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Instructive discussion of an effective block algorithm for baryon–baryon correlators

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ABSTRACT

We describe an approach for the efficient calculation of a large number of four-point correlation functions for various baryon–baryon (*BB*) channels, which are the primary quantities for studying the nuclear and hyperonic nuclear forces from lattice quantum chromodynamics. Using the four-point correlation function of a proton-Λ system as a specific example, we discuss how an effective block algorithm significantly reduces the number of iterations. The effective block algorithm is applied to calculate 52 channels of the four-point correlation functions from nucleon–nucleon to Ξ–Ξ, in order to study the complete set of isospin symmetric *BB* interactions. The elapsed times measured for hybrid parallel computation on BlueGene/Q demonstrate that the performance of the present algorithm is reasonable for various combinations of the number of OpenMP threads and the number of MPI nodes. The numerical results are compared with the results obtained using the unified contraction algorithm for all computed sites of the 52 four-point correlators.

1. Introduction

Determining how the nuclear force is described from a fundamental perspective is a challenging problem in physics. Characterising an atomic nucleus as a nucleonic many body system provides successful results although a nucleon is not a true rudimentary constituent of atomic nuclei but a composition of quarks and gluons defined in quantum chromodynamics (QCD), which is the theory of the strong interaction. For example, high-precision nucleon–nucleon (*NN*) potentials are available to describe the *NN* scattering data at low energies as well as the deuteron properties [1,2]. The energy levels of light nuclei are well reproduced by such an *NN* potential together with a three-nucleon force [3,4]. However, in contrast to the normal nuclear force, phenomenological descriptions of hyperon–nucleon (*YN*) and hyperon–hyperon (*YY*) interactions are not well constrained from experimental data because of the short life time of hyperons. The precise determination of *NN*, *YN*, and *YY* interactions has a large impact on the studies of both hypernuclei [5–7] and the hyperonic matter inside neutron stars [8–11].

Recently, a new lattice-QCD-based method for studying the interhadronic interactions has been proposed [12]. In this method, the interhadron potential can be obtained first from lattice QCD by measuring the Nambu–Bethe–Salpeter (NBS) wave function. The observables such as the phase shifts and the binding energies are calculated using the resultant potential [13]. This approach has been applied to various baryonic interactions [14–25], and has been recently extended to systems in inelastic channels [26–28]. This approach is now called HAL QCD method because almost all the recent developments cited above have been provided by the HAL QCD Collaboration. The flavour symmetry breaking is a key topic in the study of the isospin symmetric baryon–baryon (*BB*) interactions based on the 2+1 flavour lattice QCD. In such a situation, it is advantageous to calculate a large number of NBS wave functions of various *BB* channels simultaneously in a single lattice QCD calculation. Therefore, an efficient approach for performing such a computationally demanding lattice QCD calculation is crucial.

The purpose of this paper is to describe a practicable algorithm that can efficiently compute a large number of four-point correlation functions of various *BB* systems. The contraction algorithm considered in this paper is different from the unified contraction algorithm [29] and has been used to calculate the ΛN and ΣN potentials [30–32]. This is a reasonable approach for computing the various *BB* correlators efficaciously. Methods following different approach for large baryon number systems are found in Refs. [33,34]. The paper is organised as follows: Section 2 outlines a basic formulation of the HAL QCD approach. Section 3 describes an approach for calculating the four-point

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correlation function by considering the $p\Lambda$ system as an example. The present contraction algorithm is generalised to various BB systems in Section 4. In Section 5 we demonstrate the hybrid parallel computation of the four-point correlation functions. The numerical results calculated by the hybrid parallel program are compared with the results from the unified contraction algorithm in Section 6. Section 7 summarises the paper.

2. Outline of the HAL QCD method

In the study of the nuclear force using the HAL QCD approach, the equal time NBS wave function with Euclidean time t is a vital quantity, which is defined by[12,13]

$$\phi_E(\vec{r})\mathrm{e}^{-Et} = \sum_{\vec{X}} \left\langle 0 \left| B_{1,\alpha}(\vec{X}+\vec{r},t)B_{2,\beta}(\vec{X},t) \right| B=2, E \right\rangle, \tag{1}$$

where $E = \sqrt{k^2+m_{B_1}^2} + \sqrt{k^2+m_{B_2}^2}$ is the total energy in the centre of mass system of a baryon number $B=2$ state with masses m_{B_1} and m_{B_2}. $B_{1,\alpha}(x)$ ($B_{2,\beta}(x)$) denotes the local interpolating field of baryon B_1 (B_2). For simplicity, we consider a two-nucleon system in the isospin symmetric limit. Thus, $m_{B_1}=m_{B_2}=m_N$ and the $B_{1,\alpha}=p_\alpha$ ($B_{2,\beta}=n_\beta$) is the local interpolating field of proton (neutron) given by

$$p_\alpha(x) = \varepsilon_{abc}\left(u_a(x)C\gamma_5 d_b(x)\right)u_{c\alpha}(x), \qquad n_\beta(y) = -\varepsilon_{abc}\left(u_a(y)C\gamma_5 d_b(y)\right)d_{c\beta}(y), \tag{2}$$

where $u_{c\alpha}(x)$ ($d_{c\beta}(x)$) is the up (down) quark field with the colour indices denoted by a, b, and c, and the Dirac spinors denoted by α and β. The ε_{abc} is the totally anti-symmetric tensor and $C=\gamma_4\gamma_2$ is the charge conjugation matrix. For simplicity, we have suppressed the dummy spinor indices in the round brackets. Based on the NBS wave function, we define a non-local but energy-independent potential $\left(\frac{\nabla^2}{2\mu} - \frac{k^2}{2\mu}\right)\phi_E(\vec{r}) = \int d^3r'\, U(\vec{r},\vec{r}')\phi_E(\vec{r}')$ with the reduced mass $\mu = m_N/2$. An important point of the HAL QCD method is that the potential defined above gives the correct scattering phase shift of the S-matrix for all values of k in the elastic region, $E < E_{\mathrm{th}} \equiv 2m_N + m_\pi$, with the pion mass m_π, by construction. A more detailed account of the relation between the NBS wave function and the S-matrix in QCD is found in the appendix A of Ref. [13].

In lattice QCD calculations, we compute the normalised four-point correlation function defined by [20]

$$R_{\alpha\beta}^{(J,M)}(\vec{r},t-t_0) = \sum_{\vec{X}} \left\langle 0 \left| B_{1,\alpha}(\vec{X}+\vec{r},t)B_{2,\beta}(\vec{X},t)\overline{\mathcal{J}_{B_3B_4}^{(J,M)}(t_0)} \right| 0 \right\rangle \Big/ \exp\{-(m_{B_1}+m_{B_2})(t-t_0)\}, \tag{3}$$

where $\overline{\mathcal{J}_{B_3B_4}^{(J,M)}(t_0)} = \sum_{\alpha'\beta'} P_{\alpha'\beta'}^{(J,M)} \overline{B_{3,\alpha'}(t_0)B_{4,\beta'}(t_0)}$ is a source operator that creates B_3B_4 ($=pn$) states with the total angular momentum J, M. The normalised four-point function can be expressed as

$$R_{\alpha\beta}^{(J,M)}(\vec{r},t-t_0) = \sum_n A_n \sum_{\vec{X}} \left\langle 0 \left| B_{1,\alpha}(\vec{X}+\vec{r},0)B_{2,\beta}(\vec{X},0) \right| E_n \right\rangle \mathrm{e}^{-(E_n-m_{B_1}-m_{B_2})(t-t_0)} + O(\mathrm{e}^{-(E_{\mathrm{th}}-m_{B_1}-m_{B_2})(t-t_0)}), \tag{4}$$

where E_n ($|E_n\rangle$) is the eigen-energy (eigen-state) of the six-quark system and $A_n = \sum_{\alpha'\beta'} P_{\alpha'\beta'}^{(JM)} \langle E_n | \bar{B}_{4,\beta'}\bar{B}_{3,\alpha'}|0\rangle$. At moderately large $t-t_0$ where the inelastic contribution above the pion production $O(\mathrm{e}^{-(E_{\mathrm{th}}-2m_N)(t-t_0)}) = O(\mathrm{e}^{-m_\pi(t-t_0)})$ becomes exiguous, we can construct the non-local potential U through $\left(\frac{\nabla^2}{2\mu} - \frac{k^2}{2\mu}\right)R(\vec{r}) = \int d^3r'\, U(\vec{r},\vec{r}')R(\vec{r}')$. In lattice QCD calculations in a finite box, it is practical to use the velocity (derivative) expansion, $U(\vec{r},\vec{r}') = V(\vec{r},\vec{\nabla}_r)\delta^3(\vec{r}-\vec{r}')$. In the lowest few orders we have

$$V(\vec{r},\vec{\nabla}_r) = \underbrace{V_0(r) + V_\sigma(r)\vec{\sigma}_1\cdot\vec{\sigma}_2 + V_T(r)S_{12}}_{V_{LO}} + \underbrace{V_{LS}(r)\vec{L}\cdot(\vec{\sigma}_1+\vec{\sigma}_2)}_{V_{NLO}} + O(\nabla^2), \tag{5}$$

where $r=|\vec{r}|$, $\vec{\sigma}_i$ are the Pauli matrices acting on the spin space of the ith baryon, $S_{12} = 3(\vec{r}\cdot\vec{\sigma}_1)(\vec{r}\cdot\vec{\sigma}_2)/r^2 - \vec{\sigma}_1\cdot\vec{\sigma}_2$ is the tensor operator, and $\vec{L} = \vec{r}\times(-i\vec{\nabla})$ is the angular momentum operator. The first three-terms constitute the leading order (LO) potential while the fourth term corresponds to the next-to-leading order (NLO) potential. By taking the non-relativistic approximation, $E_n - m_{B_1} - m_{B_2} \simeq k_n^2/(2\mu) + O(k_n^4)$, and neglecting the V_{NLO} and the higher order terms, we obtain $\left(\frac{\nabla^2}{2\mu} - \frac{\partial}{\partial t}\right)R(\vec{r},t) \simeq V_{\mathrm{LO}}(\vec{r})R(\vec{r},t)$. For the spin singlet state, we extract the central potential as $V_C(r;J=0) = (\frac{\nabla^2}{2\mu} - \frac{\partial}{\partial t})R/R$. For the spin triplet state, the wave function is decomposed into the S- and D-wave components as

$$\begin{cases} R_{\alpha\beta}(\vec{r};\ {}^3S_1) = \mathcal{P}R_{\alpha\beta}(\vec{r};J=1) \equiv \dfrac{1}{24}\displaystyle\sum_{\mathcal{R}\in O} \mathcal{R}R_{\alpha\beta}(\vec{r};J=1), \\ R_{\alpha\beta}(\vec{r};\ {}^3D_1) = \mathcal{Q}R_{\alpha\beta}(\vec{r};J=1) \equiv (1-\mathcal{P})R_{\alpha\beta}(\vec{r};J=1). \end{cases} \tag{6}$$

Therefore, the Schrödinger equation with the LO potentials for the spin triplet state becomes

$$\begin{Bmatrix} \mathcal{P} \\ \mathcal{Q} \end{Bmatrix} \times \left\{ -\frac{\nabla^2}{2\mu} + V_0(r) + V_\sigma(r)(\vec{\sigma}_1\cdot\vec{\sigma}_2) + V_T(r)S_{12} \right\} R(\vec{r},t-t_0) = -\begin{Bmatrix} \mathcal{P} \\ \mathcal{Q} \end{Bmatrix} \times \frac{\partial}{\partial t} R(\vec{r},t-t_0), \tag{7}$$

from which the central and tensor potentials, $V_C(r;J=0) = V_0(r) - 3V_\sigma(r)$ for $J=0$, $V_C(r;J=1) = V_0(r) + V_\sigma(r)$, and $V_T(r)$ for $J=1$, can be determined.[1]

[1] The potential is obtained from the NBS wave function at moderately large imaginary time; it would be $t-t_0 \gg 1/m_\pi \sim 1.4$ fm even for the physical pion mass. Furthermore, no single state saturation between the ground state and the first excited states, $t-t_0 \gg (\Delta E)^{-1} = \left((2\pi)^2/(2\mu L^2)\right)^{-1}$, is required for the present HAL QCD