Baryonic and mesonic 3-point functions with open spin indices

M. Löffler for RQCD

June 21, 2017

Universität Regensburg

SFB TR55

Lib Hadron Analysis (LHA)

What is LHA?

A new LQCD library for efficient calculations on modern parallel architectures and on CPUs

What can be done with LHA?

BDA, MDA

Baryon Spectrum

Baryon 3pt Functions

Meson 3pt Functions

Why use LHA?

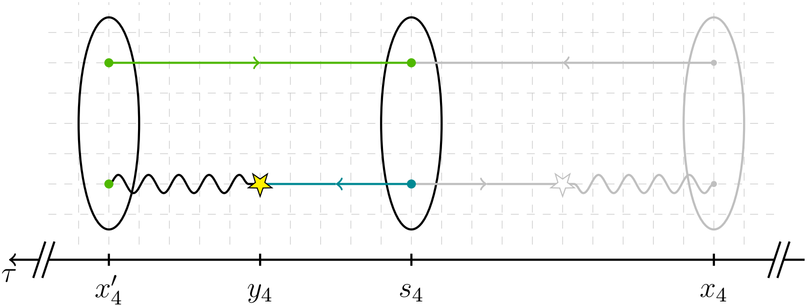
Standard implementations do not
work efficiently on new architectures

Adaptable to every physical channel within data analysis

Computation per lattice site $\rightarrow$ SIMD data layout

Parallelization scheme

Meson 3pt Functions on the Lattice using stochastic Estimators



Operators

Annihilator: $A(\mathbf{x}', x_4') = \delta_{\mathbf{ab}}\ \overline{F}_{\mathbf{A}}(\mathbf{x}', x_4')^{\boldsymbol{\alpha}}_{\mathbf{a}}\ \Gamma'^{\boldsymbol{\alpha\beta}}\ F_{\mathbf{B}}(\mathbf{x}', x_4')^{\boldsymbol{\beta}}_{\mathbf{b}}$

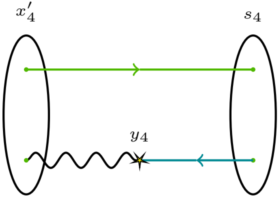
Creator: $C(\mathbf{s}, s_4) = \delta_{ba}\ \overline{F}_B(\mathbf{s}, s_4)^{\beta}_{b}\ \left(\gamma_4 \Gamma^{\dagger} \gamma_4\right)^{\beta\alpha}\ F_A(\mathbf{s}, s_4)^{\alpha}_{a}$

Current: $I(\mathbf{y}, y_4) = \delta_{\mathfrak{ab}}\ \overline{F}_{\mathfrak{A}}(\mathbf{y}, y_4)^{\mathfrak{a}}_{\mathfrak{a}}\ \Gamma^{\mathfrak{ab}}_{\mathfrak{I}}\ F_{\mathfrak{B}}(\mathbf{y}, y_4)^{\mathfrak{b}}_{\mathfrak{b}}$ (+ derivative Operators)

with $F_i \in \{L, S, C\}$ (light, strange, charm).

Γ-Structure examples:

- Scalar: $\mathbb{1}, \gamma_4$
- Pseudoscalar: γ_5, $\gamma_4\gamma_5$
- Vector: $\gamma_i, \gamma_4\gamma_i$
- Axial Vector: $\gamma_i\gamma_5$



Meson 3pt Functions - Wick Contractions

Performing the generic Wick contraction

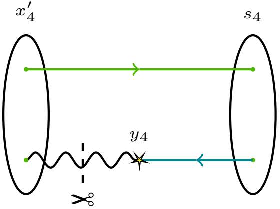
$$\langle A(x')\, I(y)\, C(s)\rangle =$$

$$= \mathrm{tr}\left[G(F_A, s, x')\ \Gamma'\ G(F_{\mathbf{B}}, x', y)\ \Gamma_{\mathfrak{J}}\ G(F_{\mathfrak{B}}, y, s)\ \Gamma\right]$$

$$= \delta_{\mathbf{ab}}\ \delta_{ab}\ \delta_{\mathfrak{ab}}\ \ (\Gamma')^{\boldsymbol{\alpha\beta}}\, (\Gamma_{\mathfrak{J}})^{\mathfrak{ab}}\, (\Gamma)^{\beta\alpha}\ \times$$
$$\times\ \ G(F_A, s, x')_{\mathbf{a}a}^{\boldsymbol{\alpha}\alpha}\ G(F_{\mathbf{B}}, x', y)_{\boldsymbol{b}\mathfrak{a}}^{\boldsymbol{\beta}\mathfrak{a}}\ G(F_{\mathfrak{B}}, y, s)_{\mathfrak{b}b}^{\mathfrak{b}\beta}$$

The stochastic all-to-all propagator

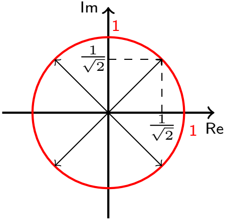
$$G(F_A, y, x')_{ba'}^{\beta\alpha'} \approx$$
$$\frac{1}{N}\sum_{i=1}^{N}\ (s_i)(F_A, y)_b^{\beta}\ \ (\eta_i^*)\ (x')_{a'}^{\alpha'}$$



Vector – Definition[1]

$$(\eta_i)\,(\mathbf{x},x_4)^{\alpha}_{a} \in \begin{cases} (\mathbb{Z}_2 \otimes \mathrm{i}\mathbb{Z}_2)/\sqrt{2} & , \quad x_4 = \textsf{sink}_{\textsf{fwd/bwd}} \\ 0 & , \quad \text{otherwise} \end{cases}$$

Vector – Properties



$$\frac{1}{N}\sum_{i=1}^{N} (\eta_i)\,(x)^{\alpha}_{a} = 0 + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

$$\frac{1}{N}\sum_{i=1}^{N} (\eta_i)\,(x)^{\alpha}_{a}\,(\eta_i^*)\,(x')^{\alpha'}_{a'} = \delta_{xx'}\;\delta_{\alpha\alpha'}\;\delta_{aa'} + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$

[1] S.-J. Dong and K.-F. Liu, "Stochastic estimation with Z(2) noise," Phys. Lett. B328 (1994) 130, hep-lat/9308015

The 3pt Function becomes

$$\langle A(x')\, I(y)\, C(s)\rangle =$$

Use that:

$$G(x,y)^{\alpha\beta}_{ab} = (\gamma_5^*)^{\beta\gamma}\; G^*(y,x)^{\gamma\delta}_{ba}\; (\gamma_5^*)^{\delta\alpha}$$

$$= \delta_{\mathbf{ab}}\, \delta_{ab}\, \delta_{\mathfrak{ab}}\; (\Gamma')^{\boldsymbol{\alpha\beta}}\, (\Gamma_{\mathfrak{I}})^{\mathfrak{ab}}\, (\Gamma)^{\beta\alpha} \;\times$$
$$\times\; G(F_A, s, x')^{\boldsymbol{\alpha}\alpha}_{\mathbf{a}a}\; G(F_{\mathbf{B}}, x', y)^{\boldsymbol{\beta}\mathfrak{a}}_{\boldsymbol{b}\mathfrak{a}}\; G(F_{\mathfrak{B}}, y, s)^{\mathfrak{b}\beta}_{\mathfrak{b}b}$$

$$= \delta_{\mathbf{ab}}\, \delta_{ab}\, \delta_{\mathfrak{ab}}\; (\Gamma')^{\boldsymbol{\alpha\beta}}\, (\Gamma_{\mathfrak{I}})^{\mathfrak{ab}}\, (\Gamma)^{\beta\alpha} \;\times$$
$$\times \underbrace{\left[\gamma_5^*\; G(F_A, x', s)^*\; \gamma_5^*\right]^{\alpha\boldsymbol{\alpha}}_{a\mathbf{a}}\; \left[\eta_i(x')\;\gamma_5^*\right]^{\boldsymbol{\beta}}_{\mathbf{b}}}_{\widehat{=}\text{ Spectator}}\; \underbrace{\left[\gamma_5^*\; s_i(F_{\mathbf{B}}, y)\right]^{\mathfrak{a}}_{\mathfrak{a}}\; G(F_{\mathfrak{B}}, y, s)^{\mathfrak{b}\beta}_{\mathfrak{b}b}}_{\widehat{=}\text{ Insertion}}$$

Meson 3pt Function - Open 3pt Function

At the end we achieve an expression for the mesonic 3pt function

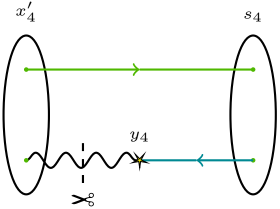
$$C^{F_A\, F_{\mathbf{B}}\, F_{\mathfrak{B}}\, \alpha\, \boldsymbol{\alpha}\, \boldsymbol{\beta}\, \mathfrak{a}\, \mathfrak{b}\, \beta}(\mathbf{p}, x_4', \mathbf{q}, y_4) = \frac{1}{N} \sum_i \; S_{i\;\;a}^{F_A\;\alpha\, \boldsymbol{\alpha}\, \boldsymbol{\beta}}(\mathbf{p}, x_4') \; I_{i\;\;a}^{F_{\mathbf{B}}\; F_{\mathfrak{B}}\; \mathfrak{a}\, \mathfrak{b}\, \beta}(\mathbf{q}, y_4)$$

$$S_{i\;\;a}^{F_A\;\alpha\, \boldsymbol{\alpha}\, \boldsymbol{\beta}}(\mathbf{p}, x_4') = \sum_{\mathbf{x}'} \; \delta_{\mathbf{ab}} \; [\gamma_5^* \; G(F_A, x', s)^* \; \gamma_5^*]_{a\mathbf{a}}^{\alpha\boldsymbol{\alpha}} \; [\eta_i(x') \; \gamma_5^*]_{\mathbf{b}}^{\boldsymbol{\beta}} \cdot e^{-i\mathbf{p}\cdot\mathbf{x}'}$$

$$I_{i\;\;a}^{F_{\mathbf{B}}\; F_{\mathfrak{B}}\; \mathfrak{a}\, \mathfrak{b}\, \beta}(\mathbf{q}, y_4) = \sum_{\mathbf{y}} \; \delta_{ab} \; \delta_{\mathfrak{a}\mathfrak{b}} \; [\gamma_5^* \; s_i(F_{\mathbf{B}}, y)]_{\mathfrak{a}}^{\mathfrak{a}} \; G(F_{\mathfrak{B}}, y, s)_{\mathfrak{b}b}^{\mathfrak{b}\beta} \cdot e^{i\mathbf{q}\cdot\mathbf{y}}$$

Contracting the spectator and insertion parts with the correct Γ-structure gives the desired result

What does this mean for computational purposes?



Meson 3pt Function - Object size

Spectator size (upper bound)

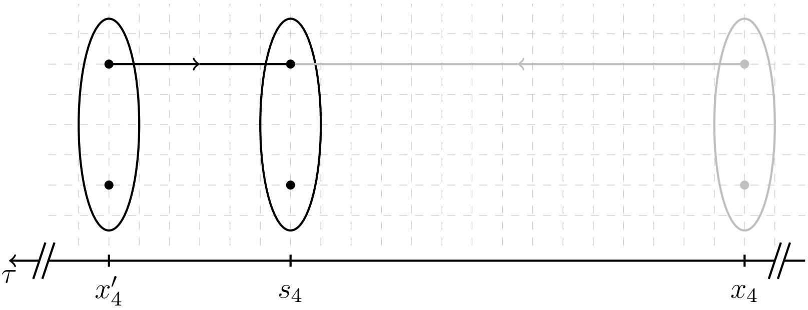
$$\text{Spectator size} = \\ \#\text{spin} \cdot \#\text{color} \cdot \#\text{stoch} \cdot \#\text{momenta} \cdot \#\text{src} \\ \cdot \text{fwd/bwd} \cdot \#\text{flavorcombinations} \cdot \#\text{noisesmearing} = \\ 64 \cdot 3 \cdot 100 \cdot 60 \cdot 4 \cdot 2 \cdot 3 \cdot 3 = \\ 8.29 \cdot 10^7 \text{ Complex Numbers} \mathrel{\hat{=}} 1.30 \text{ GB}$$

Insertion size (upper bound)

$$\text{Insertion size} = \\ \#\text{spin} \cdot \#\text{color} \cdot \#\text{stoch} \cdot \#\text{momenta} \cdot \#\text{src} \cdot \#\text{ins} \\ \cdot \#\text{derivatives} \cdot \#\text{flavorcombinations} = \\ 64 \cdot 3 \cdot 100 \cdot 60 \cdot 4 \cdot 20 \cdot (1+4) \cdot 9 = \\ 4.15 \cdot 10^9 \text{ Complex Numbers} \mathrel{\hat{=}} 64.8 \text{ GB}$$

Computation of the Spectator part (serial)

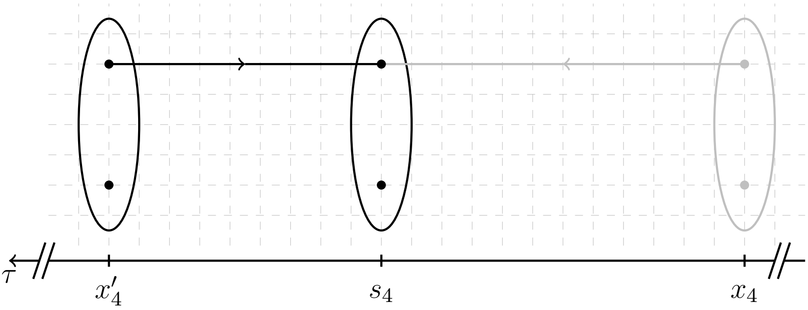
Serial loop over Source time slice s_4



Meson 3pt Functions - Parallelization

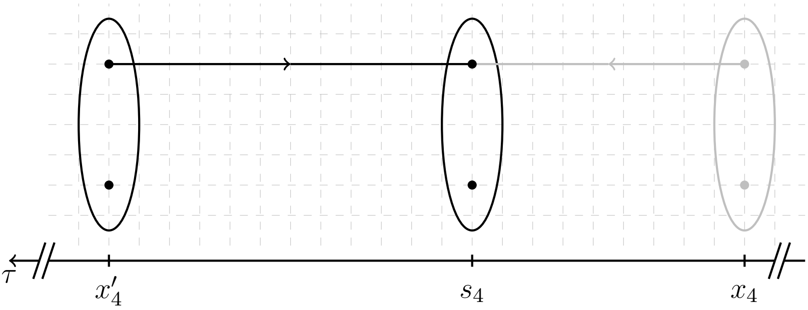
Computation of the Spectator part (serial)

Serial loop over Source time slice s_4



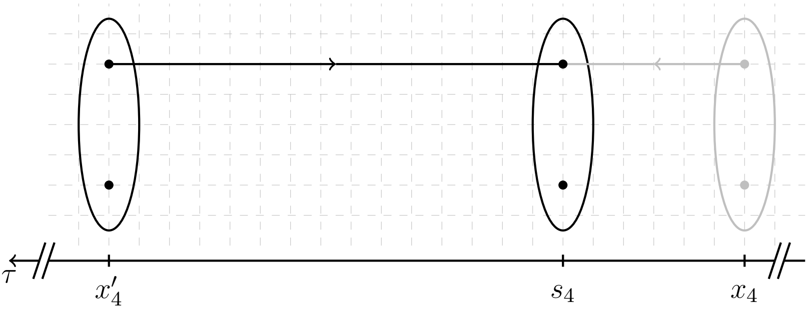
Computation of the Spectator part (serial)

Serial loop over Source time slice s_4



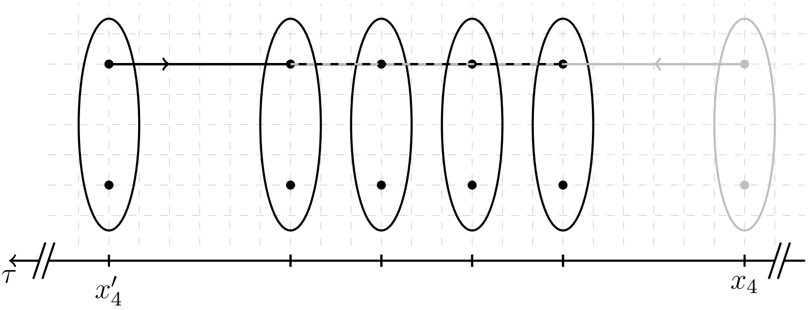
Computation of the Spectator part (serial)

Serial loop over Source time slice s_4



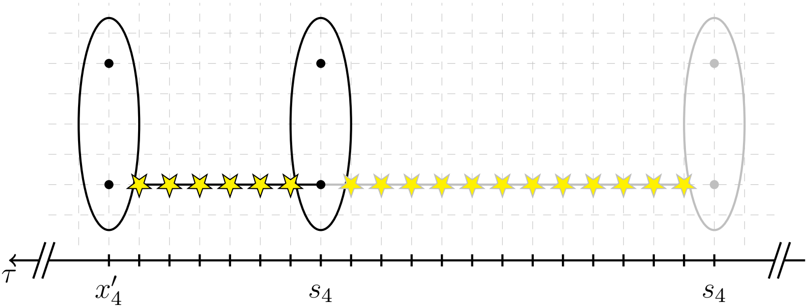
Computation of the Spectator part (parallel)

Parallel loop over Source time slice s_4



Computation of the Insertion part (parallel)

Serial outer Loop over Source time slice s_4
Parallel inner Loop over Current time slice y_4



Loop Layout

Reference implementation:

QDP++ library takes care of parallelism over lattice sites
$\rightarrow$ SIMD vectorization difficult due to its internal data layout.

LibHadronAnalysis:

Reorder loops in order to use two of the spin indices for auto-vectorization.

```
for 3 spin indices do
    for color indices a,b do
        for all sites in the local lattice do
        end
    end
end
```

Algorithm 1: Reference implementation

```
for all sites in the local lattice do
    for 1 spin index do
        for color indices a,b do
            for 2 spin indices SIMD vect. do
            end
        end
    end
end
```

Algorithm 2: LHA implementation

Machine: QPACE 3, Xeon Phi (KNL), Omni-Path, 8 nodes

Lattice Size: $32^3 \times 96$

Spec.: $S_i^{L,S} = \widetilde{G}(L, x', s)\ \widetilde{G}(S, x', s)\ \widetilde{\eta}_i(S, x')$ $(0 \leq i < 30)$

Ins.: $I_i^{S,S} = s_i(S, y)\ G(S, y, s) + \text{deriv.}$ $(0 \leq i < 30)$

Src./Snk.: $s = 30$, $x' = 16/44$

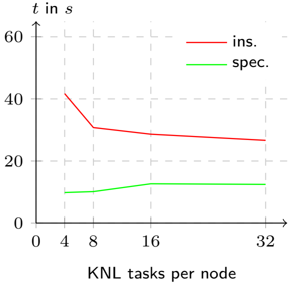


Figure 1: Contraction

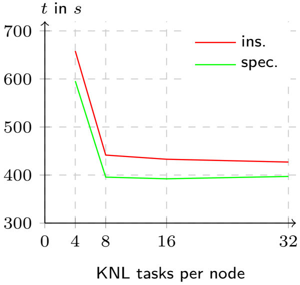


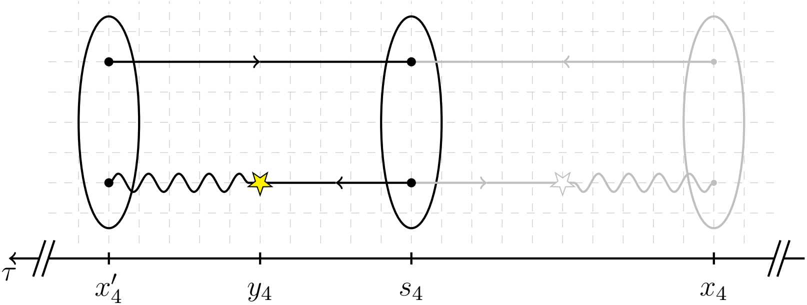
Figure 2: Total time (propagators etc.)

[2]Peter Georg: An in-depth evaluation of the Intel Omni-Path network for LQCD applications. 19/6/2017 17:00

Summary

Computation of mesonic 3pt functions by factorization into spectator and insertion parts

Highly parallelized
Using smart ordering of operator and site index loops → SIMD
'Open 3pt Function'. Analysis software is also available for the off-line contractions.



Thank you for your attention