### Nuclear correlation functions in lattice QCD

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# Ab initio approach to nuclear physics from QCD

- The Monte-Carlo evaluation of correlation functions of multibaryon systems converges slowly, requiring a large number of measurements.
- Complex many-body systems with complicated spectra.
- The number of Wick contractions, scaling as  $n_u!n_d!n_s!$
- The number of terms in the interpolating fields grows exponentially.

### In this paper

- A systematic method for the construction of nuclear interpolating fields for multibaryon systems.
- Two approaches.
- Most efficient case, it scales only polynomially in the number of quarks.
- 4He, 8Be, 12C, 16O, 28Si

## Quark level nuclear interpolating fields

- Atomic number: A
  - $n_q = 3A$  Quarks.  $\bar{\mathcal{N}}^h = \sum_{\mathbf{a}} w_h^{a_1, a_2 \dots a_{n_q}} \bar{q}(a_1) \bar{q}(a_2) \dots \bar{q}(a_{n_q}),$  (1)
  - $\overline{q}(a_i)$  Quark fields
  - $a_i$  Generic indices of the quark (color, spinor, flavor, space-time), total N possible values,  $a = \{a_1, \dots, a_{n_n}\}$
  - *h* Set of quantum numbers (momentum, angular momentum, isospin, strangeness)
  - $w_h^{a_1, a_2, \dots, a_{n_q}}$  Totally antisymmetric tensor
  - Unique terms

$$\frac{N!}{(N-n_q)!n_q!} \qquad \qquad N=12L^3$$

## Quark level nuclear interpolating fields

- Transformation properties under the symmetries of QCD
  - Color singlet
  - Parity, angular momentum, isospin, strangeness
  - Simple spatial wave function

$$\bar{\mathcal{N}}^{h} = \sum_{k=1}^{N_{w}} \tilde{w}_{h}^{(a_{1},a_{2}...a_{n_{q}}),k} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},...,i_{n_{q}}} \bar{q}(a_{i_{1}})\bar{q}(a_{i_{2}}) \dots \bar{q}(a_{i_{n_{q}}}),$$

(4)

- Reduced weights  $\tilde{w}_h^{(a_1, a_2, \dots, a_{n_q}), \kappa}$ 
  - Minimal set of nonzero numbers

Hadronic interpolating fields  

$$\bar{\mathcal{N}}^{h} = \sum_{k=1}^{M_{w}} \tilde{W}_{h}^{(b_{1},b_{2}...b_{A})} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},...,i_{A}} \bar{B}(b_{i_{1}}) \bar{B}(b_{i_{2}}) \dots \bar{B}(b_{i_{A}}),$$

- $M_W$  The number of hadronic reduced weights (5)
- $W_{h}^{b_{1},b_{2},...,b_{A}}$  Hadronic reduced weights
- $B(b_i)$  Baryon interpolating fields
  - (positive parity octet baryon)
- *b<sub>i</sub>* Generic indices (parity, angular momentum, isospin, strangeness, spatial indices)
- A single interpolating field per baryon
  - Good overlap with the single baryon ground state
  - Small number of quark level terms

#### Example

• A=2, I=J=0, S=-2

 $\Lambda^{\dagger}\Lambda^{\downarrow}$ , (6)

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

and

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

$$\begin{aligned}
\bar{\mathcal{N}}^{h} &= \sum_{k=1}^{M_{w}} \tilde{W}_{h}^{(b_{1},b_{2}...b_{A})} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},...,i_{A}} \bar{B}(b_{i_{1}}) \bar{B}(b_{i_{2}}) \dots \bar{B}(b_{i_{A}}) \\
&= \sum_{k=1}^{N_{w}} \tilde{W}_{h}^{(a_{1},a_{2}...a_{n_{q}}),k} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2}...,i_{n_{q}}} \bar{q}(a_{i_{1}}) \bar{q}(a_{i_{2}}) \dots \bar{q}(a_{i_{n_{q}}}),
\end{aligned}$$

$$\bar{B}(b) &= \sum_{k=1}^{N_{B(b)}} \tilde{W}_{b}^{(a_{1},a_{2},a_{3}),k} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},i_{3}} \bar{q}(a_{i_{1}}) \bar{q}(a_{i_{2}}) \bar{q}(a_{i_{3}}),
\end{aligned}$$
(10)

- Simple spatial wave function
  - Exponential growth of the number of terms in the nuclear interpolating fields is eliminated.
  - $N_{B(b)}$  The number of terms for single baryon interpolating field.

# A general multihadron two-point function

 $\langle \mathcal{N}_1^h(t) \bar{\mathcal{N}}_2^h(0) \rangle$ 

$$=\frac{1}{\bar{Z}}\int \mathcal{D}\mathcal{U}\mathcal{D}q\mathcal{D}\bar{q}\mathcal{N}_{1}^{h}(t)\bar{\mathcal{N}}_{2}^{h}(0)e^{-\mathcal{S}_{\text{QCD}}},\quad(11)$$

- $S_{QCD}$  QCD action
- *Z* Partition function
- DU Gluon field integration measure
- $Dq D \overline{q}$  Quark field integration measure
- *t* Euclidean time separation
- Source: simple spatial wave functions
- Sink: a plane wave basis

## Baryon building block

$$\mathcal{B}_{b}^{a_{1},a_{2},a_{3}}(\mathbf{p},t;x_{0}) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \sum_{k=1}^{N_{B(b)}} \tilde{w}_{b}^{(c_{1},c_{2},c_{3}),k} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},i_{3}} S(c_{i_{1}},x;a_{1},x_{0}) S(c_{i_{2}},x;a_{2},x_{0}) S(c_{i_{3}},x;a_{3},x_{0}),$$
(12)

- *p* Momentum (projection at the sink)
- $S(c, x, t; a, x_0, 0)$  Quark propagator
- $a_i$  combined spin-color-flavor indices
- Generalization
  - Allow the quark propagation from different source locations,  $x_0^{(1)}$ ,  $x_0^{(2)}$ ,...

$$\mathcal{B}_{b}^{a_{1},a_{2},a_{3}}(\mathbf{p},t;s_{1},s_{2},s_{3}) = \sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}} \sum_{k=1}^{N_{B(b)}} \tilde{w}_{b}^{(c_{1},c_{2},c_{3}),k} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},i_{3}} S(c_{i_{1}},\mathbf{x};a_{1},x_{0}^{(s_{1})}) S(c_{i_{2}},\mathbf{x};a_{2},x_{0}^{(s_{2})}) S(c_{i_{3}},\mathbf{x};a_{3},x_{0}^{(s_{3})}), \quad (13)$$

### Quark hadron contraction



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.

### Scaling

- Hadron blocks
  - Completely antisymmetric under all quark exchange
  - Consider only octet baryons

$$M_{w} \cdot N_{w} \frac{n_{u}! n_{d}! n_{s}!}{2^{A - n_{\Sigma^{0}} - n_{\Lambda}}},$$
(15)

• Computationally feasible for  $A \le 10$ 

#### Multibaryon contractions with determinants $M_{\mu}^{N_{\mu}} \sum_{n}^{N_{\mu}} \sum_{n}^{(a_{1},a_{2},...,a_{n_{q}}),k'} \sum_{n} \sum_{n} \sum_{ij} \sum_{j} \sum_{n} \sum_{ij} \sum_{j} \sum_{n} \sum_{ij} \sum_{j} \sum_{ij} \sum_{ij} \sum_{j} \sum_{ij} \sum_{j} \sum_{ij} \sum_{ij} \sum_{j} \sum_{ij} \sum_{ij$

$$[\mathcal{N}_{1}^{h}(t)\bar{\mathcal{N}}_{2}^{h}(0)]_{U} = \int \mathcal{D}q \mathcal{D}\bar{q} e^{-S_{\text{QCD}}[U]} \sum_{k'=1}^{N_{w}} \sum_{k=1}^{N_{w}} \tilde{w}_{h}^{\prime(a_{1}',a_{2}'...a_{n_{q}}'),k'} \tilde{w}_{h}^{(a_{1},a_{2}...a_{n_{q}}),k} \sum_{\mathbf{j}} \sum_{\mathbf{i}} \epsilon^{j_{1},j_{2},...,j_{n_{q}}} \epsilon^{i_{1},i_{2},...,i_{n_{q}}} q(a_{j_{n_{q}}}') \dots q(a_{j_{2}}') q(a_{j_{1}}') \times \bar{q}(a_{i_{1}})\bar{q}(a_{i_{2}}) \dots \bar{q}(a_{i_{n_{q}}}),$$
(16)

- Color, spinor, flavor, spatial indices
  - Primed: sink
- $\text{Unprimed: source}_{[\mathcal{N}_{1}^{h}(t)\bar{\mathcal{N}}_{2}^{h}(0)]_{U} = e^{-\mathcal{S}_{\text{eff}}[U]} \sum_{k'=1}^{N_{w}'} \sum_{k=1}^{N_{w}} \tilde{w}_{h}^{\prime(a_{1}',a_{2}'...a_{n_{q}}'),k'} \tilde{w}_{h}^{(a_{1},a_{2}...a_{n_{q}}),k} \times \sum_{\mathbf{j}} \sum_{\mathbf{i}} \epsilon^{j_{1},j_{2},...,j_{n_{q}}} \epsilon^{i_{1},i_{2},...,i_{n_{q}}} S(a_{j_{1}}';a_{i_{1}}) S(a_{j_{2}}';a_{i_{2}}) \dots S(a_{j_{n_{q}}}';a_{i_{n_{q}}}).$

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

$$\langle \mathcal{N}_{1}^{h}(t)\bar{\mathcal{N}}_{2}^{h}(0)\rangle = \frac{1}{Z} \int \mathcal{D}\mathcal{U}e^{-\mathcal{S}_{\text{eff}}} \sum_{k'=1}^{N'_{w}} \sum_{k=1}^{N'_{w}} \tilde{w}_{h}^{\prime(a'_{1},a'_{2}...a'_{n_{q}}),k'} \tilde{w}_{h}^{(a_{1},a_{2}...a_{n_{q}}),k} \times \det G(\mathbf{a}';\mathbf{a}).$$
(19)

• Total numerical cost (using LU decomposition)  $n_u^3 n_d^3 n_s^3 \times N_W' N_W$ 

### Nuclear correlation functions

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  $(4.6 \text{ fm})^3 \times 7.0 \text{ fm}$  (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 per-

- Seven source points:  $\vec{r}, \vec{r} \pm d \hat{x}, \vec{r} \pm d \hat{y}, \vec{r} \pm d \hat{z}, (d=4)$ 
  - $\vec{r}$  Arbitrary point
  - $\hat{x}, \hat{y}, \hat{z}$  Unit vectors
- 4He, 8Be, 12C, 16O, and 28Si



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

### Nuclear correlation functions

- A<20
  - Extracted energy is consistent with a system of A nucleons but large uncertainty
- 28Si
  - No flattering of the effective mass
- A clear extraction of the ground state binding energies of these systems is beyond the current work.