmode projection on the correlator was performed. Our finite volume analysis showed that the correlation function is dominated by the ground state (first excited state) in the case of $\Omega\Omega$ ($\Omega_{ccc}\Omega_{ccc}$). For both $\Omega\Omega$ and $\Omega_{ccc}\Omega_{ccc}$ systems, the spectra obtained from eigenmode-projected temporal correlators were found to be consistent with those from the HAL QCD potential. This serves as a non-trivial consistency check between Lüscher's finite volume method and the HAL QCD method, and confirms that the derivative expansion in the HAL QCD method is well converged in these systems. In addition, we conclude that the HAL QCD method can make reliable predictions regardless whether a correlator is dominated by the ground state or (first) excited state. It is particularly striking that the HAL QCD potential obtained from the correlator dominated by the first excited state can determine the binding energy of the ground state reliably.

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