Noise reduction exploration for the extraction of the neutral pion mass

(from 3-month visiting period at Humboldt University)

RC* collaboration meeting

David Albandea

Wick contraction with C* BC

- Quark-antiquark doublet formalism

$$\chi_f(x) = \begin{pmatrix} \psi_f(x) \\ \psi_f^C(x) \end{pmatrix} \qquad \chi_f(x+L\hat{k}) = K\chi_f(x) \qquad K = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_F = \frac{1}{2}\sum_f \int d^4x \; \bar{\chi}_f(x) D_f \chi_f(x)$$

- χ and $\bar{\chi}$ are not independent Grassman variables: $\bar{\chi} = (\bar{\psi}, \bar{\psi}^C) = -\chi^T C K$

⇒ non-vanishing $\langle \chi\bar{\chi} \rangle$, $\langle \bar{\chi}\bar{\chi} \rangle$, $\langle \chi\chi \rangle$

- General Wick contraction rule

$$\langle \underset{\substack{\alpha \\ c \\ r}}{\chi_f(x)} \underset{\substack{\beta \\ d \\ s}}{\chi_{f'}(y)} \rangle = -\delta_{f,f'} (CKD)^{-1}_{\substack{\alpha\beta \\ cd \\ rs}}$$

α, β : spin

c, d : color

r, s : doublet

Spectral decomposition

$$\langle 0| O(t)O^\dagger(0) |0\rangle = \sum \langle 0| O(t) |n\rangle \langle n| O^\dagger(0) |0\rangle$$

$$= \sum_n |\langle 0| O |n\rangle|^2 e^{-\Delta E_n t} \xrightarrow{t \gg 1} |\langle 0| O |0\rangle|^2 + |\langle 0| O |1\rangle|^2 e^{-\Delta E_1 t}.$$

☆ π^0 interpolating operator: $O_{\pi^0}(x) = \bar{\chi}_u(x)\gamma_5\chi_u(x) - \bar{\chi}_d(x)\gamma_5\chi_d(x)$

$$\langle O_{\pi^0}(n)\bar{O}_{\pi^0}(m)\rangle = \langle \bar{\chi}_u(n)\gamma_5\chi_u(n)\bar{\chi}_u(m)\gamma_5\chi_u(m)\rangle - \langle \bar{\chi}_u(n)\gamma_5\chi_u(n)\bar{\chi}_d(m)\gamma_5\chi_d(m)\rangle$$
$$+ u \leftrightarrow d$$

$$\langle O_{\pi^0}(x_0)\bar{O}_{\pi^0}(y_0)\rangle = -2\,\mathrm{tr}\left[\gamma_5 D_u^{-1}(x_0|y_0)\gamma_5 D_u^{-1}(y_0|x_0)\right]$$ connected

disconnected
$$\begin{cases} + \mathrm{tr}\left[\gamma_5 D_u^{-1}(x_0|x_0)\right] \mathrm{tr}\left[\gamma_5 D_u^{-1}(y_0|y_0)\right] \\ - \mathrm{tr}\left[\gamma_5 D_u^{-1}(x_0|x_0)\right] \mathrm{tr}\left[\gamma_5 D_d^{-1}(y_0|y_0)\right] + u \leftrightarrow d \end{cases}$$

Stochastic estimation of traces

- Stochastic representation of the identity matrix:

$$\left.\begin{aligned} \eta \sim \mathcal{CN}(0,1) \in \mathbb{C}^N \\ \mathbb{E}[\eta_i] = 0, \quad \mathbb{E}[\eta_i \eta_j^*] = \delta_{ij} \end{aligned}\right\} \quad \mathbb{E}[\eta\eta^\dagger] = \mathbb{I}_{N\times N}$$

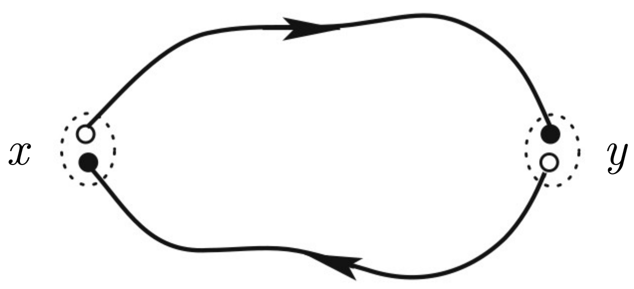
Can use this to estimate trace of a matrix (**Hutchinson algorithm**)

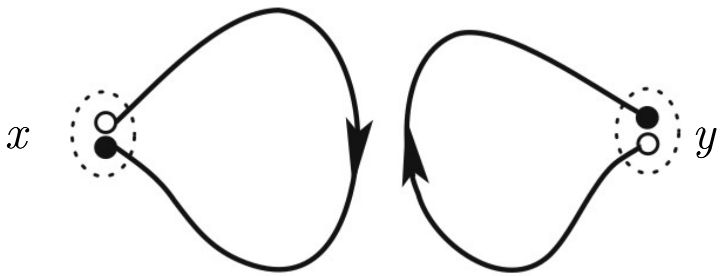
$$\mathrm{tr}\, A = \mathrm{tr}\left[A\mathbb{E}[\eta\eta^\dagger]\right] = \mathbb{E}[\eta^\dagger A \eta]$$

$$\sigma^2_{\mathrm{tr}\, A} = \mathrm{Var}[\eta^\dagger A \eta] = \mathrm{tr}\, AA^\dagger$$

- In our case $A = \gamma_5 D^{-1} \gamma_5 D^{-1}$ (connected) and $A = \gamma_5 D^{-1}$ (disconnected)

Stochastic estimation of traces





Connected pieces

$$C_{\text{conn.}}(y_0 - x_0) \supset \text{tr}\left[\gamma_5 D_u^{-1}(x_0|y_0)\gamma_5 D_u^{-1}(y_0|x_0)\right]$$

- Estimator:

$$\eta^\dagger_{(x_0)}\gamma_5 D_u^{-1}(x_0|y_0)\gamma_5 D_u^{-1}(y_0|x_0)\eta_{(x_0)}$$

- Only needs 1 inversion of D (per flavor)
- Error $\propto \dfrac{1}{\sqrt{N_{\text{src}}}}$

Disconnected pieces

$$C_{\text{disc.}}(y_0 - x_0) \supset \text{tr}\left[\gamma_5 D_u^{-1}(x_0|x_0)\right]\text{tr}\left[\gamma_5 D_u^{-1}(y_0|y_0)\right]$$

- Estimator:

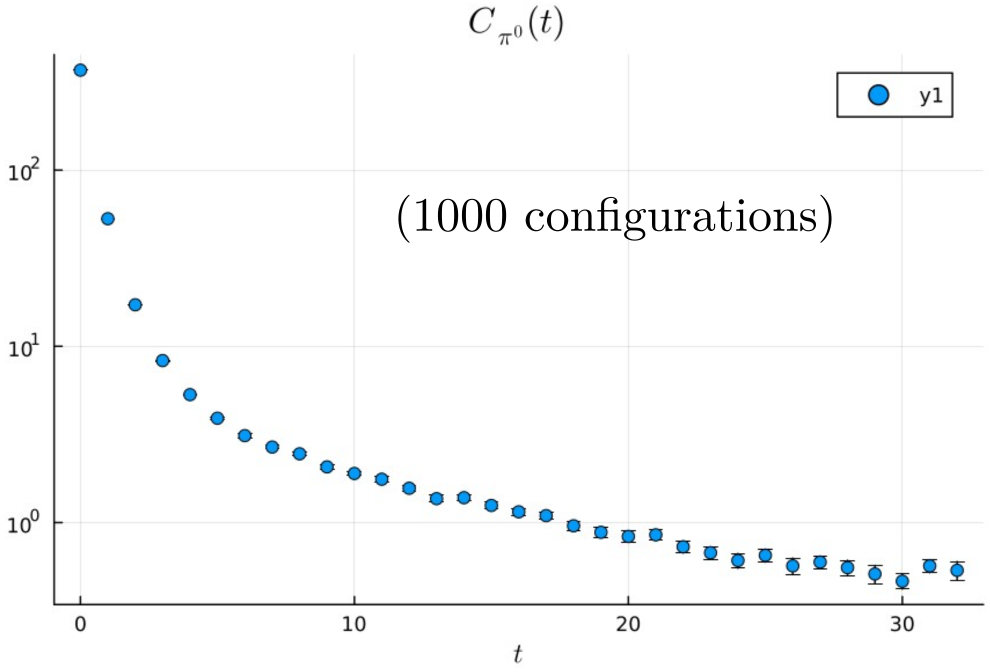
$$\eta^\dagger_{(x_0)}\gamma_5 D_u^{-1}(x_0|x_0)\eta_{(x_0)}\ \eta^\dagger_{(y_0)}\gamma_5 D_u^{-1}(y_0|y_0)\eta_{(y_0)}$$

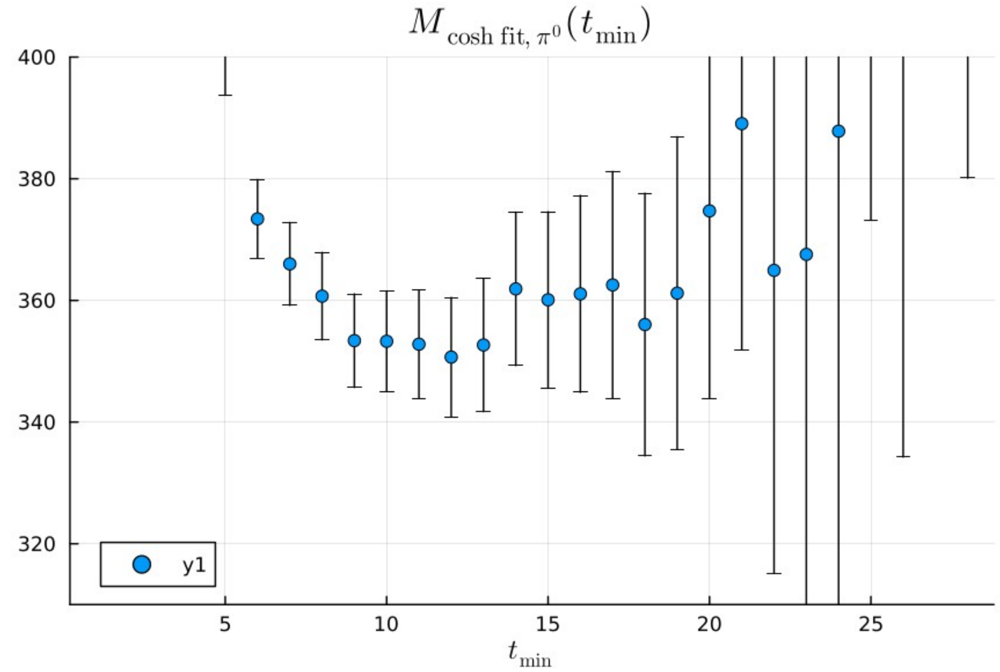
- Needs L_0+1 inversions of D
- Error $\propto \dfrac{1}{\sqrt{N_{\text{src}}^2}} = \dfrac{1}{N_{\text{src}}}$

Cheapest neutral pion mass

ensemble	lattice	β	α	κ_u	$\kappa_d = \kappa_s$	κ_c
`A360a50b324`	64×32^3	3.24	0.05	0.135560	0.134617	0.129583

a [fm]	$M_{\pi^\pm} = M_{K^\pm}$
0.05054(27)	358.6(3.7) MeV





$$C_{t_{\min}}(t) = A\cosh\left[M_{t_{\min}}\left(\frac{T}{2} - t\right)\right], \quad t \in [t_{\min}, T/2]$$

Need noise reduction techniques

- Smearing
- Increase number of sources

Smearing

- Smeared fermion fields

$$\Psi^{(S)} = (1+\omega H)^n \Psi \qquad \bar{\Psi}^{(S)} = \bar{\Psi}(1+\omega H)^n$$

H: spatial hopping operator with smeared SU(3) and U(1) gauge fields

- New Wick contraction rule

$$\langle \chi^{(S)}(x)\chi(y)\rangle = S\langle \chi(x)\chi(y)\rangle = -S(CKD)^{-1}(x,y)$$

Smearing source x

⇨ $C_{\mathrm{conn.}}(y_0 - x_0) \supset \mathrm{tr}\left[S\gamma_5 D_u^{-1}(x_0|y_0)\gamma_5 D_u^{-1}(y_0|x_0)S\right]$

⇨ $C_{\mathrm{disc.}}(y_0 - x_0) \supset \mathrm{tr}\left[S\gamma_5 D_u^{-1}(x_0|x_0)S\right]\,\mathrm{tr}\left[\gamma_5 D_u^{-1}(y_0|y_0)\right]$

Smearing

- Smeared fermion fields

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Smearing sink y

⇨ $C_{\text{conn.}}(y_0 - x_0) \supset \text{tr}\left[\gamma_5 D_u^{-1}(x_0|y_0) S S \gamma_5 D_u^{-1}(y_0|x_0)\right]$

⇨ $C_{\text{disc.}}(y_0 - x_0) \supset \text{tr}\left[\gamma_5 D_u^{-1}(x_0|x_0)\right] \text{tr}\left[S\gamma_5 D_u^{-1}(y_0|y_0) S\right]$

Smearing

- Smeared fermion fields

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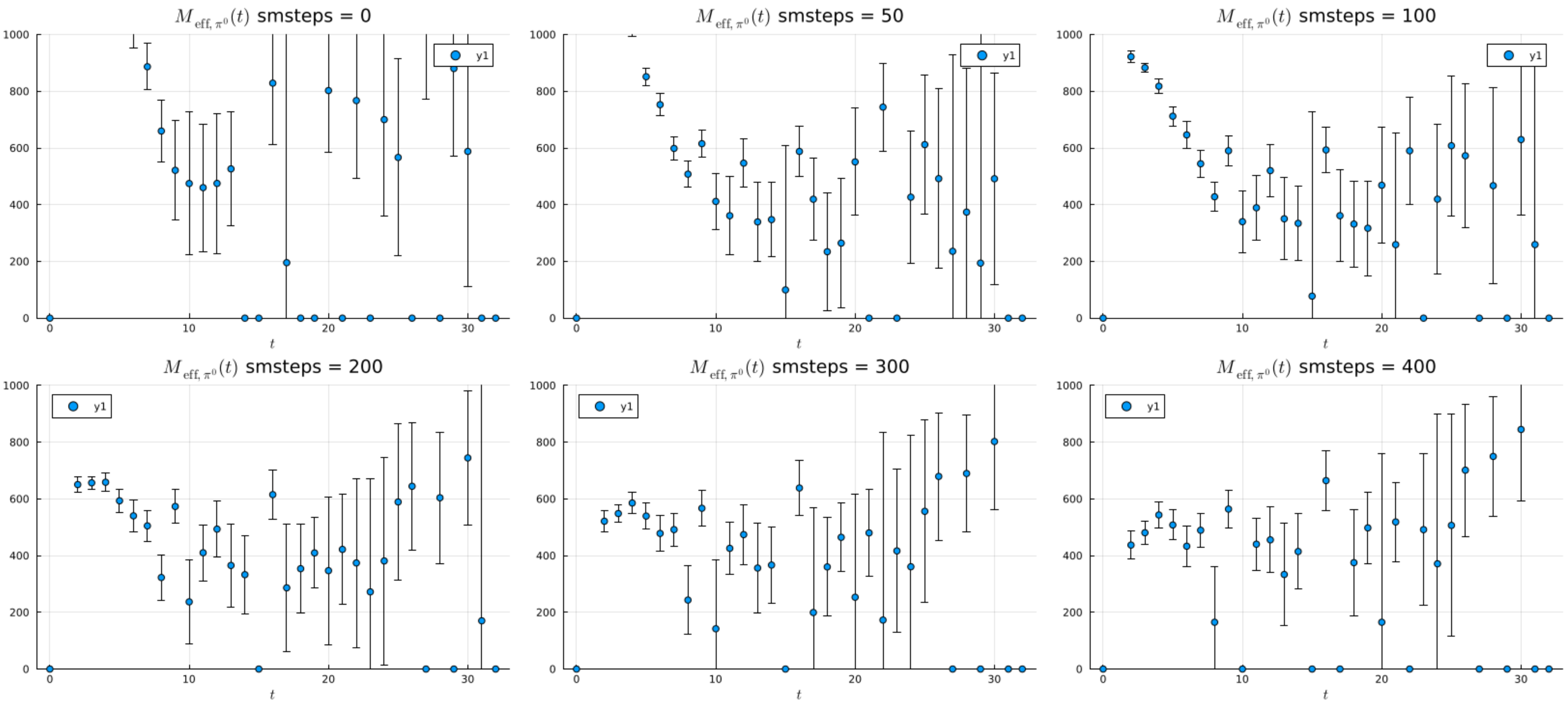
Exploration: # stochastic sources N_{src}: 1 - 200 # smearing steps n: 0 - 400

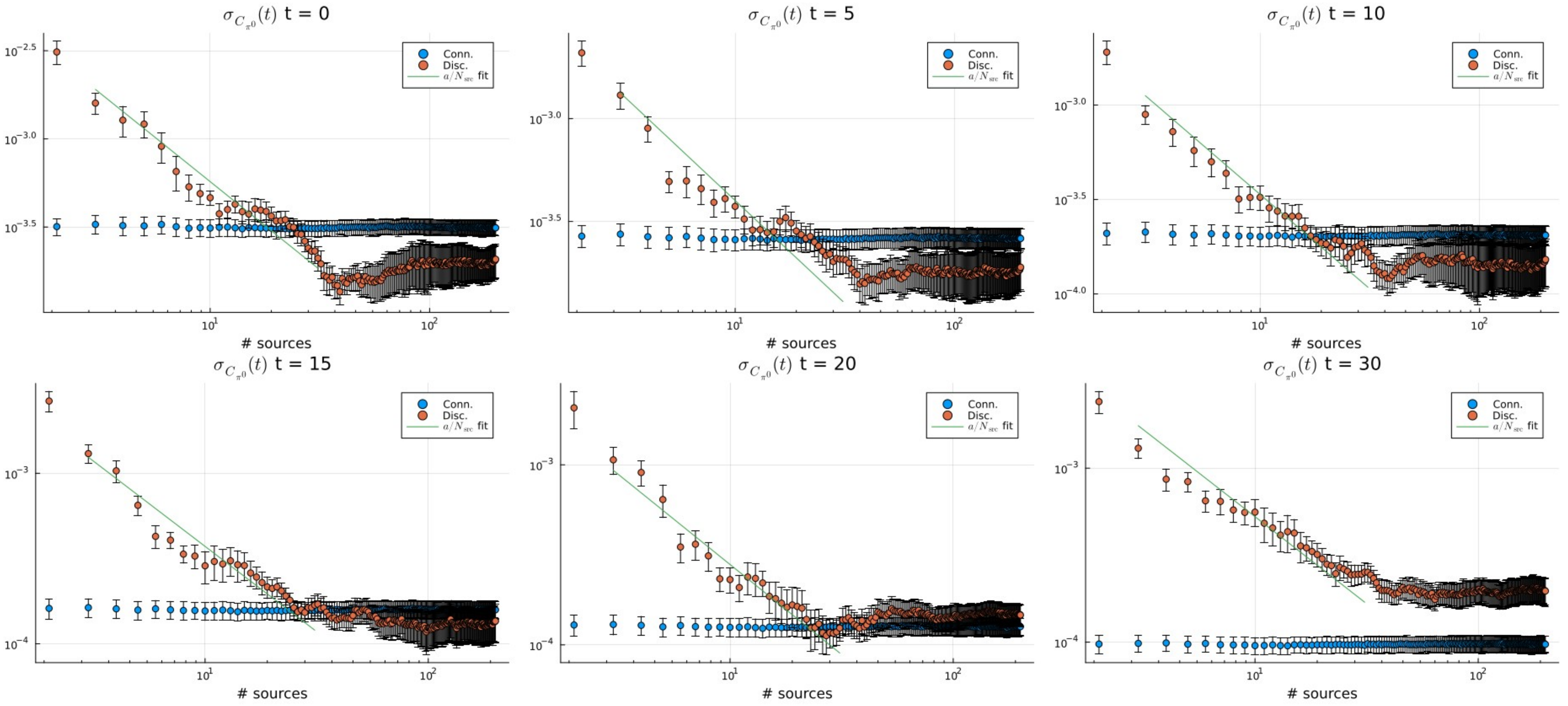
Exploration with 20 configurations

$$M_{\text{eff}}(t) = \cosh^{-1}\left[\frac{C(t+1)+C(t-1)}{2C(t)}\right]$$



☆ Plateau is extended and error is reduced

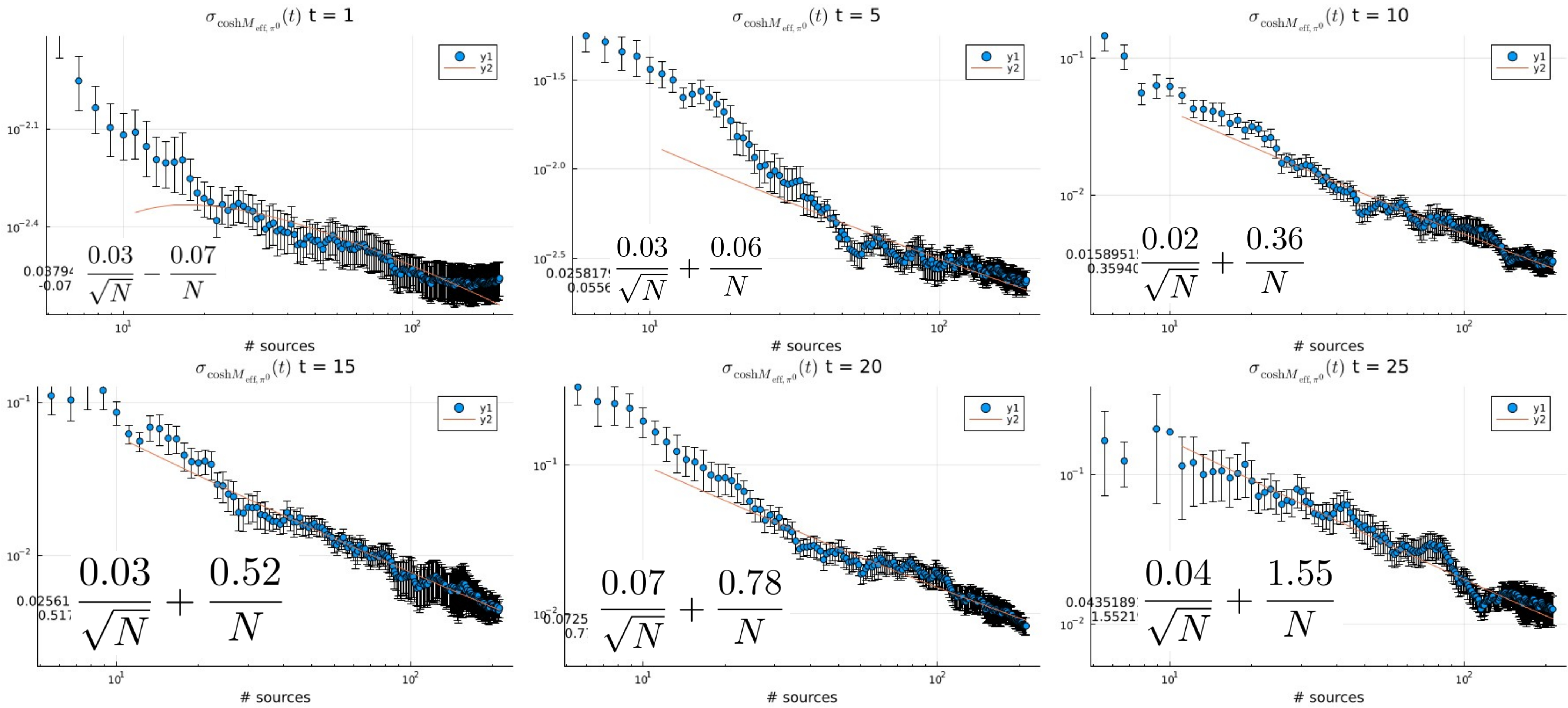
Exploration with 20 configurations



- Connected part saturates to gauge noise with few stochastic sources
- Disconnected part saturates to gauge noise after 50 stochastic sources (decaying with $1/N$)
- Connected part dominates the error for low t and >50 sources

Exploration with 20 configurations

$$M_{\text{eff}}(t) = \cosh^{-1}\left[\frac{C(t+1)+C(t-1)}{2C(t)}\right]$$



☆ Saturation to gauge noise for low t, but $1/N$ scaling for big t

⇒ Error cancellations

Conclusions & Outlook

- Smearing extends the plateau of the effective mass
- Saturation to gauge noise in the correlator is reached with 50 sources...
- ... but error of effective mass keeps decaying after 200 sources due to error cancelations
- Might be worth extracting the neutral pion mass with full statistics and a choice of number of sources and smearing steps before jumping into GEVP

Backup

Code to compute disconnected pieces at openqxd-devel/dalbandea-pi0/main/ms7.c

(code not ready for production, only for reference)

Report at rcstar/neutral-pion repository

- Total time to do the inversions of one configuration for 64 time slices, 2 flavors and 50 sources: 8.18×10^3s $\approx$ 2.5h. It took around 5h due, most probably, to the application of smearing steps (see also warning in sec. 4.2).

```
#!/bin/bash
#SBATCH -t 12:00:00
#SBATCH -n 4096 -N 43
#SBATCH -p standard96
#SBATCH -A bep00102
```