Correlation functions of atomic nuclei in Lattice QCD II

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Correlation functions of atomic nuclei

The correlation function of a nucleus with N_p protons and N_n neutrons is defined as

$$C_{N_p,N_n}(\vec{x},t) = \left\langle \prod_{i=1}^{N_p} P_{\alpha_i}(\vec{x},t) \prod_{j=1}^{N_n} N_{\alpha_j}(\vec{x},t) \prod_{k=1}^{N_p} \overline{P}_{\overline{\alpha}_k}(\vec{0},0) \prod_{l=1}^{N_n} \overline{N}_{\overline{\alpha}_l}(\vec{0},0) \right\rangle ,$$

$$P_\alpha = \varepsilon^{abc} u^a_\alpha (u^b_\beta (C\gamma_5)_{\beta\gamma} d^c_\gamma) \quad \text{and} \quad N_\alpha = \varepsilon^{abc} d^a_\alpha (u^b_\beta (C\gamma_5)_{\beta\gamma} d^c_\gamma).$$

In the last talk by Jana Günther a method was introduced to construct the correlation function recursively.

The ingredients for the recursive algorithm

Multi-baryon correlation functions can be written as

$$C(t) = \underbrace{f_{B_1}^{q_1,q_2,q_3} \dots f_{B_N}^{q_1,q_2,q_3}}_{F^{(N)}} \cdot \underbrace{\sum_{\sigma \in \Sigma} G^{B_1} \dots G^{B_N} \ \mathrm{sgn}(\sigma)}_{L^{(N)}}$$

The objects in this formula have the following meaning:

- $f_{B_i}^{q_1,q_2,q_3}$: Block of three quark propagators contracted at the sink to form a baryon.
- G^{B_i}: The spinor- and color-structure of the baryons at the source.
- F: The outer product of the $f_{B_i}^{q_1,q_2,q_3}$.
- L: The list of contributing components of F.

Both L and the antisymmerized version F_- of F can be constructed separately via a recursion:

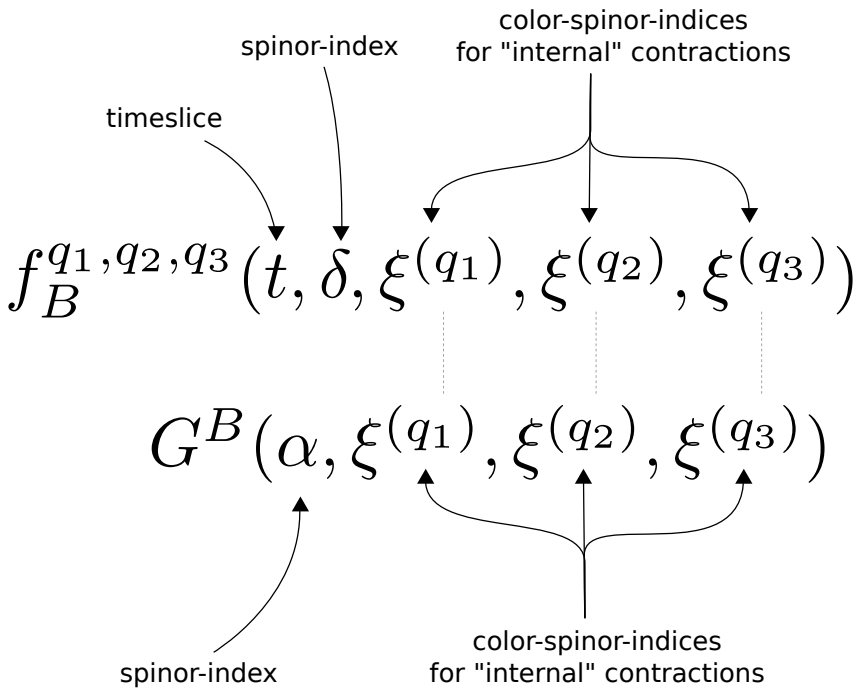
$$L^{(n+1)} = L^{(n)} \bullet G_{B_{n+1}} \qquad F_-^{(n+1)} = F_-^{(n)} \bullet f_{B_{n+1}}^{q_1,q_2,q_3}$$

Complicated multi-baron-systems

- The simplest form of the recursive algorithm can deal only with special cases, for which
  - all quarks are from a single spatial source.
  - the total number of quarks of each flavor does not exceeds 12.
- Many interesting systems do not fall into this class.
- All this restrictions can be circumvented.

More quark sources

Up to now the objects $f_B^{q_1,q_2,q_3}(t,\delta,\xi^{(q_1)},\xi^{(q_2)},\xi^{(q_3)})$ and $G^B(\alpha,\xi^{(q_1)},\xi^{(q_2)},\xi^{(q_3)})$ do not dependent of the quark sources and sinks.



More quark sources

To allow for several quark sources, the following must be changed:

1. The contractions between the objects f and G must allow for quark propagation from every baryon at the source to every baryon at the sink.
2. f and G must explicitly depend on the quark source.

The first condition can be met as follows:

- The indices ξ are promoted to color-spinor-source/-sink-indices: $\xi = \text{source/sink}(\xi) \otimes \text{spinor}(\xi) \otimes \text{color}(\xi)$.
- ξ can take $12N_{\text{source}}$ values instead of 12 values.

Projection to spin-states

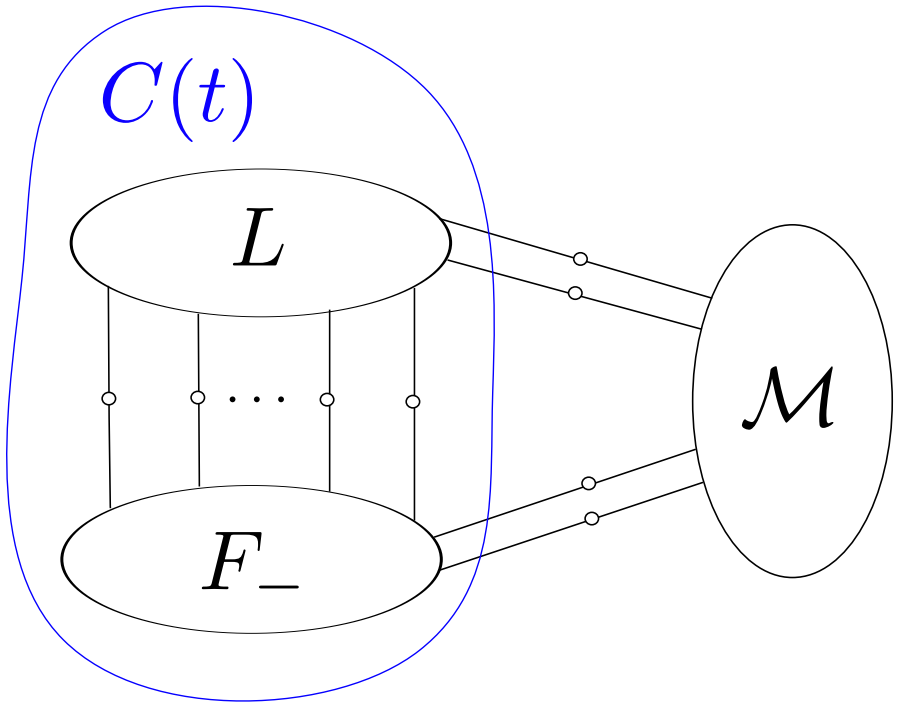
- The correlation function $[C(t)]^{\alpha_1\cdots\alpha_n}_{\delta_1\cdots\delta_n}$ has a large number of spinor component.
- In practice it is not necessary to calculate the full tensor, but only the projections of the form

$$C_{\mathcal{M}}(t) = \sum_{\alpha_i,\delta_i} [C(t)]^{\alpha_1\cdots\alpha_n}_{\delta_1\cdots\delta_n} \mathcal{M}^{\alpha_1\cdots\alpha_n}_{\delta_1\cdots\delta_n}.$$

- This can be calculated efficiently by modifying the list L:

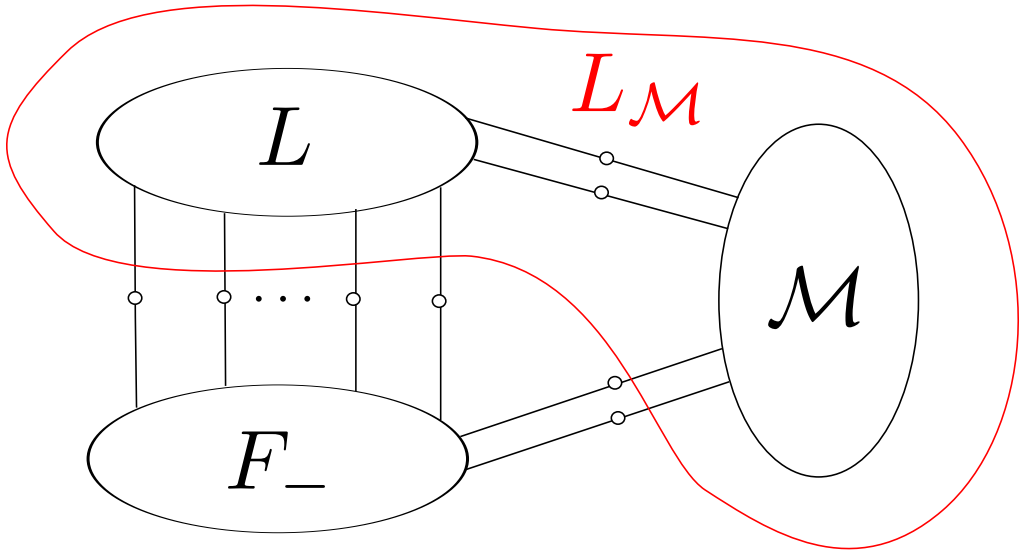
$$\begin{aligned}
&(n_{B_a}!\, n_{B_b}! \ldots)^2\, L_{\mathcal{M}}(\mathbf{A}^{(B_a)}\{\delta\}, \mathbf{A}^{(B_b)}\{\delta\}, \ldots, \mathbf{A}^{(u)}\{\xi\}, \mathbf{A}^{(d)}\{\xi\}, \mathbf{A}^{(s)}\{\xi\}) \\
= &\sum_{\mathbf{A}^{(B_a)}\{\alpha\}, \mathbf{A}^{(B_b)}\{\alpha\}, \ldots} L^{(N)}(\mathbf{A}^{(B_a)}\{\alpha\}, \mathbf{A}^{(B_b)}\{\alpha\}, \ldots, \mathbf{A}^{(u)}\{\xi\}, \mathbf{A}^{(d)}\{\xi\}, \mathbf{A}^{(s)}\{\xi\}) \\
&\times \mathcal{M}_{-}(\mathbf{A}^{(B_a)}\{\alpha\}, \mathbf{A}^{(B_b)}\{\alpha\}, \ldots, \mathbf{A}^{(B_a)}\{\delta\}, \mathbf{A}^{(B_b)}\{\delta\}, \ldots)
\end{aligned}$$

Projection to spin-states



$$C(t) = \underbrace{f_{B_1}^{q_1,q_2,q_3} \dots f_{B_N}^{q_1,q_2,q_3}}_{F^{(N)}} \cdot \underbrace{\sum_{\sigma\in\Sigma} G^{B_1} \dots G^{B_N} \ \mathrm{sgn}(\sigma)}_{L^{(N)}}$$

Projection to spin-states

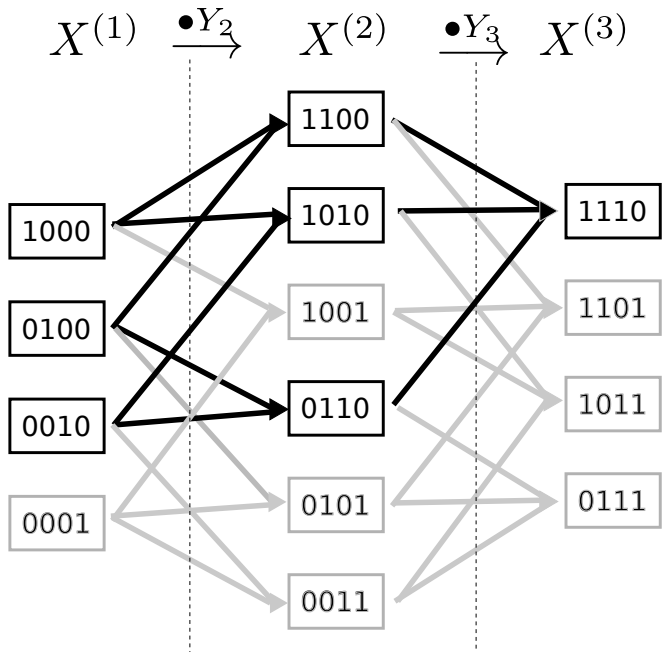


$$C(t) = \underbrace{f_{B_1}^{q_1,q_2,q_3} \dots f_{B_N}^{q_1,q_2,q_3}}_{F^{(N)}} \cdot \underbrace{\sum_{\sigma \in \Sigma} G^{B_1} \dots G^{B_N} \ \mathrm{sgn}(\sigma)}_{L^{(N)}}$$

Projection to spin-states

This approach has two advantages:

- One does not have to store the complete correlation function at any time.
- The computation of some intermediate components may not be necessary because the contraction of $\mathcal{M}$ with L cancels its contribution.



Atomic Nuclei

- QCD as the theory of strong interaction should predict the masses and properties of atomic nuclei.
- One important application of the presented algorithm is the calculation of correlation functions of atomic nuclei.
- This special case is to be presented in detail here.

Nucleon operators

For creating and annihilating of nucleons the following interpolating operators are used commonly:

$$
\begin{aligned}
P_\alpha &= \varepsilon_{abc} \left(\Gamma_1\right)_{\alpha\beta} u_{\beta;a} \left[u_{\gamma;b} (\Gamma_2)_{\gamma\delta} d_{\delta;c}\right], \\
N_\alpha &= \varepsilon_{abc} \left(\Gamma_1\right)_{\alpha\beta} d_{\beta;a} \left[u_{\gamma;b} (\Gamma_2)_{\gamma\delta} d_{\delta;c}\right] \\
\overline{P}^\alpha &= \varepsilon^{abc} \left(\Gamma_1\right)_{\alpha\beta} \overline{u}^{\beta;a} \left[\overline{u}^{\gamma;b} (\Gamma_2)^{\gamma\delta} \overline{d}^{\delta;c}\right], \\
\overline{N}^\alpha &= \varepsilon^{abc} \left(\Gamma_1\right)^{\alpha\beta} \overline{d}^{\beta;a} \left[\overline{u}^{\gamma;b} (\Gamma_2)^{\gamma\delta} \overline{d}^{\delta;c}\right]
\end{aligned}
$$

There are two important choices of the Γ_i matrices that will be discussed here:

1. The fully relativistic choice $\Gamma_1 = \mathbb{1}$ and $\Gamma_2 = C\gamma_5$.
2. The non relativistic case $\Gamma_1 = P_{nr}$ and $\Gamma_2 = C\gamma_5 P_{nr}$ with $P_{nr} = \frac{\mathbb{1}+\gamma_4}{2}$.

Recursive relations for nuclei

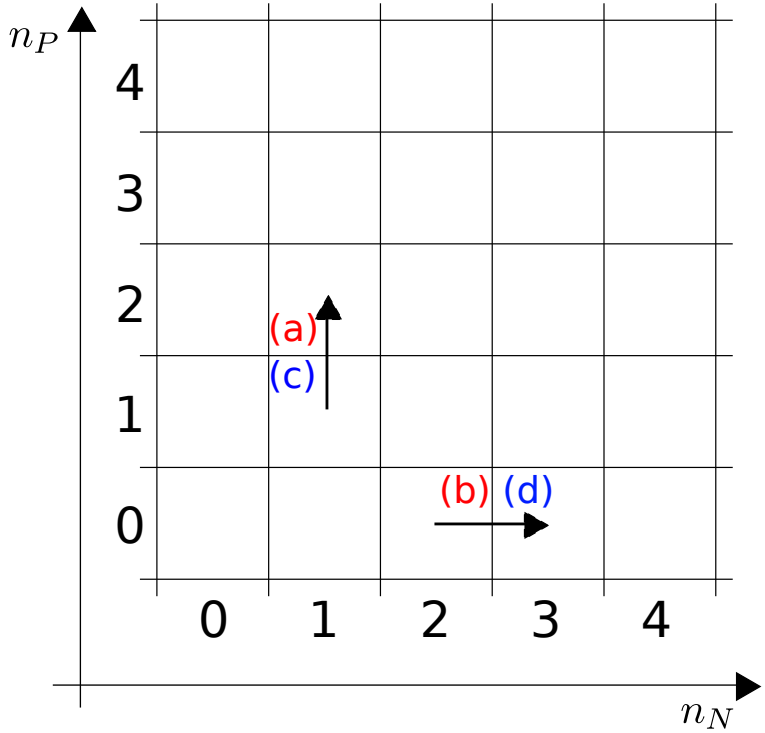
A nucleus can be defined by the number of protons N_P and the number of neutrons N_N. This yields a two dimensional recursive scheme:

$$L^{(n_P+1,n_N)} = L^{(n_P,n_N)} \bullet G_P, \quad \text{(a)}$$

$$L^{(n_P,n_N+1)} = L^{(n_P,n_N)} \bullet G_N, \quad \text{(b)}$$

$$F_-^{(n_P+1,n_N)} = F_-^{(n_P,n_N)} \bullet f_P^{u,u,d}, \quad \text{(c)}$$

$$F_-^{(n_P,n_N+1)} = F_-^{(n_P,n_N)} \bullet f_N^{d,d,u} \quad \text{(d)}$$



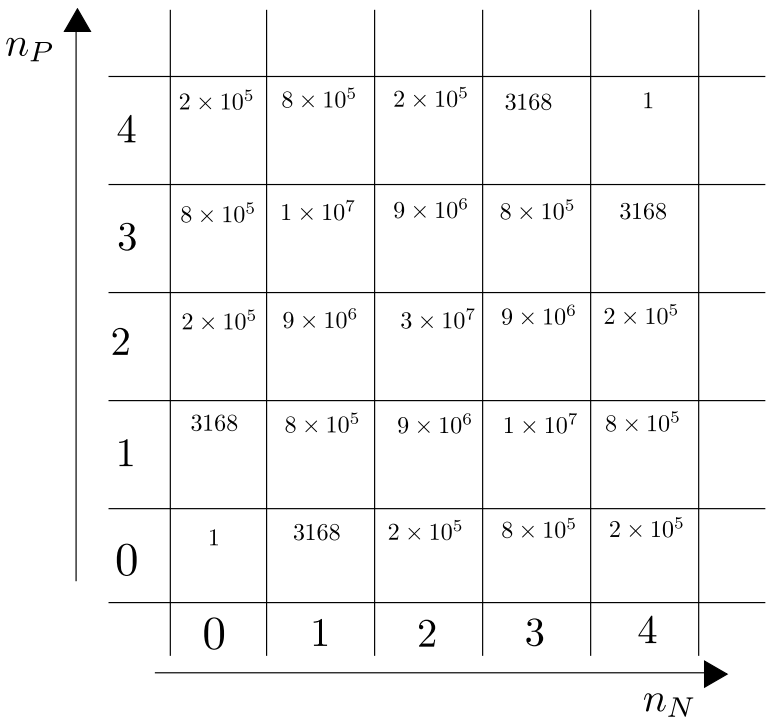
red: Recursion for the list L.
blue: Recursion for the tensor F_-.

Recursive relations for nuclei

How many components can F_- have for a given nucleus?

$$P(n_P, n_N) = C(n_P, D - n_P)C(n_N, D - n_N)$$
$$C(2n_P + n_N, 3D - 2n_P - n_N)C(n_P + 2n_N, 3D - n_P - 2n_N),$$

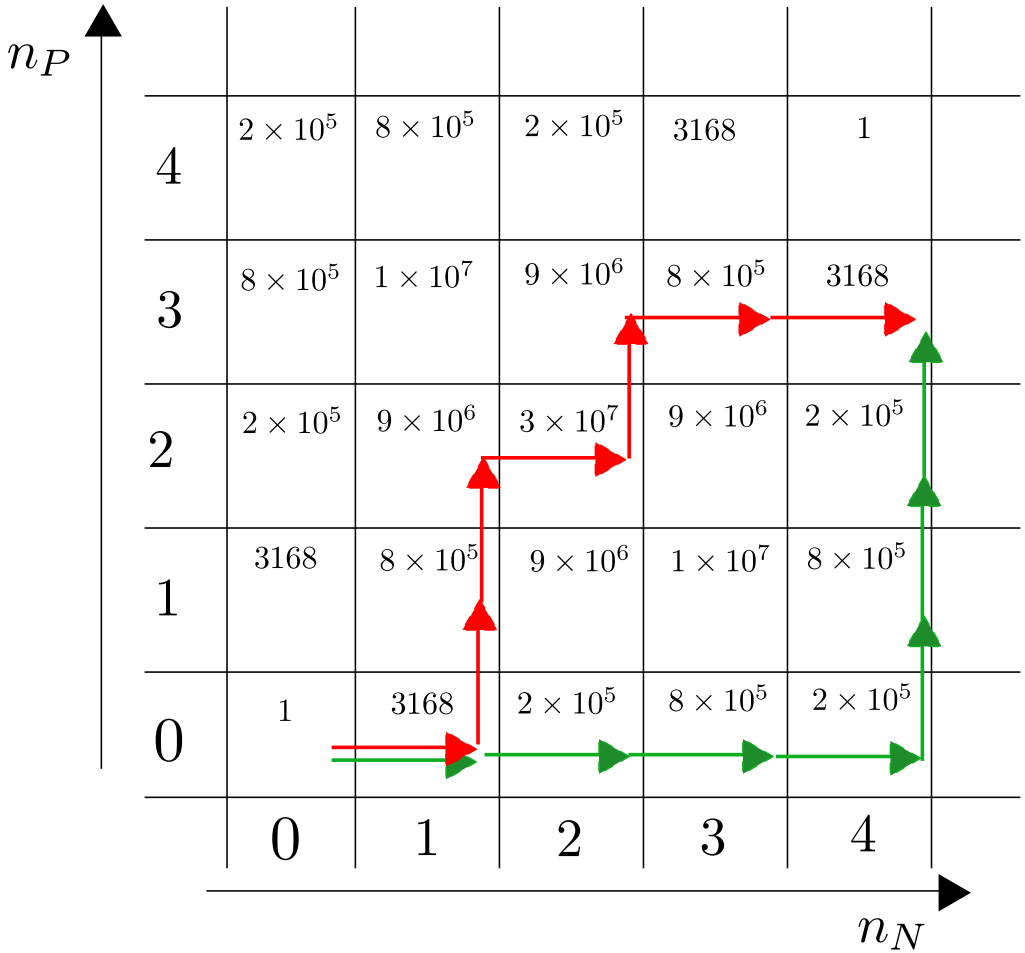
$C(n_1, n_2, \cdots) = \frac{(n_1+n_2+\cdots)!}{n_1!n_2!\cdots}$, $D \mathrel{\hat{=}}$ effective number of spinor components per quark



- This is the maximal number permitted by the antisymmetry structure.
- In practice only a fraction of this number is required.

Recursive relations for nuclei

The actual effort to calculate a given F_- depends on the chosen path.

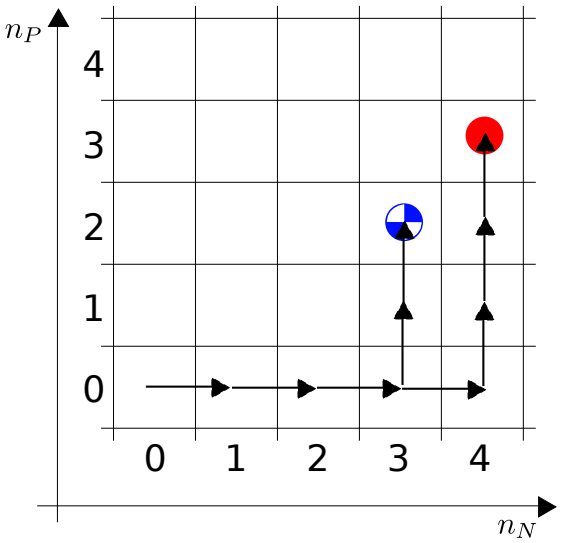


The red path is less efficient then the green one.

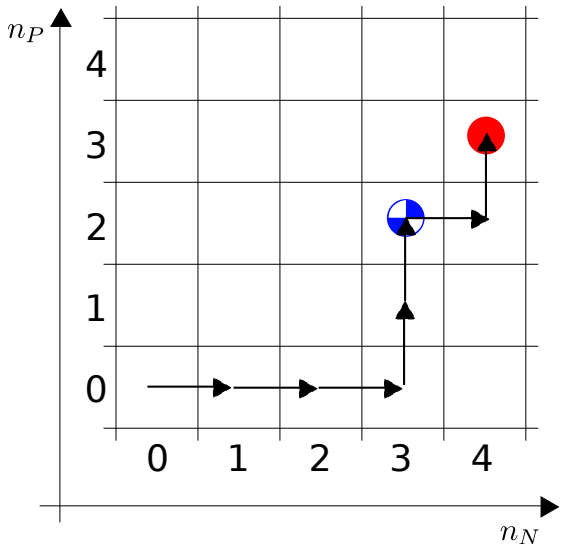
In general path which add first all baryons of one type and then the baryons of the other type are advantageous.

Recursive calculation of several nuclei

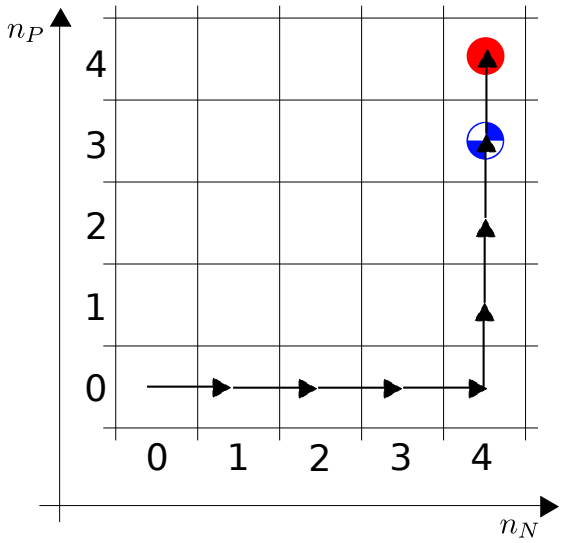
If one wants to calculate the correlation function of more then one nuclei it can be advantageous to combine the recursive operations:



10 % speedup compared with separate calculation



slower than separate calculation



47 % speedup compared with separate calculation

Comparison with naïve method

Relativistic Operators, 1 Quark source:

	N_P	N_N	No. of op.	Naïve No. of op.	η
^{3}He	2	1	19241280	5.5×10^{11}	2.9×10^4
^{4}He	2	2	531321120	5.7×10^{16}	1.1×10^8
^{6}Li	3	3	2905079520	4.9×10^{27}	1.7×10^{18}
^{7}Li	3	4	404946240	3.0×10^{33}	7.5×10^{24}
(^{8}Be)	4	4	448496928	2.8×10^{39}	6.2×10^{30}

Comparing with unified contraction algorithm

Relativistic Operators, 1 Quark source:

	N_P	N_N	η
^{3}He	2	1	3.7
^{4}He	2	2	41
^{6}Li	3	3	17500
^{7}Li	3	4	566000
(^{8}Be)	4	4	1.6×10^7

Conclusion

- An algorithm was presented that can efficiently calculate the correlation function of multi-baryon-systems.
- Several quark sources can be used.
- The projection to certain spin-states can reduce the computational effort.
- Baryons blocks can be projected to definite momentum prior to the construction of the correlation functions.
- Atomic nuclei as a special case where discussed in detail.

Thank you!

More quark sources

The usage of several quark sources can be implemented via

$$\tilde{G}^B(\chi;\xi^{(q_1)},\xi^{(q_2)},\xi^{(q_3)}) = \delta^{s(\chi),s(\xi^{(q_1)})}\delta^{s(\chi),s(\xi^{(q_2)})}\delta^{s(\chi),s(\xi^{(q_3)})} \cdot G^B(\alpha(\chi);\kappa(\xi^{(q_1)}),\kappa(\xi^{(q_2)}),\kappa(\xi^{(q_3)})),$$

$$\tilde{f}_B^{q_1,q_2,q_3}(t,\psi;\xi^{(q_1)},\xi^{(q_2)},\xi^{(q_3)}) = \sum_{\vec{x}} s_{s(\psi)}(\vec{x}) \left\langle B_{\alpha(\psi)}(\vec{x},t) \cdot q_1^{\xi^{(q_1)}} q_2^{\xi^{(q_2)}} q_3^{\xi^{(q_3)}} \right\rangle$$

where

- $s(\xi) \hat{=}$ source-/sink-part of ξ.
- $\alpha(\xi) \hat{=}$ spinor-part of ξ.
- $\kappa(\xi) \hat{=}$ spinor-color-part of ξ.

The recursive algorithm can be applied in the same way then before the introduction off additional quark sources.