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William Detmold

Kostas Orginos
William & Mary, kostas@wm.edu

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Nuclear correlation functions in lattice QCD

William Detmold[1] and Kostas Orginos[2,3]

[1]*Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[2]*Department of Physics, The College of William and Mary, Williamsburg, Virginia 23187, USA*
[3]*Jefferson Lab, Newport News, Virginia 23606, USA*

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We consider the problem of calculating the large number of Wick contractions necessary to compute states with the quantum numbers of many baryons in lattice QCD. We consider a constructive approach and a determinant-based approach and show that these methods allow the required contractions to be performed in a computationally manageable amount of time for certain choices of interpolating operators. Examples of correlation functions computed using these techniques are shown for the quantum numbers of the light nuclei, ^{4}He, ^{8}Be, ^{12}C, ^{16}O, and ^{28}Si.

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I. INTRODUCTION

The *ab initio* approach to nuclear physics from the underlying theory of the strong interactions, QCD, is hampered by the many-body nature of the nuclear problem. In principle, QCD and the electroweak interactions give rise to all the rich and complex phenomena of nuclear physics, yet it is only recently that the first QCD studies of multibaryon systems have appeared [1–8]. The reason for this is twofold. First, the Monte-Carlo evaluation of correlation functions of multibaryon systems converges slowly, requiring a large number of measurements before the necessary precision is reached (this issue will not be addressed here). Second, systems with the quantum numbers of many nucleons and hyperons are complex many-body systems with complicated spectra, and there is a multitude of physically relevant states that can be studied in QCD. Even for a given set of quantum numbers, additional complexity appears at the quark level; the number of Wick contractions required to construct systems for large atomic number grows factorially, scaling as $n_u!n_d!n_s!$ where $n_{u,d,s}$ are the numbers of up, down, and strange quarks required to construct the quantum numbers of the state in question. In many situations, this is a naive counting as there are many cancellations and contributions that are identical. However, the *a priori* identification of these simplifications is a nontrivial task. In addition to the problem of Wick contractions, the number of terms in the interpolating fields of multinucleon systems also typically grows exponentially with the size of the system. This potentially more serious problem is similar in nature to the problem of the exponential growth of nuclear wave functions faced in nuclear structure calculations where phenomenological potential models describing the low-energy nucleon-nucleon interactions are used.

In this paper, we present a systematic method for the construction of nuclear interpolating fields for multibaryon systems in lattice QCD. We demonstrate that the Grassmannian nature of the quark fields can be used to our advantage, in some cases resulting in particularly simple nuclear interpolating fields. In addition, we present two approaches that ameliorate the cost of contractions, the most efficient of which scales only polynomially in the number of quarks involved in the contraction. Using these methods we compute lattice QCD correlation functions with the quantum numbers of the light nuclei, ^{4}He, ^{8}Be, ^{12}C, ^{16}O, and ^{28}Si, demonstrating that correlation functions relevant to the study of nuclei in QCD can be constructed. A similar, but less general and less efficient, approach has been developed in Ref. [9].

II. NUCLEAR INTERPOLATING FIELDS

In order to calculate nuclear correlation functions, we first need to construct quark-level nuclear interpolating fields. This is, in principle, straightforward and, in practice, it resembles the construction of quark model wave functions for baryons [10]. A general quark-level nuclear interpolating field with atomic number A containing $n_q = 3A$ quarks (higher Fock space components can be treated but are not considered here) has the form

$$\bar{\mathcal{N}}^h = \sum_{\mathbf{a}} w_h^{a_1,a_2\ldots a_{n_q}} \bar{q}(a_1)\bar{q}(a_2)\ldots\bar{q}(a_{n_q}), \qquad (1)$$

where the $\bar{q}_{a_i}$ are the quark fields, the a_i are generic indices which combine the color, spinor, flavor, and space-time indices of the quark, and $\mathbf{a}$ is a compound index representing the n_q-plet $a_1, a_2 \ldots a_{n_q}$. Given that calculations are performed on a discrete lattice, the spatial degrees of freedom are finite and countable, and as a result we can use an integer index to describe them. Here the quark fields are all at the same time t. The index h on the nuclear interpolating field is a set of quantum numbers that identify the nuclear state, including its momentum, angular momentum, isospin, and strangeness. The Grassmannian nature of the quark field dictates that the tensor $w_h^{a_1,a_2\ldots a_{n_q}}$ is totally antisymmetric under the exchange of any two indices. If the indices a_i can have a total of N possible values, then,

ignoring the detailed flavor structure, the total number of nonvanishing terms in the above sum is

$$\frac{N!}{(N-n_q)!}. \tag{2}$$

However, many of these terms correspond to permutations of the quark fields, and the total number of unique terms (terms that are not a permutation of any other term) is

$$\frac{N!}{n_q!(N-n_q)!}. \tag{3}$$

For a generic spatial structure of the interpolating field, N corresponds to the total number of quark degrees of freedom on a time slice ($N = 12L^3$, where L is the spatial dimension of the lattice), and one may be discouraged by the feasibility of the task of building quark-level nuclear interpolating fields. However, a number of simplifying factors are omitted in the above discussion. As we consider interpolating fields with definite transformation properties under the symmetries of QCD, large numbers of terms in the nuclear interpolating field vanish. The first major reduction comes from the fact that only color singlets need to be considered. In addition, considering only interpolating fields of definite parity, angular momentum,[1] isospin, and strangeness forces several elements of the tensor $w_h^{a_1,a_2\ldots a_{n_q}}$ to vanish. Finally, the most drastic reduction of the nonzero tensor elements can be achieved using simple spatial wave functions. At this time, having recognized that only a small fraction of the terms in the sum of Eq. (1) are nonzero, as well as the fact that the tensor $w_h^{a_1,a_2\ldots a_{n_q}}$ is totally antisymmetric, we can introduce the reduced weights $\tilde{w}_h^{(a_1,a_2\ldots a_{n_q}),k}$ which are the minimal set of nonzero numbers required to completely describe the interpolating field. The n_q-plet $(a_1, a_2 \ldots a_{n_q})$ is an ordered list of indices that represents a class of terms in Eq. (1) that are all permutations of each other. The index k on the reduced weights enumerates the number of classes that the tensor $w_h^{a_1,a_2\ldots a_{n_q}}$ decomposes into. With these reduced weights, Eq. (1) can be rewritten as

$$\bar{\mathcal{N}}^h = \sum_{k=1}^{N_w} \tilde{w}_h^{(a_1,a_2\ldots a_{n_q}),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,\ldots,i_{n_q}} \bar{q}(a_{i_1})\bar{q}(a_{i_2})\ldots\bar{q}(a_{i_{n_q}}), \tag{4}$$

where N_w is the total number of reduced weights, $\mathbf{i}$ represents the n_q-plet $(i_1, i_2 \ldots i_{n_q})$, and $\epsilon^{i_1,i_2,\ldots,i_{n_q}}$ is a totally antisymmetric tensor of rank n_q with

$$\epsilon^{1,2,3,4,\ldots,n_q} = 1.$$

The above expression is the simplest form of the quark-level nuclear interpolating field and is completely described by the reduced weights. As an example, using a single-point spatial wave function, the numbers of terms contained in the simplest interpolating fields for the proton, deuteron, ^{3}He, and ^{4}He are $N_w = 9$, 21, 9, and 1, respectively.

A. Hadronic interpolating fields

Having now written down a general nuclear interpolating field with quantum numbers h, we need to calculate the reduced weights $\tilde{w}_h^{(a_1,a_2\ldots a_{n_q}),k}$ in an efficient manner. In principle, this can be achieved directly from quark fields by imposing the desired transformation properties. However, in certain cases, it is advantageous to proceed by first constructing hadronic interpolating fields from which the quark interpolating fields are derived.

The hadronic interpolating fields assume a form analogous to that of the quark interpolating fields. The baryons that make up the nucleus are also fermions; hence the general structure outlined above can be directly transcribed here. In terms of baryons, a nuclear interpolating field of a nucleus of atomic number A is

$$\bar{\mathcal{N}}^h = \sum_{k=1}^{M_w} \tilde{W}_h^{(b_1,b_2\ldots b_A)} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,\ldots,i_A} \bar{B}(b_{i_1})\bar{B}(b_{i_2})\ldots\bar{B}(b_{i_A}), \tag{5}$$

where M_w is the number of hadronic reduced weights $\tilde{W}_h^{(b_1,b_2\ldots b_A)}$, $B(b_i)$ are baryon interpolating fields, and the b_i are generic indices that include parity, angular momentum, isospin, strangeness, and spatial indices. Unlike the quark fields which are fundamental degrees of freedom, the baryon interpolating fields are composite objects; hence there is a large number of such interpolating fields for a given set of quantum numbers. For simplicity, as well as efficiency of the resulting nuclear interpolating fields, we will use a single interpolating field per baryon, selected so that it has good overlap with the single-baryon ground state, as well as being comprised of a small number of quark-level terms. The utility of the above form of the nuclear interpolating fields is twofold. First, it allows us to derive the reduced weights we need for Eq. (4). Second, interpolating fields that are derived starting from Eq. (5) may have better overlap with the nuclear ground states as it is well-known that hadronic degrees of freedom provide a successful description of much of nuclear physics.

The calculation of the reduced weights, $\tilde{W}_h^{(b_1,b_2\ldots b_A)}$, in the hadronic interpolating field is straightforward. It amounts to combining individual hadrons of given quantum numbers to build a multihadron state of definite parity, angular momentum, isospin, and strangeness. This construction can be readily automated and can be performed recursively using the known Clebsch-Gordan coefficients of SU(2) for both the spin and isospin [or SU(3) flavor if so desired].[2]

[1]For simplicity, we refer to the irreducible representation of the lattice symmetry group as angular momentum.

[2]The reader is referred to Ref. [10] for a similar construction of baryon-level wave functions from quarks.

In principle, one can use all the octet and decuplet baryons in Eq. (5); however, for most practical purposes, restricting to the positive parity octet baryons is sufficient. For example, for $A = 2$, $I = J = 0$, $S = -2$, if we restrict the spatial wave function to a single point, there are three simple hadronic interpolating fields,

$$\Lambda^{\uparrow}\Lambda^{\downarrow}, \tag{6}$$

$$\frac{1}{\sqrt{3}}[\Sigma^{+\uparrow}\Sigma^{-\downarrow} - \Sigma^{0\uparrow}\Sigma^{0\downarrow} + \Sigma^{-\uparrow}\Sigma^{+\downarrow}], \tag{7}$$

and

$$\frac{1}{2}[\Xi^{0\uparrow}n^{\downarrow} - \Xi^{-\uparrow}p^{\downarrow} - \Xi^{0\downarrow}n^{\uparrow} + \Xi^{-\downarrow}p^{\uparrow}], \tag{8}$$

where $B^{\uparrow}$ and $B^{\downarrow}$ represent the spin up and down polarizations of the baryon, B, respectively. In this example, the reduced weights can be directly read off from these equations. If we consider the case of two spatial locations, x_1 and x_2, or two momenta, $\mathbf{p_1}$ and $\mathbf{p_2}$, these simply generalize to the appropriately totally antisymmetric hadronic wave functions. For example, Eq. (6) becomes $\Lambda^{\uparrow}_1\Lambda^{\downarrow}_2 + \Lambda^{\uparrow}_2\Lambda^{\downarrow}_1$ where we make the spatial location or momentum explicit through the subscript. For further discussions of multiple-source correlation functions in the case of many-meson systems, the reader is referred to Refs. [11–13].

We have written a C++ symbolic manipulation program that generates the hadronic reduced weights using the above approach. In Ref. [8], we have used this to produce a complete basis of orthonormal interpolating fields with spatial wave functions restricted to a single point for all nuclei up to $A = 4$ and have also constructed a selection of states for $A > 4$. Generically for larger A, more complicated spatial wave functions are required because of the Pauli exclusion principle, resulting in an exponential growth of the number of possible interpolating fields as A increases (this reflects the problem faced in nuclear structure calculations as A becomes large). In certain cases, the Grassmannian nature of the quark fields is also advantageous, drastically reducing the number of nonzero reduced weights. Making use of this feature, we have been able to find particularly simple wave functions for systems as large as $A = 28$. In contrast to Ref. [9], the recursive construction of interpolating fields does not require supercomputing resources and is done on a laptop.

B. Quark interpolating fields

The reduced weights of the quark interpolating fields of Eq. (4) can be calculated by equating the two forms of the nuclear interpolating fields,

$$\begin{aligned}\bar{\mathcal{N}}^h &= \sum_{k=1}^{M_w} \tilde{W}_h^{(b_1,b_2\ldots b_A)} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,\ldots,i_A} \bar{B}(b_{i_1})\bar{B}(b_{i_2})\ldots\bar{B}(b_{i_A}) \\ &= \sum_{k=1}^{N_w} \tilde{w}_h^{(a_1,a_2\ldots a_{n_q}),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,\ldots,i_{n_q}} \bar{q}(a_{i_1})\bar{q}(a_{i_2})\ldots\bar{q}(a_{i_{n_q}}),\end{aligned} \tag{9}$$

and replacing the baryon objects by their quark interpolating fields. A single-baryon interpolating field is written in terms of quark fields as

$$\bar{B}(b) = \sum_{k=1}^{N_{B(b)}} \tilde{w}_b^{(a_1,a_2,a_3),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,i_3} \bar{q}(a_{i_1})\bar{q}(a_{i_2})\bar{q}(a_{i_3}), \tag{10}$$

where $N_{B(b)}$ is the number of terms in the single-baryon $B(b)$ interpolating field. For single-baryon interpolating fields, the weights, $\tilde{w}_b^{(a_1,a_2,a_3),k}$, have been presented in Ref. [14] (the color factors necessary for our formulation are not included in Ref. [14] but can be trivially added). The process of deriving the reduced weights $\tilde{w}_h^{(a_1,a_2\ldots a_{n_q}),k}$ from Eq. (9) can be automated, and we perform it within our symbolic manipulation program which was written in C++. An interesting feature that arises from the calculation of the reduced weights $\tilde{w}_h^{(a_1,a_2\ldots a_{n_q}),k}$ is that if we restrict ourselves to simple spatial wave functions making use of only few spatial points, then the expected exponential growth of the number of terms in the nuclear interpolating field is eliminated. A careful selection of the spatial wave functions used can control this problem, in principle, for arbitrarily large nuclei. However, restriction to a small number of quark degrees of freedom also makes it impossible to construct certain states (an example is presented in Ref. [8] where the two-baryon symmetric flavor octet was found to be inaccessible). After construction of our interpolating fields used here and in Ref. [8], an independent testing program was used to confirm that indeed the interpolating fields produced by our symbolic manipulation program have the desired transformation properties under flavor and rotation groups and are color singlets. All calculations of the reduced weights as well as the subsequent tests performed on the resulting interpolating fields were performed on a laptop computer and required an insignificant amount of computational resources.

III. TECHNIQUES FOR MULTIBARYON CONTRACTIONS

In this section, we consider how the interpolating fields constructed in the previous section can be used to generate the correlation functions of multibaryon systems. A general multihadron two-point function is given by

$$\langle \mathcal{N}_1^h(t)\bar{\mathcal{N}}_2^h(0)\rangle = \frac{1}{\mathcal{Z}}\int \mathcal{D}\mathcal{U}\mathcal{D}q\mathcal{D}\bar{q}\,\mathcal{N}_1^h(t)\bar{\mathcal{N}}_2^h(0)e^{-\mathcal{S}_{\rm QCD}}, \quad (11)$$

where $\mathcal{S}_{\rm QCD}$ and $\mathcal{Z}$ are the QCD action and partition function, respectively, and $\mathcal{D}\mathcal{U}$ and $\mathcal{D}q\mathcal{D}\bar{q}$ are the gluon and quark field integration measures, respectively. We have also introduced explicit dependence of the interpolating fields on the Euclidean time separation, t, and consider a two-point function with different creation and annihilation interpolating fields with commensurate quantum numbers. For a given choice of the interpolating fields, it is straightforward to perform the Grassmann integral over the quark fields and rewrite the correlation function in terms of the quark propagators. However, for an efficient calculation of the two-point function, we need to be mindful of the structure of the interpolating fields.

One successful class of interpolating fields for two or more hadron systems is one in which a plane wave basis at the level of the hadronic interpolating fields is used. This amounts to projecting the individual hadrons comprising the multibody system to definite momentum states, while preserving the spatial transformation properties of the overall multihadron system [1,15–21]. In this case, the complexity of the spatial wave function is such that the number of terms contributing to Eq. (4) is rather large, and hadronic interpolating fields have to be used in order to build the desired two-point function efficiently. Constructing these types of interpolating fields both at the source and the sink becomes computationally expensive because a large number of quark propagators that are required. Nevertheless, this method has been employed for meson-meson and multimeson spectroscopy [11,12,21,22]. For the case of multimeson systems, special contraction methods were required [11–13]. For multibaryon systems, the problem is more complex and will be the subject of further investigations. A further approach is to consider correlation functions in which the quark creation interpolating fields (source) have simple spatial wave functions with few degrees of freedom (for example, restricted to a few spatial locations), while using a plane wave basis for the hadronic interpolating fields at the sink. Finally, as we shall discuss below, sufficiently simple nuclear interpolating fields exist, where the number of terms contributing in Eq. (4) is small and factorization into hadrons is not computationally necessary.

A. Hadronic blocks

The quark propagator from a single source point, $x_0 = (\mathbf{x}_0, 0)$, can be used to construct baryon building blocks[3] with quantum numbers b and momentum $\mathbf{p}$ as

$$\mathcal{B}_b^{a_1,a_2,a_3}(\mathbf{p},t;x_0) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \sum_{k=1}^{N_{B(b)}} \tilde{w}_b^{(c_1,c_2,c_3),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,i_3} S(c_{i_1},x;a_1,x_0)S(c_{i_2},x;a_2,x_0)S(c_{i_3},x;a_3,x_0), \quad (12)$$

where $S(c,\mathbf{x},t;a,x_0,0)$ is the quark propagator from x_0 to $x = (\mathbf{x},t)$ and c_i, a_i are the remaining combined spin-color-flavor indices. In this notation, the sink indices are kept to the left of the source indices, and the spatial indices are displayed explicitly as they play an essential role in the construction of the block. This baryon block corresponds to the propagation of an arbitrary three-quark state from the source to the sink where it is annihilated by the prescribed baryon interpolating field. As discussed above, we have chosen to momentum project these blocks at the sink to a given momentum $\mathbf{p}$ to allow control of the total momentum of multihadron systems, although this is not necessary, and other forms of blocks can be envisaged.

We can generalize these blocks to allow the quark propagators to originate from different source locations, $x_0^{(1)}, x_0^{(2)}, \ldots$, as necessary, using

$$\mathcal{B}_b^{a_1,a_2,a_3}(\mathbf{p},t;s_1,s_2,s_3) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \sum_{k=1}^{N_{B(b)}} \tilde{w}_b^{(c_1,c_2,c_3),k} \sum_{\mathbf{i}} \epsilon^{i_1,i_2,i_3} S(c_{i_1},\mathbf{x};a_1,x_0^{(s_1)})S(c_{i_2},\mathbf{x};a_2,x_0^{(s_2)})S(c_{i_3},\mathbf{x};a_3,x_0^{(s_3)}), \quad (13)$$

where the $x_0^{(k)}$ label the source locations. These blocks can be further generalized to allow for a nontrivial single-hadron spatial wave function at the sink, but we will not consider this case further. It may also be advantageous to consider more complicated multihadron blocks similar to those implemented in Ref. [2], although the storage requirements grow rapidly with number of baryons in the block.

B. Quark-hadron contractions

Using the building blocks described above, we can consider correlation functions in which quark-level interpolating fields are used at the source and their hadronic counterparts are used at the sink.

[3]Hadronic building blocks for two-point function calculations have been used in many spectroscopy calculations in the past such as in Ref. [23], and implementations of such ideas can be found in the public domain software package chroma [24].

The contractions are performed by iterating over all combinations of source and sink interpolating field terms and connecting the source and sink with the appropriate sets of quark propagators. For a given pair of source and sink interpolating field terms, this amounts to selecting the components dictated by the source quark interpolating field from the product of blocks dictated by the hadronic sink interpolating field. The Wick contractions are implemented by performing this selection in all possible ways. This proceeds by taking the first hadron in the hadronic wave function at the sink, replacing it by the appropriate hadron block, and selecting the three free indices in all possible ways from the pool of indices dictated by the source quark interpolating field, keeping track of the appropriate permutation sign. Following this, the second baryon component in the hadronic (sink) interpolating field term is replaced with the appropriate block, and the free indices are contracted with the remaining free indices in the source quark interpolating field term in all possible ways. These first steps are illustrated in Fig. 1, and the procedure continues until all hadrons in the sink interpolating field term have been contracted, necessarily using all available quark indices at the source. The result is then multiplied by the weights of the source and sink terms under consideration and added to the correlation function (we note that the idea of using a reduced list of weights was developed independently in Ref. [9], where they are referred to as unified contraction lists). The contraction is complete after all combinations of source and sink interpolating field terms have been considered. The process described here is independent of the source and sink interpolating fields and can be applied to any correlation function. Further reductions of the total cost of the algorithm may be possible by studying the symmetry properties of a particular pair of source-sink interpolating fields. However, such reductions are not generic; hence, we do not consider them further. The procedure described has been used to perform the contractions needed for the large class of interpolating fields considered in the study of the spectrum of hypernuclei up to $A = 5$ in Refs. [8,25].

For large numbers of baryons ($A > 8$ for protons and neutrons alone), it is necessary to use multiple source locations because of the Pauli exclusion principle. In this case, the generalized blocks in Eq. (13) can be used with the algorithm presented above.

C. Scaling

From the above description, it is clear that this algorithm will in general scale as

$$M_w \cdot N_w \cdot \frac{(3A)!}{(3!)^A}, \tag{14}$$

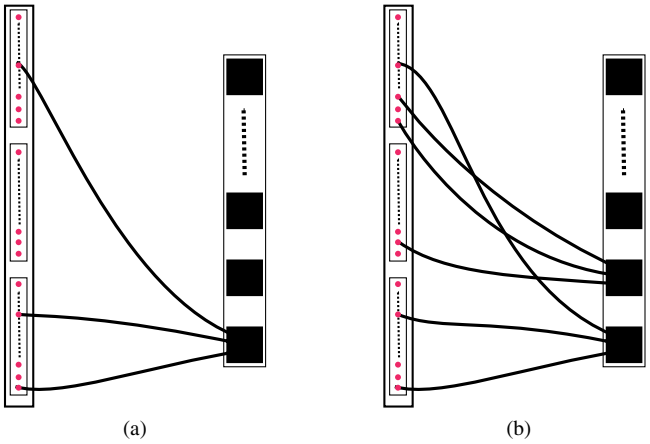

FIG. 1 (color online). Illustration of steps one and two of the quark–hadron contraction method. The small circles in the left-hand sides of the figures correspond to the quarks in the source interpolating field while the large squares and lines extending from them correspond to the hadronic blocks. The separate sets of small dots correspond to different quark flavors.

where A is the atomic number and M_w and N_w are the numbers of terms in the sink and source interpolating fields, respectively. In addition, the fact that the hadron blocks are completely antisymmetric under all quark exchanges has been taken into account. If we also take into account that the strong interactions are flavor blind and consider only octet baryon building blocks, this reduces to

$$M_w \cdot N_w \frac{n_u! n_d! n_s!}{2^{A-n_{\Sigma^0}-n_\Lambda}}, \tag{15}$$

where n_{Σ^0} and n_Λ are the numbers of Σ^0 and Λ baryons in the hadronic interpolating field and the factor in the denominator arises because all octet baryons have two quarks of the same flavor except from the Σ^0 and Λ. This algorithm can be efficiently implemented and is computationally feasible for small systems, $A \lesssim 10$. As an example of this method, a ^{4}He two-point correlation function can be computed in $\sim$0.8 sec per time slice on a single core of an Opteron 285 processor.

IV. MULTIBARYON CONTRACTIONS WITH DETERMINANTS

For larger atomic number, $A \gtrsim 10$, alternative methods are required to perform the contractions in a computationally expedient manner. It is straightforward to see how this can be done by examining the two-point functions above and making use of Wick's theorem [26]. The numerator of Eq. (11) before the integration over the gauge fields is performed is given by

$$[\mathcal{N}_1^h(t)\bar{\mathcal{N}}_2^h(0)]_U = \int \mathcal{D}q\mathcal{D}\bar{q}e^{-S_{\rm QCD}[U]} \sum_{k'=1}^{N'_w}\sum_{k=1}^{N_w} \tilde{w}_h^{\prime(a'_1,a'_2\ldots a'_{n_q}),k'} \tilde{w}_h^{(a_1,a_2\ldots a_{n_q}),k} \sum_{\mathbf{j}}\sum_{\mathbf{i}} \epsilon^{j_1,j_2,\ldots,j_{n_q}} \epsilon^{i_1,i_2,\ldots,i_{n_q}} q(a'_{j_{n_q}})\ldots q(a'_{j_2})q(a'_{j_1}) \times \bar{q}(a_{i_1})\bar{q}(a_{i_2})\ldots\bar{q}(a_{i_{n_q}}), \tag{16}$$

where the primed and unprimed indices are associated with the sink and source interpolating fields, respectively, and are composite color, spinor, flavor, and spatial indices and $[\ldots]_U$ indicates the value of the enclosed expression on a fixed gauge field. The Grassmann integral over quark fields can now be performed, resulting in the replacement of the $q\bar{q}$ pairs by elements of the quark propagator,

$$[\mathcal{N}_1^h(t)\bar{\mathcal{N}}_2^h(0)]_U = e^{-\mathcal{S}_{\rm eff}[U]} \sum_{k'=1}^{N'_w}\sum_{k=1}^{N_w} \tilde{w}_h^{\prime(a'_1,a'_2\ldots a'_{n_q}),k'} \tilde{w}_h^{(a_1,a_2\ldots a_{n_q}),k} \times \sum_{\mathbf{j}}\sum_{\mathbf{i}} \epsilon^{j_1,j_2,\ldots,j_{n_q}} \epsilon^{i_1,i_2,\ldots,i_{n_q}} S(a'_{j_1};a_{i_1})S(a'_{j_2};a_{i_2})\ldots S(a'_{j_{n_q}};a_{i_{n_q}}), \tag{17}$$

where $S_{\rm eff}[U]$ denotes the pure gauge part of the QCD action together with the logarithm of the determinant of the Dirac matrix. The above expression of Wick's theorem, illustrated in Fig. 2, can be written in terms of the determinant of a matrix G, whose matrix elements are given by

$$G(\mathbf{a}';\mathbf{a})_{j,i} = \begin{cases} S(a'_j;a_i) & \text{for } a'_j \in \mathbf{a}' \text{ and } a_i \in \mathbf{a} \\ \delta_{a'_j,a_i} & \text{otherwise} \end{cases}, \tag{18}$$

where, as before, $\mathbf{a}' = (a'_1, a'_2 \ldots a'_{n_q})$ and $\mathbf{a} = (a_1, a_2 \ldots a_{n_q})$. Note also that the nontrivial block of the matrix $G(\mathbf{a}';\mathbf{a})$ is of size $n_q \times n_q$; hence, for computing its determinant, we only need to consider this block. For this reason, in the following discussion, the matrix $G(\mathbf{a}';\mathbf{a})$ denotes only this small nontrivial block.

Making use of this definition, the full nuclear correlation function can be written as

$$\langle \mathcal{N}_1^h(t)\bar{\mathcal{N}}_2^h(0)\rangle = \frac{1}{\mathcal{Z}}\int \mathcal{D}\mathcal{U}e^{-\mathcal{S}_{\rm eff}} \sum_{k'=1}^{N'_w}\sum_{k=1}^{N_w} \tilde{w}_h^{\prime(a'_1,a'_2\ldots a'_{n_q}),k'} \tilde{w}_h^{(a_1,a_2\ldots a_{n_q}),k} \times \det G(\mathbf{a}';\mathbf{a}). \tag{19}$$

The determinant of a matrix of size n_q can be evaluated in n_q^3 operations (for example via LU decomposition) instead of the naive $n_q!$ operations,[4] so making use of this representation of the nuclear correlation function is numerically advantageous. Furthermore, because of the flavor blindness of the strong interaction, the matrix $G(\mathbf{a}';\mathbf{a})$ is block diagonal; as a result, the determinant calculation breaks into a product of smaller determinants, one for each flavor.

Given the reduced weights determined above and the appropriate quark propagators, the implementation of Eq. (19) is very fast, scaling polynomially with the number of terms in the source and sink quark-level interpolating fields as well as the number of quarks per flavor. The total cost of this form of contractions scales as

$$n_u^3 n_d^3 n_s^3 \times N'_w N_w, \tag{20}$$

where N'_w N_w are the number of terms in the sink and source quark interpolating fields, respectively. As a result, if we can construct interpolating fields with a sufficiently small number of terms, correlation functions with a very

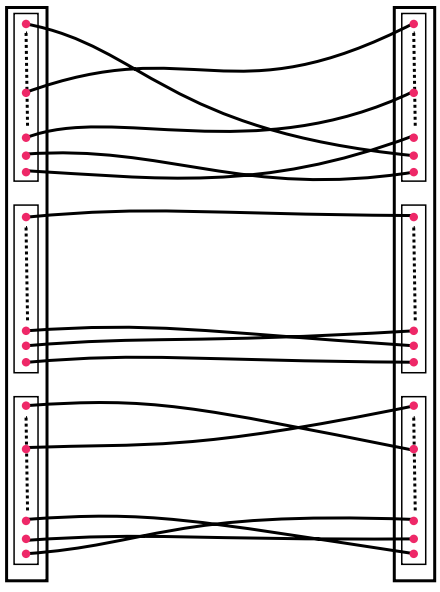

FIG. 2 (color online). Illustration of the quark determinant level contraction with each of the three sub-blocks listing the up, down, and strange quarks of the wave function term, respectively. Within each flavor of quark, all possible contractions are performed by forming a determinant of the matrix of quark propagators as described in the text.

[4]The expectation of polynomial scaling of contractions was noted by D. B. Kaplan in Ref. [27]. However, the scaling of N_w and N'_w with the atomic number A is generically exponential.

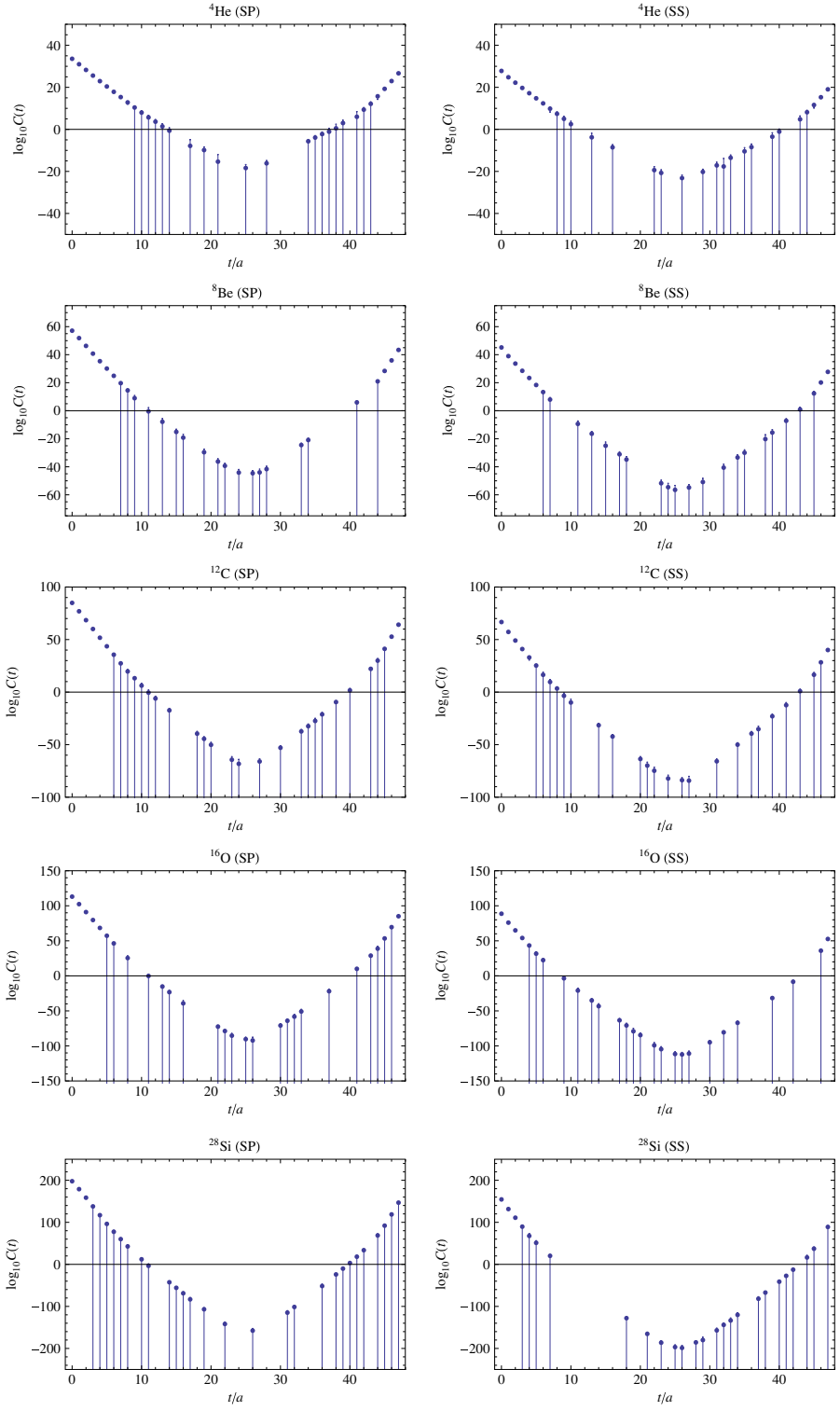

FIG. 3 (color online). Correlation functions for nuclear systems, ^{4}He, ^{8}Be, ^{12}C, ^{16}O, and ^{28}Si. In each row, correlators based on both smeared-point and smeared-smeared quark propagators are shown.

large atomic number A can be constructed. It should be noted that for generic interpolating operators, N'_w and N_w can grow exponentially with the size of the system, but specific examples can be found where this is not the case.

V. NUCLEAR CORRELATION FUNCTIONS

We have performed preliminary studies to investigate the numerical efficiency of these methods. Results for the quark-hadron approach have been presented in

Ref. [8], and here we focus on the determinant-based approach. Calculations are performed on an ensemble of gauge configurations generated with a tadpole-improved Lüscher-Weisz gauge action and a clover fermion action with tadpole-improved tree-level clover coefficient. The gauge links entering the fermion action are stout smeared, with $\rho = 0.125$. Three flavors of quarks with masses corresponding to the physical strange quark mass were used. The lattice spacing, $a \sim 0.145$ fm, and the dimensions of the lattice are $L^3 \times T = 32^3 \times 48$, corresponding to a physical volume of $(4.6\text{ fm})^3 \times 7.0$ fm (further details will be presented elsewhere [28]). We have performed a large number of measurements from spatially distinct sources on an ensemble of about 250 gauge configurations well separated in hybrid Monte Carlo evolution time. All calculations are performed in double precision, and care is taken to preserve the dynamic range of correlation functions by rescaling quark propagators before contractions are performed.

The determinant-based method has the potential to calculate nuclear correlation functions of very large nuclei. The most general interpolating fields for a multinucleon system has a large number of terms. This number grows exponentially with the number of quarks. However, restricting the spatial part of the interpolating field to few points can reduce the number of nonzero weights sufficiently so that the resulting correlation functions can be computed efficiently. Here, instead of a single-point source that we used in Ref. [8], we use seven points. These points are $\vec{r}$, $\vec{r} \pm d\hat{x}$, $\vec{r} \pm d\hat{y}$, and $\vec{r} \pm d\hat{z}$ where $\vec{r}$ is an arbitrary point on our lattice and $\hat{x}$, $\hat{y}$, and $\hat{z}$ are the unit vectors in the principal lattice directions and d is a displacement length which is chosen to be $d = 4$ in this work. Given that there exists a single-point ^{4}He interpolating field that contains only one term, we place such ^{4}He interpolating fields on some (or all) of the seven points used in our construction. Given that we are interested in the lowest angular momentum state, the spatial part of the interpolating field is projected onto the A_1 irreducible representation of the cubic group. Using our symbolic manipulation program, we perform all the necessary reductions so that the interpolating field contains the minimal number of terms. Furthermore, with our simplest $A = 2$ and $A = 3$ interpolating fields, we can build in the same manner any nucleus up to $A = 28$. Larger nuclei will require more than seven points; however, by extending this approach, in principle, contractions for any A are possible if an appropriately large number of points is used. For the tests presented here, we chose the simplest possible interpolating fields that we can construct. The symbolic manipulations required to produce the interpolating fields are performed on a laptop and take an insignificant amount of computer time.

In Fig. 3, the logarithms of correlation functions are shown for correlators with the quantum numbers of the light nuclei, ^{4}He, ^{8}Be, ^{12}C, ^{16}O, and ^{28}Si. Error bars that reach the lower axis of the plots indicate that the correlator has fluctuations that are negative at one standard deviation. The extracted energies for each of the atomic number $A < 20$ systems are consistent with a system of A nucleons but with large uncertainties at present (for ^{28}Si, no flattening of the effective mass is seen before the signal is lost). Given the large number of near-threshold energy levels expected in these complex nuclear systems (see Ref. [8] for an example for $A = 4$), a clean extraction of the ground state binding energies of these systems is beyond the current work. In addition, the baryon number density of the larger systems (0.3 fm^{-3} for ^{28}Si) is substantial, and volume effects are expected to be significant. It will be necessary to use larger volumes, increase greatly the statistical precision, and improve the interpolating operators that we have used in order to obtain the binding energies and excitation spectra of these systems. Nevertheless, this study demonstrates the computational feasibility of lattice QCD calculations of light nuclei.

VI. CONCLUSIONS AND OUTLOOK

In this work, we have discussed a systematic way of constructing interpolating fields for multibaryon systems. In addition, we have investigated the issue of performing the Wick contractions with these interpolating fields in lattice QCD (see Ref. [9] for related work). We have shown that there are approaches that enable calculations of systems with a very large number of nuclei that are computationally feasible and demonstrated their effectiveness by calculating correlators with a baryon number up to $A = 28$. Given the expected spectra of such complex systems, significant advances are required in order to extract ground state energies from these correlators. Finally, the methods described here may prove useful in calculations of QCD at nonzero baryon density, where projection onto a given baryon number is required.

We note that Ref. [9] presents a related investigation of contractions for multihadron systems which has some overlap with the discussions in Sec. III. However, our algorithms differ in a number of important regards. First, the generation of weight factors in Eq. (9) is performed recursively in our approach, requiring insignificant amounts of computer time in comparison to the supercomputing resources required in the brute-force approach of Ref. [9]. For certain choices of interpolating fields,[5] our algorithms also scale polynomially for all values of the baryon number A and bypass the limitations to $A = 8$ for nonstrange systems discussed in Ref. [9].

[5]Interpolating fields with number of terms N_w that does not grow with the baryon number A exist for all values of A.

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