

Isospin breaking corrections to the mass of the Ω^- baryon

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Second LatticeNET workshop



Summary

- **Isospin breaking**
- **QCD+QED** with C^* boundary conditions
- **Baryon** masses on the lattice
- Connected and partially connected contributions
 - 1. 3-quark connected contributions:** past measurements and HLRN allocation
 - 2. 1-quark connected contributions:** computation and testing

Isospin symmetry breaking

Isospin symmetry is the symmetry in the exchange between the **up** and **down quarks**

In **QCD** is an **approximate** symmetry: there is a small difference between m_u and m_d (**strong isospin breaking**)

In **QCD+QED** the symmetry is also broken by the difference in the electric charges $q_u = \frac{2}{3}e$ and $q_d = -\frac{1}{3}e$ (**electromagnetic isospin breaking**)

QCD+QED on the lattice

In an era where measurements aim to 1% precision both the coupling to QED and the strong isospin breaking have to be taken into account in QCD lattice simulations

The **coupling to QED** is challenging on the lattice due to the need to impose boundary conditions, in the standard case of **periodic boundary conditions** in space we can look at Gauss law:

$$Q = \int_0^L dx^3 \rho(x) = \int_0^L dx^3 \nabla \cdot E(x) = 0 \quad (1)$$

No interpolating operator can have a superposition with a charged state and we can't measure masses of charged hadrons

C^* boundary conditions

One solution comes from C^* boundary conditions, consisting in the charge conjugation of quark and gauge fields when crossing the boundaries of the lattice

This choice preserves locality, gauge and translational invariance

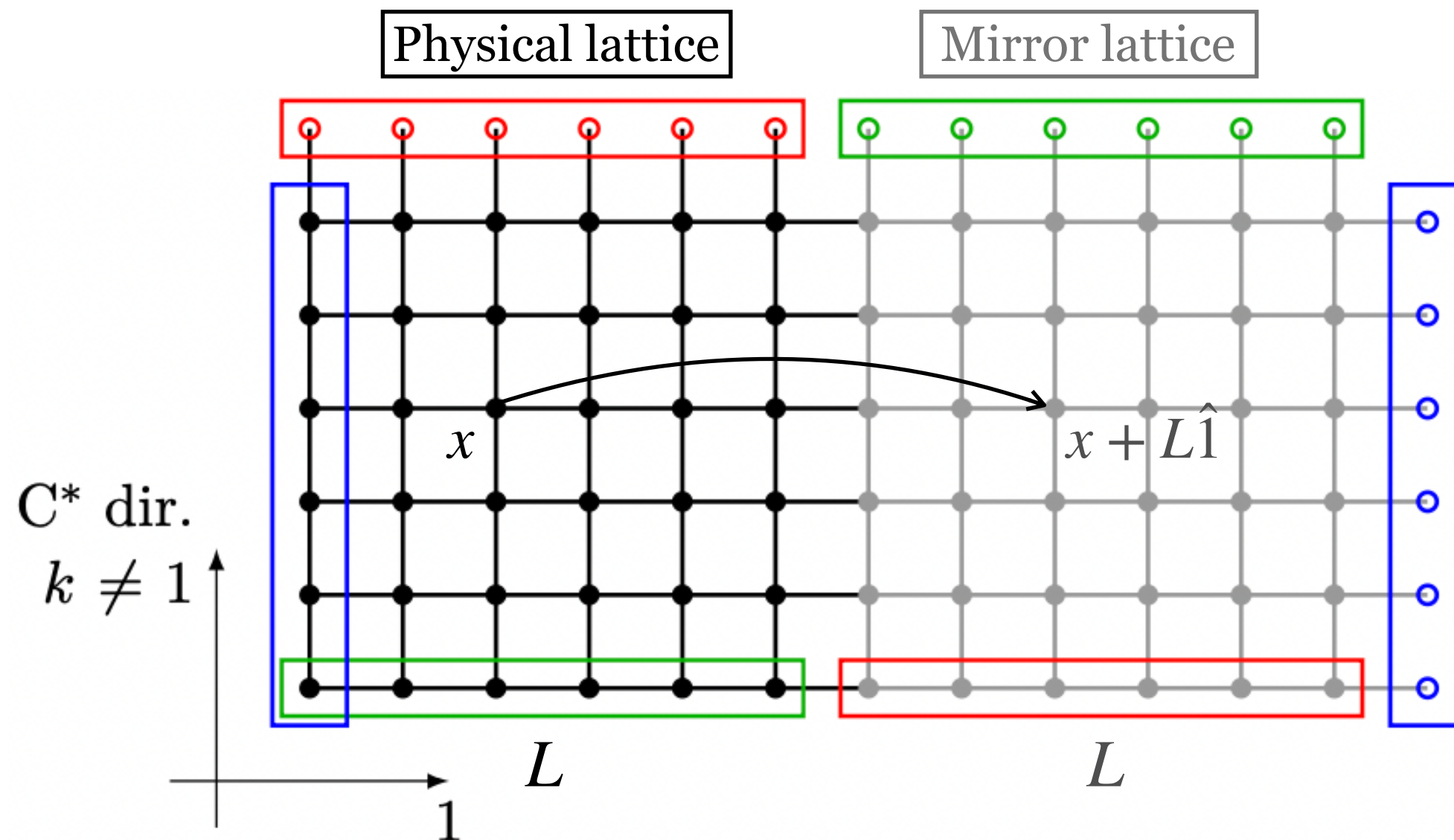
In this case we obtain for **Gauss law**:

$$Q = \int_0^L dx^3 \rho(x) = \int_0^L dx^3 \nabla \cdot E(x) \neq 0$$

Since the electric field changes sign under charge conjugation and becomes anti-periodic

C^* boundary conditions

In the *openQxD* code these boundary conditions are implemented through the **orbifold construction**



From: Isabel Campos et al. “openQ*D code: a versatile tool for QCD+QED simulations”. In: The European Physical Journal C (Mar. 2020).

C^* boundary conditions

With C^* boundary conditions there are **additional contributions to quark propagators**:

$$\overbrace{\langle q_a^A(x) \bar{q}_b^B(y) \rangle} = D^{-1}(x, y)_{ab}^{AB} \quad (1)$$

$$\overbrace{\langle q_a^A(x) q_b^{B,T}(y) \rangle} = - D^{-1}(x, y + L\hat{1})_{ad}^{AB} C_{db} \quad (2)$$

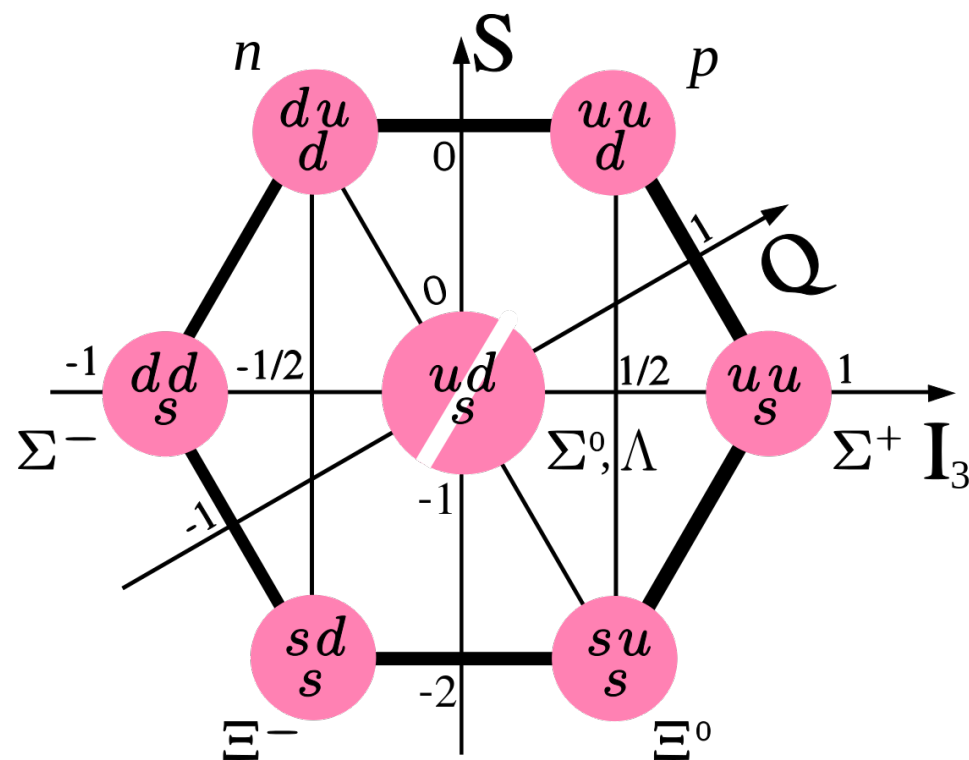
$$\overbrace{\langle \bar{q}_a^{A,T}(x) \bar{q}_b^B(y) \rangle} = C_{ad} D^{-1}(x + L\hat{1}, y)_{db}^{AB} \quad (3)$$

This is the reason for the presence of additional contractions in **baryonic two-point functions**

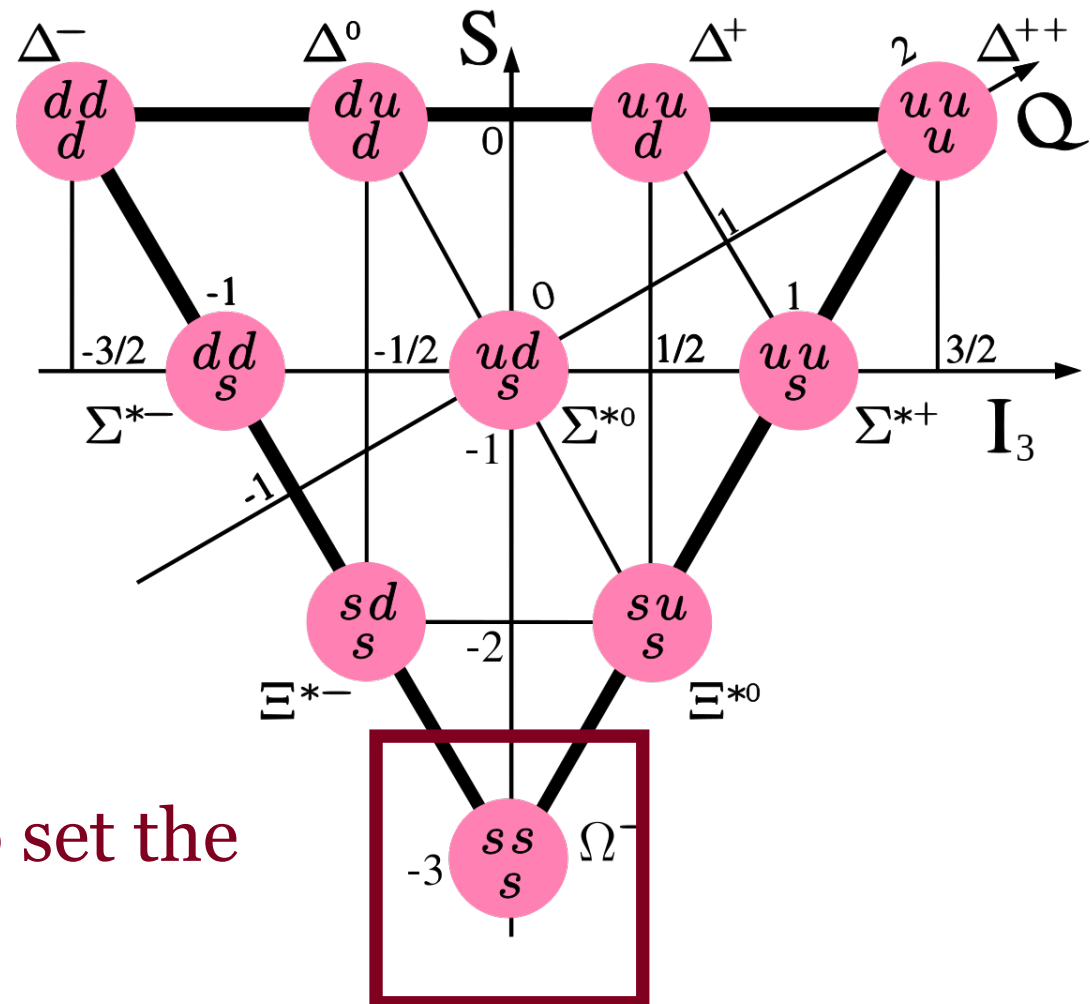
Baryon masses on ensembles with C* BC

Baryons are hadrons composed of **three valence quarks**

Baryon octet



Baryon decuplet



the Ω^- baryon has been used to set the scale of lattice simulations

Baryon masses on the lattice

To measure baryon masses on the lattice we have to define **interpolating operators**

$$v_{\Omega^-}^{m;d}(x) = \sum_{\substack{abc \\ ABC}} W_{abc}^{d;m} \epsilon^{ABC} \psi_c^C(x) \psi_a^A(x) \psi_b^B(x) \quad (1)$$

$$\bar{v}_{\Omega^-}^{m;d}(x) = \sum_{\substack{abc \\ ABC}} \bar{W}_{abc}^{d;m} \epsilon^{ABC} \bar{\psi}_b^B(x) \bar{\psi}_a^A(x) \bar{\psi}_c^C(x)$$

Where

$$W_{abc}^{d;m} = P_{dc}^{ml} \Gamma_{ab}^l + P_{db}^{ml} \Gamma_{ac}^l + P_{da}^{ml} \Gamma_{cb}^l \quad (2)$$

$$\bar{W}_{abc}^{d;m} = P_{cd}^{ml} \Gamma_{ab}^l + P_{bd}^{ml} \Gamma_{ac}^l + P_{ad}^{ml} \Gamma_{cb}^l$$

$$P^{ml} = [\delta^{ml} Id_{4 \times 4} - \frac{1}{3} \gamma^m \gamma^l]$$

$$\Gamma^l = C \gamma^l \quad (3)$$

Baryon masses on the lattice

Constructing the **two-point correlation function at zero momentum** and measuring its exponential decay at large time separation we can obtain the mass of the interpolated state

$$C_{\Omega^-}(x_0) = \sum_{\substack{dd' \\ m}} \sum_{\mathbf{x}} P_{dd'}^+ v_{\Omega^-}^{m;d}(x) \bar{v}_{\Omega^-}^{m;d'}(0) \quad (1)$$

Where:

$$P^+ = \frac{1 + \gamma^0}{2} \quad (2)$$

Due to C^* boundary conditions the two point function has contributions from two kind of diagrams: **3-quark connected** and **1-quark connected**

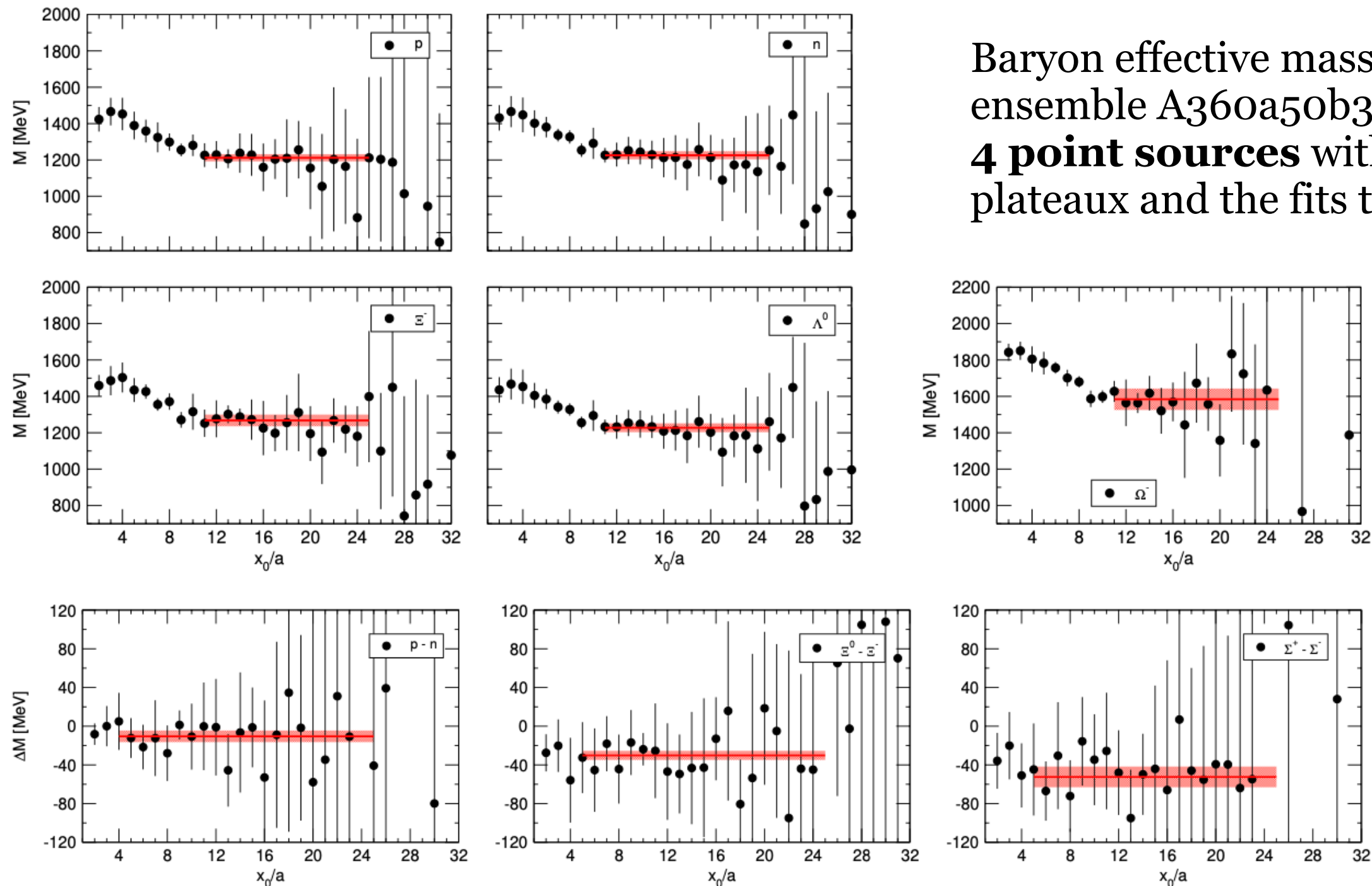
3-quark connected contributions

The two space-time points are connected by **three quark propagators**, we obtain these contributions also in the standard case of periodic boundary conditions in space

$$C_{\Omega-}(x_0) = \sum_{\substack{d'd \\ m}} \sum_{\substack{\alpha bc \\ \alpha' b' c'}} \sum_{\mathbf{x}} \sum_{\substack{ABC \\ A'B'C'}} \left[\bar{W}_{a'b'c'}^{d';m} P_{dd'}^+ W_{abc}^{d;m} \epsilon^{ABC} \epsilon^{A'B'C'} \overline{\psi_a^A(x)} \bar{\psi}_{a'}^{A'}(0) \right. \\ \left. \overline{\psi_b^B(x)} \bar{\psi}_{b'}^{B'}(0) \overline{\psi_c^C(x)} \bar{\psi}_{c'}^{C'}(0) \right] \quad (1)$$

All the inversions are performed using point sources

3-quark connected contributions

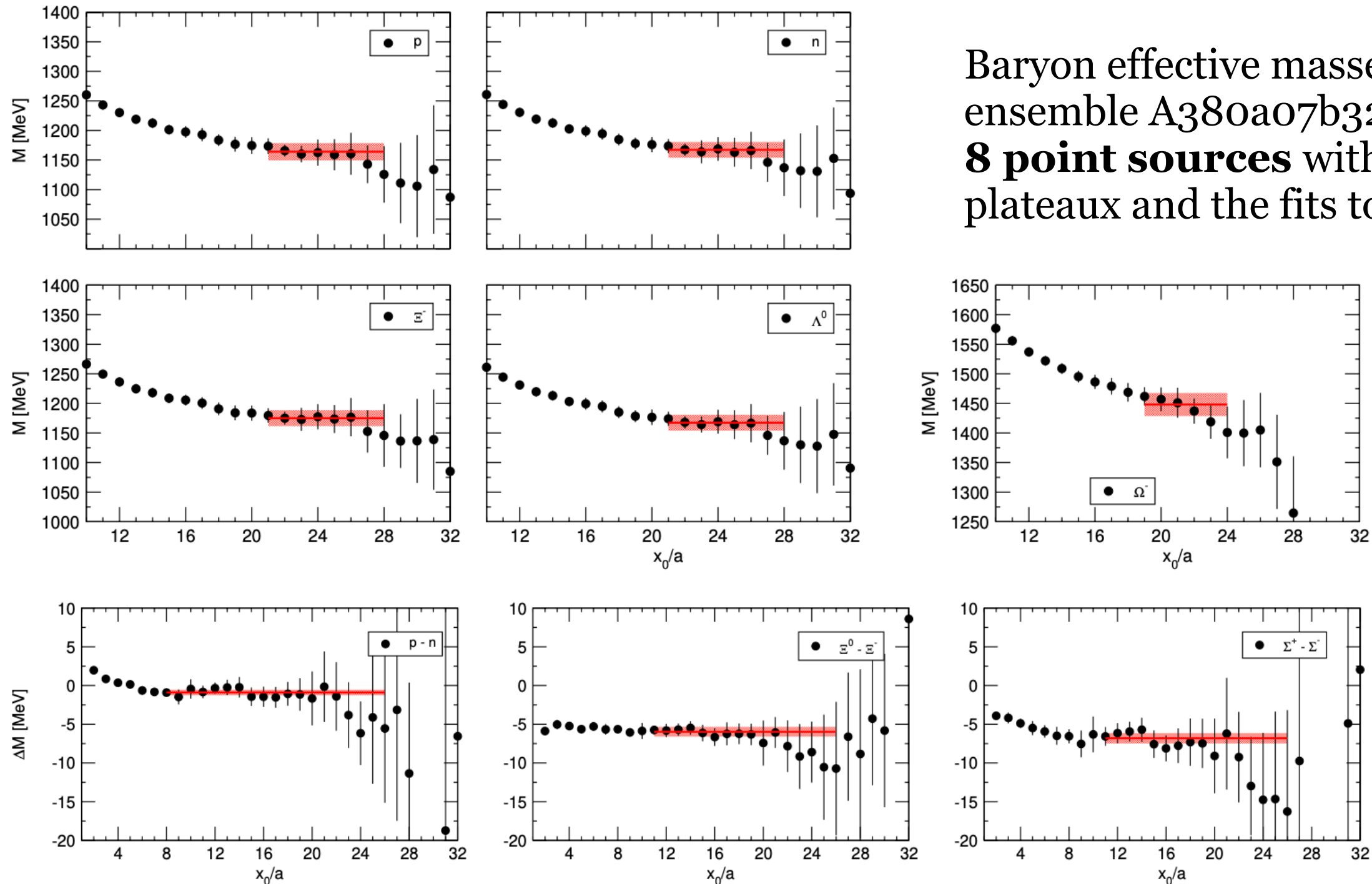


Baryon effective masses for the ensemble A360a50b324+RW2 for **4 point sources** with the selected plateaux and the fits to a constant.

From L. Bushnaq et al. “First results on QCD+QED with C* boundary conditions”. In Journal of high energy physics (Mar. 2023)

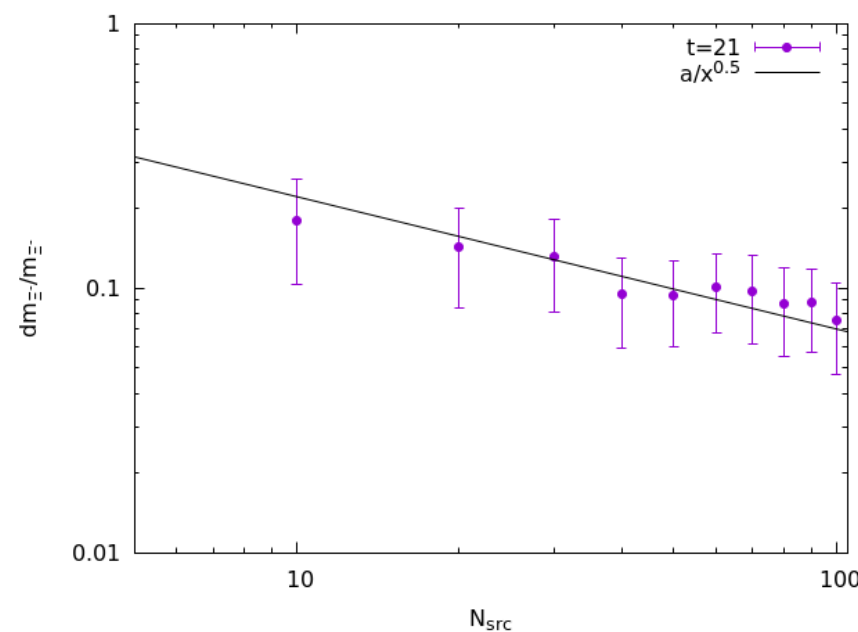
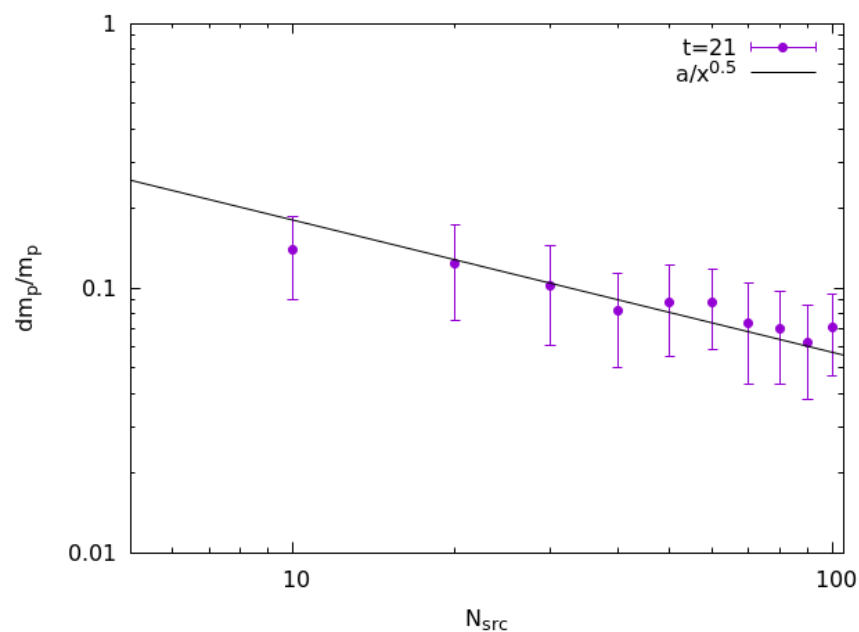
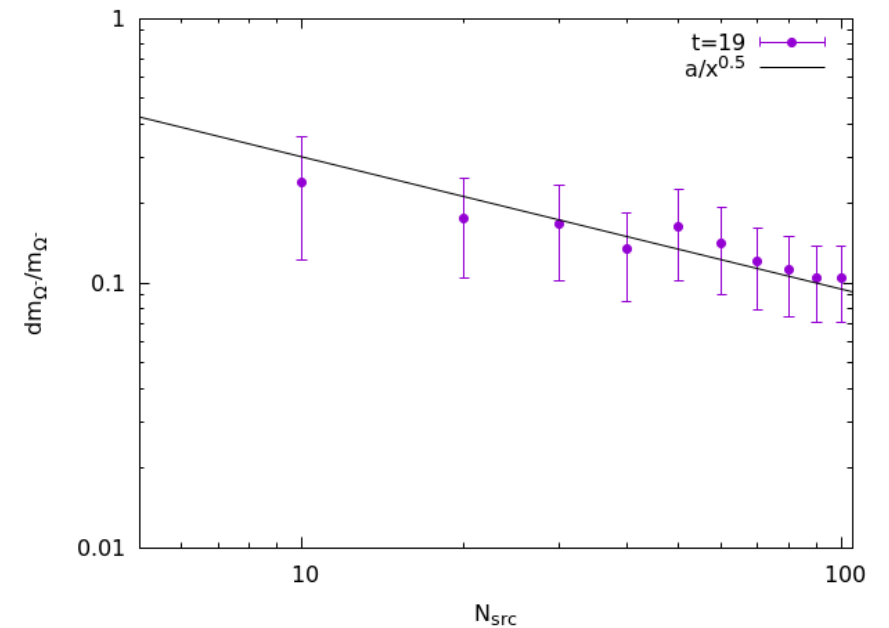
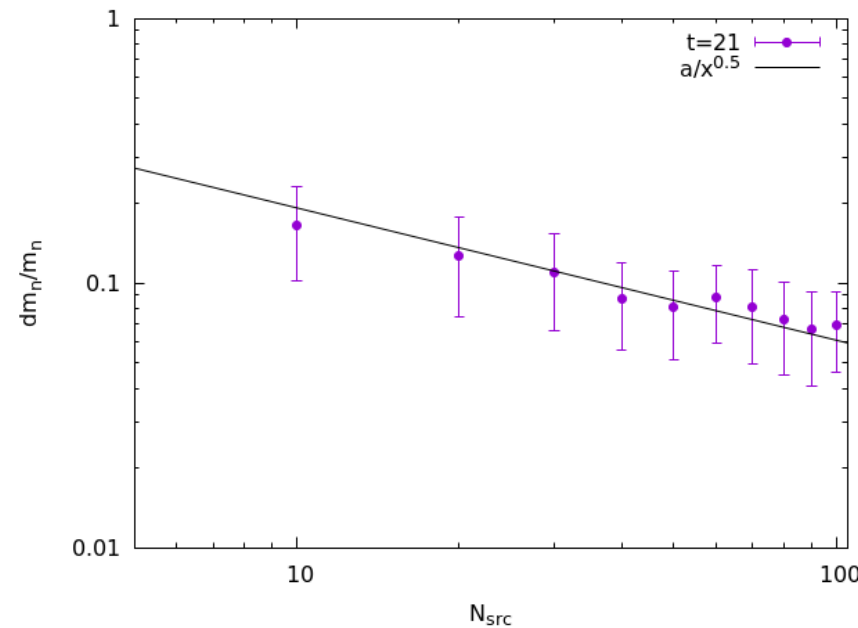
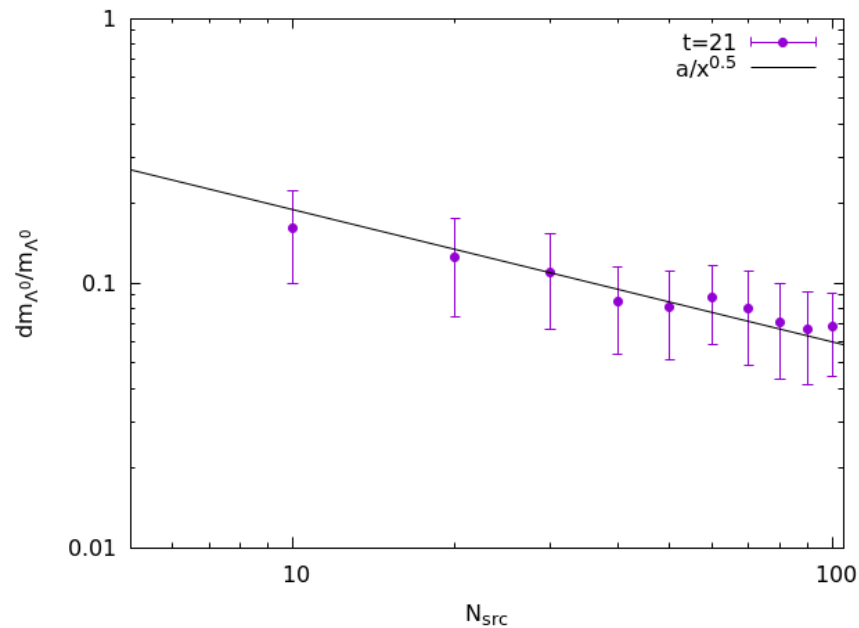
3-quark connected contributions

Baryon effective masses for the ensemble A380a07b324+RW1 for **8 point sources** with the selected plateaux and the fits to a constant.



From L. Bushnaq et al. “First results on QCD+QED with C* boundary conditions”. In Journal of high energy physics (Mar. 2023)

3-quark connected contributions



Relative error on baryon effective masses for 40 configurations spaced 50 of the ensemble A380a07b324+RW1 as a function of the number of point sources with a fit to $\frac{a}{\sqrt{N_{src}}}$ at fixed t

We start to approach the gauge noise for 90 sources

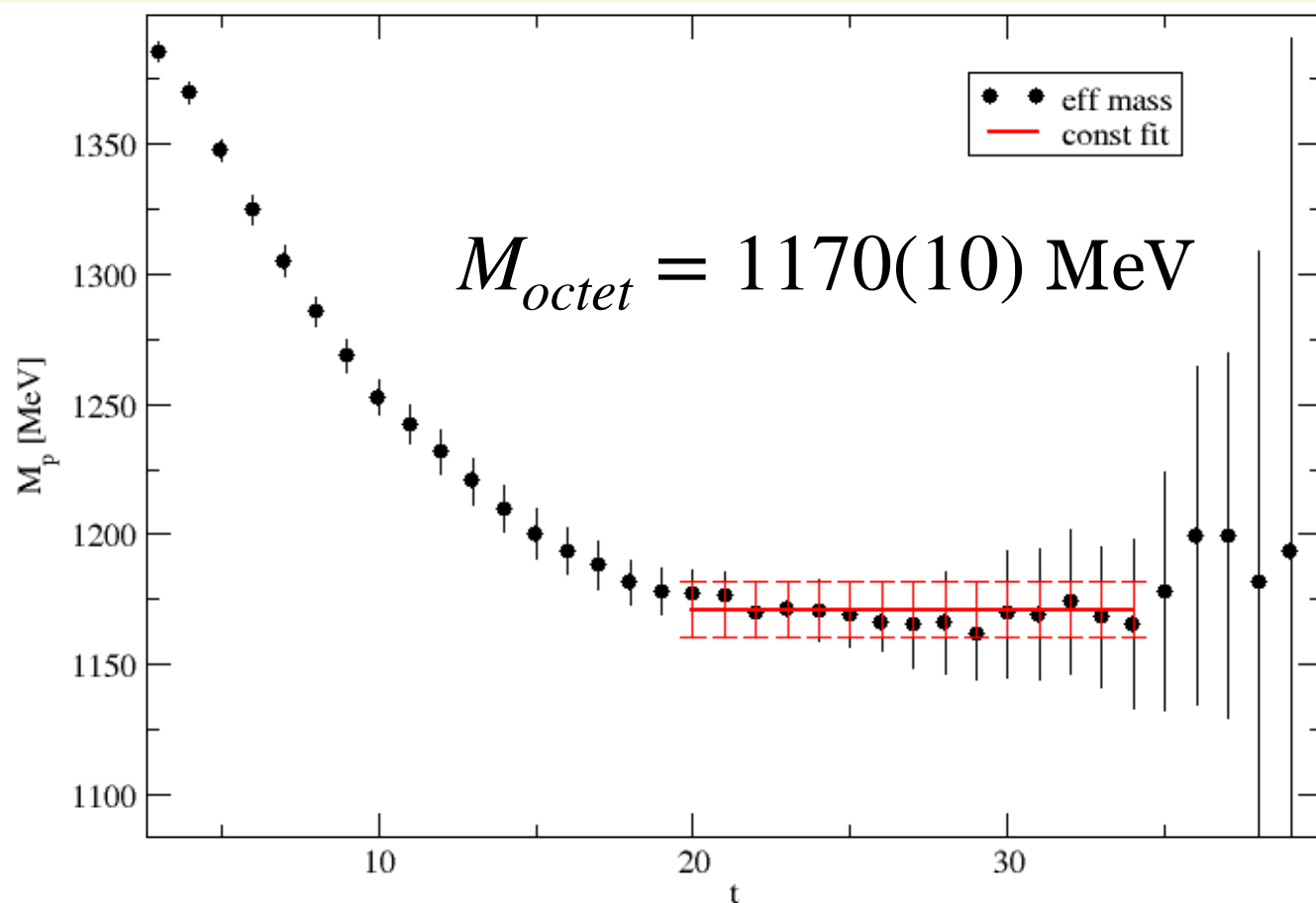
3-quark connected contributions

Motivated by the previous plots we decided to increase the number of point sources used in the measurements up to 100 or 150

Project in new **HLRN allocation**, where we were granted **89.46 Mcore-h**

Distribute between **three ensembles**: 2 QCD and 1 QCD+QED

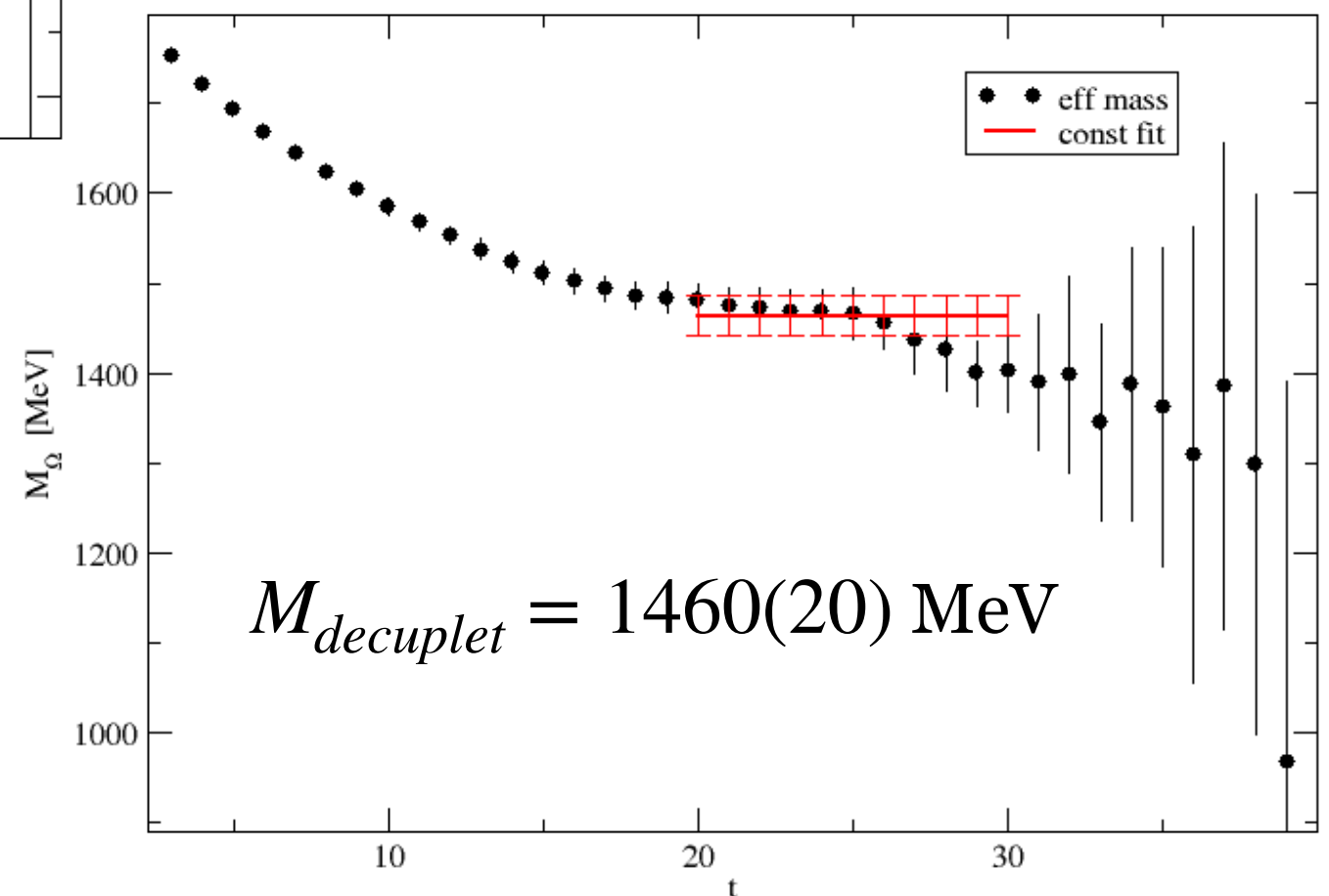
3-quark connected contributions: preliminary



Only two non degenerate masses
because at the SU(3) symmetric
point

First results for **B400a00b324**

QDC ensemble
large volume: 80x48x48x48
1000 configurations
10 point sources



1-quark connected contributions

1-quark connected contributions are a finite-volume effect due to C^* boundary conditions, obtained when we consider quark-quark and antiquark-antiquark propagators.

The two space-time points are connected by 1 quark propagator only

$$C_{\Omega^-}(x_0) = - \sum_{\substack{d'd \\ m}} \sum_{\substack{abc \\ \alpha'b'c'}} \sum_{\mathbf{x}} \sum_{\substack{ABC \\ A'B'C'}} \left[\bar{W}_{a'b'c'}^{d';m} P_{dd'}^+ W_{abc}^{d;m} \epsilon^{A'B'C'} \epsilon^{ABC} \overbrace{\bar{\psi}_{a'}^{A'}(0) \bar{\psi}_{b'}^{B'}(0)} \right. \\ \left. \overbrace{\psi_c^C(x) \bar{\psi}_{c'}^{C'}(0)} \overbrace{\psi_b^B(x) \psi_a^A(x)} \right] \quad (1)$$

1-quark connected contributions

$$C_{\Omega^-}(x_0) = - \sum_{\substack{d'd \\ m}} \sum_{\substack{\alpha abc \\ \alpha' a'b'c'}} \sum_{\mathbf{x}} \sum_{\substack{ABC \\ A'B'C'}} \left[\bar{W}_{a'b'c'}^{d';m} P_{dd'}^+ W_{abc}^{d;m} \epsilon^{ABC} \epsilon^{A'B'C'} \right] \quad (1)$$

$$C_{a'\alpha'} \left[D^{-1}(L\hat{1}, 0)_{\alpha'b'}^{A'B'} D^{-1}(x, 0)_{cc'}^{CC'} \right] \left[D^{-1}(x, x + L\hat{1})_{b\alpha}^{BA} \right] C_{\alpha a}$$

The result is obtained with a combination of point sources and stochastic sources inversions

1-quark connected contributions

Point sources

$$\eta(z)_{V\nu}^{(A\alpha)} = \delta_{VA}\delta_{\nu\alpha}\delta_{0,z} \quad \xi(z)_{A'\alpha'}^{(B'b')} = D^{-1}(z; z')_{\alpha'\nu}^{A'V} \eta(z')_{V\nu}^{(B'b')} \quad (1)$$

Stochastic sources

Using the identity:

$$\frac{1}{N_s} \sum_n \chi(x)_a^{(n)\dagger A} \chi(y)_b^{(n)B} = \delta_{AB}\delta_{ab}\delta_{xy} \quad (2)$$

$$D^{-1}(x; x + L\hat{1})_{b\alpha}^{BA} = \frac{1}{N_s} \sum_n [D^{-1}\chi^{(n)}]_b^B(x) \chi^{\dagger(n)}(x + L\hat{1})_\alpha^A \quad (3)$$

1-quark connected contributions

Defining:

$$T_{a'b'c',abc} = \sum_{\substack{d'd\alpha'\alpha \\ m}} \bar{W}_{\alpha'b'c'}^{d';m} P_{dd'}^+ W_{abc}^{d;m} C_{\alpha'a'} C_{a\alpha} \quad (1)$$

$$C(x_0) = - \sum_{\substack{abc \\ a'b'c'}} \sum_{\mathbf{x}} \sum_{\substack{ABC \\ A'B'C'}} \left[T_{a'b'c',abc} \epsilon^{ABC} \epsilon^{A'B'C'} \xi(L\hat{1})_{A'a'}^{(B'b')} \xi(x)_{Cc}^{(C'c')} \right. \\ \left. \frac{1}{N_s} \sum_n [D^{-1} \chi^{(n)}](x)_b^B \chi^{\dagger(n)}(x + L\hat{1})_a^A \right] \quad (2)$$

$$= - \sum_{\substack{abc \\ a'b'c'}} \sum_{\mathbf{x}} \sum_{\substack{ABC \\ A'B'C'}} \left[\underbrace{T_{a'b'c',abc}}_{\text{Projection in analysis}} \underbrace{\Psi_{\Omega-}(x_0)_{abc,a'b'c'}}_{\text{Computed in the code}} \right] \quad (3)$$

Projection in analysis

Computed in the code

1-quark connected contributions: check programs

It is possible to test the results of the measurements checking that they present the correct properties, we are considering:

1. Gauge invariance



2. Tree level result



3. Translational invariance



1-quark connected contributions: check of gauge invariance

Check invariance under a **random gauge transformation** $G(x)$

Apply the gauge transformation to **sources** and **gauge fields**:

Gauge fields $U(x) \rightarrow U^G(x) \quad (1)$

Dirac operator $D^{-1}(U, x, y) \rightarrow D^{-1}(U^G, x, y) = G(x)D^{-1}(U, x, y)G^\dagger(y) \quad (2)$

Stochastic source $\chi(x) \rightarrow G(x)\chi(x) = \chi^G(x) \quad (3)$

Point source $\eta^{(y)}(z) \rightarrow G(z)\eta^{(y)}(z)G^\dagger(y) = Id_{3 \times 3}\delta_{yz} = \eta^{(y)}(z) \quad (4)$

We can prove these transformation rules by applying the transformation to the two-point function and seeing that all the transformations cancel

1-quark connected contributions: check of gauge invariance

The check consists in comparing the result with and without applying the gauge transformation up to machine precision

$$\Psi_{\Omega-(x_0)abc,a'b'c'}[U, \chi, \eta] \stackrel{?}{=} \Psi_{\Omega-(x_0)abc,a'b'c'}[U^G, \chi^G, \eta] \quad (1)$$

The code passes this check



1-quark connected contributions: check of tree level result

This check consists in performing the measurements for **free fermions** (trivial gauge fields), in this case the Dirac operator is trivial in colour indices:

$$D^{-1}(x, y)^{AB}_{ab} = D^{-1}(x, y)_{ab} \delta^{AB} \quad (1)$$

And the tree level result is zero by construction:

$$\sum_{\substack{ABC \\ A'B'C'}} \epsilon^{ABC} \epsilon^{A'B'C'} \delta^{AB} \delta^{CC'} \delta^{A'B'} = 0 \quad (2)$$

1-quark connected contributions: check of tree level result

We can then perform the measurements with trivial gauge fields and compare with the expected result

$$\Psi_{\Omega^-(x_0)abc,a'b'c'}[Id_{SU(3)\times U(1)},\chi,\eta] \stackrel{?}{=} 0 \quad (1)$$

The code passes this check



1-quark connected contributions: check of translational invariance

This check relies on the property of the Dirac operator under a **translation of the gauge fields**:

$$U(x) \rightarrow U(x + S) = U^{(S)}(x) \quad (1)$$

$$D^{-1}(U; x, y) \rightarrow D^{-1}(U^{(S)}; x, y) = D^{-1}(U; x + S, y + S) \quad (2)$$

We can use the identity for the Dirac operator:

$$D^{-1}(U^{(S)}; x - S, y - S) = D^{-1}(U; x, y) \quad (3)$$

1-quark connected contributions: check of translational invariance

The check consists in comparing the result with and without applying the translation up to machine precision

$$\Psi_{\Omega^-(x_0)abc,a'b'c'}[U, \chi, \eta] \stackrel{?}{=} \Psi_{\Omega^-(x_0)abc,a'b'c'}[U^{(S)}, \chi^{(-S)}, \eta^{(-S)}] \quad (1)$$



Computed using
 $D^{-1}(U^{(S)}; x - S, y - S)$

Not finalized yet



Future plans

1. 3-quark connected:

- **Finalize the measurements** for the three ensembles, using all configurations and increasing the number of sources in steps of 10 up to 100/150, while checking the behaviour of the error

2. 1-quark connected:

- End the testing process via **translational invariance**
- Start running the code on small statistics for A400a00b324 ensemble and **compare the size of the two kinds of contributions**

Back up slides: proof of fermion propagators

$$\langle q_a^A(x) q_b^{B,T}(y) \rangle = - D^{-1}(x, y + L\hat{1})_{ad}^{AB} C_{db} \quad (1)$$

$$\begin{aligned} \overline{\langle q_a^A(x) q_b^{B,T}(y) \rangle} &= \langle q_a^A(x) C[q_b^{B,T}(y + L\hat{1})] \rangle \quad (2) \\ &= - \langle q_a^A(x) \bar{q}_d^B(y + L\hat{1}) C_{db} \rangle \\ &= - D^{-1}(x, y + L\hat{1})_{ad}^{AB} C_{db} \end{aligned}$$

Back-up slides: 3-quark connected contributions

Project in new **HLRN allocation**, where we were granted **89.46 Mcore-h**

Distributed between **two QCD ensembles**, cheaper since only 2 baryon masses are non degenerate, and where we can extend the measurements with the Rome123 method to include the coupling to QED:

1. **B400a00b324**: a QCD ensemble with a volume of $80 \times 96 \times 48^2$, larger with respect to previous measurements, 1000 configurations and 100 sources
2. **A400a00b324**: another QCD ensemble the same pion mass and volume $64^2 \times 32^2$, also useful for finite-volume effects evaluation, 2000 configurations and 150 sources

Back-up slides: 3-quark connected contributions

A **QCD+QED** ensemble, more expensive since we have 5 non degenerate masses for our ensemble with $m_d = m_s$

A418a02b324 with a value of $\alpha_B = 0.02$, not used in previous measurements, 2000 configurations and 100 sources

Back-up slides: 3-quark connected contributions

Some details of the ensembles and measurements:

- $O(a)$ improved Wilson fermions with one SW term for QCD gauge fields and one for QED gauge fields
- $a \simeq 0.05$ fm for all the ensembles considered
- Scale setting using the CLS determination of $\sqrt{8t_0} = 0.415$ fm
- Wilson flow gauge smearing
- Gaussian fermion smearing

Back-up slides: check of gauge invariance

$$\Psi_{\Omega-}(x_0)_{abc,a'b'c'} = \sum_{\substack{HLIDF \\ A'B'C'D'E'F'H'I'}} \sum_{\mathbf{x}} \epsilon^{ABC} \epsilon^{A'B'C'} G^\dagger(0)^{A'I'} G^\dagger(0)^{F'B'} G^\dagger(0)^{H'C'} G(x)^{AH} G(x)^{BL} G(x)^{CI} D^{-1}(U, L\hat{1}, 0)^{I'F'} D^{-1}(U, x, 0)^{IH'} D^{-1}(U, x, v)^{LF} \chi(v)^F \chi^\dagger(x + L\hat{1})^H \quad (1)$$

Using the property:

$$\epsilon^{ABC} G(x)^{AH} G(x)^{BL} G(x)^{CI} = \epsilon^{HLI} \det[G] = \epsilon^{HLI} \quad (2)$$

$$\epsilon^{A'B'C'} G^\dagger(0)^{A'I'} G^\dagger(0)^{F'B'} G^\dagger(0)^{H'C'} = \epsilon^{I'F'H'} \det[G] = \epsilon^{I'F'H'}$$

We obtain the same result as without performing the gauge transformation

Back-up slides: check of gauge invariance of stochastic inversions

Same strategy but considering only the part involving stochastic sources

$$\Theta^{(n)}(x)^C = \sum_{ABD} \epsilon^{ABC} D^{-1}(x, v)^{BD} \chi^{(n)}(v)^D \left[\chi^{\dagger(n)}(x + L\hat{1}) \right]^A C \quad (1)$$



$$\Theta^{(G,n)}(x)^C = \sum_{\substack{ABD \\ EFM}} \epsilon^{ABC} G(x)^{AM} G(x)^{BE} D^{-1}(x, v)^{BF} \chi^{(n)}(v)^F \chi^{\dagger(n)}(x + L\hat{1})^M \quad (2)$$

Using again $\epsilon^{ABC} G(x)^{AH} G(x)^{BL} G(x)^{CI} = \epsilon^{HLI} \quad (3)$

We get:

$$\Theta^{(G,n)}(x)^C = G^*(x)^D \Theta^{(n)}(x)^D \quad (4)$$

Back-up slides: check of gauge invariance of stochastic inversions

The check consists in testing that the gauge transformed result follows the expected transformation rule

$$G^*(x)^D \Theta^{(n)}(x)^D [U, \chi] \stackrel{?}{=} \Theta^{(n)}(x)^C [U^G, \chi^G]$$

The code passes this check

