1 Contractions and diagrams for the light quark sector

1.1 Contractions for 2-point correlation functions

1.1.1 Correlators of type $M - M$

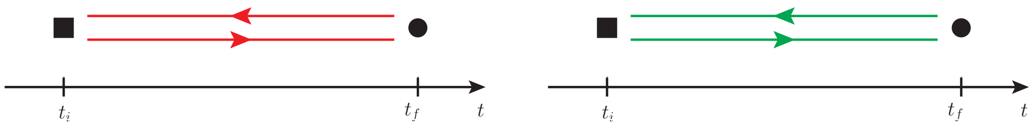

Figure 1: **Fully quark-connected diagrams of type** $M - M$ with arbitrary (local) single-meson operators at source and sink; left: built from forward propagators (red); right: built from stochastic propagators (green) emanatiing from source timeslice.

Singly quark-disconnected diagrams do not contribute for isospin quantum numbers $I = 1,\ I_3 = 0$ due to $SU(2)$ isospin symmetry.

Calculation with point-source propagators we only consider diagrams for up quarks.

$$\begin{aligned}
&C_{M-M}\left(t_{f_1}, t_{i_1}; \vec{p}_{f_1}, \vec{x}_{i_1}; \Gamma_{J,f_1}, \Gamma_{J,i_1}\right) \\
&= \sum_{\vec{x}_{f_1}} \langle \bar{u}(t_{f_1}, \vec{x}_{f_1})\, \Gamma_{J,f_1}\, u(t_{f_1}, \vec{x}_{f_1})\, \bar{u}(t_{i_1}, \vec{x}_{i_1})\, \Gamma_{J,i_1}\, u(t_{i_1}, \vec{x}_{i_1}) \rangle_f^c\, \mathrm{e}^{i\vec{p}_{f_1}\vec{x}_{f_1}} \qquad (1) \\
&= -\sum_{\vec{x}_{f_1}} \mathrm{Tr}\left(S_{f_1,i_1}\, \Gamma_{J,i_1}\, S_{i_1,f_1}\, \Gamma_{J,f_1}\right) \mathrm{e}^{i\vec{p}_{f_1}\vec{x}_{f_1}} \\
&= -\sum_{\vec{x}_{f_1}} \mathrm{Tr}\left(\left(\gamma_5\ (J\,S\,J)_{f_1,i_1}\ \gamma_5\right)^{\tilde{\dagger}}\ \Gamma_{f_1}\ (J\,S\,J)_{f_1,i_1}\ \Gamma_{i_1}\right) \mathrm{e}^{i\vec{p}_{f_1}\vec{x}_{f_1}}
\end{aligned}$$

We use the notation $\Gamma_{J,l}$ for the Γ-vertex $J\,\Gamma_l\,J$ including the smearing operator J for $l \in \{i_1, f_1\}$. Note, that $(S\,J)_{\cdot,i_1}$ is the propagator obtained from the smeared point source at site x_{i_1}.

In QLUA we calculate $-C_{M-M}\left(t_{f_1}, t_{i_1}; \vec{p}_{f_1}, \vec{x}_{i_1}; \Gamma_{f_1}, \Gamma_{i_1}\right)$, i.e. **without the -1 from the closed fermion loop**. There is no Fourier transform in the source location $\vec{x}_{i_1}$; this phase has to be added at analysis time.

Calculation with stochastic timeslice source and one-end-trick Here we use timeslice sources $\xi(t_{i_1}, \alpha)$ for source timeslice t_{i_1} and spin component α, with

$$\xi\left(t_{i_1}, \alpha\right)_{t,\vec{x},\beta,b} = \delta_{t,t_{i_1}}\, \delta_{\alpha,\beta}\, \xi\left(t_{i_1}\right)_{\vec{x},b} \qquad (2)$$

This source is multiplied with a momentum phase and smeared with smearing operator J, which leads to source

$$\xi\,(t_{i_1}, \alpha, J, \vec{p})_{t,\vec{x},\beta} = \delta_{t,t_{i_1}}\ \delta_{\alpha,\beta}\ J(\vec{x},\vec{y})\,\mathrm{e}^{i\vec{p}\vec{y}}\,\xi\,(t_{i_1})_{\vec{y}} \tag{3}$$

and the stochastic timeslice propagator

$$\phi\,(t_{i_1}, \alpha, J, \vec{p}) = D^{-1}\,\xi\,(t_{i_1}, \alpha, J, \vec{p}) \tag{4}$$

The correlator follows as

$$\begin{aligned} &C_{M-M}\,(t_{f_1}, t_{i_1}; \vec{p}_{f_1}, \vec{p}_{i_1}; \Gamma_{f_1}, \Gamma_{i_1}) \\ &= -\sum_{\vec{x}_{f_2}} (\Gamma_{i_1}\,\gamma_5)_{\alpha\beta}\ (J\,\phi\,(t_{i_1}, \beta, J, 0))^{\dagger}_{\vec{x}_{f_1}}\ \gamma_5\,\Gamma_{f_1}\,J\,\phi\,(t_{i_1}, \alpha, J, \vec{p}_{i_1})_{\vec{x}_{f_1}}\ \mathrm{e}^{i\vec{p}_{f_1}\vec{x}_{f_1}} \end{aligned} \tag{5}$$

In QLUA we calculate $-C_{M-M}\,(t_{f_1}, t_{i_1}; \vec{p}_{f_1}, \vec{p}_{i_1}; \Gamma_{f_1}, \Gamma_{i_1})$, i.e. **without the -1 from the closed fermion loop**. The Fourier transform in the source location $\vec{x}_{i_1}$ is performed implicitly, no further phase has to be added.
We contract for the choices

- $\Gamma_{i_1} \in \{\gamma_i,\ \gamma_0\,\gamma_i,\ \gamma_5\}$
- $\Gamma_{f_1} \in \{\gamma_i,\ \gamma_0\,\gamma_i,\ \gamma_5\}$
- all momentum combinations for $\vec{p}_{i_1}$, $\vec{p}_{f_1}$

1.1.2 Correlators of type $MxM - M$

Singly and **doubly quark-disconected diagrams** do not contribute for isospin quantum numbers $I = 1$, $I_3 = 0$ due to $SU(2)$ isospin symmetry.
We contract

$$\begin{aligned} &C_{MxM-M}\,(t_{f_1}, t_{i_1}, t_{i_2}; \vec{p}_{f_1}, \vec{p}_{i_2}, \vec{x}_{i_1}; \Gamma_{J,f_1}, \Gamma_{J,i_2}) \\ &= -\sum_{\vec{x}_{f_1}} \mathrm{Tr}\left(\left(\gamma_5\ (J\,S\,J)_{f_1,i_1}\ \gamma_5\right)^{\dagger}\ \Gamma_{f_1}\ \left(J\,T\,(t_{i_2}, \vec{p}_{i_2}; \Gamma_{J,i_2})\ J\right)_{f_1,i_1}\ \Gamma_{i_1}\right)\ \mathrm{e}^{i\vec{p}_{f_1}\vec{x}_{f_1}} \end{aligned} \tag{6}$$

Here, $(T(\ldots)\,J)_{\cdot,i_1}$ is the sequential propagator obtained from a smeared point source.

In QLUA **without factor -1 from closed fermion loop**. No Fourier transform in $\vec{x}_{i_1}$, phase has to be added at analysis time.

We contract for the choices

- $\Gamma_{i_1} = \Gamma_{i_2} = \gamma_5$
- $\Gamma_{f_1} \in \{\gamma_i,\ \gamma_0\,\gamma_i\}$
- all momentum combinations for $\vec{p}_{i_1}$, $\vec{p}_{i_2}$, $\vec{p}_{f_1}$

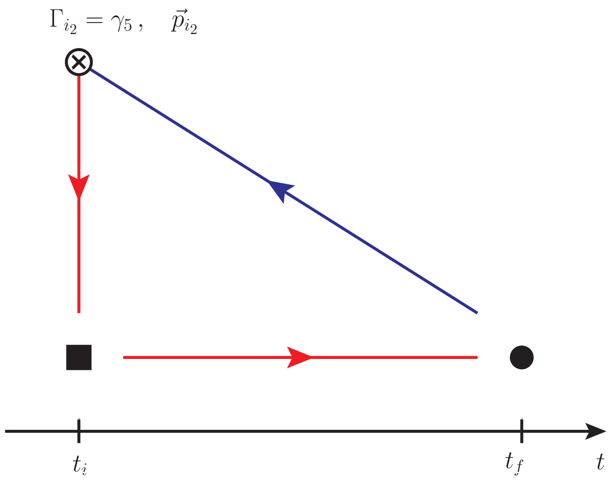

Figure 2: **Fully quark-connected diagrams of type** $MxM - M$ (triangle diagrams) with 2 free vertices (Γ_{i_1}, Γ_{f_2}) built from a propagator (red) and and sequential propagator through the source timeslice (blue); the Dirac structure in the sequential vertex is fixed to $\Gamma_{i_2} = \gamma_5$.

1.1.3 Correlators of type $MxM - MxM$

Diagrams of **higher degree of quark-disconnectedness "singly"** do not contribute.

Calculation of the direct diagram Obtained from product of correlators in eqs. (1) and (5) using $\Gamma_l = \gamma_5$ for all $l \in i_1, i_2, f_1, f_2$.

Calculation of the box diagram Using the stochastic timeslice propagators to connect f_1 and f_2, we can decompose the box diagram contraction

$$C^{\mathrm{box}}_{MxM-MxM} = \mathrm{Tr}\left(T_{f_2 i_1}\left(t_{i_2};\vec{p}_{i_2};\Gamma_{J,i_2}\right)\,\Gamma_{J,i_1}\left(p_{i_1}\right)\,\gamma_5\,S^{\tilde{\dagger}}_{f_1 i_1}\,\gamma_5\,\Gamma_{J,f_1}\left(p_{f_1}\right)\,\phi\left(f_2\right)_{f_1}\,\xi\left(f_2\right)^{\tilde{\dagger}}_{f_2}\,\Gamma_{J,f_2}\left(p_{f_2}\right)\right)\,. \tag{7}$$

We use the notation

$$\Gamma_{J,l}\left(p_l\right)_{x,y} = J\left(\vec{x},\vec{x}'\right)\,\Gamma_l\,\mathrm{e}^{i\vec{p}_l(\vec{x}'-\vec{y}')}\,\mathbb{1}_{\mathrm{col}}\,J^{\dagger}\left(\vec{y}',\vec{y}\right)\,\delta_{t_x,t_l}\,\delta_{t_x,t_y} \tag{8}$$

and $l \in \{i_1, i_2, f_1, f_2\}$. The operation $(\quad)^{\tilde{\dagger}}$ refers to the spin-color adjoint object.

$$\begin{array}{rcll} S_{f_1,i_1} & = & S_{x_{f_1},x_{i_1}} & \text{forward propagator from source at } x_{i_1} \\ T\left(\ldots\right)_{f_2,i_1} & = & T\left(\ldots\right)_{x_{f_2},x_{i_1}} & \text{sequential propagator} \\ \xi\left(f_2\right)_{f_2} & = & \xi\left(f_2\right)_{x_{f_2}} & \text{stochastic source on timeslice } t_{f_2} \\ \phi\left(f_2\right)_{f_1} & = & \phi\left(f_2\right)_{x_{f_1}} & \text{stochastic propagator from timeslice } t_{f_2} \end{array} \tag{9}$$

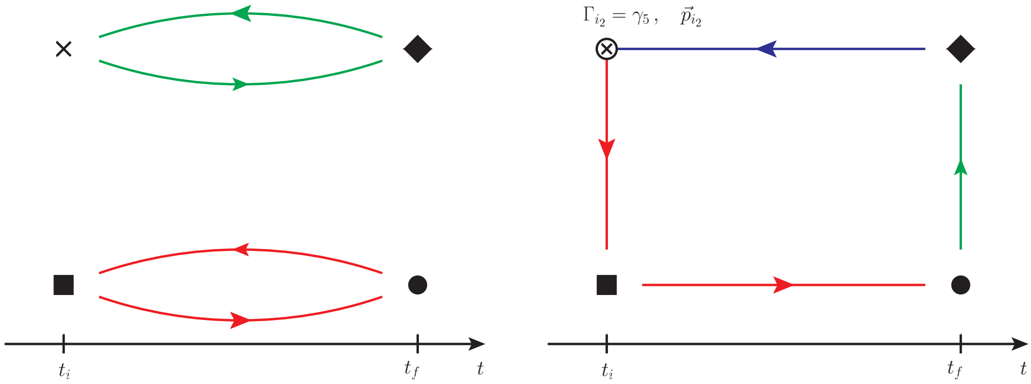

Figure 3: Left: **Singly quark-disconnected diagram of type** $MxM - MxM$ (direct diagram) with 4 free vertices built from propagators (red) and and stochastic propagators (green); the same contractions will give the diagrams of type $M - M$ diagrams (single meson at source and sink) in Fig. [1]; right: **Fully quark-connexted diagram Box diagram of type** $MxM - MxM$ (box diagram) with 3 free vertices built from propagator (red), sequential propagator (blue, through the source timeslice) and stochastic propagator (green) at final time.

$\Gamma_{i_1}(p_{i_1})$ does not carry the subscript J, since the point sources for for S_{f_1,i_1} and $T_{f_2,i_1}(p_{i_2})$ have been smeared before the inversions. x_{i_1} is the source location and $\vec{x}_{i_1}$ is not summed over. The momentum p_{i_1} is fixed by multiplying the contraction with the phase factor $\mathrm{e}^{i\vec{p}_{i_1}\vec{x}_{i_1}}$, which depends only on the momentum vector $\vec{p}_{i_1}$.
We thus need the two objects

$$\eta^r_\xi\left(t_{f_2}, t_{i_1}; \vec{p}_{f_2}, \vec{p}_{i_2}; \vec{x}_{i_1}; \Gamma_{J,f_2}, \Gamma_{J,i_2}\right)_{\alpha,a} = \sum_{\vec{x}_{f_2}} \left(J\,\xi^r\left(f_1\right)\right)^\dagger_{f_2} \Gamma_{f_2}\left(p_{f_2}\right)\,\left(J\,T\left(p_{i_2}\right)\,J\right)_{f_2,i_1} \quad (10)$$

$$\eta^r_\phi\left(t_{f_1}, t_{i_1}; \vec{p}_{f_1}; \vec{x}_{i_1}; \Gamma_{J,f_1}\right)_{\alpha,a} = \sum_{\vec{x}_{f_1}} \left(J\,S\,J\right)^\dagger_{f_1,i_1}\,\gamma_5\,\Gamma_{f_1}\left(p_{f_1}\right)\,\left(J\,\phi^r\left(f_1\right)\right)_{f_1} \quad (11)$$

For the box diagram in the ρ-correlation matrix we have the following simplifications

- $\Gamma_l = \gamma_5$ for all $l \in \{i_1, i_2, f_1, f_2\}$;
- $t_{f_1} = t_{f_2} = t_f$ sink timeslice;
- $t_{i_1} = t_{i_2} = t_i$ source timeslice.

The second property allows us to fill two *L:DiracFermions*s with the timeslices $\xi\left(t_f\right)_{t_f}$ and $\phi\left(t_f\right)_{t_f}$, respectively. Given one source time, we can then evaluate the box diagram for all sink timeslices in one call to the contraction routine.

For a specific choice of $\{p_l \,|\, l \in \{i_2, f_1, f_2\}\}$ we then calculate

$$C^{\text{box}}_{MxM-MxM}\,(t_f, t_i; \vec{p}_{f_1}, \vec{p}_{f_1}, \vec{p}_{i_1}, \vec{p}_{i_2})$$
$$= -\sum_{\alpha,\beta} \sum_{a,b} (\Gamma_{i_1})^{ab}_{\alpha\beta}\; \eta^r_\phi\,(t_{f_1}, t_{i_1}; \vec{p}_{f_1}; \vec{x}_{i_1}; \Gamma_{J,f_1})_{\beta,b}\; \eta^r_\xi\,(t_{f_2}, t_{i_1}; \vec{p}_{f_2}, \vec{p}_{i_2}; \vec{x}_{i_1}; \Gamma_{J,f_2}, \Gamma_{J,i_2})_{\alpha,a}\; \mathrm{e}^{i\vec{p}_{i_1}\vec{x}_{i_1}}\,. \tag{12}$$

We contract for $0 \le t_f - t_i \le t_{\text{max}}$ and all momentum combinations at source i_2 (sequential source) and sinks f_1, f_2. The Fourier transform in $\vec{x}_{i_1}$ (point source location) is not done at contraction time. The phase factor to set $\vec{p}_{i_1}$ must be added at analysis time.

With the current number of source locations and *dt_source_sink_2pt* in QLUA we can in principle contract for any sink time t_f.

1.2 Contractions for 3-point correlation functions

1.2.1 Correlators of type $M - J - M$

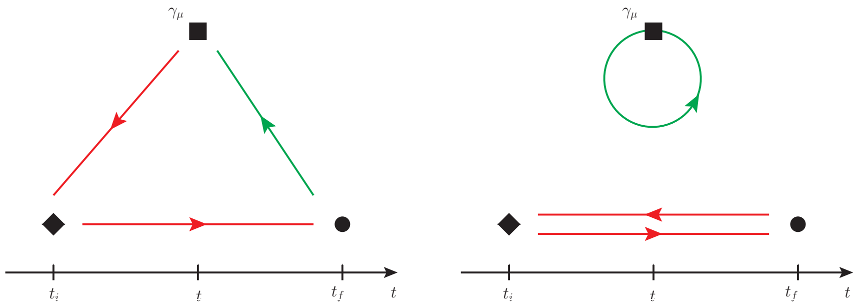

Figure 4: Left: **fully quark-connected diagram of type** $M - J - M$ built from forward (red) and stochastic (green) propagators); single-meson operator at source and sink; right: **singly quark-disconnected diagram of type** $M - J - M$ built from forward and stochastic propagators; the stochastic propagator in the left diagram differs from the one in the loop in the right diagram due to different smearing.

The 3-point functions are calculated for each sink time separately.

The decomposition of the contraction for left diagram in figure [4] reads

$$\begin{aligned}
&C_{M-J-M}\left(t_f, t_i; \vec{p}_{f_1}, \vec{q}, \vec{p}_{i_1}; \Gamma_{J,f_1}, \Gamma_c, \Gamma_{J,i_1}\right) \\
&= -\mathrm{Tr}\left(S_{f_1 i_1}\,\Gamma_{J,i_1}\left(\vec{p}_{i_1}\right)\,\gamma_5\,S^{\tilde{\dagger}}_{ci}\,\gamma_5\,\Gamma_c\left(\vec{q}\right)\,S_{cf}\,\Gamma_{J,f_1}\left(\vec{p}_{f_1}\right)\right) \qquad (13)\\
&= -\mathrm{Tr}\left(S_{fi}\,\Gamma_{J,i_1}\left(\vec{p}_{i_1}\right)\,\gamma_5\,S^{\tilde{\dagger}}_{ci}\,\gamma_5\,\Gamma_c\left(\vec{q}\right)\,\phi^r\left(f_1\right)_c\,\xi^r\left(f_1\right)^{\tilde{\dagger}}_{f_1}\,\Gamma_{J,f_1}\left(\vec{p}_{f_1}\right)\right)\\
&= -\left[\left(J\,\xi^r\left(f_1\right)_{f_1}\right)^{\tilde{\dagger}}\,\Gamma_{f_1}\left(\vec{p}_{f_1}\right)\,\left(J\,S\,J\right)_{f_1,i_1}\right]\,\Gamma_{i-1}\left(\vec{p}_{i_1}\right)\,\gamma_5\,\left[\left(S\,J\right)^{\tilde{\dagger}}_{ci_1}\,\gamma_5\,\Gamma_c\left(\vec{q}\right)\,\phi^r\left(f_1\right)_c\right]\\
&= -\sum_{\alpha,\beta}\sum_{a,b}\left(\Gamma_{i_1}\,\gamma_5\right)^{ab}_{\alpha\beta}\,\eta^r_\phi\left(t_f, t_i; \vec{q}, \vec{x}_{i_1}; \Gamma_c\right)_{\beta,b}\,\eta^r_\xi\left(t_f, t_i; \vec{p}_{f_1}, \vec{x}_{i_1}; \Gamma_{J,f_1}\right)_{\alpha,a}\,\mathrm{e}^{i\vec{p}_{i_1}\vec{x}_{i_1}}
\end{aligned}$$

with the fields

$$\eta^r_\phi\left(t_f, t_i; \vec{q}, \vec{x}_{i_1}; \Gamma_c\right) = \sum_{\vec{x}_c}\,\left(S\,J\right)^{\tilde{\dagger}}_{ci_1}\,\gamma_5\,\Gamma_c\,\phi^r\left(f_1\right)_c\,\mathrm{e}^{i\vec{q}\vec{x}_c} \qquad (14)$$

$$\eta^r_\xi\left(t_f, t_i; \vec{p}_{f_1}, \vec{x}_{i_1}; \Gamma_{J,f_1}\right) = \sum_{\vec{x}_{f_1}}\,\left(J\,\xi^r\left(f_1\right)_{f_1}\right)^{\tilde{\dagger}}\,\Gamma_{f_1}\,\left(J\,S\,J\right)_{f_1,i_1}\,\mathrm{e}^{i\vec{p}_{f_1}\vec{x}_{f_1}}\,. \qquad (15)$$

For the diagrams of type $M-J-M$ one needs both the sink-smeared and sink-unsmeared forward propagators (always from a smeared source).

We contract for the choices

1. $\Gamma_{i_1} \in \{\gamma_i,\, \gamma_0\,\gamma_i\}$
2. $\Gamma_{f_1} = \gamma_5$
3. $\Gamma_c = \gamma_c$ and $\Gamma_c = \gamma_c\,\gamma_i\,\bar{\nabla}_i$ with $\gamma_c \in \{\gamma_\mu,\, \gamma_\mu\,\gamma_5\}$
4. all combinations of $\vec{q}$ (momentum of current insertion) and $\vec{p}_{f_1}$ (momentum of final state)
5. pre-set number of $t_{f_1} = t_f$ (final timeslice), which given a source location sets the source-sink time separation

1.2.2 Correlators of type $MxM - J - M$

Other **diagrams of degree singly quark-disconnected or higher** do not contribute for isospin $I = 1$, $I_3 = 0$.
We use the version on the right-hand side of figure [6].

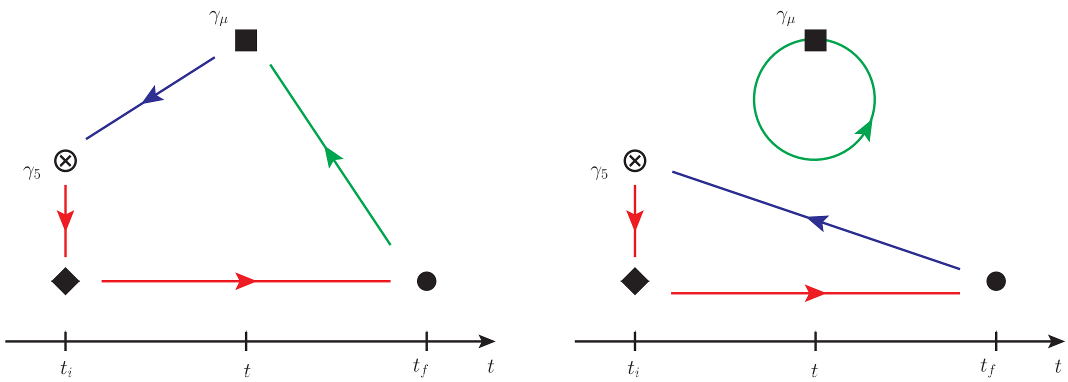

Figure 5: Left: **fully quark-connected diagram of type** $MxM - J - M$ built from forward (red), sequential (blue) and stochastic (green) propagarors; right: **singly quark-disconnected diagram of type** $MxM - J - M$; the stochastic propagator in the diagram is unsmeared.

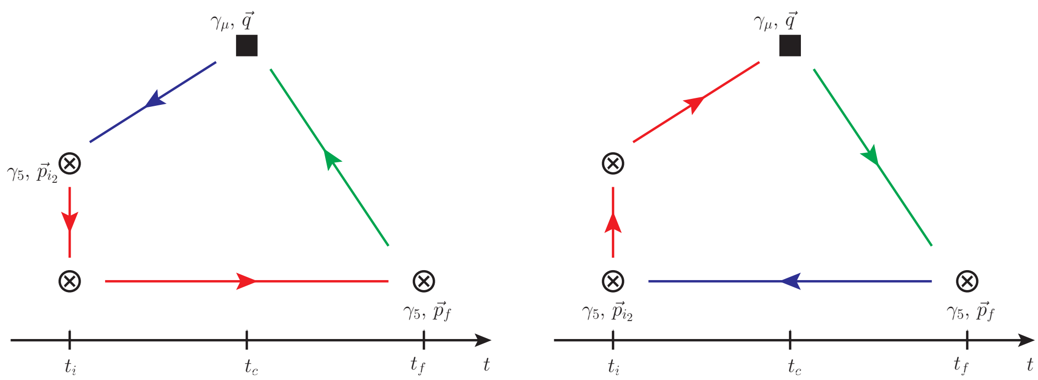

Figure 6: Comparison of two ways to calculate the box diagram of type $MxM - J - M$.

$$
\begin{aligned}
&C^{\mathrm{box}}_{MxM-J-M}\left(t_f, t_i; \vec{p}_{f_1}, \vec{q}, \vec{p}_{i_1}, \vec{p}_{i_2}; \Gamma_c\right) && (16)\\
&= -\mathrm{Tr}\left(T_{f_1 i_1}\, \Gamma_{J,i_1}\left(\vec{p}_{i_1}\right)\, \gamma_5\, S^{\tilde{\dagger}}_{c i_1}\, \gamma_5\, \Gamma_c\left(\vec{q}\right)\, S_{cf}\, \Gamma_{J,f_1}\left(\vec{p}_f\right)\right) && (17)\\
&= -\mathrm{Tr}\left(T_{f i_1}\, \Gamma_{J,i_1}\left(\vec{p}_{i_1}\right)\, \gamma_5\, S^{\tilde{\dagger}}_{c i_1}\, \gamma_5\, \Gamma_c\left(\vec{q}\right)\, \phi^r\left(f_1\right)_c\, \xi^r\left(f_1\right)^{\tilde{\dagger}}_f\, \Gamma_{J,f_1}\left(\vec{p}_{f_1}\right)\right)\\
&= -\left[\left(J\,\xi^r\left(f_1\right)\right)^{\tilde{\dagger}}_{f_1}\, \Gamma_{f_1}\left(\vec{p}_{f_1}\right)\, \left(J\,T\,J\right)_{f_1,i_1}\right]\, \Gamma_{i_1}\left(\vec{p}_{i_1}\right)\, \gamma_5\, \left[\left(S\,J\right)^{\tilde{\dagger}}_{c,i_1}\, \gamma_5\, \Gamma_c\left(\vec{q}\right)\, \phi^r\left(f\right)_c\right]\\
&= -\left(\Gamma_{i_1}\left(p_{i_1}\right)\, \gamma_5\right)^{ab}_{\alpha\beta}\, \eta^r_\xi\left(t_f, t_i; \vec{p}_{f_1}, \vec{p}_{i_2}, \vec{x}_{i_1}; \Gamma_{f_1}, \Gamma_{i_2}\right)_{\alpha,a}\, \eta^r_\phi\left(t_f, t_i; \vec{q}, \vec{x}_{i_1}; \Gamma_c\right)_{\beta,b}
\end{aligned}
$$

with fields

$$
\eta^r_\xi\left(t_f, t_i; \vec{p}_{f_1}, \vec{p}_{i_2}, \vec{x}_{i_1}; \Gamma_{f_1}, \Gamma_{i_2}\right) = \sum_{\vec{x}_{f_1}} \left(J\,\xi^r\left(f_1\right)\right)^{\tilde{\dagger}}_{f_1}\, \Gamma_{f_1}\left(\vec{p}_{f_1}\right)\, \left(J\,T\,J\right)_{f_1,i_1}\, \mathrm{e}^{i\vec{p}_{f_1}\vec{x}_{f_1}} \tag{18}
$$

$$
\eta^r_\phi\left(t_f, t_i; \vec{q}, \vec{x}_{i_1}; \Gamma_c\right) = \sum_{\vec{x}_c} \left(S\,J\right)^{\tilde{\dagger}}_{c,i_1}\, \gamma_5\, \Gamma_c\, \phi^r\left(f\right)_c\, \mathrm{e}^{i\vec{q}\vec{x}_c}\,. \tag{19}
$$

We have the following restrictions

- $\Gamma_{f_1} = \gamma_5 = \Gamma_{i_1} = \Gamma_{i_2}$
- Γ_c as in 1.2.1
- all momentum combinations for $\vec{p}_{f_1}$, $\vec{p}_{i_2}$

The Fourier tranform in $\vec{x}_{i_1}$ (point source location) is not carried out at contraction time; the phase has to be added at analysis time. In QLUA we do **not include the factor -1 for the closed fermion loop**.

The next diagram is the crossed box diagram in figure [7]. Using the one-end trick we

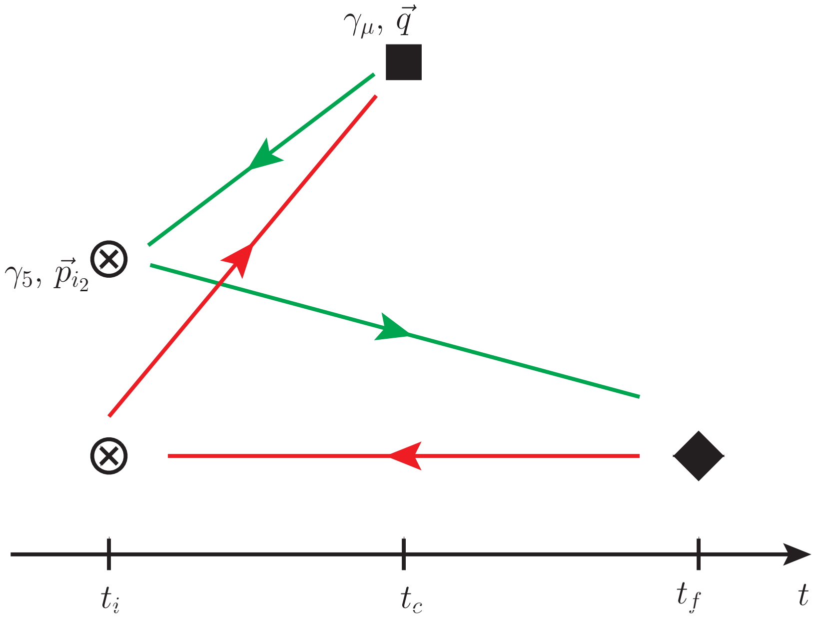

Figure 7: $MxM-J-M$ crossed box diagram; forward propagators are in red, stochastic propagators are in green.

write the correlator as

$$C^{\text{crossed box}}_{MxM-J-M}\left(t_f, t_i; \vec{p}_{f_1}, \vec{q}, \vec{p}_{i_1}, \vec{p}_{i_2}; \Gamma_c\right) \tag{20}$$
$$= -\mathrm{Tr}\left(S_{f_1,i_1}\,\Gamma_{J,i_1}\left(\vec{p}_{i_1}\right)\,S_{i_1,c}\,\Gamma_c\left(\vec{q}\right)\,\phi^r\left(i_2,\vec{p}_{i_2},\alpha\right)_c\,\left(\Gamma_{J,i_2}\,\gamma_5\right)_{\alpha\beta}\,\phi^r\left(i_2,0,\beta\right)^{\dagger}_{f,}\,\gamma_5\,\Gamma_{J,f}\left(\vec{p}_f\right)\right)$$
$$= -\sum_{\alpha,\beta}\sum_{a,b,\gamma,\delta}\left(\Gamma_{i_1}\right)^{ab}_{\gamma\delta}\,\eta^r_\phi\left(t_c,t_i;\vec{q},\vec{p}_{i_2};\vec{x}_{i_1}\Gamma_c;\alpha\right)^b_\delta\,\eta^r_{\bar{\phi}}\left(t_f,t_i;\vec{p}_f;\vec{x}_{i_1}\Gamma_f;\beta,\gamma\right)^a_\gamma\,\mathrm{e}^{i\vec{p}_{i_1}\vec{x}_{i_1}}\,\left(\Gamma_{i_2}\,\gamma_5\right)_{\alpha\beta}$$

with fields

$$\eta^r_\phi\left(t_c,t_i;\vec{q},\vec{p}_{i_2};\vec{x}_{i_1}\Gamma_c;\alpha\right) = \left(S_{c,i_1}\,J\right)^{\dagger}\,\Gamma_c\,\phi^r\left(i_2,\vec{p}_{i_2},\alpha\right)_c\,\mathrm{e}^{i\vec{q}\vec{x}_c} \tag{21}$$
$$\eta^r_{\bar{\phi}}\left(t_f,t_i;\vec{p}_f;\vec{x}_{i_1}\Gamma_f;\beta\right) = \left(J\,\phi^r\left(i_2,0,\beta\right)\right)^{\dagger}_f\,\gamma_5\,\Gamma_f\,\left(J\,S\right)_{f,i_1}\,\mathrm{e}^{i\vec{p}_f\vec{x}_f} \tag{22}$$

Here $\phi^r\left(i_2,\vec{p}_{i_2},\alpha\right)$ is a stochastic timeslice propagator for the one-end-trick with momentum set to $\vec{p}_{i_2}$ and non-zero source spin component α. We then have

$$\phi^r\left(i_2,\vec{p}_{i_2},\alpha\right)_x = \left(S\,J\right)(x,y)\,\eta^r\left(i_2,\vec{p}_{i_2},\alpha\right)_y \tag{23}$$
$$\eta^r\left(i_2,\vec{p}_{i_2},\alpha\right)_{y,\beta,b} = \mathrm{e}^{i\vec{p}_{i_2}\vec{y}}\,\delta_{t_y,t_{i_2}}\,\delta_{\beta,\alpha}\,\eta^r\left(i_2\right)_{\vec{y},b} \tag{24}$$

such that we have the expectation value

$$
\begin{aligned}
&\mathrm{E}\left[\phi^{r}\left(i_{2}, \vec{p}_{i_{2}}, \alpha\right)_{x_{c}, \gamma, a}\left(\Gamma_{J, i_{2}} \gamma_{5}\right)_{\alpha \beta} \phi^{r}\left(i_{2}, 0, \beta\right)_{x_{f}, \delta, b}^{\tilde{\dagger}}\right] \qquad (25)\\
&=(S\, J)\left(x_{c}, y\right)_{\gamma \lambda}^{a c} \mathrm{e}^{i \vec{p}_{i_{2}} \vec{y}} \delta_{t_{y}, t_{i_{2}}} \delta_{\lambda, \alpha} \mathrm{E}\left[\eta^{r}\left(i_{2}\right)_{\vec{y}, c} \eta^{r}\left(i_{2}\right)_{\vec{z}, d}^{*}\right] \delta_{t_{z}, t_{i_{2}}} \delta_{\beta, \kappa}(S\, J)\left(x_{f}, z\right)_{\delta \kappa}^{b d *}\left(\Gamma_{c} \gamma_{5}\right)_{\alpha \beta} \\
&=(S\, J)\left(x_{c}, y\right)_{\gamma \lambda}^{a c} \mathrm{e}^{i \vec{p}_{i_{2}} \vec{y}} \delta_{t_{y}, t_{i_{2}}} \delta_{\lambda, \alpha} \delta_{\vec{y}, \vec{z}} \delta_{c, d} \delta_{t_{z}, t_{i_{2}}} \delta_{\beta, \kappa}(S\, J)\left(x_{f}, z\right)_{\delta \kappa}^{b d *}\left(\Gamma_{c} \gamma_{5}\right)_{\alpha \beta} \\
&=(S\, J)\left(x_{c} ; t_{i_{2}}, \vec{y}\right)_{\gamma \alpha}^{a c} \mathrm{e}^{i \vec{p}_{i_{2}} \vec{y}}(S\, J)\left(x_{f} ; t_{i_{2}}, \vec{y}\right)_{\delta \beta}^{b c *}\left(\Gamma_{c} \gamma_{5}\right)_{\alpha \beta} \\
&=(S\, J)\left(x_{c} ; t_{i_{2}}, \vec{y}\right)_{\gamma \alpha}^{a c} \mathrm{e}^{i \vec{p}_{i_{2}} \vec{y}}\left(\Gamma_{c} \gamma_{5}\right)_{\alpha \beta}(S\, J)^{\dagger}\left(t_{i_{2}}, \vec{y} ; x_{f}\right)_{\beta \delta}^{c b} \\
&=\left((S\, J)\left(x_{c} ; t_{i_{2}}, \vec{y}\right) \mathrm{e}^{i \vec{p}_{i_{2}} \vec{y}} \Gamma_{c}\,(J\, S)\left(t_{i_{2}}, \vec{y} ; x_{f}\right) \gamma_{5}\right)_{\gamma \delta}^{a b} .
\end{aligned}
$$

The propagators ϕ^r used in the equations above are the same we use the direct $MxM - MxM$ diagram.

For more efficiency we use the alternative distribution of the sequential source momentum $\vec{p}_{i_2}$ and calculate

- $\eta_{\bar{\phi}} \longleftarrow \phi\,(i_2, \vec{p}_{i_2}, \alpha)$ and
- $\eta_{\phi} \longleftarrow \phi\,(i_2, 0, \alpha)$,

which gives $N_{\Gamma_c} \times N_{\vec{p}_c}$ combinations for η_ϕ and $N_{\vec{p}_{i_2}} \times N_{\vec{p}_f}$ combinations for $\eta_{\bar{\phi}}$. Doing that *we write the sequential source momentum label using the negative sequential source momentum*, because for given $\vec{p}_{i_2}$, what enters the correlator is the phase $\mathrm{e}^{-i\vec{x}_{i_2}\vec{p}_{i_2}}$ due to Hermitean conjugate in the definition (22).

2 Contractions and diagrams for the heavy-light quark sector

2.1 Contractions for 2-point correlation functions

For $M - M$ with piont source propagators or one-end-trick these are the same contractions here, just replace one of the two propagators with a heavy quark propagator.

2.2 Contractions for 3-point correlation functions

The difference in contractions for the heavy-light system compared to the light-light system is the change of the stochastic timeslice propagator ϕ. For the heavy-light system, this must be the heavy quark propagator.

3 Timings

object	time / seconds	number	total time / seconds
$\chi_l^\dagger\, T$	2.008 (6)	$N_{\mathrm{src}} \times N_{p_{i_2}} \times N_{\mathrm{sample}}$	2602
$S_l^\dagger\, \phi_l$	1.82 (2)	$N_{\mathrm{src}} \times N_{\mathrm{coh}} \times N_{\mathrm{sample}}$	175
combine	0.069 (2)	$N_{\mathrm{src}} \times N_{\mathrm{coh}} \times N_{p_{i_2}} \times N_{\mathrm{sample}}$	180
Σ			$2957\,\mathrm{s} \lesssim 1.0\,\mathrm{h}$

object	time / seconds	number	total time / seconds
S_l	23.7 (1.5)	$N_{\text{src}} \times N_{\text{coh}}$	190
S_c	24.4 (3)	$N_{\text{src}} \times N_{\text{coh}}$	195
S_b	12.5 (2)	$N_{\text{src}} \times N_{\text{coh}}$	100
ϕ_l	1.85 (2)	$N_{\text{sink}} \times N_{\text{sample}}$	2131
ϕ_c	1.964 (4)	$N_{\text{sink}} \times N_{\text{sample}}$	2263
ϕ_b	1.042 (2)	$N_{\text{sink}} \times N_{\text{sample}}$	1200
T	24.7 (1.1)	$N_{\text{src}} \times N_{p_{i_2}}$	2668
Σ			$8747\,\text{s} \lesssim 2.5\,\text{h}$

object	time per object / seconds	number	total time / seconds
fwd_light_dgc_phi_light	15.49 (0.00)	$N_{\text{dt}} \times N_{\text{sample}}$	558
fwd_light_dgc_phi_charm	15.50 (0.07)		558
fwd_light_gc_phi_bottom	15.30 (0.17)		551
fwd_light_gc_phi_light	15.44 (0.02)	$N_{\text{dt}} \times N_{\text{sample}}$	556
fwd_light_gc_phi_charm	15.52 (0.05)		559
fwd_light_dgc_phi_bottom	15.18 (0.16)		546
xibar_light_fwd_light	2.60 (0.02)	$N_{\text{dt}} \times N_{\text{sample}}$	94

xibar_charm_fwd_light	2.44 (0.04)		88
xibar_bottom_fwd_light	2.44 (0.04)		88
xibar_light_seq_light	2.48 (0.13)	$N_{\rm dt} \times N_{p_{i_2}} \times N_{\rm sample}$	2411
xibar_charm_seq_light	2.62 (0.13)		2547
xibar_bottom_seq_light	2.77 (0.13)		2692
Σ			$11248\,{\rm s} \lesssim 3.5\,{\rm h}$

For the esitmated times we use our standard values

- $N_{\rm sample} = 12$;
- $N_{p_{i_2}} = 27$;
- $N_{\rm dt} = 3$;
- $N_{\rm src} = 4$;
- $N_{\rm coh} = 2$;
- $N_{\rm sink} = N_{\rm sink}\left(N_{\rm src}, N_{\rm coh}, N_{\rm sink}^{(2pt)}\right) = T$ for $N^{(2pt)} = 24$.

We arrive at a walltime of $\lesssim 7\,{\rm h}$ (including at least about 10 % fluctuation for the timings) on 768 cores, which means it needs $\lesssim 768\,{\rm cores} \times 7\,{\rm h} \times 2 = 10445\,{\rm core\ h}$ on Edison. We can straightforwardly bundle up calculations for several configurations to get the discount of 0.6, which means about 6270 core h per configuration.

Given the approximately 9 Mio core h we have, this would abount to more than 1000 configurations.
Relevant changes in the contraction scripts are:

- factorization of diagrams (split up by stochastic propagator and source);
- due to $dt_{\rm source-sink}/a \leq 12$ and $N_{\rm src} \times N_{\rm coh} = 8 = T/12$ for the 3-point functions the contractions are done for all source locations and all relevant sink times simultaneously;

- the *combine* step, to build the final diagram *is taken out of the contraction scripts* (now *invert_contract_v4.qlua*); the final combination of the factors of the diagram can be done straighforwardly on a single-core desktop or the like

3.0.1 Queuing times

32 nodes	704 nodes
4-01:46:57	0-22:22:32
	2-01:25:39
	2-01:32:20