

Hermitizing the HAL QCD potential in the derivative expansion

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A formalism is given to hermitize the HAL QCD potential, which needs to be non-Hermitian except for the leading-order (LO) local term in the derivative expansion as the Nambu–Bethe–Salpeter (NBS) wave functions for different energies are not orthogonal to each other. It is shown that the non-Hermitian potential can be hermitized order by order to all orders in the derivative expansion. In particular, the next-to-leading order (NLO) potential can be exactly hermitized without approximation. The formalism is then applied to a simple case of $\Xi\Xi(^1S_0)$ scattering, for which the HAL QCD calculation is available to the NLO. The NLO term gives relatively small corrections to the scattering phase shift and the LO analysis seems justified in this case. We also observe that the local part of the hermitized NLO potential works better than that of the non-Hermitian NLO potential. The Hermitian version of the HAL QCD potential is desirable for comparing it with phenomenological interactions and also for using it as a two-body interaction in many-body systems.
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1. Introduction

Lattice quantum chromodynamics (QCD) is a successful non-perturbative method to study hadron physics from the underlying degrees of freedom, i.e., quarks and gluons. Masses of single stable hadrons obtained from lattice QCD show good agreement with the experimental results, and even hadron interactions have been recently explored in lattice QCD. Using the Nambu–Bethe–Salpeter (NBS) wave function, linked to the S-matrix in QCD [1–9], the hadron interactions have mainly been investigated by two methods: the finite volume method [1] and the HAL QCD potential method [5–7]. Theoretically the two methods in principle give the same results for the scattering phase shifts between two hadrons, while in practice they sometimes show different numerical results for two-baryon systems, whose origin has been clarified recently in Refs. [10,11].

The HAL QCD method utilizes the NBS wave function in the non-asymptotic (interacting) region, and extracts the non-local but energy-independent potentials from the space and time dependences of the NBS wave function. Physical observables such as phase shifts and binding energies are then calculated by solving the Schrödinger equation in infinite volume using the obtained potentials, since the asymptotic behavior of the NBS wave function is related to the T-matrix element and thus to the phase shifts [9]. In practice, the non-local potential is given by the form of the derivative expansion, which is truncated by the first few orders [12].

While the HAL QCD method has been successfully applied to a wide range of two- (or three-) hadron systems at heavy pion masses [13–28] as well as at the nearly physical mass [29–35], there are some subtleties or issues in the method. One is the theoretical treatment of the bound states in this method, which has been recently clarified in Ref. [36]. In this paper, we consider the other issue, the non-hermiticity of the potential in the HAL QCD method. We show in Sect. 2 that the non-Hermitian potential defined in the derivative expansion can be made Hermitian order by order in the derivative expansion. In particular, a non-Hermitian potential that contains the second derivative at most can be made exactly Hermitian, while non-Hermitian potentials with higher-order derivatives than second order can be shown to be made Hermitian potentials, using the mathematical induction for the order of the derivative expansion. In Sect. 3, we apply our method to a non-Hermitian HAL QCD potential for $\Xi\Xi$ in lattice QCD [12], which consists of local and second- or first-order derivative terms. We show that the exactly hermitized potential gives the same scattering phase shifts as those from the original non-Hermitian potential but the contribution from its derivative term is smaller than that from the original derivative term. A summary and the conclusion to this paper are given in Sect. 4.

2. Hermitizing the non-Hermitian potential

In this section, we propose a method to hermitize the non-Hermitian Hamiltonian order by order in terms of derivatives. We consider the non-Hermitian Hamiltonian for the relative coordinate of two identical particles without spin, which is given by

$$H = H_0 + \sum_{n=0}^{\infty} V_n, \quad H_0 = -\frac{1}{m}\nabla^2, \quad (1)$$

where V_n is the potential with n -derivatives, and m is the mass of the particle, so that the reduced mass is given by $m/2$. The explicit form of V_n is denoted as

$$V_n := \frac{1}{n!} V_l^{i_1 i_2 \dots i_n} \nabla_{i_1} \nabla_{i_2} \dots \nabla_{i_n}, \quad (2)$$

where the local function $V_l^{i_1 i_2 \dots i_n}$ is symmetric under exchanges of indices $i_1 i_2 \dots i_n$ and summations over repeated indices are implicitly assumed. In this paper, we assume that the above derivative expansion is convergent. See Appendix A for some arguments. Except the local potential V_0 , the other $V_{n>0}$ are non-Hermitian. Note also that the $\vec{r}$ -dependence of V_n is implicit.

Since $H_0 + V_0$ is Hermitian, we first consider V_1 and V_2 , which is the next-to-leading (first) order, and more generally V_{2n-1} and V_{2n} as the n th order, for the hermitizing problem, and introduce

$$U_n := V_{2n} + V_{2n-1}. \quad (3)$$

The reason to treat V_{2n} and V_{2n-1} together will be clear later. In terms of the derivative expansion for the potential, V_0 is of leading order while V_1 and V_2 are of next-to-leading, so that V_0 is much larger in size than V_1 or V_2 at low energies.

2.1. $n = 1$ case

At $n = 1$, the Hamiltonian is given by

$$H^{(1)} = H_0 + V_0 + U_1, \quad (4)$$

where the $n = 1$ potential U_1 is rewritten as

$$U_1 = \tilde{V}_2 + \tilde{V}_1, \quad \tilde{V}_2 := \frac{1}{2} \nabla_i V_2^{ij} \nabla_j, \quad \tilde{V}_1 := \tilde{V}_1^i \nabla_i, \quad \tilde{V}_1^i := V_1^i - \frac{1}{2} \left(\nabla_j V_2^{ji} \right). \quad (5)$$

Here $\tilde{V}_2$ is Hermitian, while $\tilde{V}_1$ is not.

The corresponding Schrödinger equation is given by

$$H^{(1)} \psi = E \psi, \quad (6)$$

which transforms to

$$\tilde{H}^{(1)} \phi = E \phi, \quad \tilde{H}^{(1)} = R_1^{-1} H^{(1)} R_1, \quad (7)$$

by the change of the wave function that $\psi := R^{(1)} \phi$ with a local function $R^{(1)} = R_1$, where

$$\tilde{H}^{(1)} = H_0 + \tilde{V}_0 + \tilde{V}_2 + \left\{ \tilde{V}_1^i - \frac{2}{m} R_1^{-1} \nabla^i R_1 + V_2^{ij} R_1^{-1} \nabla_j R_1 \right\} \nabla_i, \quad (8)$$

$$\tilde{V}_0 = V_0 - \frac{1}{m} R_1^{-1} \nabla^2 R_1 + V_1^i R_1^{-1} \nabla_i R_1 + \frac{1}{2} V_2^{ij} \left(R_1^{-1} \nabla_i \nabla_j R_1 \right). \quad (9)$$

By demanding the condition that

$$\tilde{V}_1^i - \frac{2}{m} R_1^{-1} \nabla^i R_1 + V_2^{ij} R_1^{-1} \nabla_j R_1 = 0, \quad (10)$$

$\tilde{H}^{(1)}$ becomes Hermitian as $\tilde{H}^{(1)} = H_0 + \tilde{V}_0 + \tilde{V}_2$, where

$$\tilde{V}_0 = V_0 - \frac{1}{2} \left(\nabla_i \tilde{V}_1^i \right) + \frac{m}{4} \tilde{V}_1^i \left(\delta^{ij} - \frac{m}{2} V_2^{ij} \right)^{-1} \tilde{V}_1^j, \quad (11)$$

$$R_1^{-1} \nabla_i R_1 = \frac{m}{2} \left(\delta^{ij} - \frac{m}{2} V_2^{ij} \right)^{-1} \tilde{V}_1^j. \quad (12)$$

In the rotationally symmetric case such that

$$\tilde{V}_1^i(\vec{r}) := \hat{r}^i \tilde{V}_1(r), \quad V_2^{ij}(\vec{r}) := V_{2a}(r) \hat{r}^i \hat{r}^j + V_{2b}(r) \delta^{ij}, \quad R_1(\vec{r}) := R_1(r) \quad (13)$$

with $r := |\vec{r}|$ and $\hat{r}^i := r^i/r$, we have

$$\frac{d R_1(r)}{d r} = \frac{m}{2} \frac{\tilde{V}_1(r)}{1 - \frac{m}{2} V_2(r)} R_1(r), \quad V_2 := V_{2a} + V_{2b}, \quad (14)$$

which can be solved as

$$R_1(r) = \exp \left[\frac{m}{2} \int_{r_\infty}^r \frac{\tilde{V}_1(s)}{1 - \frac{m}{2} V_2(s)} d s \right], \quad (15)$$

where we assume $V_1(r) = 0$ and $R_1(r) = 1$ at sufficiently large $r \geq r_\infty$. Thus the Hermitian local potential $\tilde{V}_0$ becomes

$$\tilde{V}_0 = V_0 - \frac{\tilde{V}_1}{r} - \frac{1}{2} \tilde{V}_1' + \frac{m}{4} \frac{\tilde{V}_1^2}{1 - \frac{m}{2} V_2}, \quad \tilde{V}_1 := V_1 - \frac{V_{2a}}{r} - \frac{V_{2a}' + V_{2b}'}{2}, \quad (16)$$

where the prime ' means the derivative with respect to r .

2.2. $n = 2$ case

In the previous subsection, we show that the non-Hermitian potential at $n = 1$ can be made Hermitian without any approximations. In this subsection, we proceed to the next order, the $n = 2$ case, where some truncations are required for a number of derivatives, as we will see.

The $n = 2$ Hamiltonian is given by

$$H^{(2)} = H^{(1)} + U_2, \quad (17)$$

where the $n = 2$ potential U_2 can be written as

$$U_2 = \frac{1}{4!} \nabla_i \nabla_j U_{2,4}^{ijkl} \nabla_k \nabla_l + \frac{1}{3!} U_{2,3}^{ijk} \nabla_i \nabla_j \nabla_k + \frac{1}{2!} \nabla_i U_{2,2}^{ij} \nabla_j + U_{2,1}^i \nabla_i \quad (18)$$

$$:= U_{2,4} + U_{2,3} + U_{2,2} + U_{2,1}, \quad (19)$$

and $U_{2,4}$ and $U_{2,2}$ are Hermitian, while $U_{2,3}$ and $U_{2,1}$ are not. In terms of the original V_4 and V_3 , we have

$$U_{2,4}^{ijkl} := V_4^{ijkl}, \quad U_{2,3}^{ijk} := V_3^{ijk} - \frac{1}{2} \nabla_l V_4^{ijkl}, \quad U_{2,2}^{ij} := -\frac{2}{4!} (\nabla_k \nabla_l V_4^{ijkl}), \quad U_{2,1}^i := \frac{1}{4!} (\nabla_j \nabla_k \nabla_l V_4^{ijkl}). \quad (20)$$

2.2.1. General case

The change of the wave function $\psi = R^{(2)}\phi$ at $n = 2$ is given by

$$R^{(2)} = R_1(1 + R_2), \quad R_2 := R_{2,0} + R_{2,2}, \quad (21)$$

where the $n = 1$ term R_1 has already been determined in the previous subsection, while the $n = 2$ term R_2 contains the local function $R_{2,0}$ without derivatives and $R_{2,2}$ with second derivatives as

$$R_{2,2} := \frac{1}{2!} R_{2,2}^{ij} \nabla_i \nabla_j. \quad (22)$$

As will be seen later, we can make $H^{(2)}$ Hermitian without the first derivative term, $R_{2,1}$.

The transformed Hamiltonian $\tilde{H}_2$ is given by

$$\begin{aligned} \tilde{H}^{(2)} &:= (R^{(2)})^{-1} H^{(2)} R^{(2)} \simeq (1 - R_2) R_1^{-1} (H^{(1)} + U_2) R_1 (1 + R_2) \\ &\simeq \tilde{H}^{(1)} + R_1^{-1} U_2 R_1 + [\tilde{H}^{(1)}, R_2], \quad \tilde{H}^{(1)} = H_0 + \tilde{V}_0 + \tilde{V}_2 := \tilde{V}_0 + H_{1,2}, \end{aligned} \quad (23)$$

where $\tilde{H}^{(1)}$ is already made Hermitian by R_1 and we neglect higher-order terms such as $O(R_2^2)$ and $O(R_2 H_2)$.

We first consider $\tilde{U}_2 := R_1^{-1} U_2 R_1$, which is evaluated as

$$\tilde{U}_2 = U_{2,4} + \tilde{U}_{2,3} + \tilde{U}_{2,2} + \tilde{U}_{2,1} + \tilde{U}_{2,0}, \quad (24)$$

where $\tilde{U}_{2,n}$ consists of n th derivative terms, and $\tilde{U}_{2,2}$ can be taken to be Hermitian while $\tilde{U}_{2,0}$ is always Hermitian. (Note that $U_{2,4}$ is defined to be Hermitian.) Explicit forms of $\tilde{U}_{2,n}$ in terms of $U_{2,l}$ are too complicated and unnecessary for our argument hereafter.

Similarly we can write

$$X_0 := [\tilde{H}^{(1)}, R_{2,0}] = X_{0,1} + X_{0,0}, \quad (25)$$

$$X_2 := [\tilde{H}^{(1)}, R_{2,2}] = X_{2,3} + X_{2,2} + X_{2,1} + X_{2,0}, \quad (26)$$

where n in $X_{k,n}$ represents the number of derivatives, and $X_{k,2n}$ is taken to be Hermitian. Explicitly, we have

$$X_{2,3} := \frac{1}{3!} X_{2,3}^{ijk} \nabla_i \nabla_j \nabla_k, \quad X_{2,2} := \frac{1}{2!} \nabla_i X_{2,2}^{ij} \nabla_j, \quad X_{2,1} := X_{2,1}^i \nabla_i, \quad (27)$$

$$X_{2,3}^{ijk} = \left[H_{1,2}^{il} (\nabla_l R_{2,2}^{jk}) - R_{2,2}^{il} (\nabla_l H_{1,2}^{jk}) \right] + 2 \text{ permutations}, \quad (28)$$

$$X_{2,2}^{ij} = -R_{2,2}^{il} (\nabla_k \nabla_l H_{1,2}^{kj}) + \frac{1}{2} \left\{ H_{1,2}^{kl} (\nabla_k \nabla_l R_{2,2}^{ij}) + (\nabla_k H_{1,2}^{kl}) (\nabla_l R_{2,2}^{ij}) - R_{2,2}^{kl} (\nabla_k \nabla_l H_{1,2}^{ij}) \right\}, \quad (29)$$

$$X_{2,1}^i = -R_{2,2}^{ij} (\nabla_j \tilde{V}_0) - \frac{1}{4} R_{2,2}^{kl} (\nabla_j \nabla_k \nabla_l H_{1,2}^{ij}) - \frac{1}{2} (\nabla_j X_{2,2}^{ij}), \quad (30)$$

$$X_{2,0} = -\frac{1}{2} R_{2,2}^{ij} (\nabla_i \nabla_j \tilde{V}_0), \quad (31)$$

and

$$X_{0,1} = H_{1,2}^{ij} (\nabla_j R_{2,0}) \nabla_i, \quad X_{0,0} = \frac{1}{2} H_{1,2}^{ij} (\nabla_i \nabla_j R_{2,0}) + \frac{1}{2} (\nabla_i H_{1,2}^{ij}) (\nabla_j R_{2,0}), \quad (32)$$

where $H_{1,2}$ is defined in Eq. (23).

The transformed Hamiltonian becomes

$$\tilde{H}^{(2)} = \tilde{H}^{(1)} + U_{2,4} + \tilde{U}_{2,3} + \tilde{U}_{2,2} + \tilde{U}_{2,1} + \tilde{U}_{2,0} + X_{2,3} + X_{2,2} + X_{2,1} + X_{2,0} + X_{0,1} + X_{0,0}. \quad (33)$$

To remove non-Hermitian third derivative terms, $R_{2,2}$ must satisfy

$$\tilde{U}_{2,3}^{ijk} + X_{2,3}^{ijk} = 0, \quad (34)$$

which becomes a linear first-order partial differential equation for $R_{2,2}$. Once $R_{2,2}$ is determined from this equation, $X_{2,2}$, $X_{2,1}$, and $X_{2,0}$ are completely fixed. To remove non-Hermitian first derivative terms, $R_{2,0}$ must satisfy

$$\tilde{U}_{2,1}^i + X_{2,1}^i + H_{1,2}^{ij} (\nabla_j R_{2,0}) = 0, \quad (35)$$

which again becomes a linear first-order partial differential equation for $R_{2,0}$, so that we can easily solve it to fix $X_{0,0}$.

We finally obtain

$$\tilde{H}^{(2)} = \tilde{H}^{(2)} + U_{2,4} + \tilde{U}_{2,2} + \tilde{U}_{2,0} + X_{2,2} + X_{2,0} + X_{0,0}, \quad (36)$$

which is manifestly Hermitian at $n = 2$.

2.2.2. $R_{2,2}$ and $R_{2,0}$ for the rotationally symmetric case

In order to demonstrate that the equations for $R_{2,2}$ and $R_{2,0}$ can be solved, we explicitly determine $R_{2,2}$ and $R_{2,0}$ for the rotationally symmetric case.

For this case, we have

$$\tilde{U}_{2,3}^{ijk} := V_{3a}(r) \hat{r}^i \hat{r}^j \hat{r}^k + V_{3b}(r) \left\{ \hat{r}^i \delta^{jk} + \hat{r}^j \delta^{ki} + \hat{r}^k \delta^{ij} \right\}, \quad \tilde{U}_{2,1}^i := V_1(r) \hat{r}^i, \quad (37)$$

$$H_{1,2}^{ij} := H_{2a}(r) \hat{r}^i \hat{r}^j + H_{2b}(r) \delta^{ij}, \quad R_{2,2}^{ij} := R_{2a}(r) \hat{r}^i \hat{r}^j + R_{2b}(r) \delta^{ij}, \quad R_{2,0} := R_{2,0}(r), \quad (38)$$

which lead to

$$X_{2,3}^{ijk} = 3X_{3a}(r)\hat{r}^i\hat{r}^j\hat{r}^k + X_{3b}(r)\left\{\hat{r}^i\delta^{jk} + \hat{r}^j\delta^{ki} + \hat{r}^k\delta^{ij}\right\}, \quad (39)$$

$$X_{3a} := (H_{2a} + H_{2b})R'_{2a} - (R_{2a} + R_{2b})H'_{2a} - \frac{2}{r}(R_{2a}H_{2b} - H_{2a}R_{2b}), \quad (40)$$

$$X_{3b} := (H_{2a} + H_{2b})R'_{2b} - (R_{2a} + R_{2b})H'_{2b} + \frac{2}{r}(R_{2a}H_{2b} - H_{2a}R_{2b}). \quad (41)$$

Thus Eq. (34) gives

$$H_{2+}R'_{2a} - H'_{2a}R_{2+} - \frac{2}{r}(R_{2a}H_{2b} - H_{2a}R_{2b}) = \frac{V_{3a}}{3}, \quad (42)$$

$$H_{2+}R'_{2b} - H'_{2b}R_{2+} + \frac{2}{r}(R_{2a}H_{2b} - H_{2a}R_{2b}) = V_{3b} \quad (43)$$

with $R_{2+} := R_{2a} + R_{2b}$ and $H_{2+} := H_{2a} + H_{2b}$, which is simplified as

$$H_{2+}R'_{2+} - H'_{2+}R_{2+} = \frac{V_{3+}}{3}, \quad V_{3+} := V_{3a} + 3V_{3b}. \quad (44)$$

This equation can be easily solved as

$$R_{2+} = C(r)H_{2+}(r), \quad C(r) := \int_{r_\infty}^r ds \frac{V_{3+}(s)}{3H_{2+}(s)^2}, \quad (45)$$

where we assume the s -integral to be finite. In other words, singularities of the integrand between $0 < s < r_\infty$ are all integrable. From the original equations, individual terms are given by

$$R_{2a}(r) = C(r)H_{2a}(r) + \frac{r^2}{3} \int_{r_\infty}^r ds \frac{H_{2b}(s)V_{3a}(s) - 3H_{2a}(s)V_{3b}(s)}{s^2H_{2+}^2(s)}, \quad (46)$$

$$R_{2b}(r) = C(r)H_{2b}(r) + \frac{r^2}{3} \int_{r_\infty}^r ds \frac{3H_{2a}(s)V_{3b}(s) - H_{2b}(s)V_{3a}(s)}{s^2H_{2+}^2(s)}. \quad (47)$$

Once $R_{2,2}(\vec{r})$ is determined, Eq. (30) fixes $X_{2,1}^i$ and Eq. (35) becomes

$$V_1(r) + X_1(r) + H_{2+}(r)R'_{2,0}(r) = 0, \quad (48)$$

which can be solved as

$$R_{2,0}(r) = - \int_{r_\infty}^r ds \frac{V_1(s) + X_1(s)}{H_{2+}(s)}, \quad (49)$$

where

$$X_{2,1}^i := X_1(r)\hat{r}^i, \quad (50)$$

and $X_1(r)$ is expressed in terms of $\tilde{V}_0$, H_{2a} , H_{2b} , V_{3a} , and V_{3b} .

2.3. All orders

We now argue that we can make the total Hamiltonian Hermitian order by order in the derivative expansion. The total Hamiltonian is given in the derivative expansion as

$$H = H_0 + V_0 + \sum_{l=1}^{\infty} U_l, \quad U_l := V_{2l} + V_{2l-1}, \quad (51)$$

while the n th-order Hamiltonian is denoted as

$$H^{(n)} = H_0 + V_0 + \sum_{l=1}^n U_l. \quad (52)$$

In previous subsections, we have already shown that $H^{(1)}$ and $H^{(2)}$ can be made Hermitian. As before, we make the even-derivative terms Hermitian by introducing lower derivative terms, so that

$$U_n = \sum_{k=1}^{2n} U_{n,k}, \quad U_{n,2k} : \text{Hermitian}, \quad (53)$$

where k of $U_{n,k}$ represents the number of derivatives in these terms, while n corresponds to the order of this term. Throughout this subsection, we use similar notations for other quantities such as $F_{n,k}$, which is the n th-order term with k derivatives, and is Hermitian for even k .

The transformation operator R is expanded as

$$R = R_1 \left(1 + \sum_{l=2}^{\infty} R_l \right), \quad (54)$$

where R_n is expanded in terms of even numbers of derivatives as

$$R_n := \sum_{k=0}^{n-1} R_{n,2k}. \quad (55)$$

In order to prove that H can be made Hermitian order by order, we use mathematical induction. We have already seen that H_1 and H_2 can be made Hermitian by R_1 and $R_1(1 + R_2)$, respectively.

We next assume that H_n can be made Hermitian by $R^{(n)} = R_1(1 + \sum_{l=2}^n R_l)$ at the n th order as

$$\tilde{H}^{(n)} := (R^{(n)})^{-1} H^{(n)} R^{(n)} \simeq \sum_{k=0}^n \tilde{H}_{2k}^{(n)} + \Delta \tilde{H}_{n+1}, \quad (56)$$

where $\tilde{H}_{2k}^{(n)}$ are all Hermitian with $2k$ derivatives and contain terms whose orders are less than or equal to n , while $\Delta \tilde{H}_{n+1}$ is non-Hermitian at $(n+1)$ th order and consists of terms such as

$$\left(\prod_{i=1}^s R_{k_i} \right) \times R_1^{-1} U_l R_1 \times (1 \text{ or } R_m), \quad s = 0, 1, 2, \dots,$$

for $1 < k_i, l, m \leq n$ with the constraint $\sum_{i=1}^s (k_i - 1) + (l - 1) + (m - 1) = n$. Therefore, the maximum number of derivatives in $\Delta \tilde{H}^{(n+1)}$ is $2 \sum_{i=1}^s (k_i - 1) + 2l + 2(m - 1) = 2(n + 1)$, so that we can write

$$\Delta \tilde{H}_{n+1} = \sum_{k=0}^{2(n+1)} \Delta \tilde{H}_{n+1,k}, \quad (57)$$

where k denotes the number of derivatives in $\Delta \tilde{H}_{n+1,k}$, which is Hermitian for even k .

We now consider the transformed Hamiltonian at the $(n+1)$ th order as

$$\tilde{H}^{(n+1)} := \left(R^{(n+1)} \right)^{-1} H^{(n+1)} R^{(n+1)} \simeq \left(R^{(n)} \right)^{-1} H^{(n)} R^{(n)} + \tilde{U}_{n+1} + \left[\tilde{H}^{(1)}, R_{n+1} \right], \quad (58)$$

where the second term is evaluated as

$$\tilde{U}_{n+1} := R_1^{-1} U_{n+1} R_1 = \sum_{k=0}^{2(n+1)} \tilde{U}_{n+1,k}, \quad (59)$$

while the third term becomes

$$\left[\tilde{H}^{(1)}, R_{n+1} \right] = \sum_{k=0}^n X_{n+1}[k], \quad X_{n+1}[k] := \left[\tilde{H}^{(1)}, R_{n+1,2k} \right] = \sum_{l=1}^{2k+1} X_{n+1,l}[k]. \quad (60)$$

Using the assumption of mathematical induction in Eq. (56), we have

$$\begin{aligned} \tilde{H}^{(n+1)} &= \sum_{k=0}^n \left(\tilde{H}_{2k}^{(n)} + \sum_{l=1}^k X_{n+1,2l}[k] \right) + \sum_{k=0}^{n+1} \left(\Delta \tilde{H}_{n+1,2k} + \tilde{U}_{n+1,2k} \right) \\ &\quad + \sum_{k=0}^n \left(\Delta \tilde{H}_{n+1,2k+1} + \tilde{U}_{n+1,2k+1} + \sum_{l=0}^k X_{n+1,2l+1}[k] \right). \end{aligned} \quad (61)$$

Using $n+1$ unknown $R_{n+1,2k}$ with $k = 0, 1, \dots, n$, we can remove non-Hermitian contributions in $\tilde{H}^{(n+1)}$ (the second line in Eq. (61)), as shown below.

We first remove $(2n+1)$ th-order derivative terms in the second line by requiring

$$\Delta \tilde{H}_{n+1,2n+1} + \tilde{U}_{n+1,2n+1} + X_{n+1,2n+1}[n] = 0, \quad (62)$$

which fixes $R_{n+1,2n}$.

The next condition becomes

$$\Delta \tilde{H}_{n+1,2n-1} + \tilde{U}_{n+1,2n-1} + X_{n+1,2n-1}[n] + X_{n+1,2n-1}[n-1] = 0, \quad (63)$$

where $X_{n+1,2n-1}[n]$ is already determined completely from $R_{n+1,2n}$. Therefore, the above equation determines $R_{n+1,2n-2}$ in $X_{n+1,2n-1}[n-1]$.

Repeating this procedure, we can remove all non-Hermitian contributions as follows. For general $k = 0, 1, 2, \dots, n$, we have

$$\Delta \tilde{H}_{n+1,2k+1} + \tilde{U}_{n+1,2k+1} + \sum_{l=k+1}^n X_{n+1,2k+1}[l] + X_{n+1,2k-1}[k] = 0, \quad (64)$$

where $\sum_{l=k+1}^n X_{n+1,2k+1}[l]$ has already been determined from $R_{n+1,2l}$ with $l = n, n-1, n-2, \dots, k+1$.

Thus the above condition fixes $R_{n+1,2k}$ in $X_{n+1,2k-1}[k]$. Therefore it is shown that $H^{(n+1)}$ can be made Hermitian as

$$\tilde{H}^{(n+1)} = \sum_{k=0}^n \left(\tilde{H}_{2k}^{(n)} + \sum_{l=1}^k X_{n+1,2l}[k] \right) + \sum_{k=0}^{n+1} \left(\Delta \tilde{H}_{n+1,2k} + \tilde{U}_{n+1,2k} \right). \quad (65)$$

The proof that non-Hermitian H can be made Hermitian order by order is thus completed by mathematical induction.

We note here that the n th-order Hamiltonian, given by Eqs. (2) and (3), contains $2n+1$ new unknown functions to be extracted from the NBS wave functions generated by lattice QCD calculations. Thus,

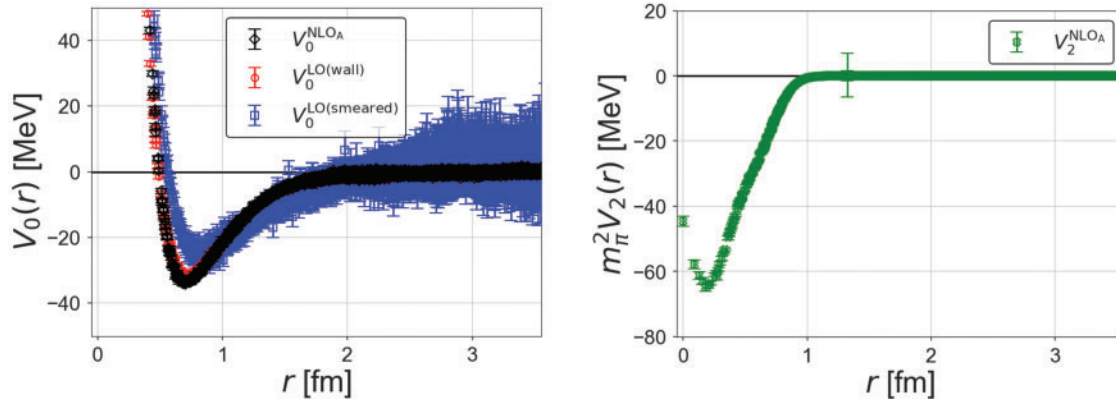


Fig. 1. NLO potentials without V_1 (NLO_A): (Left) $V_0^{\text{NLO}_A}(r)$ (black open diamonds), together with $V_0^{\text{LO}}(r)$ from the wall source (red open circles) and the smeared source (blue open squares). (Right) $V_2^{\text{NLO}_A}(r)$ multiplied by m_π^2 (green open crosses).

in order to perform the n th-order analysis, we need a total of $(n+1)^2$ NBS wave functions, which must be independent beyond numerical uncertainties. This may give rise to severe limitations in applying the present formalism to the cases where the higher-order terms are important. In the next section we will see that, in the case of $\Xi\Xi(^1S_0)$ scattering, the LO potential already gives a good approximation for the scattering phase shift, while the NLO corrections to the phase shift gradually appear as the energy increases.

3. Hermitizing the NLO potential for the $\Xi\Xi(^1S_0)$ system

In this section, we actually apply the method in Sect. 2 to lattice QCD data. We consider the $\Xi\Xi(^1S_0)$ system, whose potential is much more precise than those for NN or $N\Lambda$ thanks to the presence of more strange quarks in the system, in order to make the NLO analysis numerically possible. The potential for the $\Xi\Xi(^1S_0)$ was calculated on 2+1 flavor QCD ensembles [37] at $a = 0.09$ fm on a 64^4 lattice 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. See Ref. [12] for more details.

The rotationally symmetric potential in the previous section for the $n = 1$ case can be rewritten as

$$V(\vec{r}, \nabla) = V_0(r) + V_1(r) \hat{r}^i \nabla_i + V_2(r) \nabla^2 + V_3(r) \vec{L}^2, \quad (66)$$

where the expression in the previous section is recovered by replacing

$$V_1(r) \rightarrow V_1(r) - \frac{V_{2a}(r)}{r}, \quad V_2(r) \rightarrow \frac{1}{2} (V_{2a}(r) + V_{2b}(r)), \quad V_3(r) \rightarrow \frac{V_{2a}(r)}{2r^2}. \quad (67)$$

Since the $V_3(r)$ term does not contribute to the S-wave scattering, we ignore this term in the present analysis. Having only two NBS wave functions, one from the wall source, the other from the smeared source, available from the previous calculation [12], we consider two different extractions of potentials, one with $V_1(r) = 0$ (NLO_A), the other with $V_2(r) = 0$ (NLO_B), in the present analysis.

3.1. NLO_A : NLO analysis without V_1

We first consider the NLO_A potential for $\Xi\Xi(^1S_0)$,

$$V^{\text{NLO}_A}(\vec{r}, \nabla) = V_0^{\text{NLO}_A}(r) + V_2^{\text{NLO}_A}(r) \nabla^2, \quad (68)$$

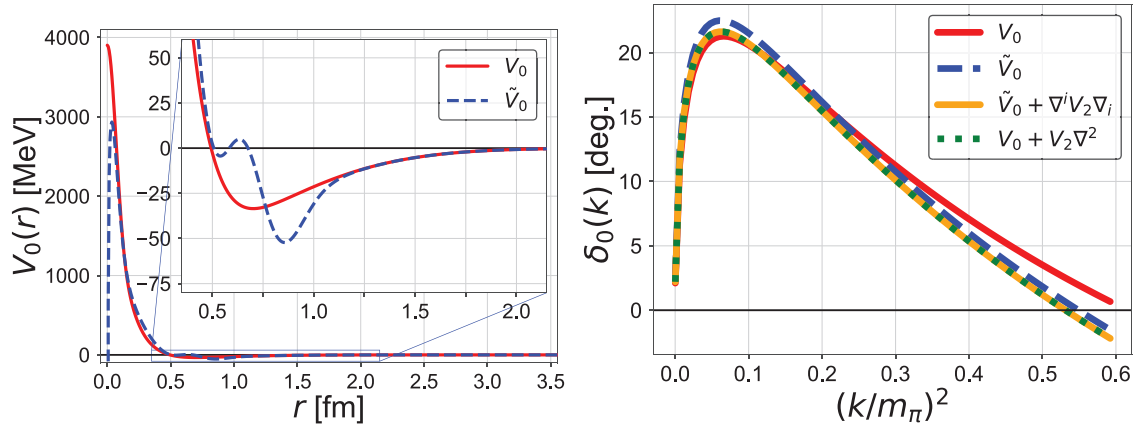


Fig. 2. (Left) $\tilde{V}_0^{\text{NLO}_A}(r)$ (blue dashed line) for $\Xi\Xi(^1S_0)$ together with $V_0^{\text{NLO}_A}(r)$ (red solid line). (Right) Scattering phase shifts for $\Xi\Xi(^1S_0)$ from $V_0^{\text{NLO}_A}$ (red solid line), $\tilde{V}_0^{\text{NLO}_A}$ (blue dashed line), $V^{\text{NLO}_A}(\vec{r}, \nabla)$ (green dotted line), and $\tilde{V}^{\text{NLO}_A}(\vec{r}, \nabla)$ (yellow solid line).

where $V_0^{\text{NLO}_A}(r)$, together with $V_0^{\text{LO(wall)}}(r)$ from the wall source and $V_0^{\text{LO(smeared)}}(r)$ from the smeared source, are plotted in Fig. 1 (left), and $m_\pi^2 V_2^{\text{NLO}_A}(r)$ is given in Fig. 1 (right). Small differences between $V_0^{\text{NLO}_A}(r)$ and $V_0^{\text{LO(wall)}}(r)$ are observed at short distance, due to contributions from $V_2^{\text{NLO}_A}(r)$, which is non-zero only at $r < 1$ fm.

According to the procedure in Sect. 2, we can make this non-Hermitian potential Hermitian as

$$\tilde{V}^{\text{NLO}_A}(\vec{r}, \nabla) = \tilde{V}_0^{\text{NLO}_A}(r) + \nabla^i V_2^{\text{NLO}_A}(r) \nabla_i, \quad (69)$$

where

$$\tilde{V}_0^{\text{NLO}_A}(r) = V_0^{\text{NLO}_A}(r) + \frac{(V_2^{\text{NLO}_A})'(r)}{r} + \frac{(V_2^{\text{NLO}_A})''(r)}{2} + \frac{m_\Xi}{4} \frac{\{(V_2^{\text{NLO}_A})'(r)\}^2}{1 - m_\Xi V_2^{\text{NLO}_A}(r)}. \quad (70)$$

Here $\tilde{V}_0$ is calculated from the fitted functions for $V_0^{\text{NLO}_A}(r)$ and $V_2^{\text{NLO}_A}(r)$ in Ref. [12], together with the first and second derivatives of V_2 analytically calculated from the fitted function. We compare $\tilde{V}_0^{\text{NLO}_A}(r)$ with $V_0^{\text{NLO}_A}(r)$ in Fig. 2 (left), while we plot the phase shifts of the $\Xi\Xi(^1S_0)$ obtained with $\tilde{V}_0^{\text{NLO}_A}(r)$, $V_0^{\text{NLO}_A}(r)$, $V^{\text{NLO}_A}(\vec{r}, \nabla)$, and $\tilde{V}^{\text{NLO}_A}(\vec{r}, \nabla)$ in Fig. 2 (right). For visibility, only central values are given here. Errors of $\tilde{V}_0^{\text{NLO}_A}$ are comparable to those of $V_0^{\text{NLO}_A}$, which can be seen in Fig. 1 (left). We notice that the leading-order term $V_0^{\text{NLO}_A}$ of the original non-Hermitian NLO_A potential describes the behavior of the scattering phase shift rather well at low energy but shows some deviation from the NLO_A result at high energies, while the local term $\tilde{V}_0^{\text{NLO}_A}$ of the hermitized NLO_A potential describes the scattering phase shift in a wider energy range, $0 \leq (k/m_\pi)^2 \leq 0.6$ with small deviations around the turning point at $(k/m_\pi)^2 \simeq 0.1$. Of course, the non-Hermitian NLO_A potential $V^{\text{NLO}_A}(\vec{r}, \nabla)$ and the hermitized NLO_A potential $\tilde{V}^{\text{NLO}_A}(\vec{r}, \nabla)$ give identical results at all energies by construction.

3.2. NLO_B: NLO analysis without V_2

We next consider the NLO analysis without V_2 (NLO_B), whose potential is given by

$$V^{\text{NLO}_B}(\vec{r}, \nabla) = V_0^{\text{NLO}_B}(r) + V_1^{\text{NLO}_B}(r) \hat{r}^i \nabla_i. \quad (71)$$

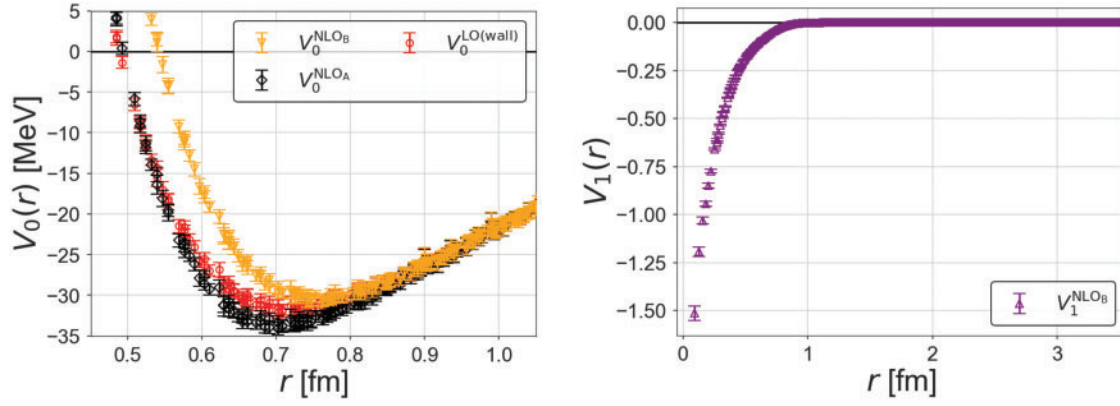


Fig. 3. (Left) $V_0^{\text{NLO}_B}(r)$ (yellow open triangles) as a function of r at short distances, together with $V_0^{\text{LO(wall)}}(r)$ (red open circles) and $V_0^{\text{NLO}_A}(r)$ (black open triangles). (Right) $V_1^{\text{NLO}_B}(r)$ (purple open triangles).

Figure 3 (left) shows $V_0^{\text{NLO}_B}(r)$ (yellow open triangles), together with $V_0^{\text{LO(wall)}}(r)$ (red open circles) and $V_0^{\text{NLO}_A}(r)$ (black open triangles), at $0.45 \text{ fm} \leq r \leq 1.05 \text{ fm}$, while Fig. 3 (right) gives $V_1^{\text{NLO}_B}(r)$ (purple open triangles) at $r \leq 3.5 \text{ fm}$. Unlike $V_0^{\text{NLO}_A}(r)$, $V_0^{\text{NLO}_B}(r)$ deviates greatly from $V_0^{\text{LO(wall)}}(r)$ at short distances.

According to the procedure in Sect. 2, we convert this non-Hermitian NLO_B potential to a local Hermitian potential $\tilde{V}_0^{\text{NLO}_B}(r)$, where

$$\tilde{V}_0^{\text{NLO}_B}(r) = V_0^{\text{NLO}_B}(r) - \frac{V_1^{\text{NLO}_B}(r)}{r} - \frac{1}{2}(V_1^{\text{NLO}_B})'(r) + \frac{m\Xi}{4}(V_1^{\text{NLO}_B}(r))^2, \quad (72)$$

which is shown in Fig. 4 (left) by the blue dotted line, together with $V_0^{\text{LO(wall)}}(r)$ (red solid line) and $V_0^{\text{NLO}_B}(r)$ (yellow dashed line). The attractive pocket of $\tilde{V}_0^{\text{NLO}_B}(r)$ around $r \simeq 0.6 \text{ fm}$ is much deeper than that of $V_0^{\text{LO(wall)}}(r)$ or $V_0^{\text{NLO}_B}(r)$. Figure 4 (right) compares the scattering phase shifts $\delta_0(k)$ among $V_0^{\text{LO(wall)}}(r)$ (red solid circles), $V_0^{\text{NLO}_B}(r)$ (yellow solid down-triangles), $V_0^{\text{NLO}_A}(r)$ (black solid diamonds), $V^{\text{NLO}_B}(\vec{r}, \nabla)$ (purple solid up-triangles), $V^{\text{NLO}_A}(\vec{r}, \nabla)$ (green crosses), and $\tilde{V}_0^{\text{NLO}_B}(r)$ (blue open squares). By construction, $\tilde{V}_0^{\text{NLO}_B}(r)$ and $V^{\text{NLO}_B}(\vec{r}, \nabla)$ give identical results, which also agree well with $\delta_0(k)$ from $V_0^{\text{NLO}_A}(r)$. As mentioned before, $V_0^{\text{LO(wall)}}(r)$ and $V_0^{\text{NLO}_A}(r)$ give good approximations at low energy but show small deviations as energies increase. However, $\delta_0(k)$ from $V_0^{\text{NLO}_B}(r)$ deviates from others even at low energies. Finally it is noted that two different NLO potentials, $V^{\text{NLO}_A}(\vec{r}, \nabla)$ (green solid crosses) and $V^{\text{NLO}_B}(\vec{r}, \nabla)$ (purple solid up-triangles), agree well even at high energies, though the first derivative term ($V_1^{\text{NLO}_B}(r)$) has larger effects than the second derivative term ($V_2^{\text{NLO}_A}(r)$) on the scattering phase shift.

4. Summary and concluding remarks

The HAL QCD potential expressed as an energy-independent non-local potential is known to be non-Hermitian due to the nature of the Nambu–Bethe–Salpeter (NBS) wave function used to extract it: While the leading-order (LO) term in the derivative expansion of the potential is local and Hermitian, the higher-order terms are in general non-Hermitian. In this paper, we have formulated a way of hermitizing it in the derivative expansion. Since the hermitized potential can be expressed to contain only an even number of derivatives, we classify the first- and second-order derivative terms as the next-to-leading order (NLO) and in general $(2n - 1)$ and $2n$ derivative terms as the n th order. Starting from the NLO terms, which can be made Hermitian exactly, we have shown that the higher-order

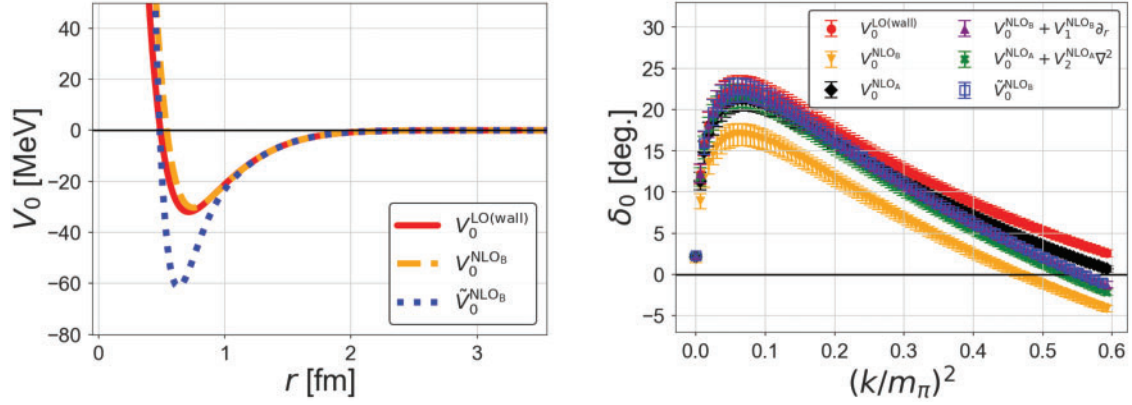


Fig. 4. (Left) $\tilde{V}_0^{\text{LOB}}(r)$ (blue dotted line) for $\Xi\Xi(^1S_0)$ together with $V_0^{\text{LO(wall)}}(r)$ (red solid line) and $V_0^{\text{NLOB}}(r)$ (yellow dashed line). (Only central values are plotted for visibility.) (Right) Scattering phase shifts $\delta_0(k)$ for $\Xi\Xi(^1S_0)$ from $V_0^{\text{LO(wall)}}(r)$ (red solid circles), $V_0^{\text{NLOB}}(r)$ (yellow solid down-triangles), $V_0^{\text{NLOA}}(r)$ (black solid diamonds), $V_0^{\text{NLOB}}(\vec{r}, \nabla)$ (purple solid up-triangles), $V_0^{\text{NLOA}}(\vec{r}, \nabla)$ (green crosses), and $\tilde{V}_0^{\text{NLOB}}(r)$ (blue open squares).

terms can be hermitized order by order to all orders using mathematical induction in the derivative expansion.

In order to see the feasibility of our formalism, we applied it to the case of $\Xi\Xi(^1S_0)$ scattering for which two independent NBS wave functions were available from the lattice QCD calculations [12]. Since two NBS wave functions are insufficient for the full NLO analysis, which requires three unknown functions, $V_0(r)$, $V_1(r)$, and $V_2(r)$, we carried out two NLO analyses, one without V_1 (NLO_A) and the other without V_2 (NLO_B). Although the two hermitized potentials, $\tilde{V}^{\text{NLOA}}$ and $\tilde{V}^{\text{NLOB}}$, look very different, the former containing a second-order derivative term while the latter is purely local, they give essentially the same phase shifts within the uncertainties of the calculations. This agreement indicates that the obtained NLO phase shift can be regarded approximately as the yet unknown exact one. By comparing it to the LO phase shifts obtained in Ref. [12], we find that the LO phase shift from the NBS wave function with the wall source is very similar to the NLO phase shift at low energies while it is slightly larger at higher energies. The LO analysis with the wall source is thus well justified for the $\Xi\Xi(^1S_0)$ scattering.

While the non-Hermitian potential is fine as long as we are interested in two-body observables such as scattering amplitudes and binding energies, the Hermitian version is more convenient for a comparison with phenomenological interactions and also for using it as a two-body interaction in many-body systems.

Appendix A. Convergence of the derivative expansion for non-local potentials

In this appendix, we briefly discuss an issue with the convergence of the derivative expansion for non-local potentials.

Let us consider a non-local potential $V(\mathbf{x}, \mathbf{y})$, which can be expressed in terms of the derivative expansion as

$$V(\mathbf{x}, \mathbf{y}) = \sum_{n=0}^{\infty} \frac{1}{n!} V_l^{i_1 i_2 \dots i_n}(\mathbf{x}) \nabla_{i_1} \nabla_{i_2} \dots \nabla_{i_n} \delta^{(3)}(\mathbf{x} - \mathbf{y}), \quad (\text{A.1})$$

where no symmetry is assumed for generality.

Applying this potential to a plane wave $e^{i\mathbf{k}\cdot\mathbf{x}}$, we obtain

$$\bar{V}(\mathbf{x}, \mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{x}} \equiv \int d\mathbf{y} V(\mathbf{x}, \mathbf{y}) e^{i\mathbf{k}\cdot\mathbf{y}} = \sum_{n=0}^{\infty} \frac{i^n}{n!} V_l^{i_1 i_2 \dots i_n}(\mathbf{x}) k_{i_1} k_{i_2} \dots k_{i_n} e^{i\mathbf{k}\cdot\mathbf{x}} \quad (\text{A.2})$$

$$= e^{i\mathbf{k}\cdot\mathbf{x}} \int d\mathbf{r} V(\mathbf{x}, \mathbf{x} + \mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} = e^{i\mathbf{k}\cdot\mathbf{x}} \sum_{n=0}^{\infty} \int d\mathbf{r} V(\mathbf{x}, \mathbf{x} + \mathbf{r}) \frac{i^n}{n!} (\mathbf{k} \cdot \mathbf{r})^n. \quad (\text{A.3})$$

By equating Eqs. (A.2) and (A.3), we have

$$V_l^{i_1 i_2 \dots i_n}(\mathbf{x}) = \int d\mathbf{r} V(\mathbf{x}, \mathbf{x} + \mathbf{r}) r_{i_1} r_{i_2} \dots r_{i_n} \equiv V_l(\mathbf{x}) \langle r_{i_1} r_{i_2} \dots r_{i_n} \rangle_{\mathbf{x}}, \quad (\text{A.4})$$

where we define the n th moment of non-locality, $\langle r_{i_1} r_{i_2} \dots r_{i_n} \rangle_{\mathbf{x}}$, satisfying $\langle 1 \rangle_{\mathbf{x}} = 1$, and $V_l(\mathbf{x})$ is the term at $n = 0$ (the local term) in the derivative expansion (A.1). Then $\bar{V}(\mathbf{x}, \mathbf{k})$ can be expanded as

$$\bar{V}(\mathbf{x}, \mathbf{k}) = V_l(\mathbf{x}) \sum_{n=0}^{\infty} \frac{i^n}{n!} \langle (\mathbf{k} \cdot \mathbf{r})^n \rangle_{\mathbf{x}}. \quad (\text{A.5})$$

The convergence of the sum in Eq. (A.5) is guaranteed if the absolute magnitude of the n th moment of non-locality grows more slowly than $n^{\alpha n}$ with $\alpha < 1$ as $n \rightarrow \infty$, though the convergence rate depends on $\mathbf{x}$ and $\mathbf{k}$, reflecting the detail for the non-locality of $V(\mathbf{x}, \mathbf{x} + \mathbf{r})$. It is clear that the sum converges as $\mathbf{k} \rightarrow 0$. The convergence of the derivative expansion applied to a wave function, which can be expressed as a superposition of plane waves, is usually guaranteed, though the convergence rate depends on the nature of the wave function. In practice, for instance, the importance of the NLO terms can be estimated from $|\mathbf{k}| |\langle \mathbf{r} \rangle_{\mathbf{x}}|$ or $\mathbf{k}^2 |\langle \mathbf{r}^2 \rangle_{\mathbf{x}}|$, where $\mathbf{k}$ is the local wave number.

If the total energy is small enough, the wave function is expanded by plane waves with small $|\mathbf{k}|$ only. As the total energy increases, higher-order terms become important to cause slower convergence, and even may cease to converge at some energy, depending on the non-locality of $V(\mathbf{x}, \mathbf{x} + \mathbf{r})$. In this paper, we assume that the non-locality of potentials is mild enough for the derivative expansion to converge.

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