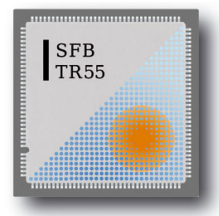
Details of a Staggered Fermion Data Analysis

Maximilian Ammer

BERGISCHE
UNIVERSITÄT
WUPPERTAL

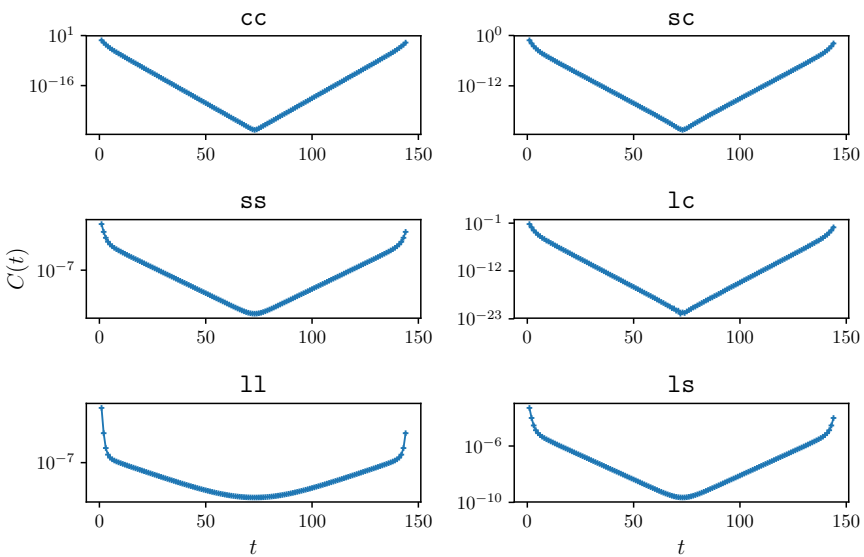


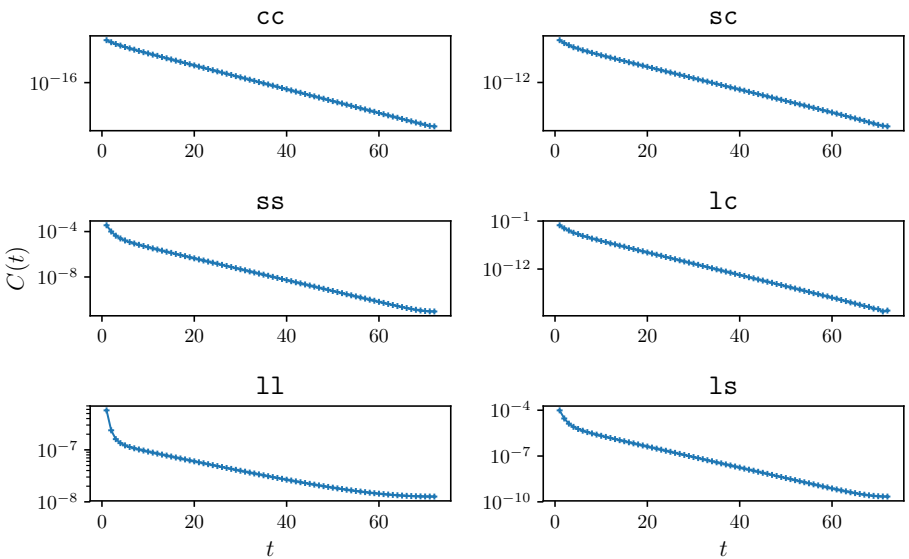
Data

- Data generated by BMWC, analysis in collaboration with Stephan Dürr
- Staggered Fermion simulation with $N_f = 2 + 1 + 1$
- Analysis of one ensemble with $\beta = 4.0126$ ($a \approx 0.063$ fm) close to the physical point
- Analysis of the six pseudo-scalar channels (`ll`, `ss`, `cc`, `ls`, `lc`, `sc`)
- Extraction of effective masses and effective decay constants in lattice units

Data

- Correlator data ($N \times T = 441 \times 144$ matrices)
- Symmetrize to reduce noise (discarding value at $t = 0$)





$$\rightarrow C(t) = \frac{1}{N} \sum_{i=1}^{N} C_i(t), \qquad t \in \{1, 2, \ldots, T/2 = 72\}$$

Blocking

To calculate statistical errors and covariances:

- Block data to minimize auto-correlation between configurations:

$$N = n_{(\mathrm{bins})} \cdot l_{\mathrm{bin}} + n_{\mathrm{disc}}$$

- Average each block:

$$C_i^{\mathrm{bl}}(t) = \frac{1}{l_{\mathrm{bin}}} \sum_{j=(i-1)\cdot l_{\mathrm{bin}}+1}^{i\cdot l_{\mathrm{bin}}} C_j(t)$$

- Jackknife resampling:

$$C_i^{\mathrm{jk}}(t) = \frac{1}{n-1} \sum_{j\neq i}^{n} C_j^{\mathrm{bl}}(t)$$

- Jackknife errors:

$$\tilde{\sigma}_C(t)^2 = (n-1) \cdot \langle (C_i^{\mathrm{jk}}(t) - \langle C_i^{\mathrm{jk}}(t) \rangle_n)^2 \rangle_n$$

- Compensate for discarded configurations:

$$\sigma_C(t) = \sqrt{\tfrac{N-n_{\mathrm{disc}}}{N}} \cdot \tilde{\sigma}_C(t).$$

Blocking

- Choose block size:

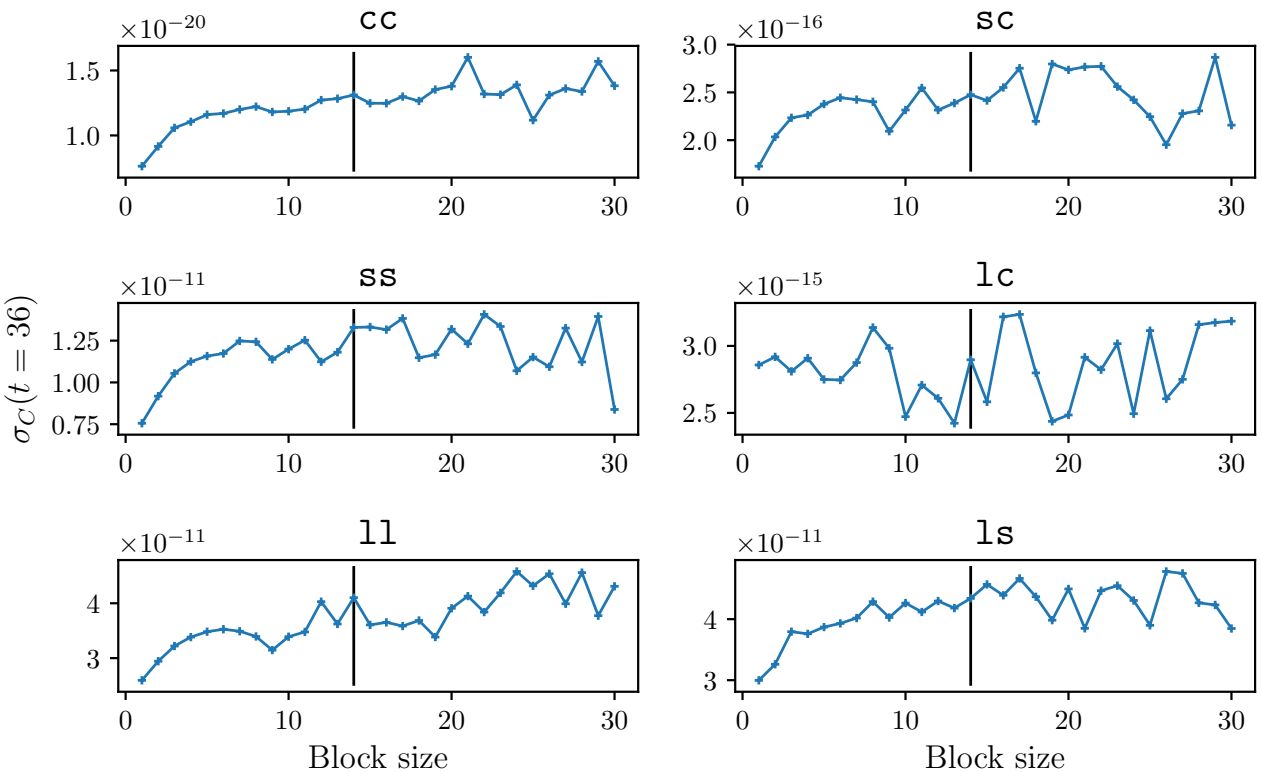


Figure: Jackknife errors of $C(t = 36)$ for different block sizes.

- Here $l_{\text{bin}} = 14$ was chosen
  $\rightarrow$ errors close to errors from Γ-method (`UWerr`).

Local definitions of M_{eff} and F_{eff}

Assuming a single decaying exponential for the correlator:

$$C(t) = Fe^{-Mt}$$

- Local effective mass in terms of discretized derivative:

$$M_{\text{eff}}^{(\text{ld})}(t) := \frac{\ln C(t-a) - \ln C(t)}{a} \qquad \text{(left derivative)}$$

$$M_{\text{eff}}^{(\text{rd})}(t) := \frac{\ln C(t) - \ln C(t+a)}{a} \qquad \text{(right derivative)}$$

$$M_{\text{eff}}^{(\text{cd})}(t) := \frac{\ln C(t-a) - \ln C(t+a)}{2a} \qquad \text{(central derivative).}$$

- Local effective decay constant:

$$F_{\text{eff}}^{(\text{cd})}(t) := \frac{C(t)}{e^{-M_{\text{eff}}^{(\text{cd})}(t)\cdot t}}.$$

Including backwards running contribution from periodic boundary conditions:

$$C(t) = F\left(e^{-Mt} + e^{-M(T-t)}\right) = 2Fe^{-M\frac{T}{2}}\cosh\left(M\left(\frac{T}{2} - t\right)\right)$$

- Local effective mass according to *Beane et al* [1] :

$$M_{\text{eff}}^{(\text{acosh})}(t) := \frac{1}{a}\cosh^{-1}\left(\frac{C(t-a) + C(t+a)}{2C(t)}\right).$$

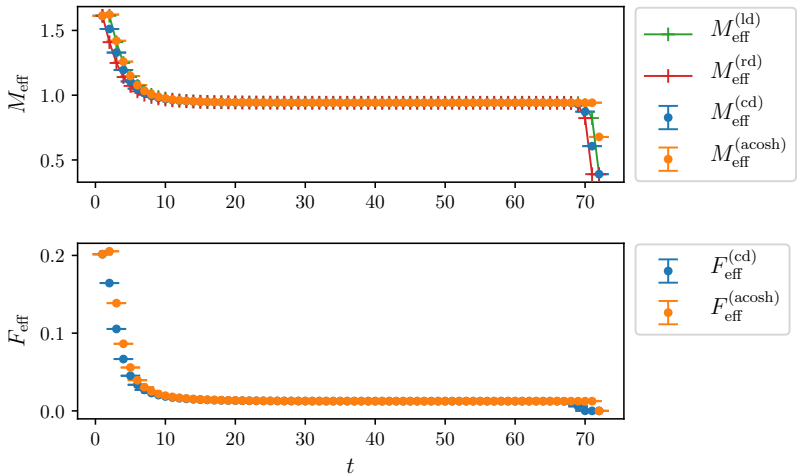
- Then the effective decay constant is given by:

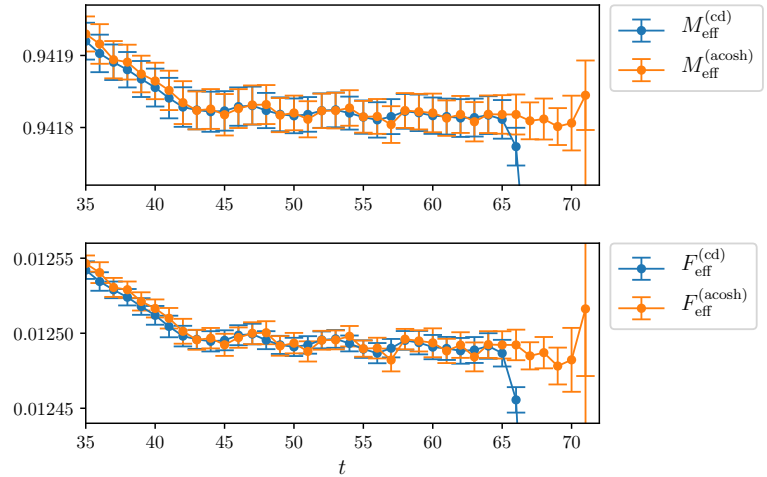
$$F_{\text{eff}}^{(\text{acosh})}(t) := \frac{C(t)}{e^{-M_{\text{eff}}^{(\text{acosh})}(t)\cdot t} + e^{-M_{\text{eff}}^{(\text{acosh})}(t)\cdot(T-t)}}.$$

[1] Phys. Rev. D 86, 094509 (2012)

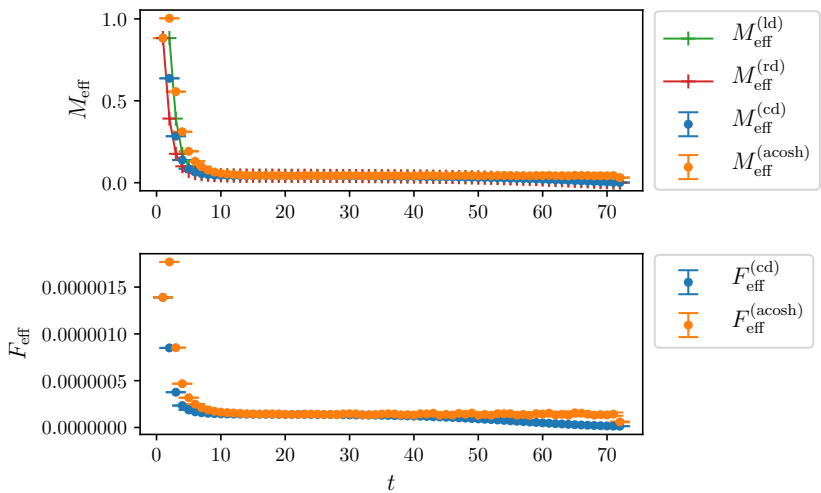
Local definitions of M_{eff} and F_{eff}

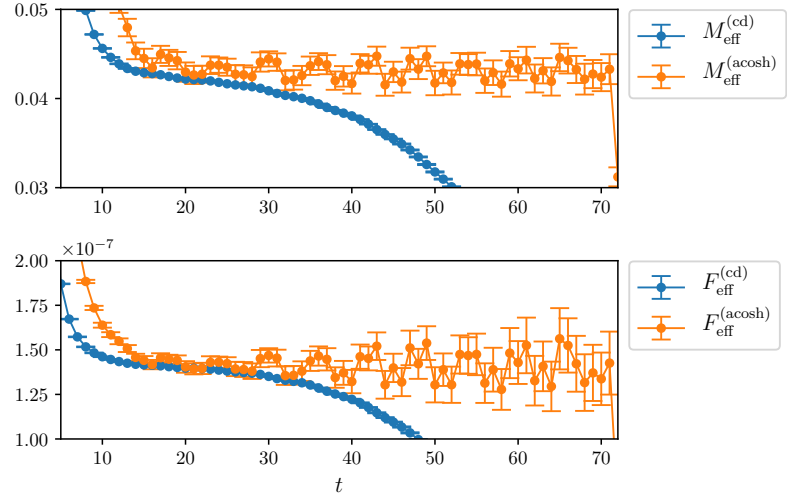
- cc-channel:





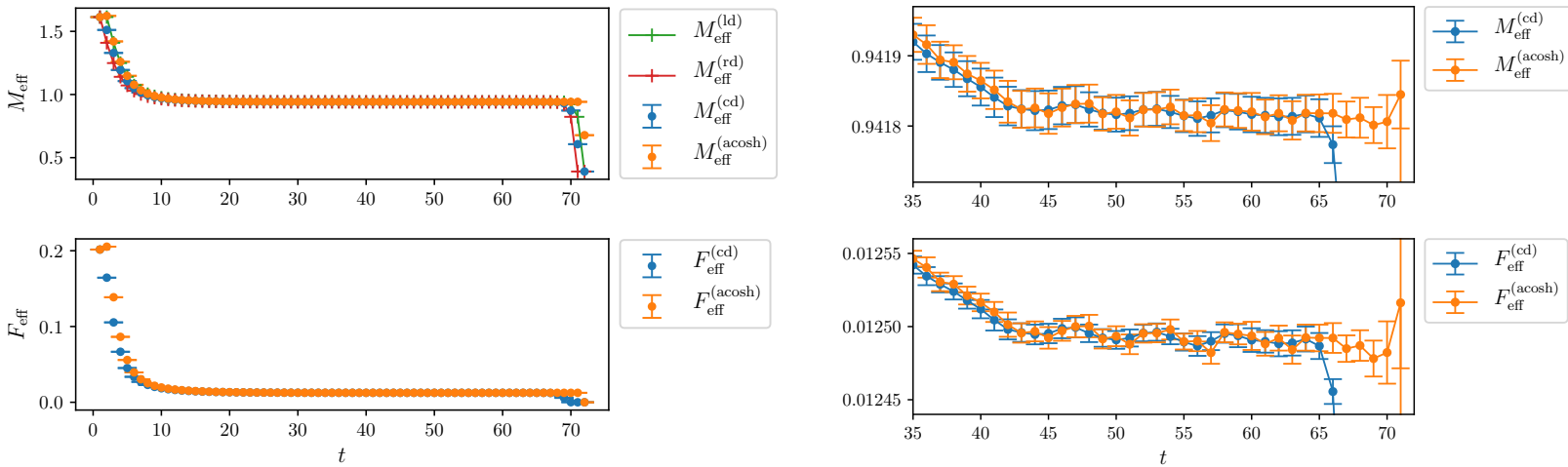
- ll-channel:



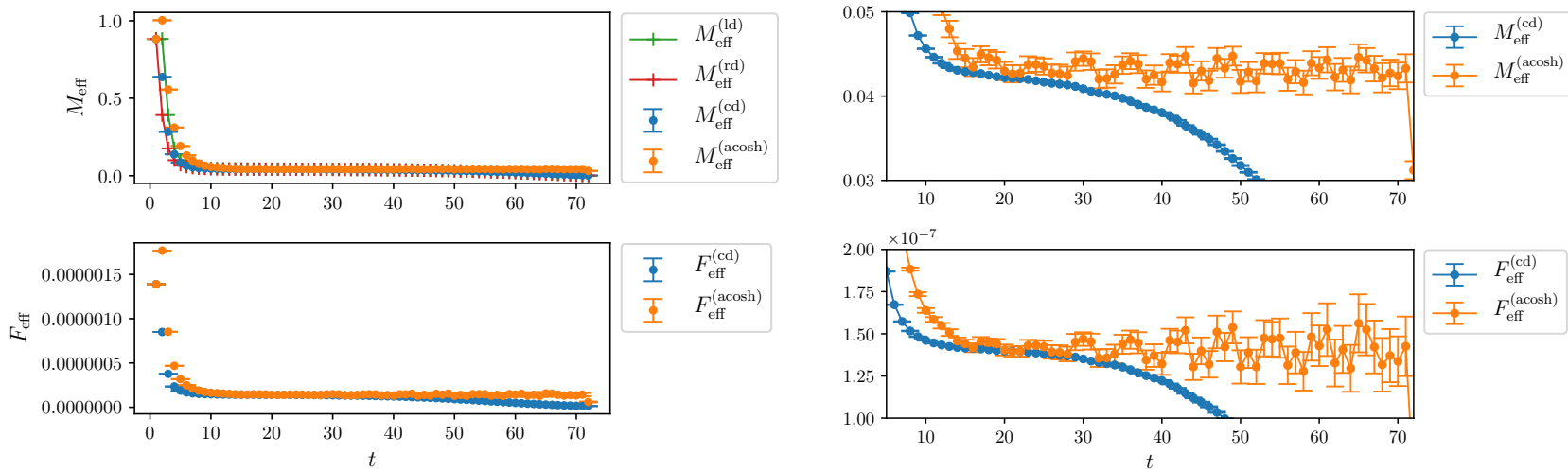


Local definitions of M_{eff} and F_{eff}

- cc-channel: ($\rightarrow$ use either defintion)

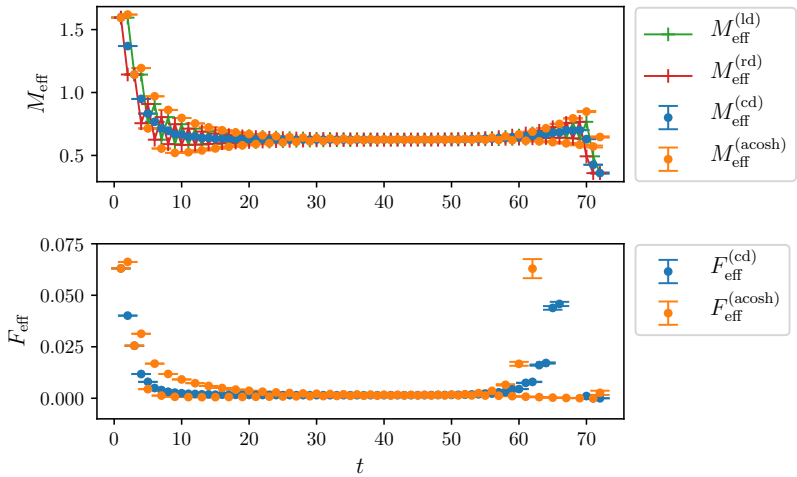


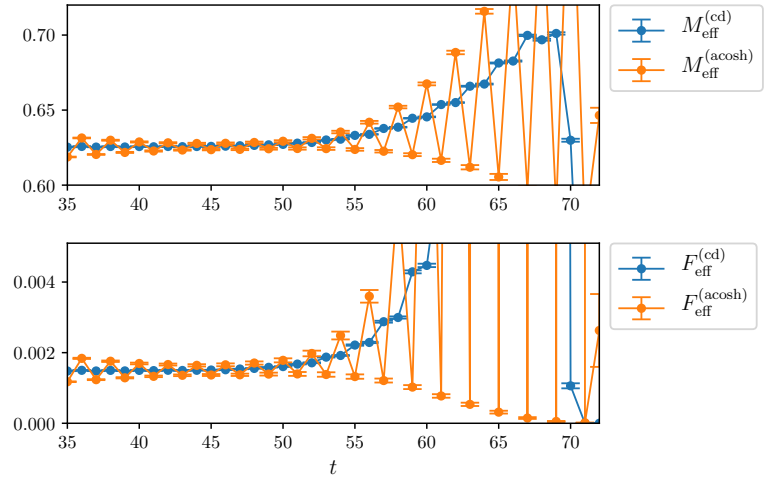
- ll-channel: ($\rightarrow$ use $M_{\text{eff}}^{(\text{acosh})}$)



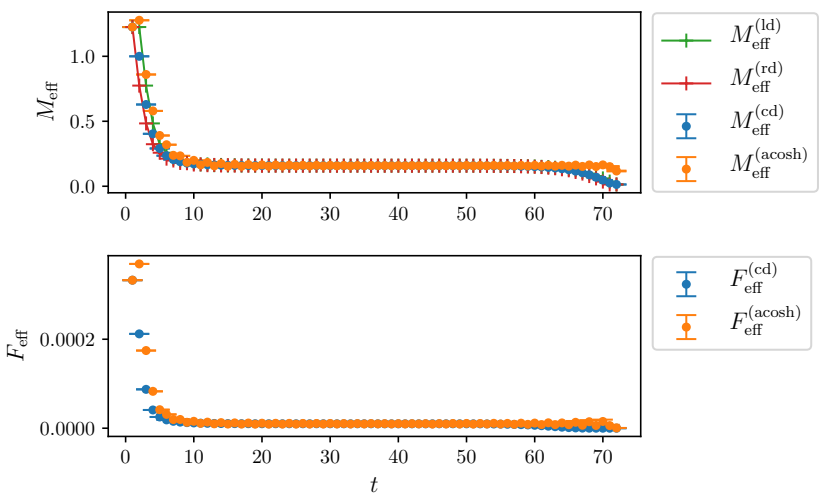
Local definitions of M_{eff} and F_{eff}

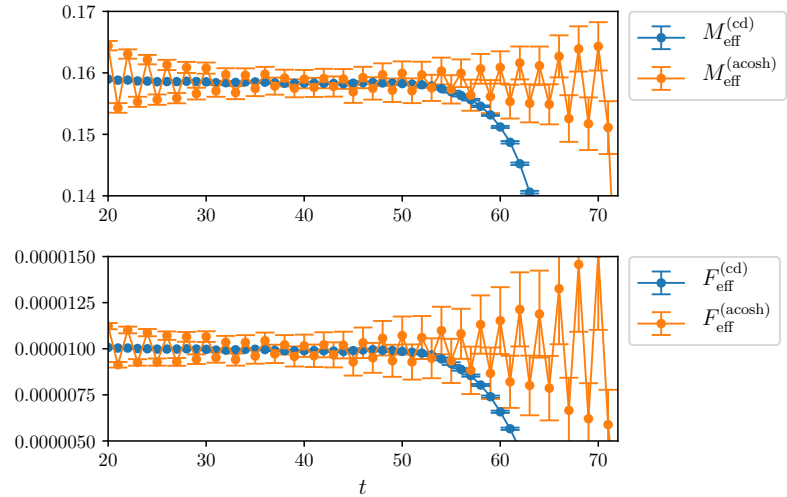
- sc-channel:





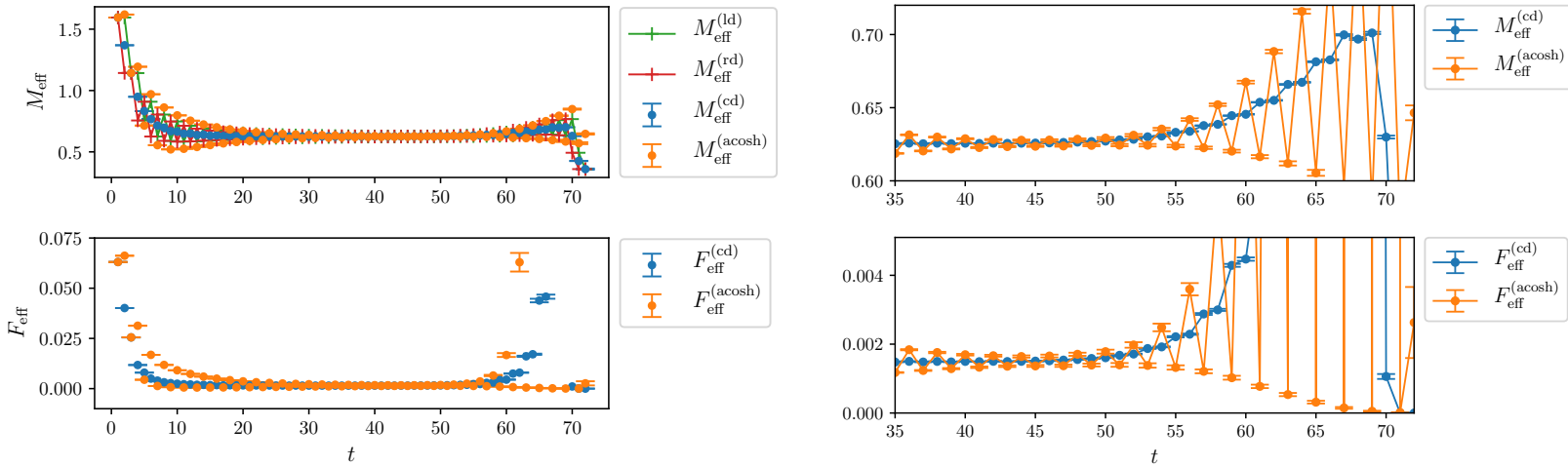
- ls-channel:



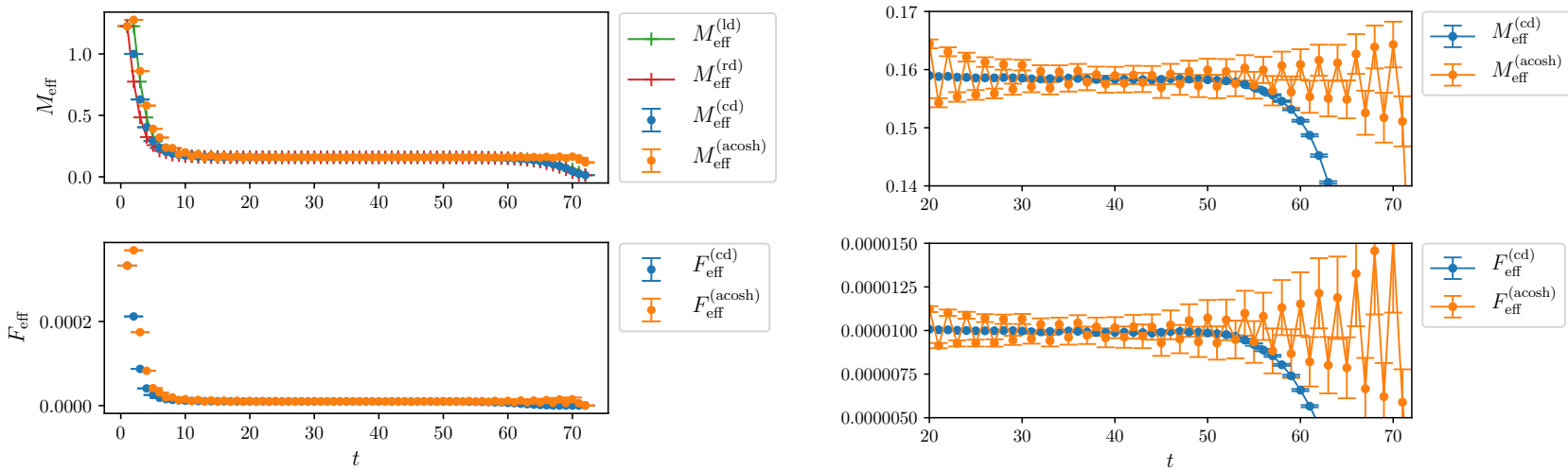


Local definitions of M_{eff} and F_{eff}

- sc-channel: ($\rightarrow$ use $M_{\mathrm{eff}}^{(\mathrm{cd})}$)

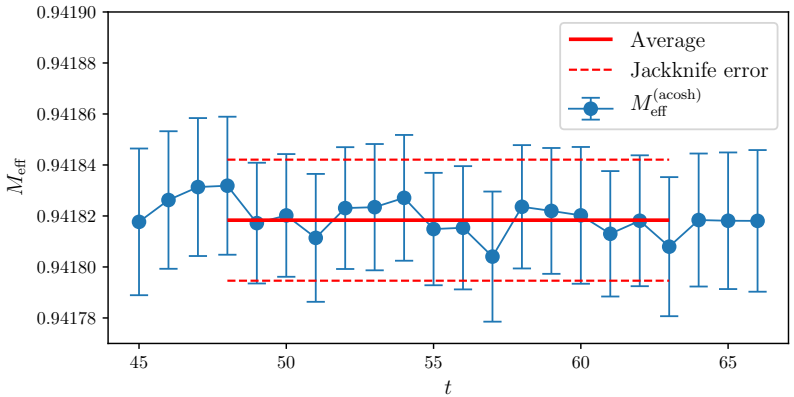


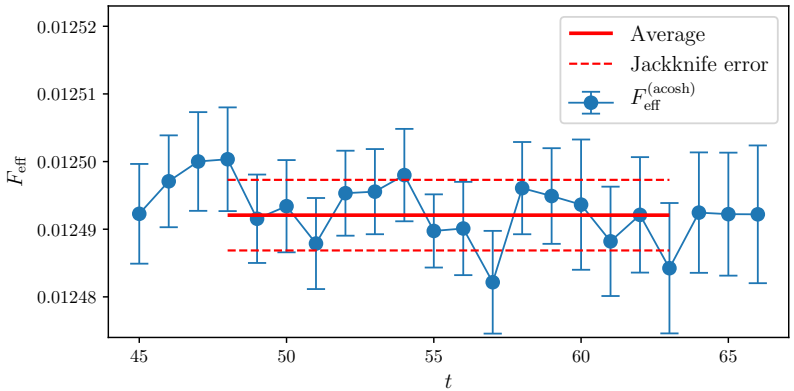
- ls-channel: ($\rightarrow$ use $M_{\mathrm{eff}}^{(\mathrm{acosh})}$)



Fit functions for $M_{\text{eff}}(t)$ and $F_{\text{eff}}(t)$

- First average inside mass plateau:



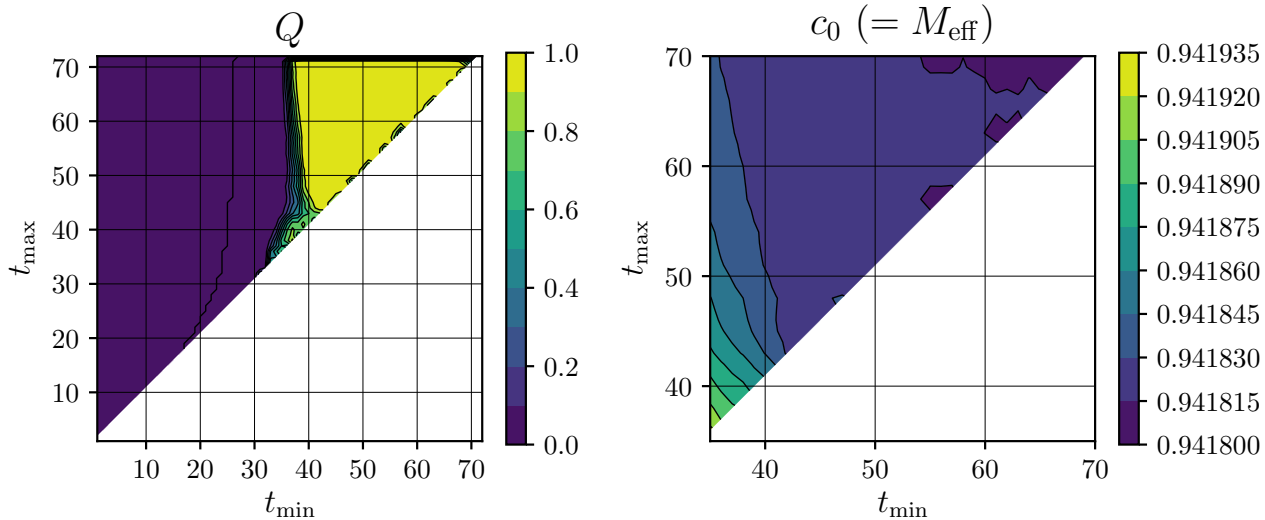


Fit functions for $M_{\mathrm{eff}}(t)$ and $F_{\mathrm{eff}}(t)$

- First average inside mass plateau:
- Fitting a constant:
  - Fit function: $f(t) = c_0$

Fit functions for $M_{\mathrm{eff}}(t)$ and $F_{\mathrm{eff}}(t)$

- First average inside mass plateau:
- Fitting a constant:
  - Fit function: $f(t) = c_0$
  - Determine suitable fit window $\rightarrow [t_{\mathrm{min}}, t_{\mathrm{max}}] = [48, 63]$



$$Q = \frac{\Gamma\left(\frac{m}{2}, \frac{\chi^2}{2}\right)}{\Gamma\left(\frac{m}{2}\right)} = \frac{\int_{\frac{\chi^2}{2}}^{\infty} \tau^{\frac{m}{2}-1} e^{-\tau} d\tau}{\int_0^{\infty} \tau^{\frac{m}{2}-1} e^{-\tau} d\tau}, \qquad m = (t_{max} - t_{min} + 1) - n_{par}.$$

Fit functions for $M_{\text{eff}}(t)$ and $F_{\text{eff}}(t)$

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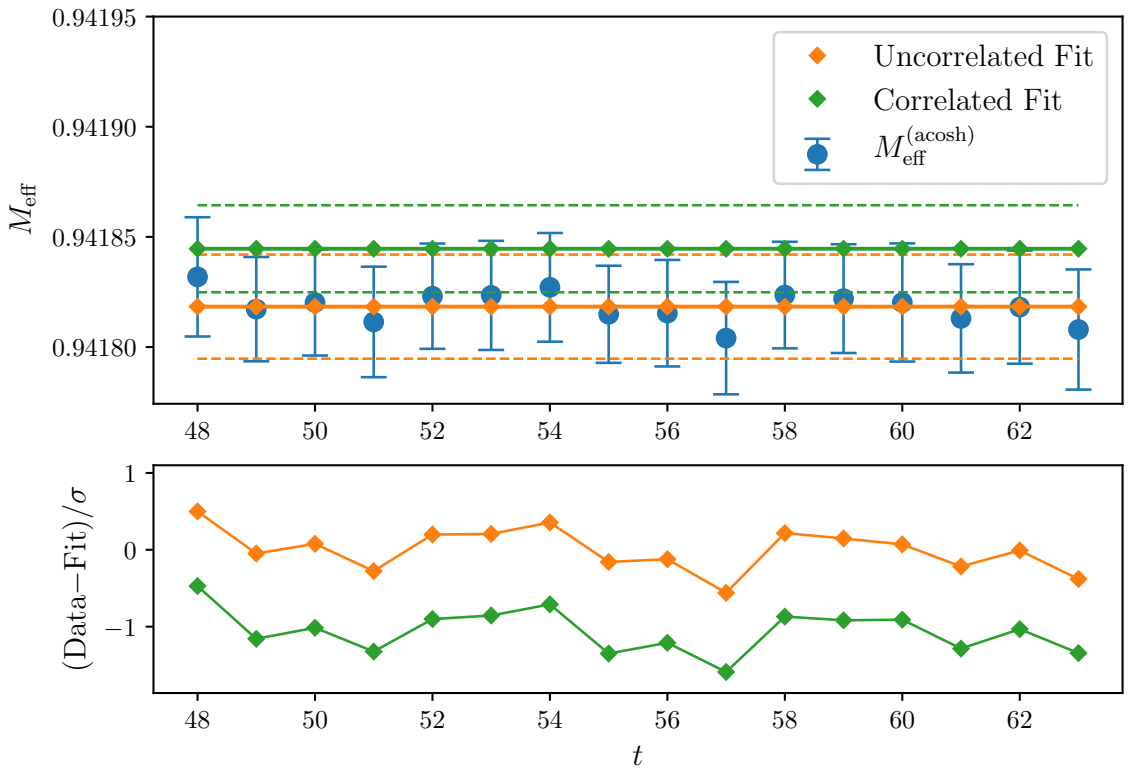
  - Uncorrelated fit
  - Correlated fit



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  - Uncorrelated fit
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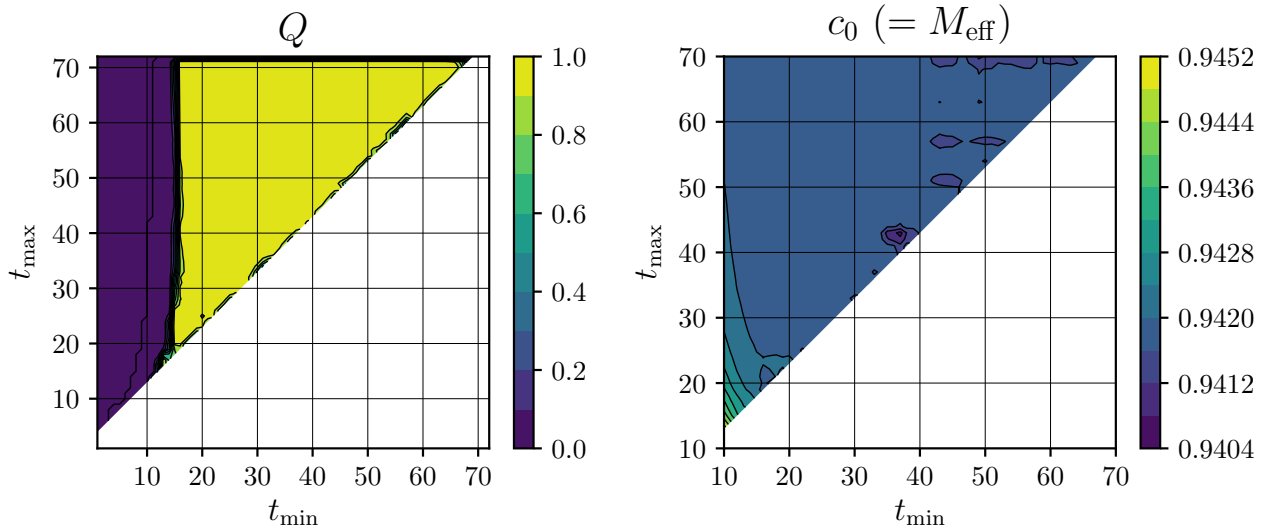
  - Perform fits on all n Jackknife samples and calculate error of fit parameters:

$$\sigma^2_{c_0} = \frac{n-1}{n} \sum_i^n (c_0^i - c_0)^2 \quad \cdot \frac{N - n_{\mathrm{disc}}}{N}$$

- Fitting a constant plus an exponential:
  - Fit function: $f(t) = c_0 + c_1 e^{-c_2 t}$
  - Determine suitable fit window $\rightarrow [t_{\mathrm{min}}, t_{\mathrm{max}}] = [32, 58]$



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Fit functions for $M_{\mathrm{eff}}(t)$ and $F_{\mathrm{eff}}(t)$

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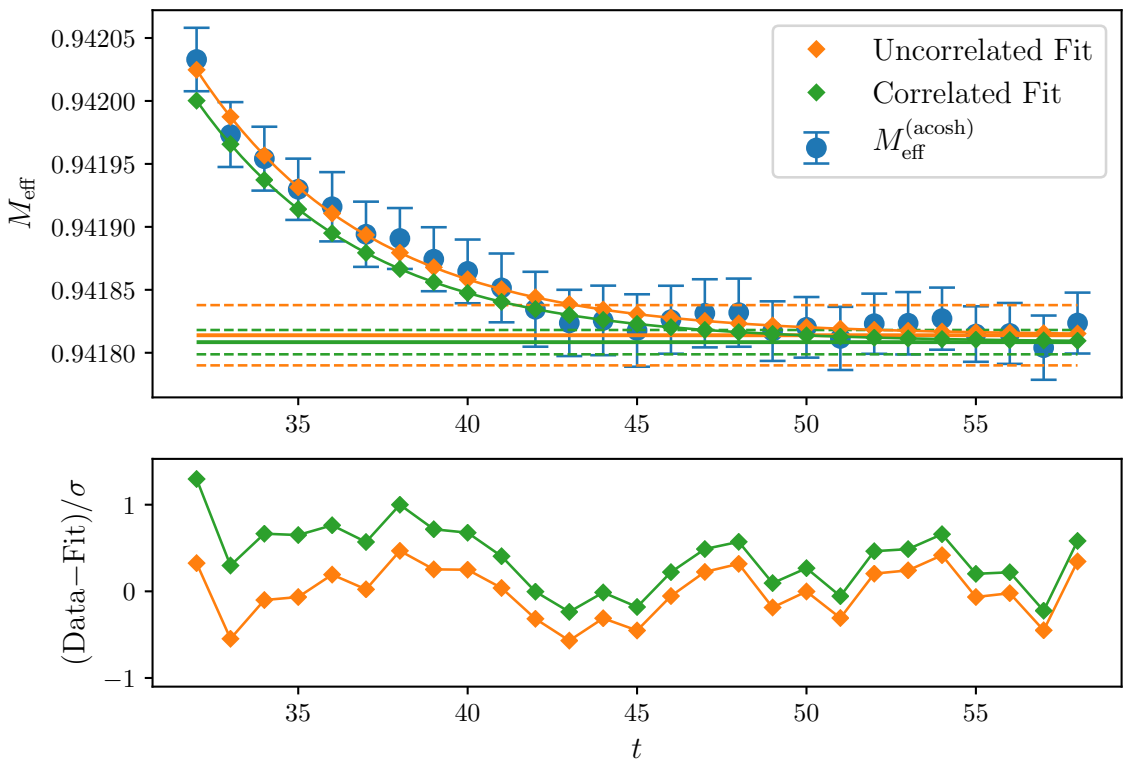
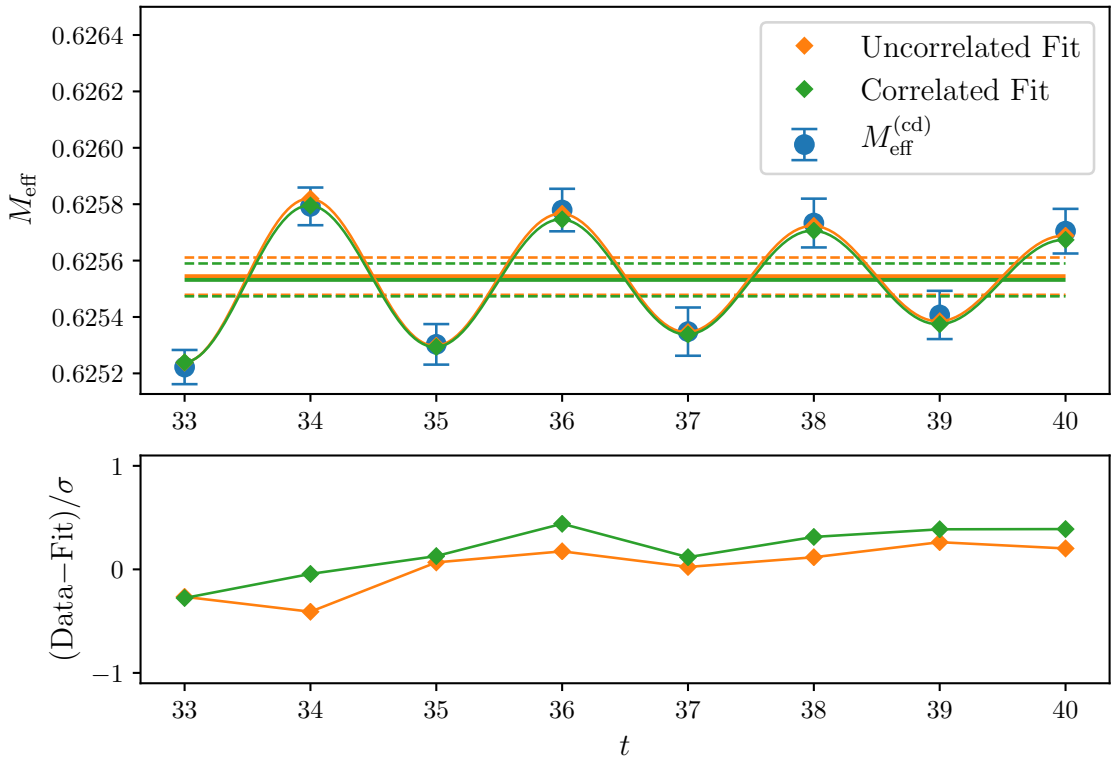


Fit functions for $M_{\text{eff}}(t)$ and $F_{\text{eff}}(t)$

For `sc,lc,ls`-channels fit staggered oscillations with extra cos-terms:

- Fit function $f(t) = c_0 + c_1 e^{-c_2 t} \cos(\pi t)$:



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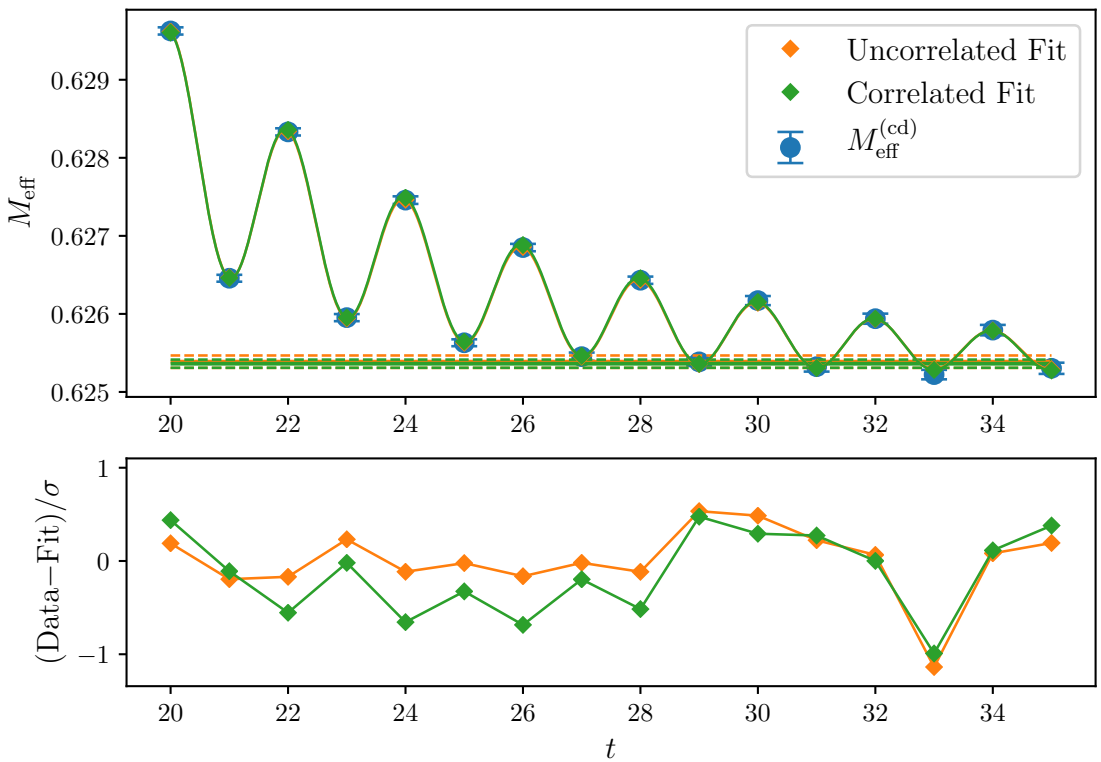
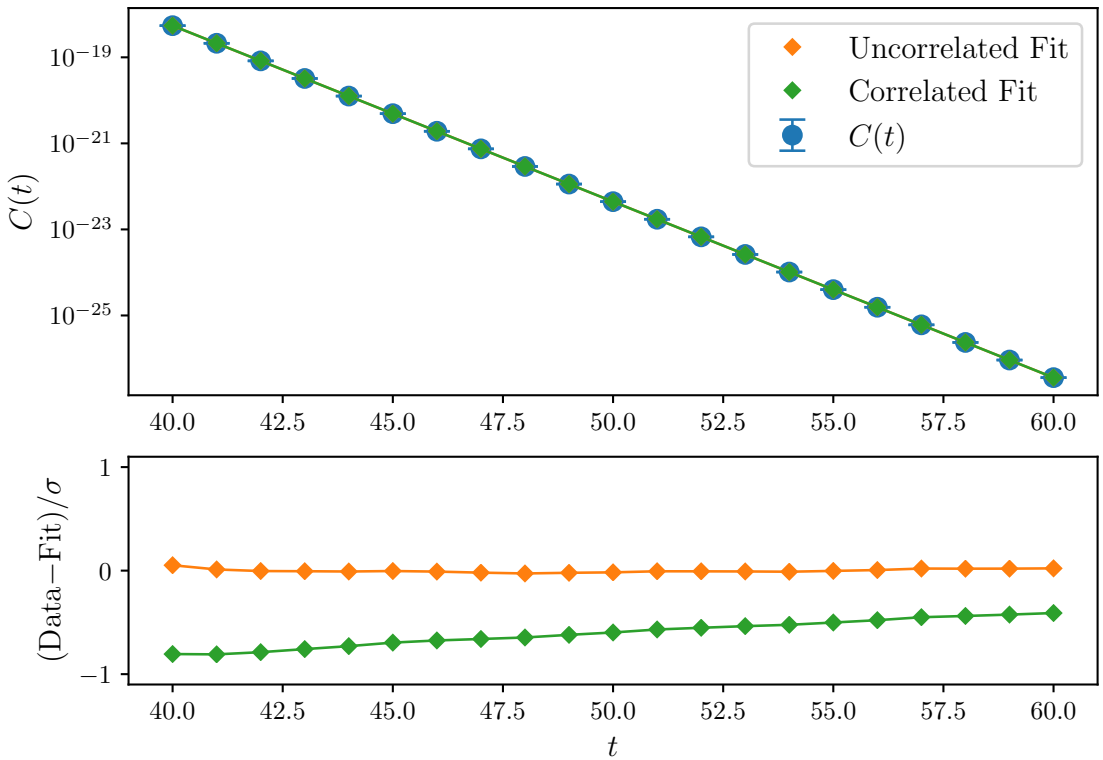
- Fit function $f(t) = c_0 + c_1 e^{-c_2 t} \cos(\pi t)$:
- Fit function $f(t) = c_0 + c_1 e^{-c_2 t} + c_3 e^{-c_4 t} \cos(\pi t)$:



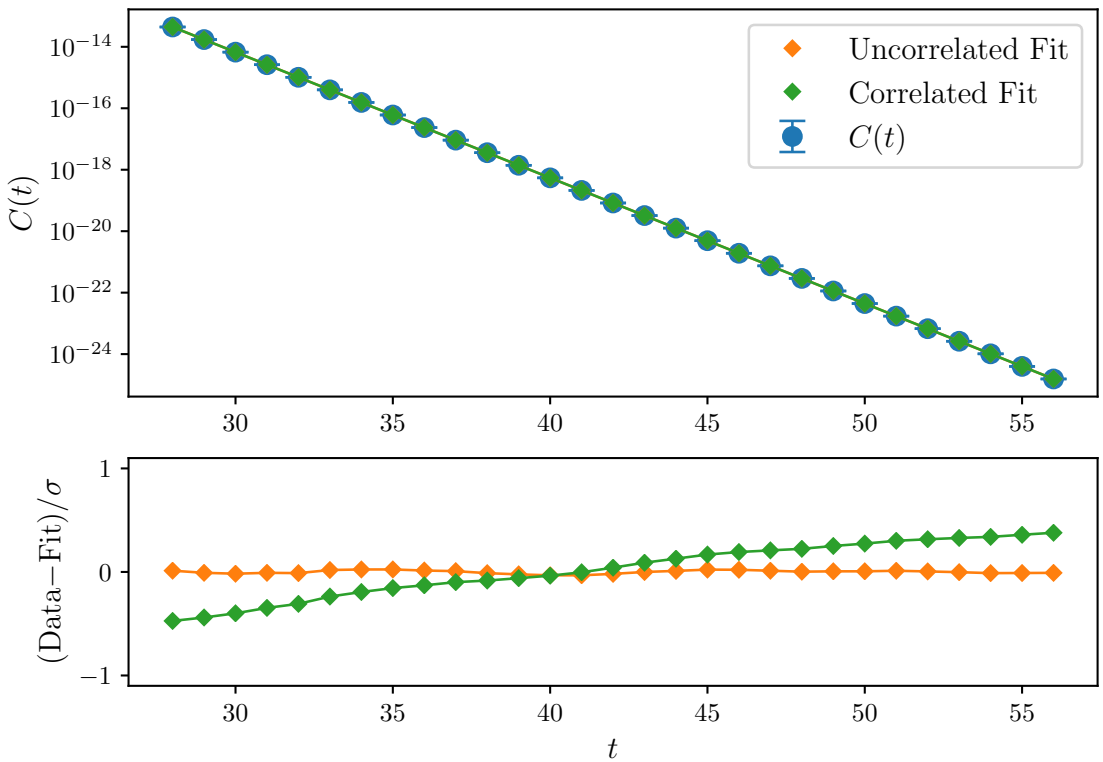
Fitting the Correlator

- `cc,ss,ll`-channel: fit one, two or more cosh-functions.
- Fit function $f(t) = c_0 \left(e^{-c_1 t} + e^{c_1 (t-T)}\right)$



Fitting the Correlator

- `cc,ss,ll`-channel: fit one, two or more cosh-functions.
- Fit function $f(t) = c_0 \left(e^{-c_1 t} + e^{c_1 (t-T)}\right) + c_2 \left(e^{-c_3 t} + e^{c_3 (t-T)}\right)$
- Impose $c_1 < c_3$



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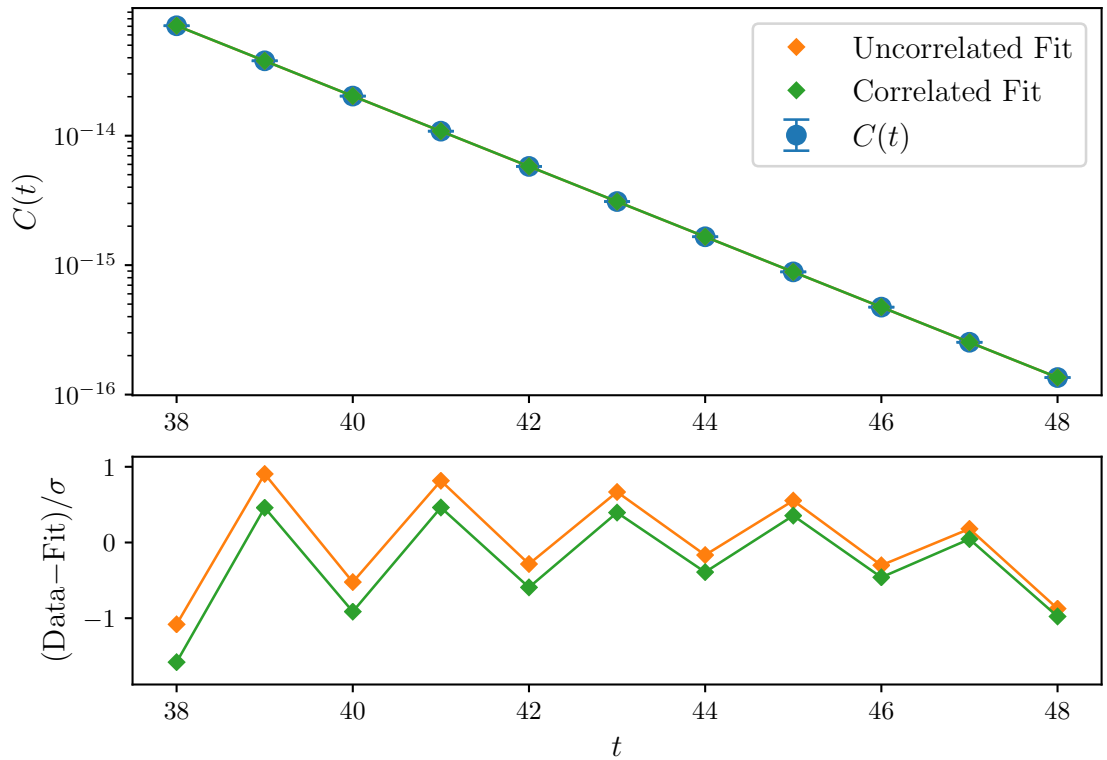

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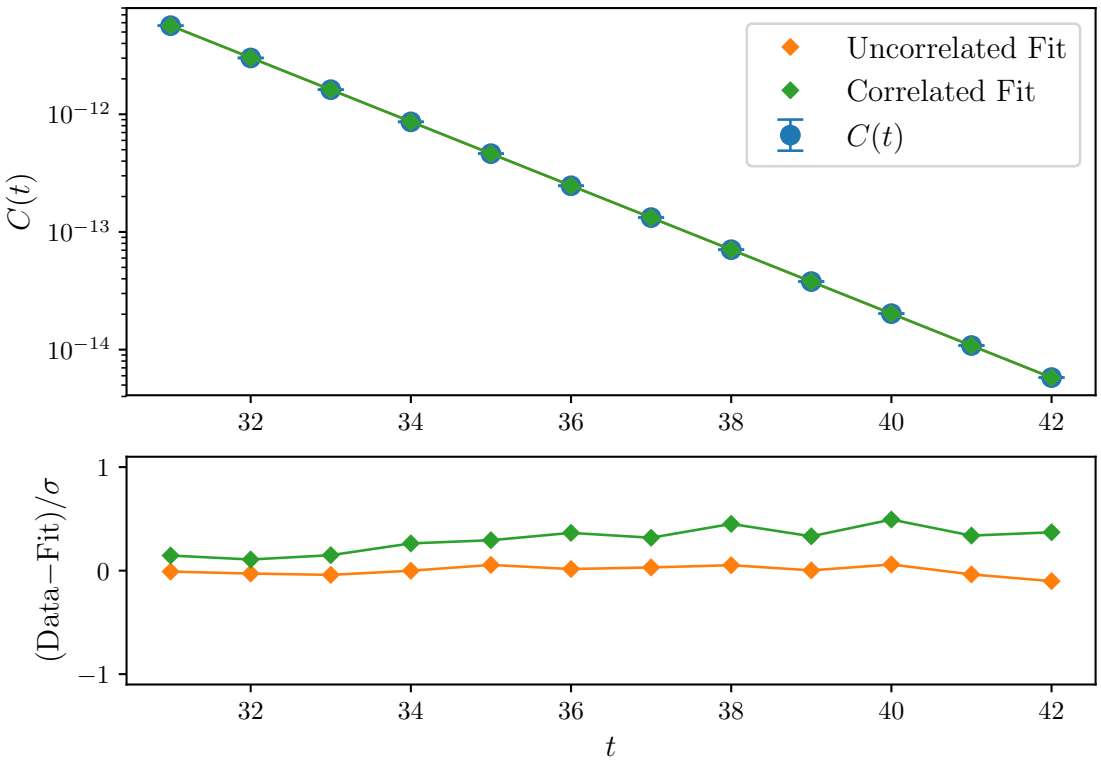
- `sc`,`lc`,`ls`-channel: fit one, two or more cosh-functions plus cos-term.
- Fit function $f(t) = c_0 \left(e^{-c_1 t} + e^{c_1 (t-T)}\right) + c_2 e^{-c_3 t} \cos(\pi t)$



Fitting the Correlator

- `sc,lc,ls`-channel: fit one, two or more cosh-functions plus cos-term.
- Fit function
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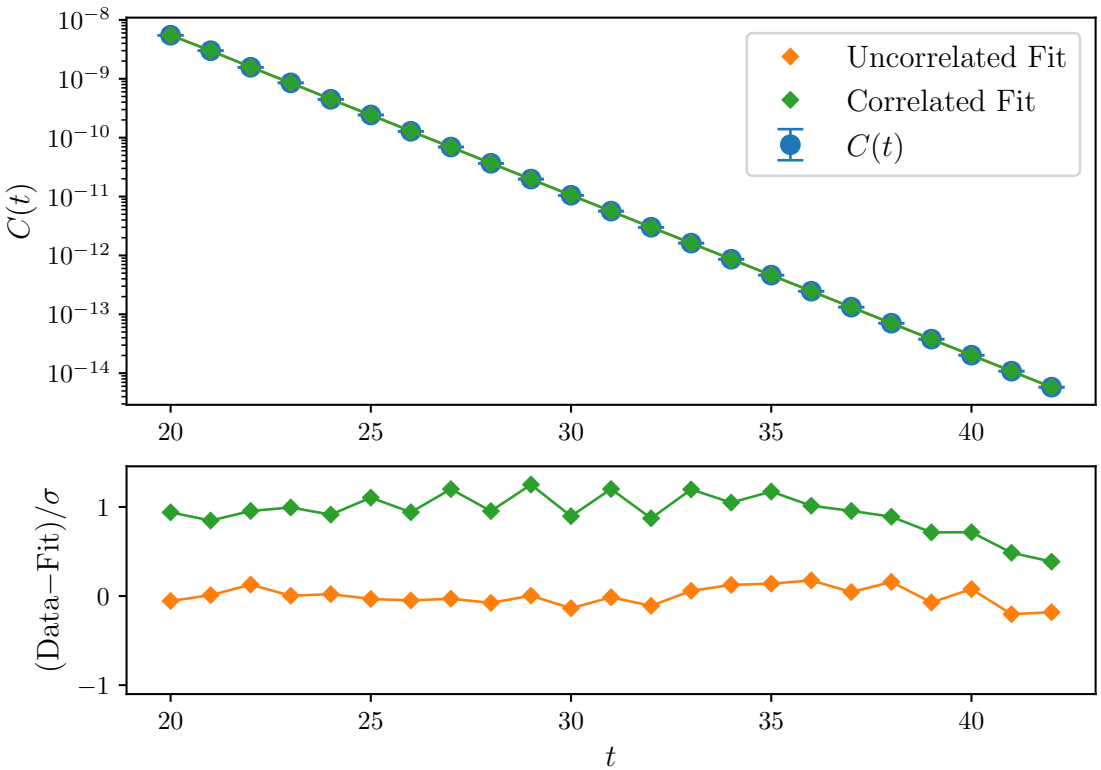
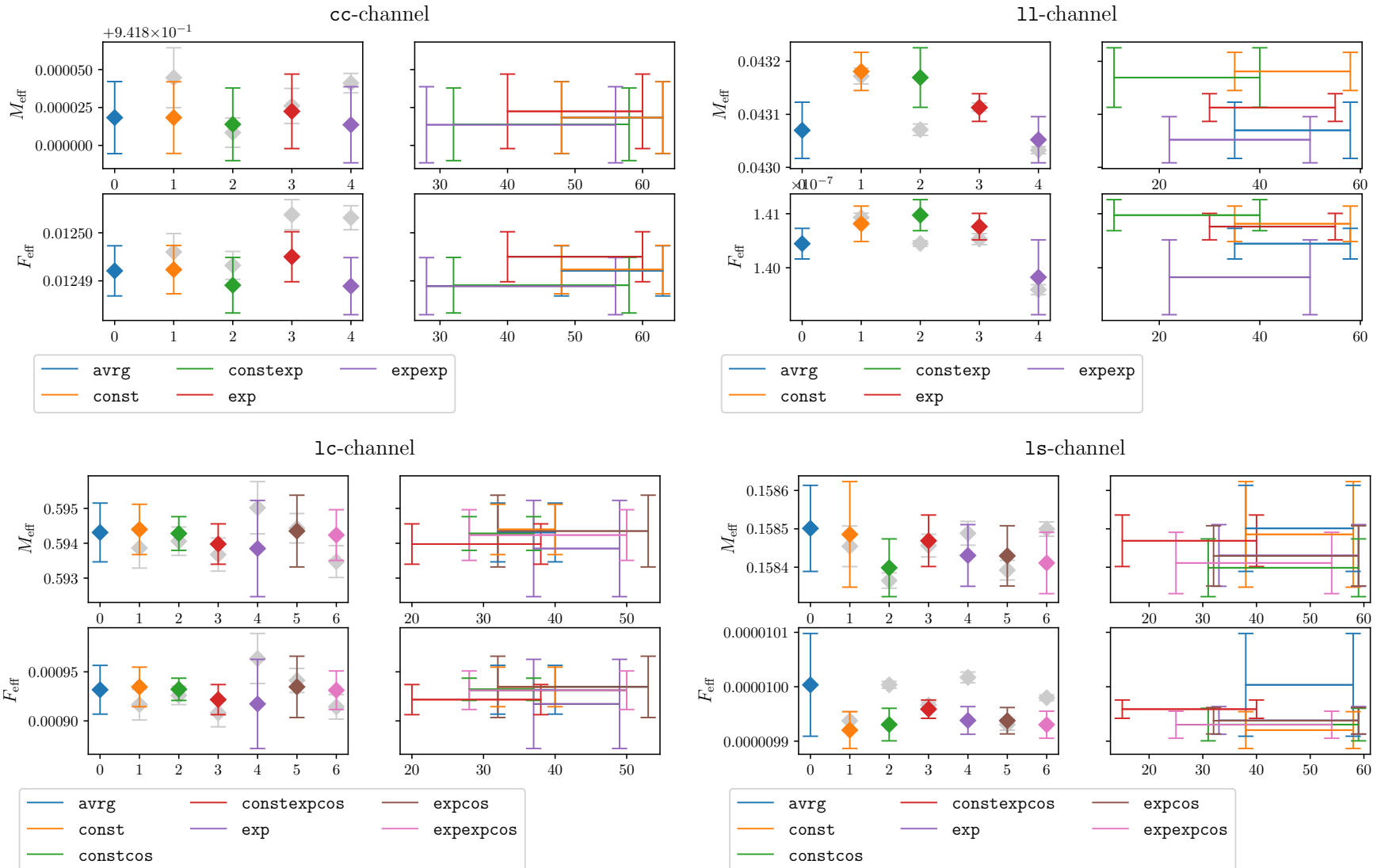


Summary of all fits



Covariance matrices of all channels

- Covariance matrix of uncorrelated fits:

	cc-$M_{\rm eff}$	cc-$F_{\rm eff}$	ss-$M_{\rm eff}$	ss-$F_{\rm eff}$	ll-$M_{\rm eff}$	ll-$F_{\rm eff}$	sc-$M_{\rm eff}$	sc-$F_{\rm eff}$	lc-$M_{\rm eff}$	lc-$F_{\rm eff}$	ls-$M_{\rm eff}$	ls-$F_{\rm eff}$
cc-$M_{\rm eff}$	6.29e-10											
cc-$F_{\rm eff}$	1.24e-10	3.53e-11										
ss-$M_{\rm eff}$	9.59e-10	2.16e-10	3.61e-09									
ss-$F_{\rm eff}$	9.21e-13	1.98e-13	3.34e-12	4.02e-15								
ll-$M_{\rm eff}$	1.83e-10	3.57e-11	9.52e-10	7.24e-13	1.90e-09							
ll-$F_{\rm eff}$	2.21e-15	5.91e-16	5.30e-15	2.78e-18	2.63e-14	4.80e-19						
sc-$M_{\rm eff}$	1.21e-09	2.65e-10	2.67e-09	2.38e-12	-1.19e-10	-5.49e-15	5.23e-09					
sc-$F_{\rm eff}$	3.54e-11	8.75e-12	7.81e-11	7.97e-14	-1.03e-11	-1.73e-16	2.09e-10	9.63e-12				
lc-$M_{\rm eff}$	6.32e-09	1.06e-09	1.23e-08	1.52e-11	2.86e-09	-1.64e-14	1.72e-08	6.19e-10	5.29e-07			
lc-$F_{\rm eff}$	1.54e-10	2.46e-11	2.93e-10	3.71e-13	5.35e-11	-6.69e-16	4.55e-10	1.73e-11	1.41e-08	3.86e-10		
ls-$M_{\rm eff}$	1.08e-09	2.54e-10	3.53e-09	2.79e-12	1.67e-09	1.39e-14	2.93e-09	9.20e-11	2.69e-08	7.03e-10	6.39e-09	
ls-$F_{\rm eff}$	3.31e-13	7.81e-14	7.47e-13	6.78e-16	4.24e-13	4.67e-18	7.68e-13	2.70e-14	9.12e-12	2.47e-13	1.75e-12	6.17e-16

- Covariance matrix of correlated fits:

	cc-$M_{\rm eff}$	cc-$F_{\rm eff}$	ss-$M_{\rm eff}$	ss-$F_{\rm eff}$	ll-$M_{\rm eff}$	ll-$F_{\rm eff}$	sc-$M_{\rm eff}$	sc-$F_{\rm eff}$	lc-$M_{\rm eff}$	lc-$F_{\rm eff}$	ls-$M_{\rm eff}$	ls-$F_{\rm eff}$
cc-$M_{\rm eff}$	4.09e-11											
cc-$F_{\rm eff}$	1.48e-11	6.23e-12										
ss-$M_{\rm eff}$	3.25e-13	1.40e-13	5.19e-13									
ss-$F_{\rm eff}$	1.92e-16	8.19e-17	2.89e-16	1.61e-19								
ll-$M_{\rm eff}$	-6.08e-12	-8.21e-13	3.05e-13	1.70e-16	4.35e-11							
ll-$F_{\rm eff}$	-6.31e-17	-4.44e-17	2.99e-19	1.37e-22	4.06e-16	8.60e-21						
sc-$M_{\rm eff}$	8.22e-11	2.57e-11	-8.82e-13	-4.13e-16	-7.09e-12	-3.41e-17	1.69e-09					
sc-$F_{\rm eff}$	2.53e-12	8.57e-13	2.62e-14	1.78e-17	-3.35e-13	-1.98e-18	6.03e-11	2.33e-12				
lc-$M_{\rm eff}$	-4.62e-10	-2.95e-10	-4.32e-12	-2.26e-15	-9.97e-10	-3.69e-15	3.31e-09	9.76e-11	2.09e-07			
lc-$F_{\rm eff}$	-1.15e-11	-8.03e-12	-2.90e-13	-1.54e-16	-3.20e-11	-1.42e-16	8.15e-11	2.35e-12	5.64e-09	1.56e-10		
ls-$M_{\rm eff}$	3.88e-12	3.11e-12	-8.49e-13	-5.17e-16	2.74e-11	2.79e-16	1.04e-10	3.78e-12	1.85e-10	1.19e-12	3.49e-10	
ls-$F_{\rm eff}$	-2.77e-15	-9.86e-16	-6.66e-16	-3.80e-19	4.51e-15	1.18e-20	-1.62e-15	3.39e-16	2.15e-13	4.85e-15	6.68e-14	2.62e-17

Sample Covariance Matrix:

$$\mathrm{Cov}_C(t,t') = (n-1)\left\langle \Big(C_i(t) - \langle C_i(t)\rangle\Big)\Big(C_i(t') - \langle C_i(t')\rangle\Big)\right\rangle \cdot \frac{N - n_{\mathrm{disc}}}{N}$$

$$\mathrm{Cov}_C(t,t) = \sigma_C^2(t)$$

Correlated fitting $\Leftrightarrow$ minimizing χ^2_{cor}

$$\chi^2_{\mathrm{cor}} = \sum_{t,t'=t_{\mathrm{min}}}^{t_{\mathrm{max}}} \big(f(t) - C(t)\big)\mathrm{Cov}_C^{-1}(t,t')\big(f(t') - C(t')\big)$$

Uncorrelated fitting $\Leftrightarrow$ minimizing χ^2_{uncor}

$$\chi^2_{\mathrm{uncor}} = \sum_{t=t_{\mathrm{min}}}^{t_{\mathrm{max}}} \frac{\big(f(t) - C(t)\big)^2}{\sigma_C^2(t)}$$

Known Issues with correlated fitting (see e.g. *C. Michaels '93*[2],*Seibert '93*[3]...):

- Only trustworthy for $p = t_{\max} - t_{\min} \ll n$ (here $p = 10 \sim 30$, $n = 31$).
- Otherwise underestimates errors.
- Singular behaviour for $p > n$.
- Very badly conditioned for $p \approx n$ (here cond $\approx 10^{12} \sim 10^{30}$).
  $\rightarrow$ Numerical inversion introduces large biases.

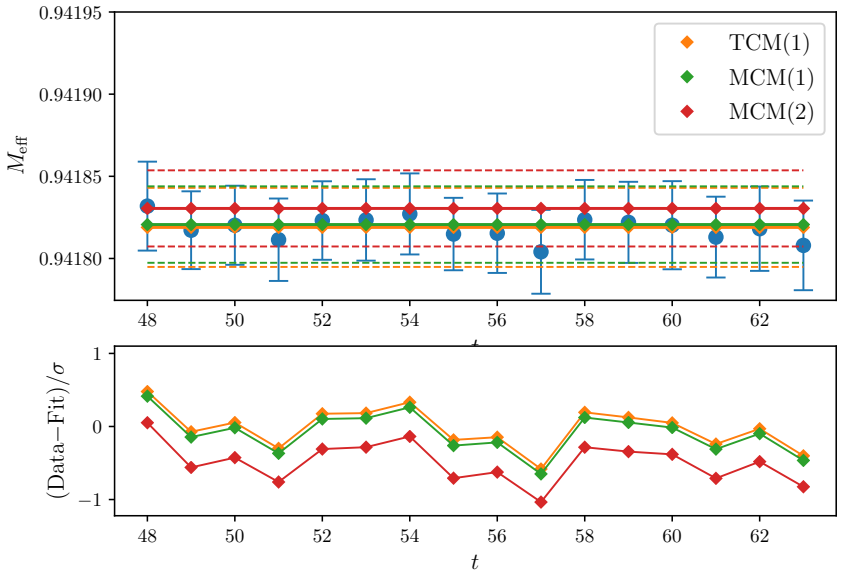
[2] hep-lat/9310026
[3] hep-lat/9305014

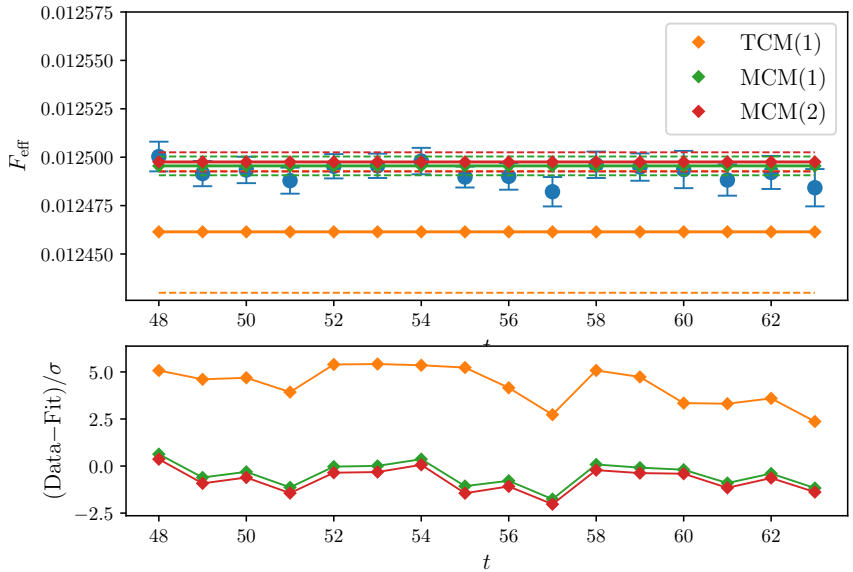
Methods to modify/truncate the covariance matrix:

- TCM(i)-Method: Truncate Covariance Matrix, keep only i off-diagonals.
  - Resulting matrix is no longer positive (semi-)definite.
  - Very unreliable for fixed i.
- MCM(i)-Method: Remove all but the i largest singular values of the correlation matrix.
  - For $i = 1$ result is often very close to uncorrelated fit.
  - For $i \leq 2$ result is often close to or worse than correlated fit.
- Many more ...

Modified Covariance Matrices

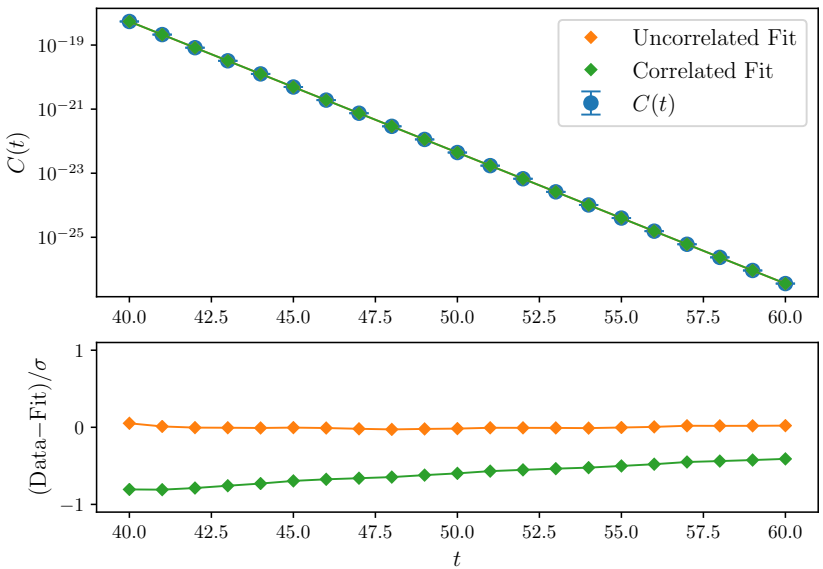
Examples: (cc-channel, constant fits)

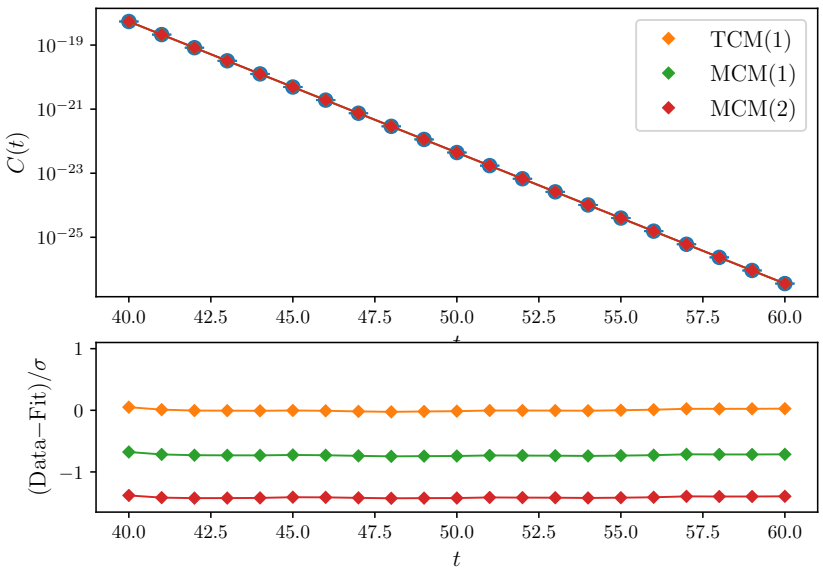




Modified Covariance Matrices

Examples: (cc-channel, one cosh-function fit)

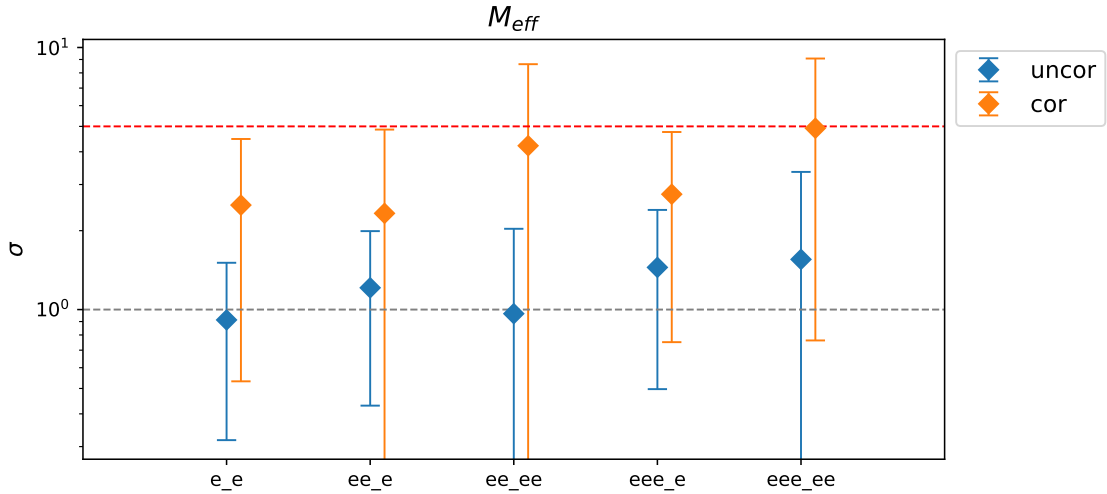




Is correlated fitting necessary?

Test fitting methods on synthetic correlator data:

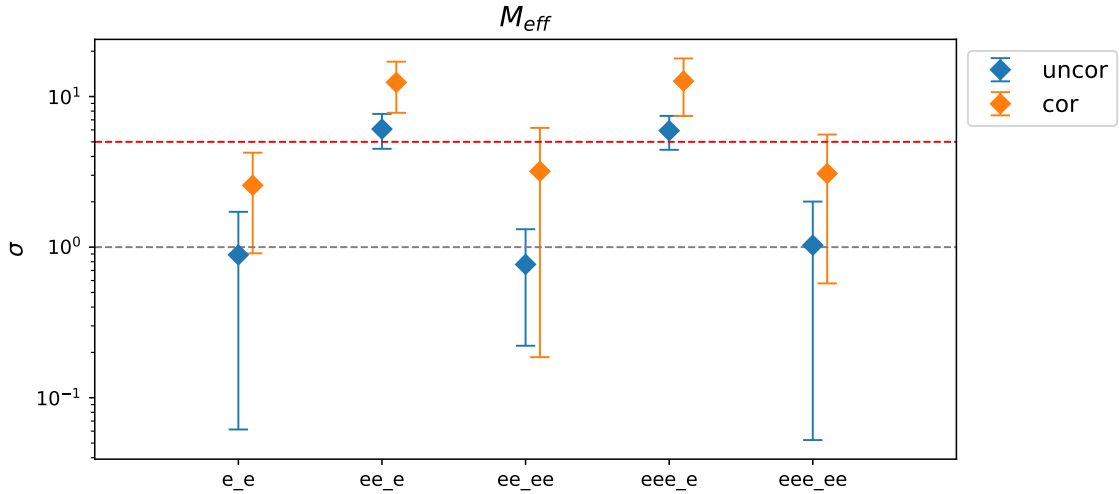
- Data with normally distributed uncorrelated noise:



Is correlated fitting necessary?

Test fitting methods on synthetic correlator data:

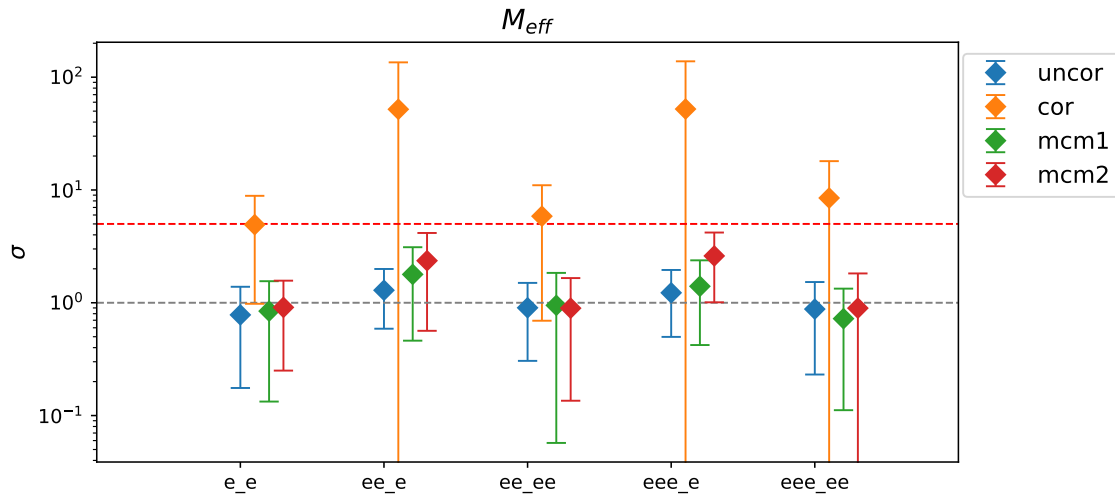
- Data with normally distributed uncorrelated noise:
- Data with correlated noise (adding normally distributed noise to noise from neighboring time-slice):



Is correlated fitting necessary?

Test fitting methods on synthetic correlator data:

- Data with normally distributed uncorrelated noise:
- Data with correlated noise (adding normally distributed noise to noise from neighboring time-slice):
- Data with correlated noise ("multiplying" normally distributed noise with covariance of real data):



Is correlated fitting necessary?

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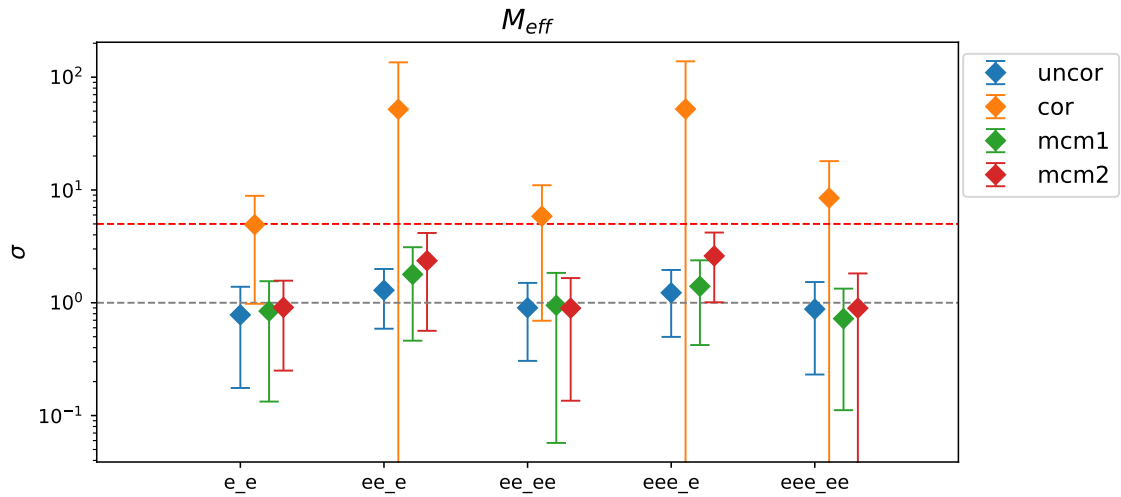

→ Uncorrelated fitting appears to produce best results.
→ Always include (at least) the first excited state in correlator fits.
→ Modification/truncation methods do not improve on uncorrelated fits.

Thank you.