Scale Setting from a combination of Wilson and Wtm quarks

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IFIC UV-CSIC

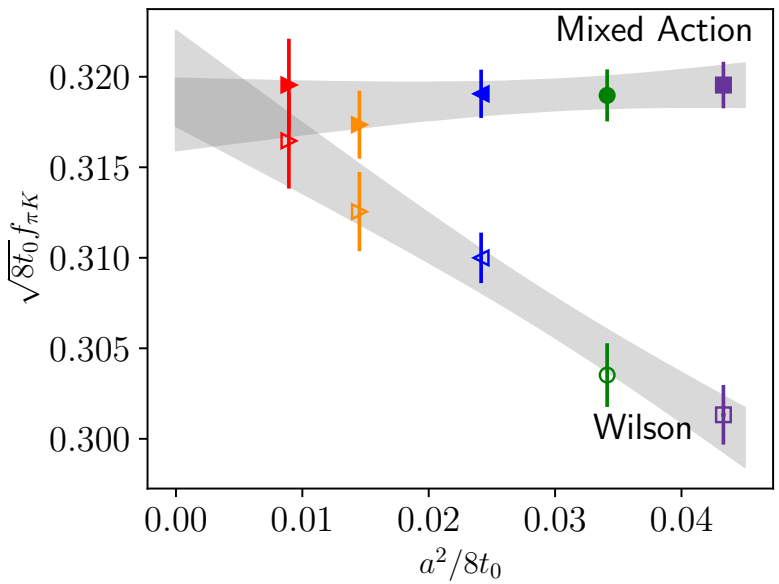
ECT* Trento workshop on scale setting

This work is partially supported by CNS2022-136005

Introduction

Introduction

- Scale setting $[f_{\pi,K}]$ from two valence regularizations
  - ⇝ Wilson unitary
  - ⇝ Wtm mixed action
- Different cutoff effects
  - ⇝ Heavily constrain continuum limit



$$m_\pi = m_K, \; m_K^2 + \tfrac{1}{2} m_\pi^2 \equiv phys.$$

Setup

Wilson fermions

- CLS ensembles

  [Bruno et al.,1411.3982],

  [Mohler et al.,1712.04884]

- $N_f = 2 + 1$

- Non-perturbatively $\mathcal{O}(a)$-improvement
- OBC in time for gauge fields

  [Lüscher, Schaefer, 1105.4749]

$$D_{\mathrm{W}}^{\mathrm{I}} = \frac{1}{2}\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - \frac{a}{2}\nabla_\mu^*\nabla_\mu + \frac{i}{4}\, a c_{sw} \sigma_{\mu\nu} \hat{F}_{\mu\nu} + \boldsymbol{m}$$

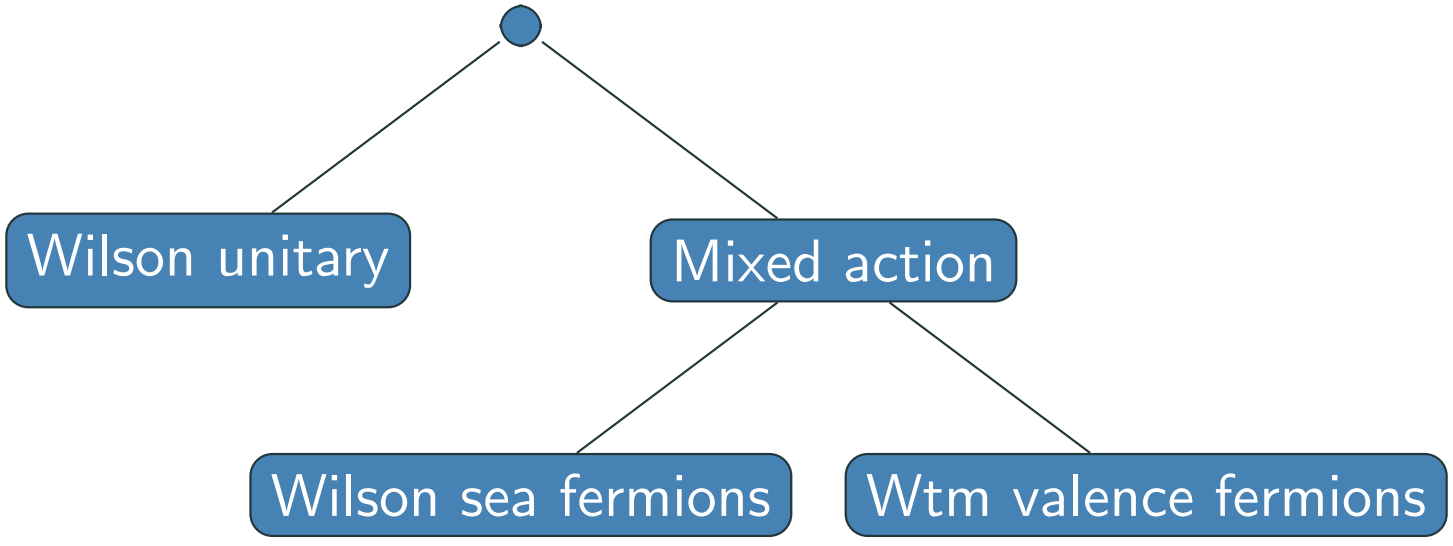
Wtm fermions

$$D_{\mathrm{Wtm}} = D_{\mathrm{W}}^{\mathrm{I}} + i\gamma_5 \boldsymbol{\mu}$$

⇝ Automatic $\mathcal{O}(a)$-improvement at maximal twist: $\frac{m_q^{\mathrm{R}}}{\mu_q^{\mathrm{R}}} = 0$

[Frezzotti et al. [ALPHA] hep-lat/0101001], [Frezzotti, Rossi, hep-lat/0306014]

Setup

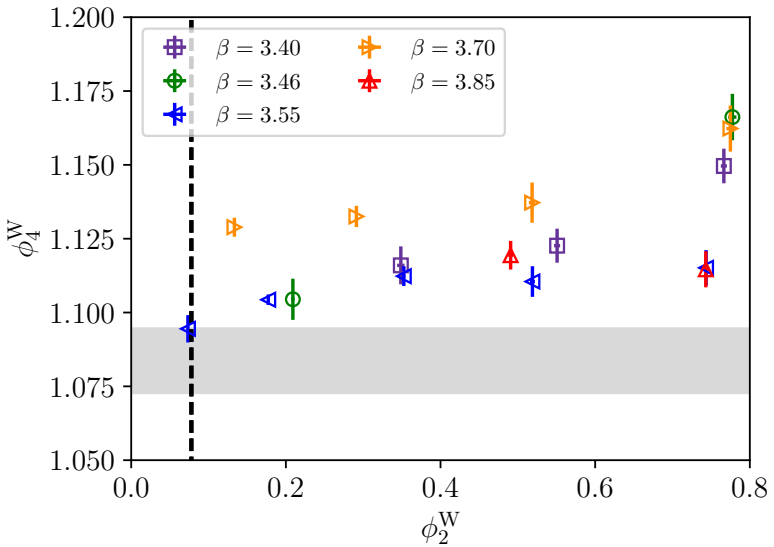

Wilson unitary
Mixed action
Wilson sea fermions
Wtm valence fermions

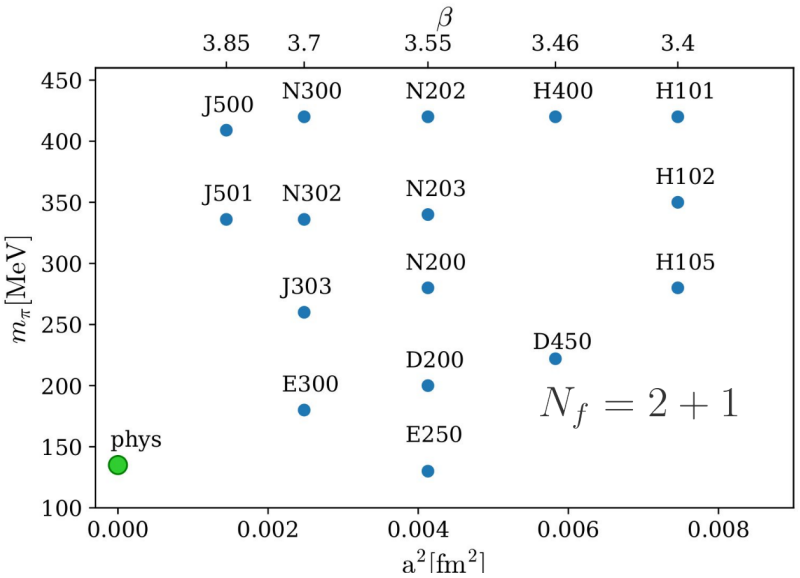
Wilson unitary setup

- Chiral trajectory $\mathrm{tr}(M_q) = 2m_{ud} + m_s \approx \mathrm{const.}$

  ⇝ Renormalized chiral trajectory $\phi_4 = 8t_0\left(m_K^2 + \frac{1}{2}m_\pi^2\right) = \mathrm{const.}$

  [Bruno, Korzec, Schaefer, 1608.08900] $\qquad \phi_2 \equiv 8t_0 m_\pi^2$





⇝ Iterative procedure in t_0^{ph} needed for physical point definition ϕ_2^{ph}, ϕ_4^{ph}

Wilson unitary setup

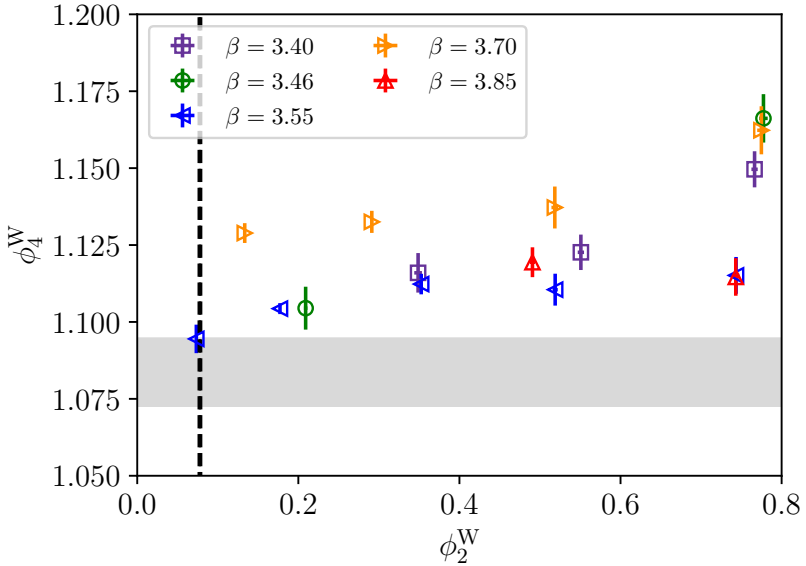
β	a [fm]	id	L/a	T/a	m_π [MeV]	m_K [MeV]	$m_\pi L$	MDU	N_{cnfg}
3.40	0.085	H101r000	32	96	426	426	5.8	4004	1001
		H101r001	32	96	426	425	5.8	4036	1009
		H102r001	32	96	360	446	4.9	3988	997
		H102r002	32	96	360	446	4.9	4032	1008
		H105r001	32	96	286	470	3.9	3788	947
		H105r002	32	96	286	470	3.9	4168	1042
		H105r005	32	96	286	470	3.9	3348	837
3.46	0.075	H400r001	32	96	429	429	5.2	2020	505
		H400r002	32	96	429	429	5.2	2160	540
		D450r011	64	128	221	483	5.4	4000	250
3.55	0.063	N202r001	48	128	418	418	6.5	3596	899
		N203r000	48	128	350	448	5.4	3024	756
		N203r001	48	128	350	448	5.4	3148	787
		N200r000	48	128	288	470	4.4	3424	856
		N200r001	48	128	288	470	4.4	3424	856
		D200r000	64	128	204	488	4.2	8004	2001
		E250r001	96	192	131	497	4.0	4000	100
...	...	...	...	...	...	...	...	...	...

blue ensembles: periodic b.c.

Wilson unitary setup

β	a [fm]	id	L/a	T/a	m_π [MeV]	m_K [MeV]	$m_\pi L$	MDU	N_{cnfg}
...	...	...	...	...	...	...	...	...	...
3.70	0.049	N300r002	48	128	427	427	5.1	6084	1521
		N302r001	48	128	350	457	4.2	8804	2201
		J303r003	64	192	261	481	4.1	8584	1073
		E300r001	96	192	177	499	4.2	4540	227
3.85	0.038	J500r004	64	192	418	418	5.2	6288	198
		J500r005	64	192	418	418	5.2	5232	130
		J500r006	64	192	418	418	5.2	3096	94
		J501r001	64	192	339	453	4.3	6536	371
		J501r002	64	192	339	453	4.3	4560	248
		J501r003	64	192	339	453	4.3	4296	168

Wilson unitary setup: mass-shifts

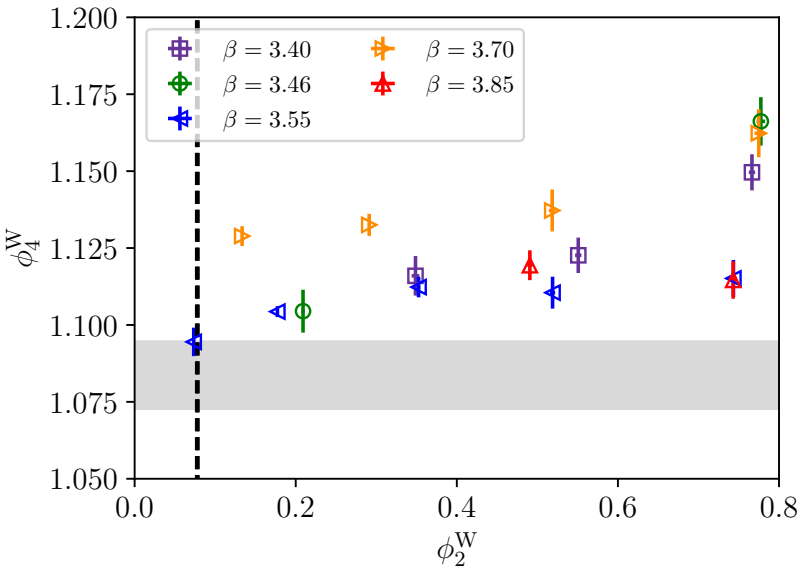


- Chiral trajectory
  $\mathrm{tr}(M_q) = 2m_{ud} + m_s \approx \mathrm{const.}$
- $\phi_2 = 8t_0 m_\pi^2$, $\phi_4 = 8t_0 m_K^2 + \frac{1}{2}\phi_2$
- $\phi_4 = \mathrm{const.} \equiv \phi_4^{\mathrm{ph}}$
- Small mass-shifts ($\leq 8\%$)
  [Bruno, Korzec, Schaefer, 1608.08900]

$$O(m_s') = O(m_s) + \delta m_s \frac{dO}{dm_s}|_{m_s},$$

$$\frac{dO}{dm_q} = \sum_i \frac{\partial O(\langle P_i \rangle)}{\partial \langle P_i \rangle} \left[\left\langle \frac{\partial P_i}{\partial m_q} \right\rangle - \left\langle P_i \frac{\partial S}{\partial m_q} \right\rangle + \langle P_i \rangle \left\langle \frac{\partial S}{\partial m_q} \right\rangle \right]$$

Wilson unitary setup: mass-shifts

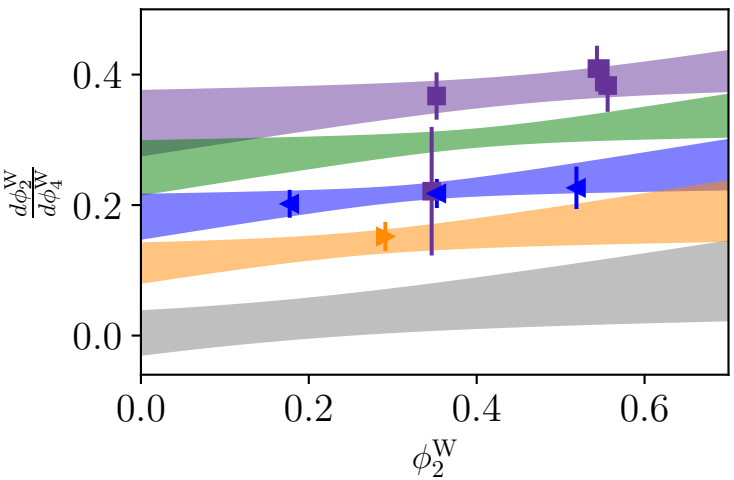


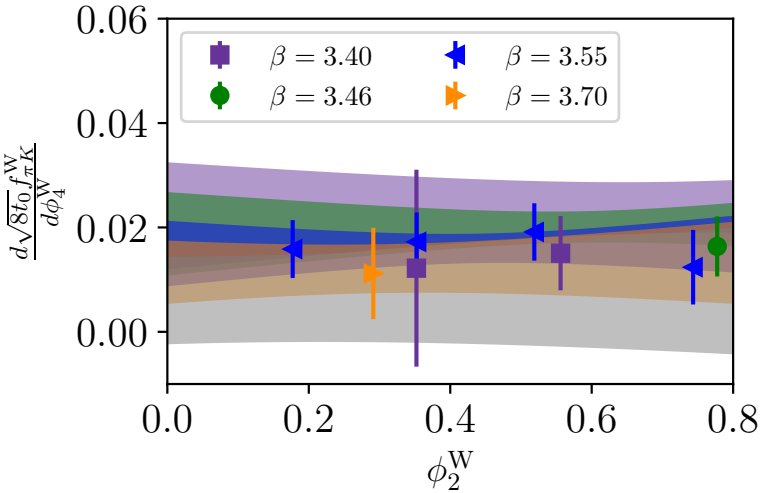
- Chiral trajectory
  $\mathrm{tr}(M_q) = 2m_{ud} + m_s \approx \mathrm{const.}$
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- $\phi_4 = \mathrm{const.} \equiv \phi_4^{\mathrm{ph}}$
- Small mass-shifts ($\leq 8\%$)
  [Strassberger et al., 2112.06696]

$$O(\phi_4^{\mathrm{W,ph}}) = O(\phi_4^{\mathrm{W}}) + \left(\phi_4^{\mathrm{W,ph}} - \phi_4^{\mathrm{W}}\right) \frac{dO}{d\phi_4^{\mathrm{W}}}$$

Wilson unitary setup: mass-shifts

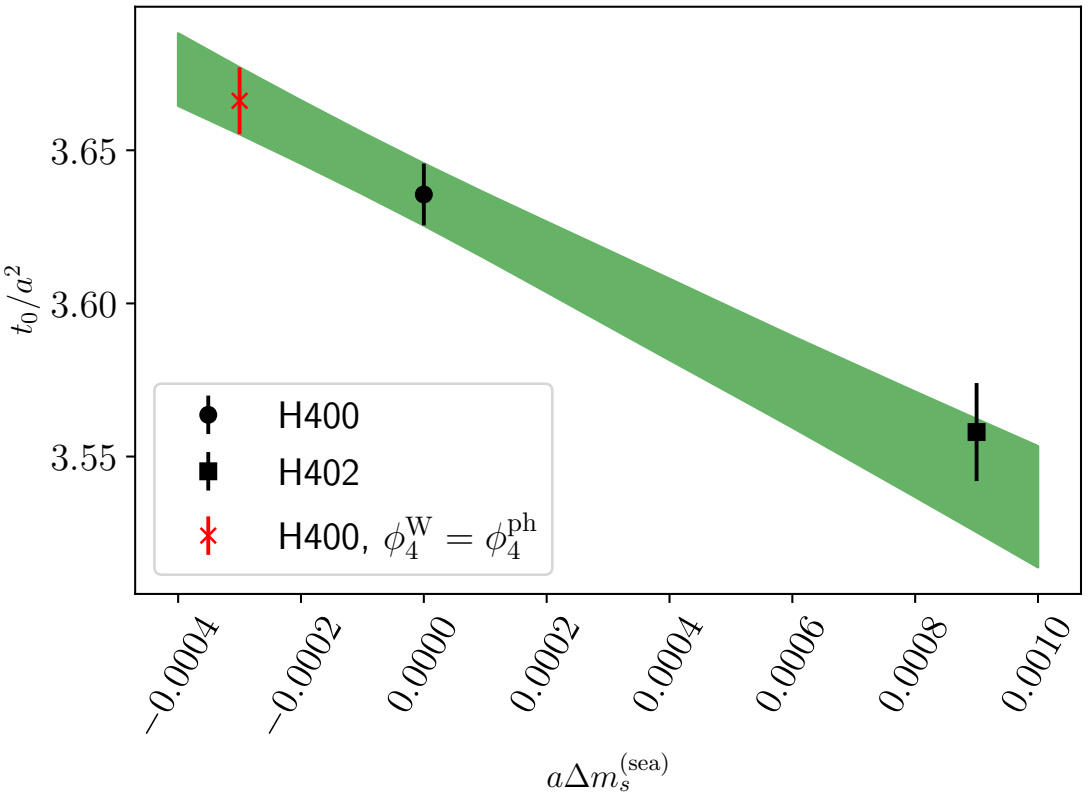
- Compute derivatives $dO/d\phi_4^{\mathrm{W}}$ for each ensemble
  - ⇝ Global fit derivatives [B. Strassberger, PhD thesis]





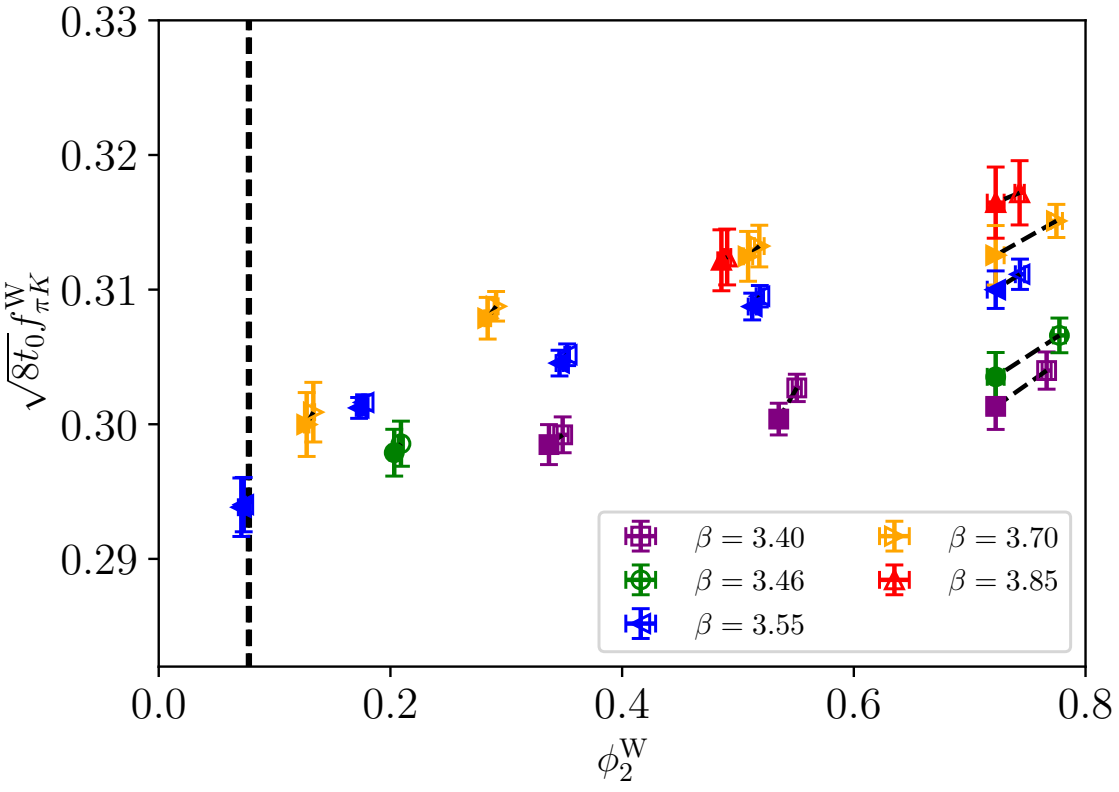
$\mathrm{p-value} \sim 0.5$ [Bruno, Sommer, 2209.14188]

Wilson unitary setup: mass-shifts



$$O(\phi_4^{\mathrm{W,ph}}) = O(\phi_4^{\mathrm{W}}) + \left(\phi_4^{\mathrm{W,ph}} - \phi_4^{\mathrm{W}}\right) \frac{dO}{d\phi_4^{\mathrm{W}}}$$

Wilson unitary setup: mass-shifts

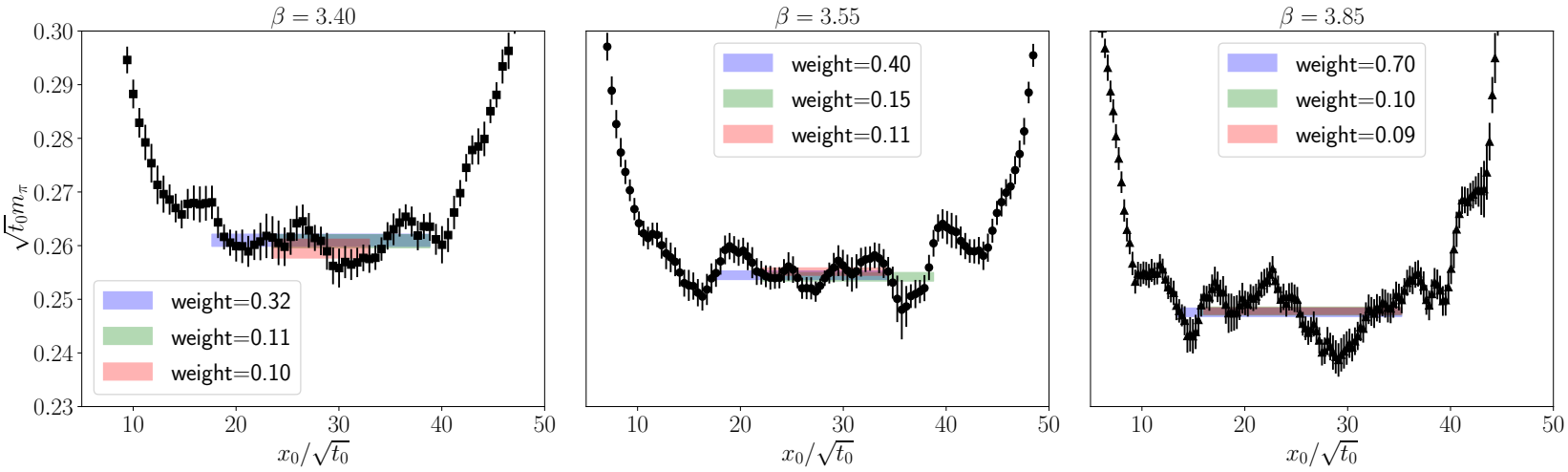


$$O(\phi_4^{\mathrm{W,ph}}) = O(\phi_4^{\mathrm{W}}) + \left(\phi_4^{\mathrm{W,ph}} - \phi_4^{\mathrm{W}}\right) \frac{dO}{d\phi_4^{\mathrm{W}}}$$

Wilson unitary setup

- OBC in time for gauge fields: avoid topology freezing

[Lüscher, Schaefer, 1105.4749] $m_\pi \approx 360$ MeV



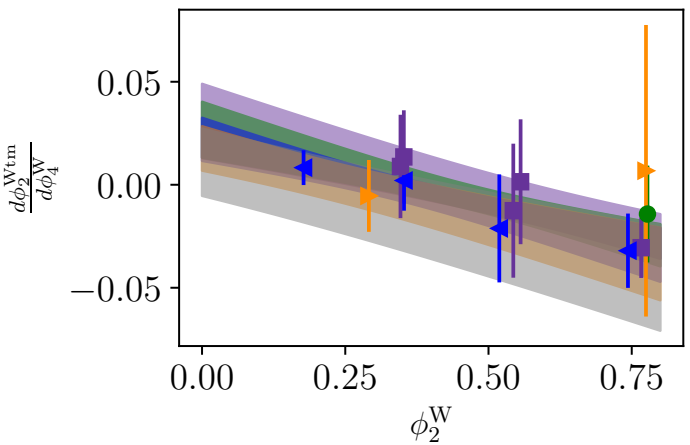
- Plateau extraction through model average
  1. Fit to a constant
  2. Vary fit/plateau range
  3. $\mathrm{TIC} = \chi^2 - 2\left\langle \chi^2 \right\rangle \to \mathrm{W} \propto \exp\left(-0.5 \times \mathrm{TIC}\right)$ [Frison, 2302.06550], [Bruno,Sommer, 2209.14188]
  4. $m_\pi = \sum_i m_\pi^{(i)} W^{(i)}$, $\sigma^2_{\mathrm{syst}}[m_\pi] = \left(\sum_i m_\pi^{(i)} W^{(i)}\right)^2 - \sum_i m_\pi^{2,(i)} W^{(i)}$

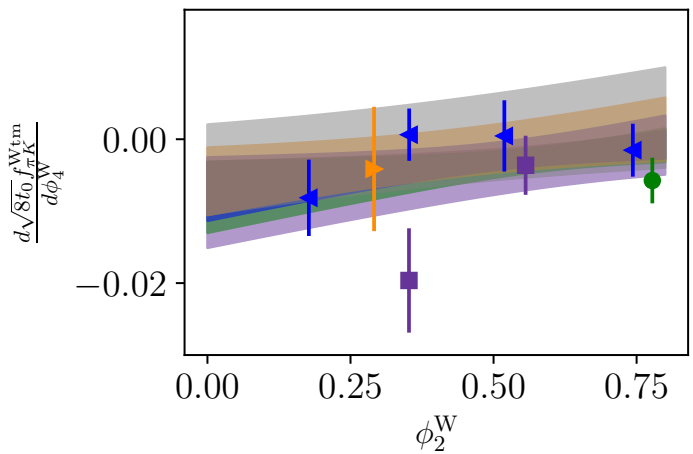
Mixed action setup: sea sector

- Mass-shift sea quark masses

$$O^{\mathrm{Wtm}}(\phi_4^{\mathrm{W,ph}}) = O^{\mathrm{Wtm}}(\phi_4^{\mathrm{W}}) + \left(\phi_4^{\mathrm{ph}} - \phi_4^{\mathrm{W}}\right) \frac{dO^{\mathrm{Wtm}}}{d\phi_4^{\mathrm{W}}},$$

$$\frac{dO^{\mathrm{Wtm}}}{dm_q^{(\mathrm{sea})}} = \sum_i \frac{\partial O^{\mathrm{Wtm}}(\langle P_i \rangle)}{\partial \langle P_i \rangle} \left[\cancel{\left\langle \frac{\partial P_i}{\partial m_q^{(\mathrm{sea})}} \right\rangle} - \left\langle P_i \frac{\partial S}{\partial m_q^{(\mathrm{sea})}} \right\rangle + \langle P_i \rangle \left\langle \frac{\partial S}{\partial m_q^{(\mathrm{sea})}} \right\rangle \right]$$

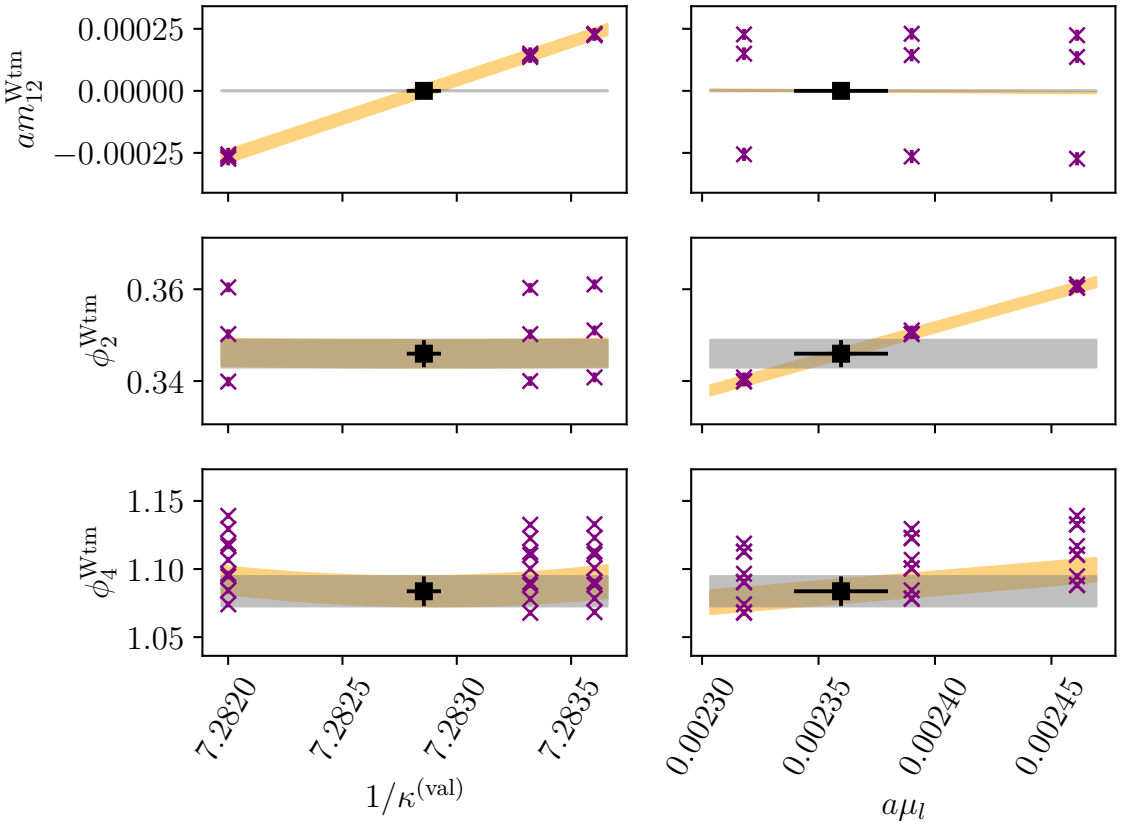




$$\mathrm{p-value} \sim 0.15$$

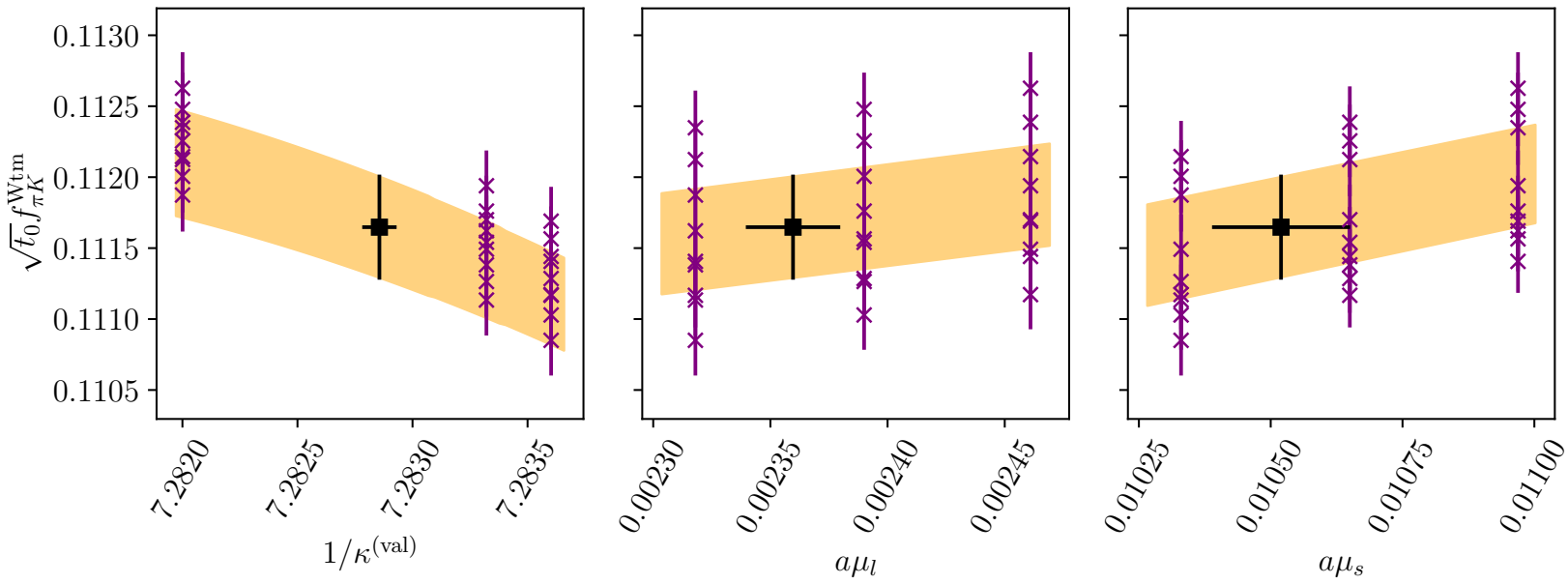
Mixed action setup: valence sector

- Match valence & sea quark masses through $m_{\pi,K}$
  ⇝ recover unitarity in the continuum, $\phi_4 \equiv \phi_4^{\mathrm{ph}}$
- Tune to maximal twist through vanishing PCAC quark mass
  ⇝ $am_{12}^{\mathrm{Wtm}} = 0$



Mixed action setup: valence sector

⇝ Interpolate $f_{\pi,K}$ to matching and maximal twist point



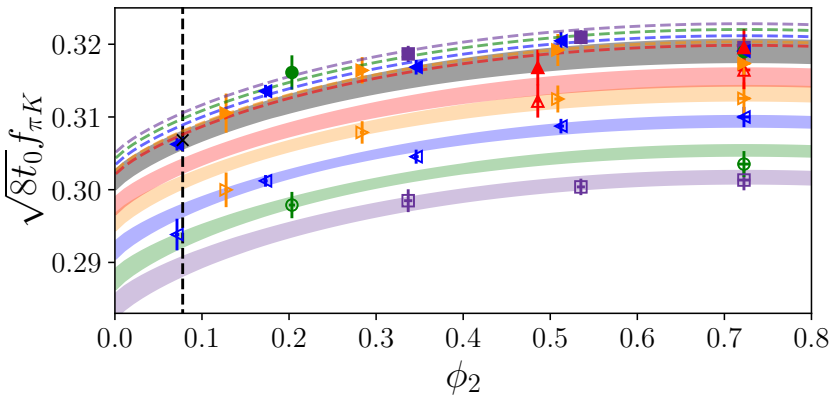
Scale setting

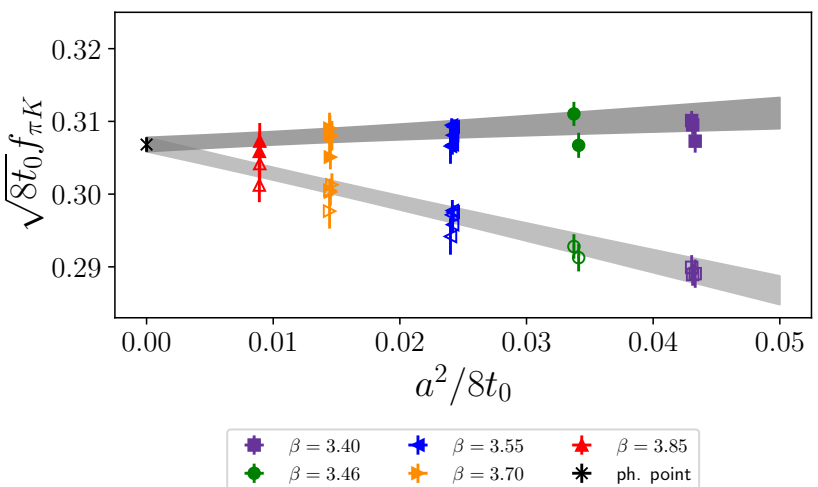
Scale setting

- Set the scale through $\sqrt{t_0} f_{\pi K}$ [Bruno, Korzec, Schaefer, 1608.08900]
  - ▷ $m_{\pi,K}^{\mathrm{isoQCD}}$ to define the physical point
  - ▷ $f_{\pi K}^{\mathrm{isoQCD}} = \frac{2}{3}\left(f_K + \frac{1}{2} f_\pi\right)^{\mathrm{isoQCD}}$ to set the scale
  - ▷ isoQCD $\rightarrow$ Edinburgh consensus, FLAG24 + f_K^{isoQCD}
- Two regularizations: Wilson unitary & Wtm mixed action
  - ▷ Different cutoff effects

    ⇝ Control continuum limit
  - ▷ Increased statistical precision by combining both data sets
- Model variation over chiral-continuum limit
  - ▷ Various choices: TIC, AIC, ...
  - ▷ Systematic uncertainty

Chiral-continuum extrapolation: test model





- SU(3) χPT
- $\mathcal{O}(a^2)$ cutoff effects
- All data included
  - ⇝ penalize coarsest lattice spacing & heaviest pion

⇝ $\mathrm{p} - \mathrm{value} = 0.8$

Model variation

- Chiral extrapolation
  - ▷ SU(3), SU(2) χPT
  - ▷ Taylor expansion
    $p_1 + p_2\,(\phi_2 - \phi_2^{\mathrm{sym}})^2 +$
    $p_3\,(\phi_2 - \phi_2^{\mathrm{sym}})^4$
- Cutoff effects
  - ▷ $\mathcal{O}(a^2)$, $\mathcal{O}(a^2 + a^2\phi_2)$,
    $\mathcal{O}(a^2\alpha_{\mathrm{S}}^{\Gamma})$ [Husung, 2206.03536]
- Data cuts
  - ▷ $\beta \leq 3.40$
  - ▷ $\beta \leq 3.46$
  - ▷ $m_\pi \geq 420$ MeV
  - ▷ $m_\pi \geq 420$ MeV, $\beta \leq 3.40$
  - ▷ $m_\pi L \leq 4.1$

- Average:

$$\mathrm{W} \propto \exp\left(-0.5 \times \mathrm{IC}\right),$$

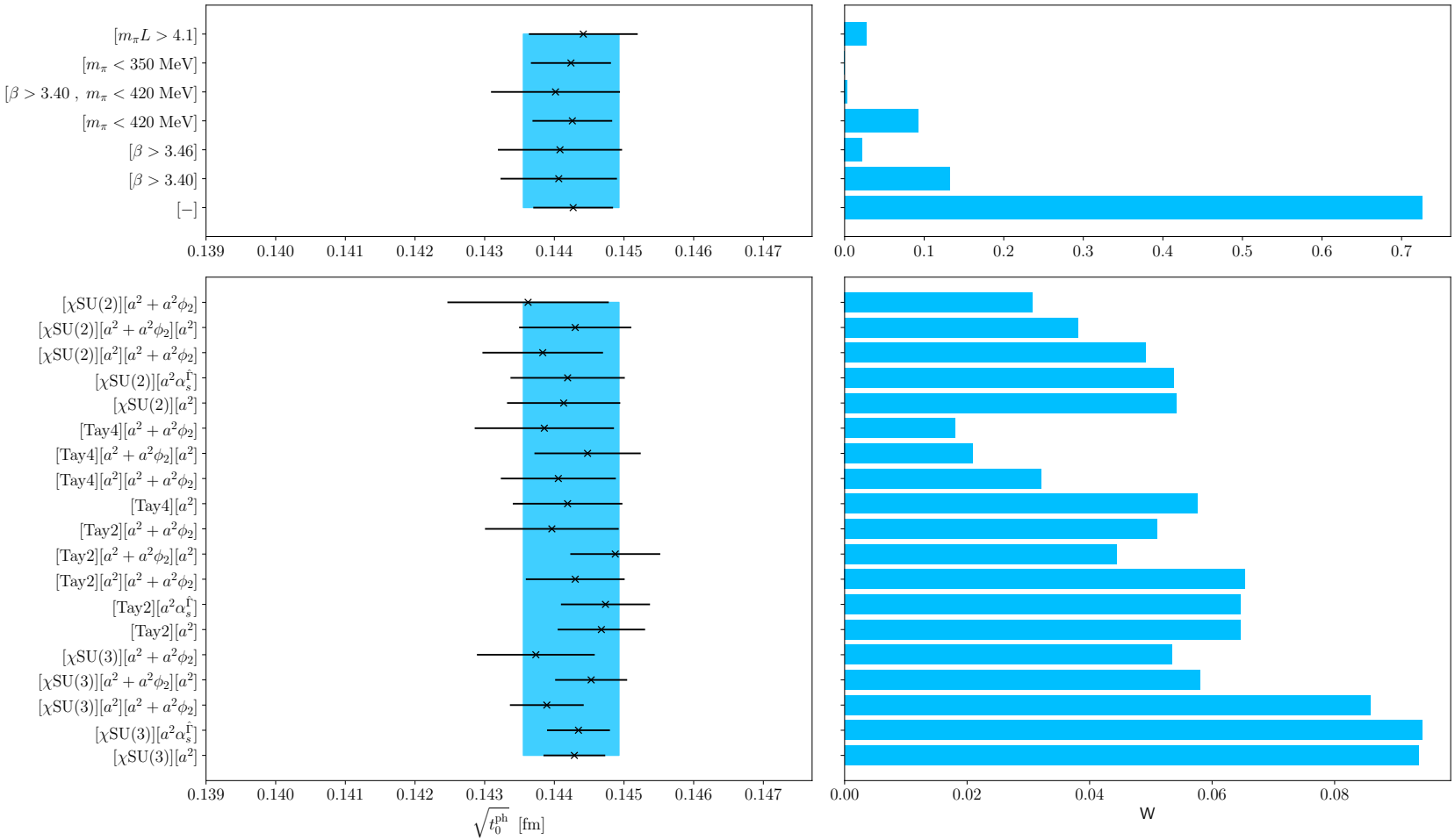
$$\sqrt{t_0^{\mathrm{ph}}} = \sum_i \sqrt{t_0^{\mathrm{ph,(i)}}}\, w^{(\mathrm{i})},$$

$$\sigma^2[\sqrt{t_0^{\mathrm{ph}}}] = \sqrt{t_0^{\mathrm{ph}}}^2 - \left(\sum_i \sqrt{t_0^{\mathrm{ph,i)}}}^2\, w^{(\mathrm{i})}\right),$$

$$\mathrm{IC} \to \mathrm{TIC} = \chi^2 - 2\left\langle \chi^2 \right\rangle,$$

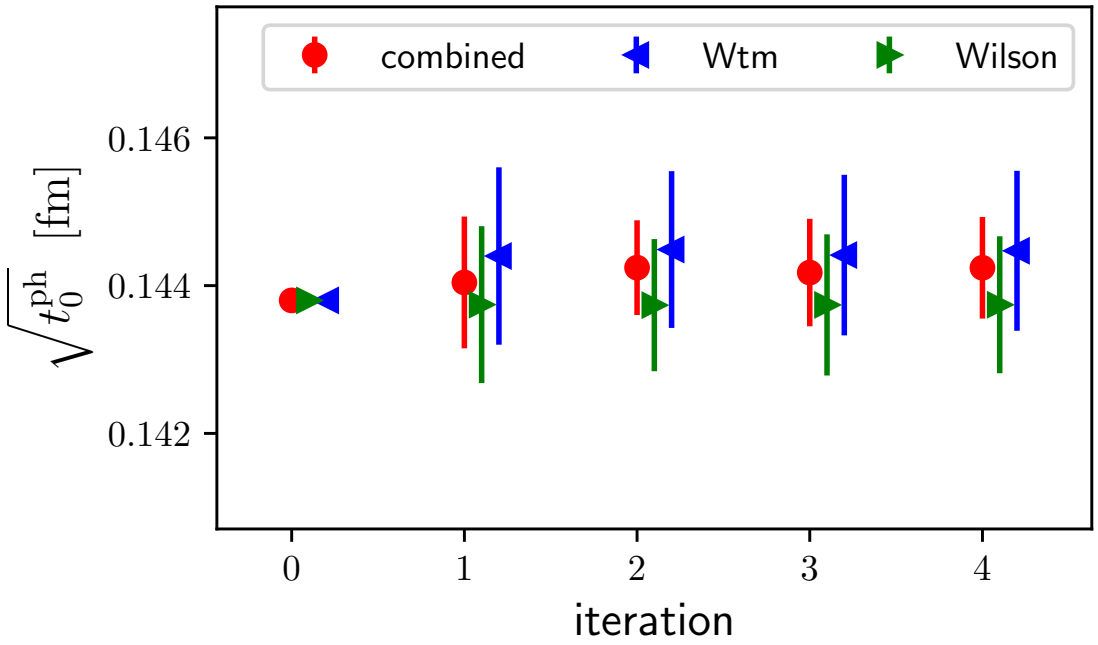
⇝ other IC's are explored...

Model average: TIC



$$\mathrm{p-value_{min}} = 0.44,\ \mathrm{p-value_{max}} = 0.97$$

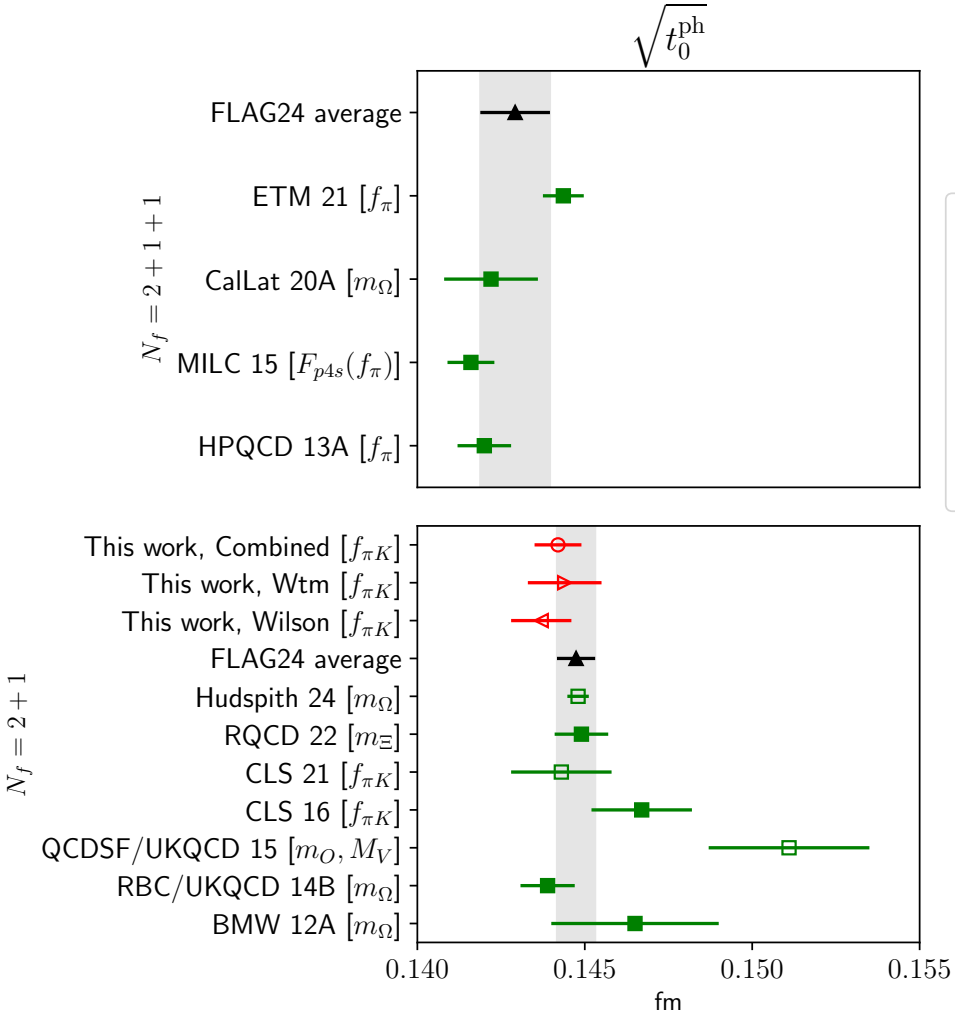
Iterative determination of t_0^{ph}

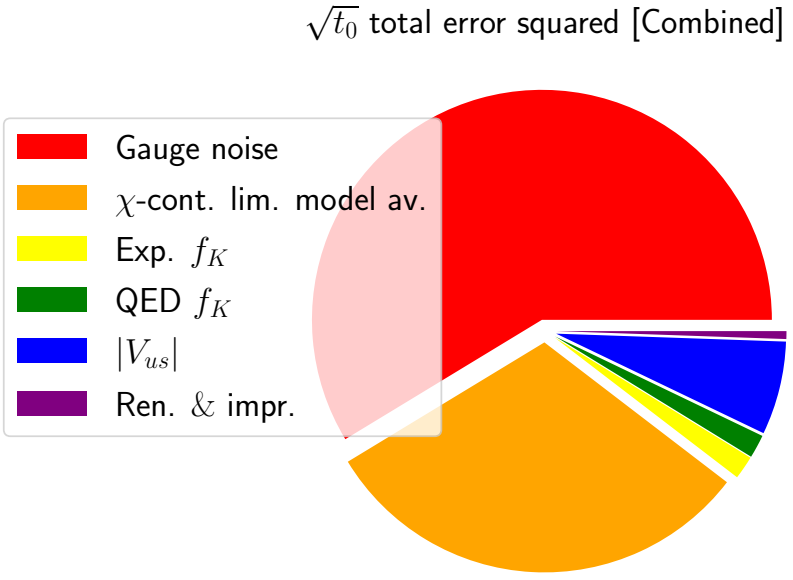


⇝ Needed for physical point definition ϕ_2^{ph}, ϕ_4^{ph}

Results

[PRELIMINARY]





$$\sqrt{t_0^{\rm ph}} = 0.1442(6)_{\rm stat}(4)_{\rm syst}[7]_{\rm tot}\ \text{fm}$$

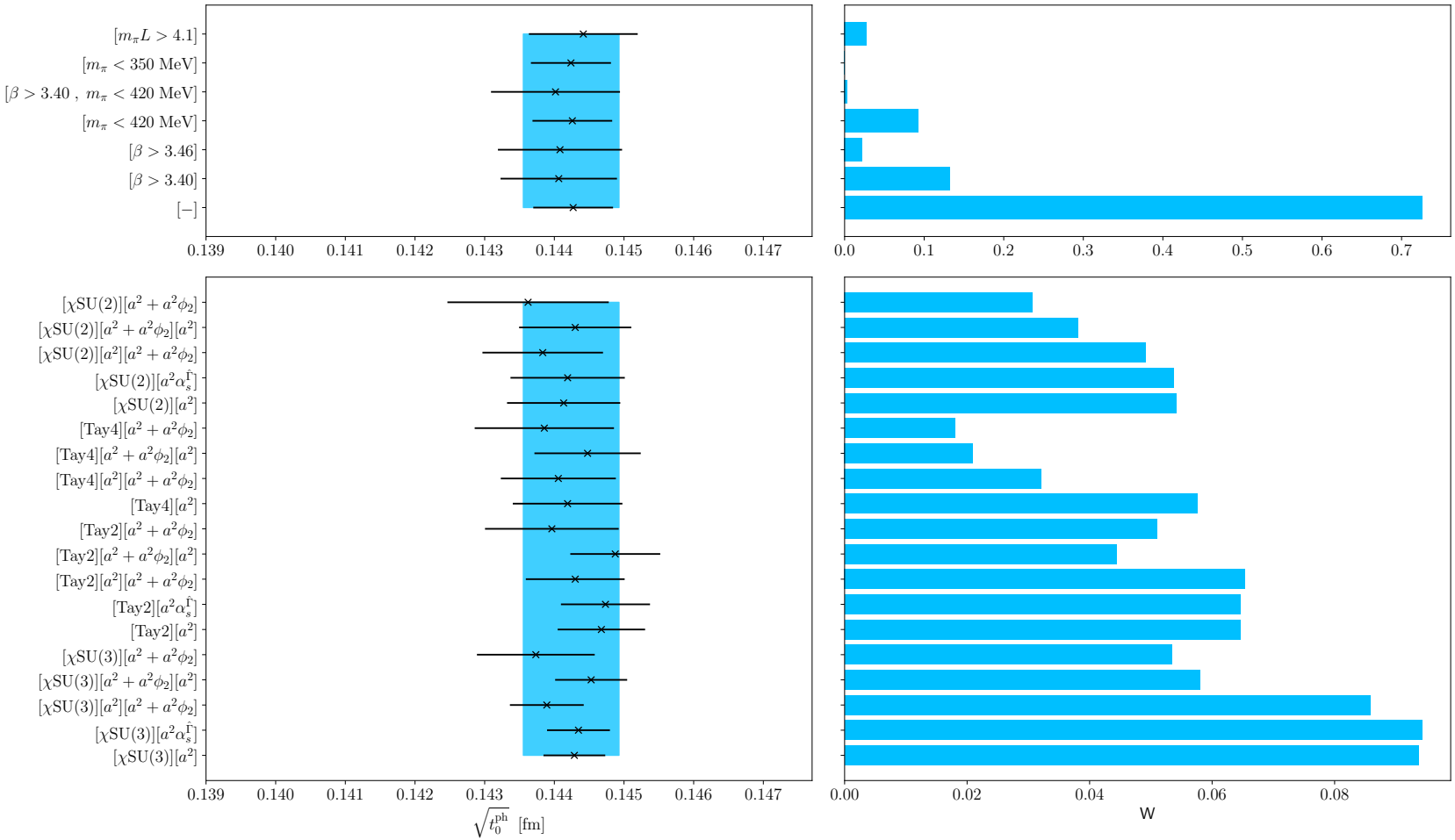
ADerrors.jl, $\Gamma-$method

[U. Wolff, hep-lat/0306017]

[A. Ramos, 1809.01289, 2012.11183]

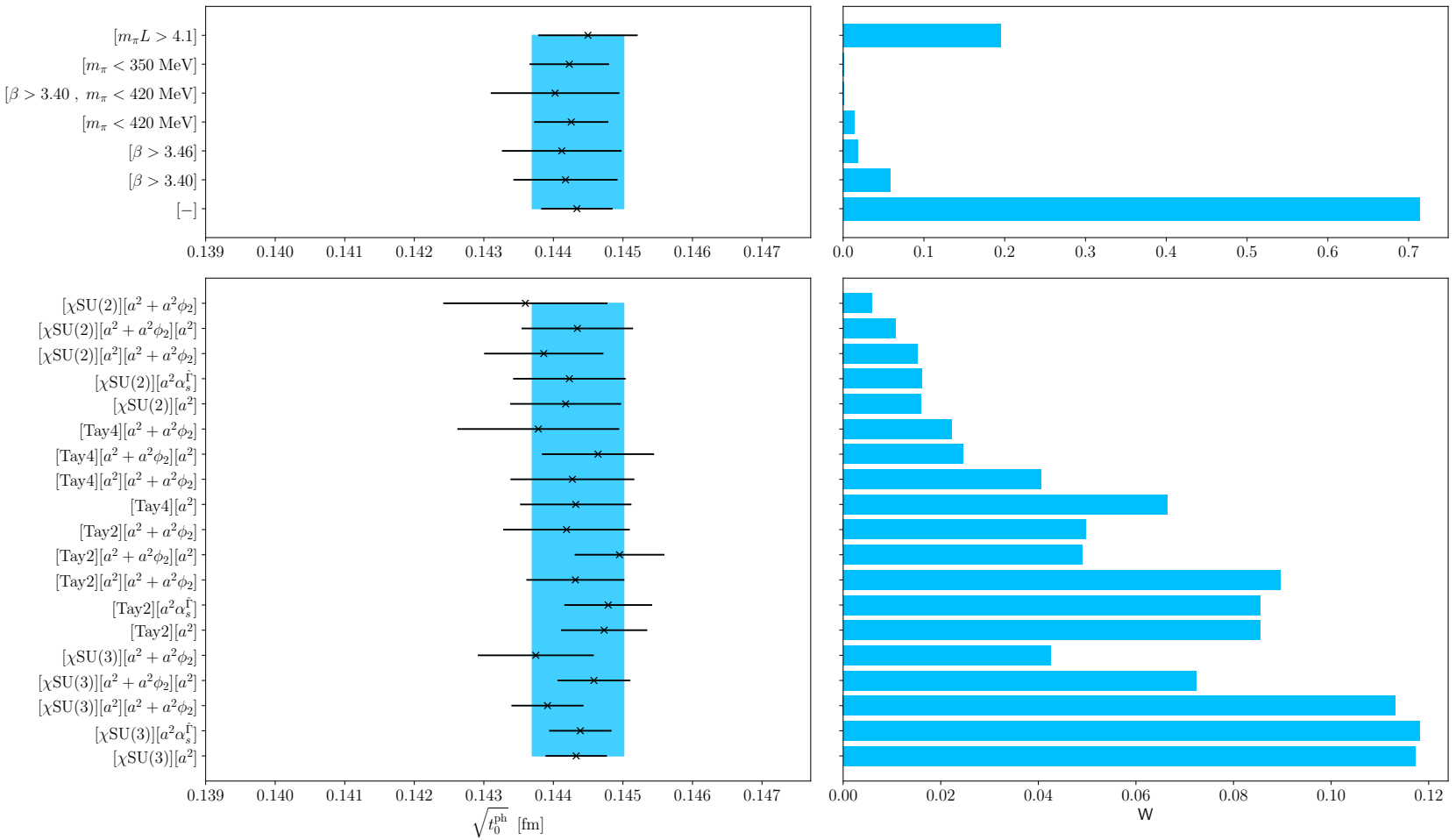
IC variations: TIC, Combined

$\mathrm{TIC} = \chi^2 - 2\langle\chi^2\rangle$, Combined



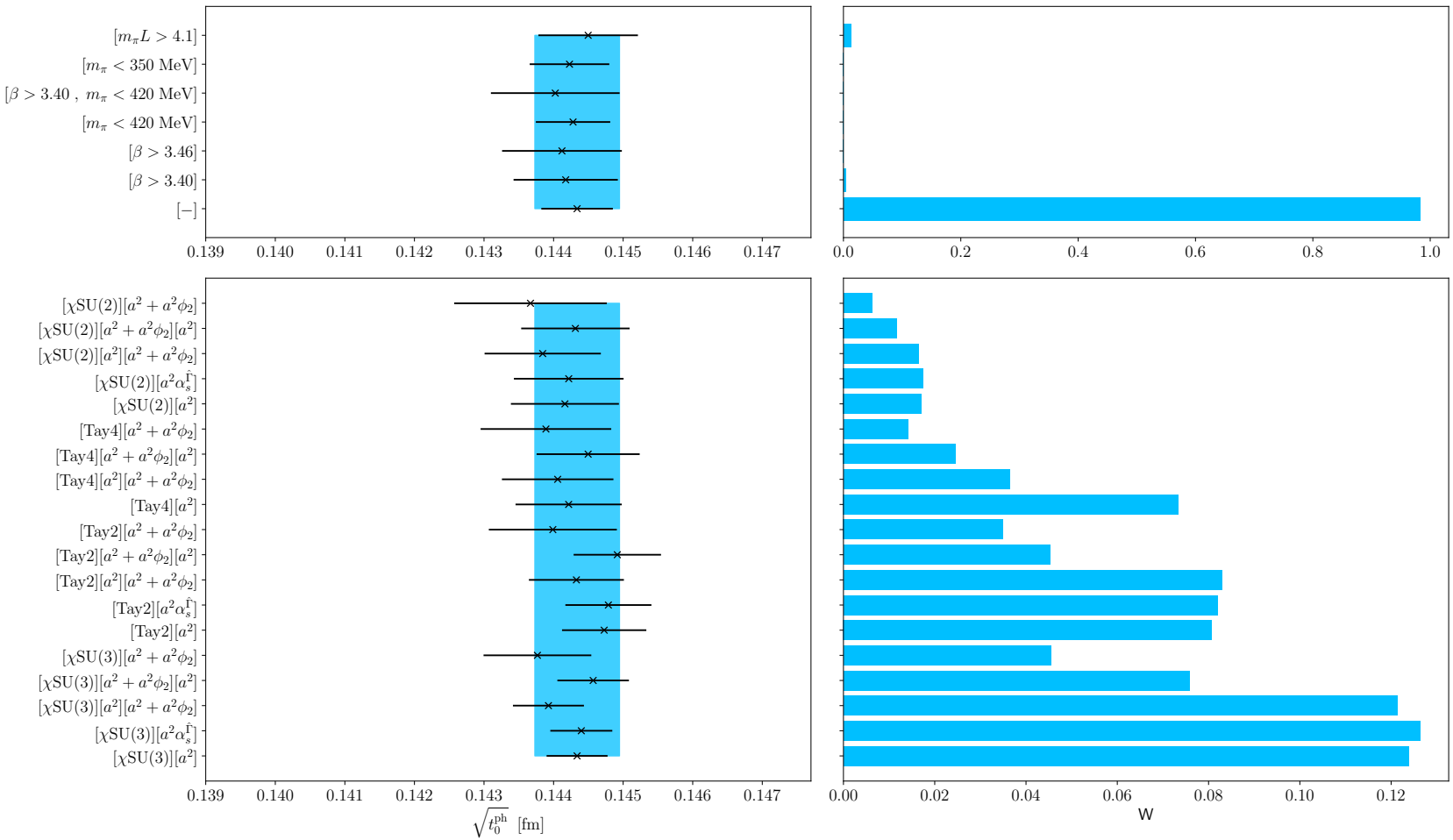
IC variations: $\mathrm{AIC}^{\mathrm{sub}}$, Combined

$$\mathrm{AIC}^{\mathrm{sub}} = \chi^2 + 2n_{\mathrm{param}} + n_{\mathrm{cut}},\ \text{Combined}$$ [E. Neil, J. Sitison, 2305.19417]



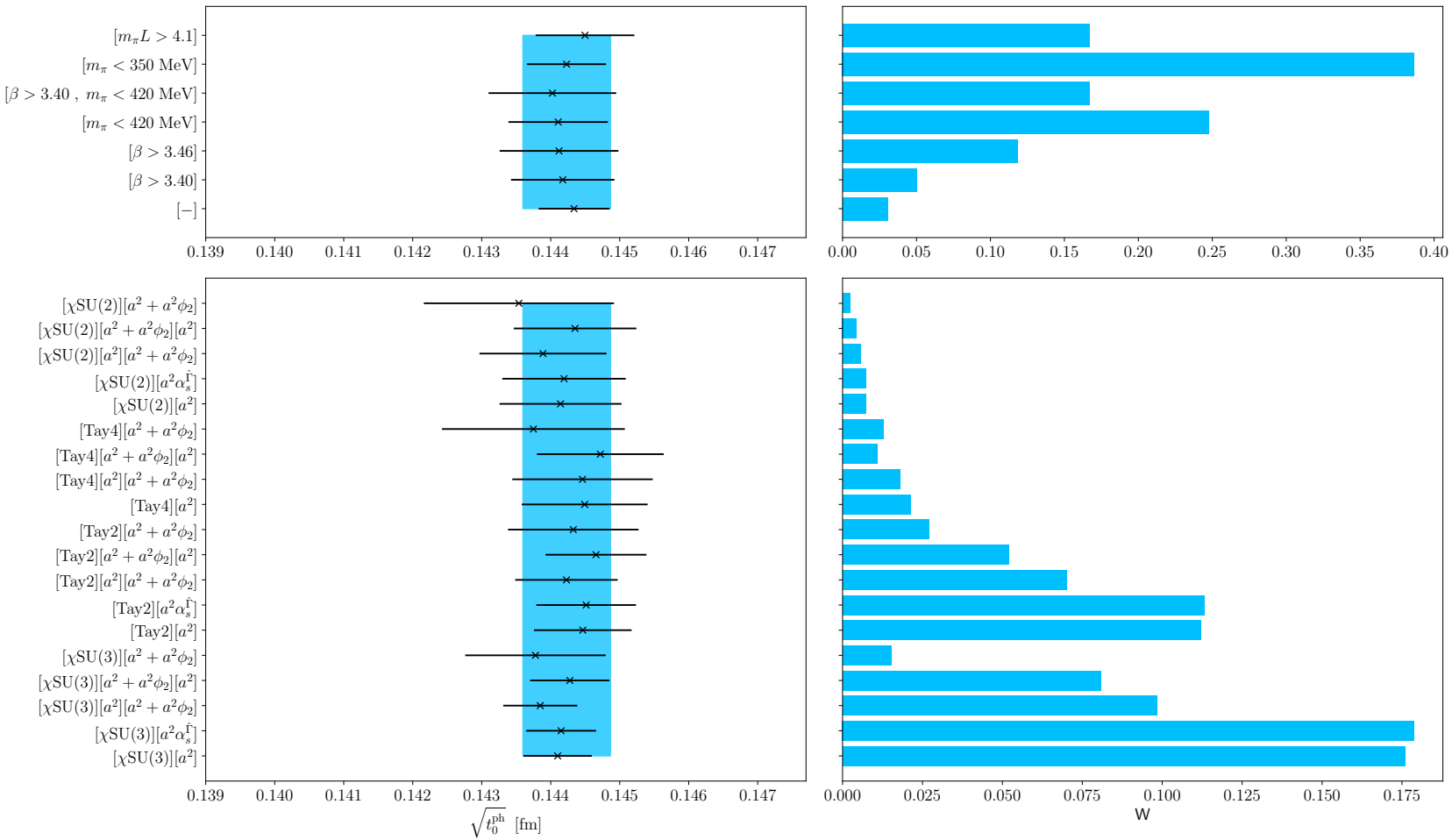
IC variations: $\mathrm{AIC}^{\mathrm{perf}}$, Combined

$$\mathrm{AIC}^{\mathrm{perf}} = \chi^2 + 2n_{\mathrm{param}} + 2n_{\mathrm{cut}},\ \text{Combined}$$ [E. Neil, J. Sitison, 2305.19417]

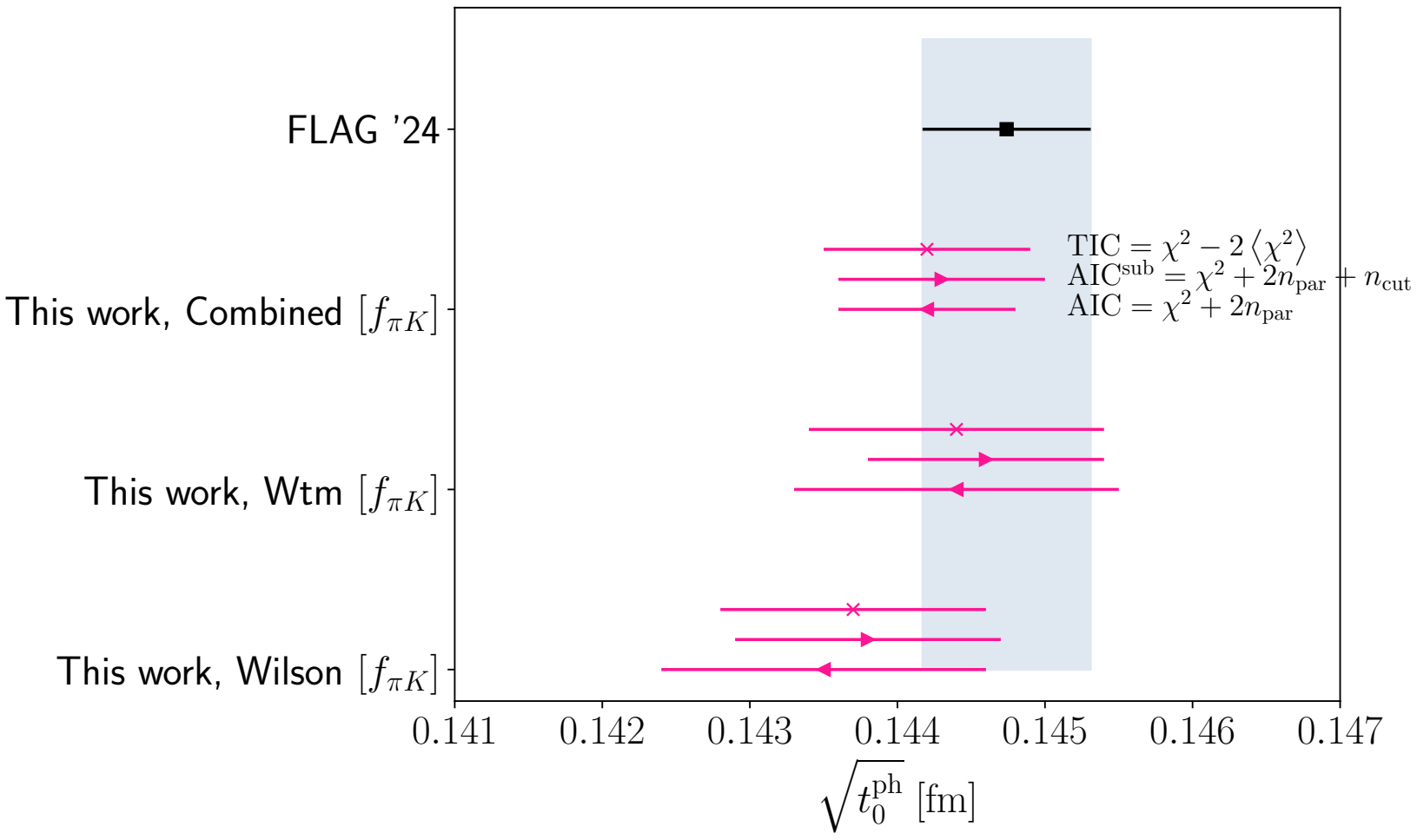


IC variations: AIC, Combined

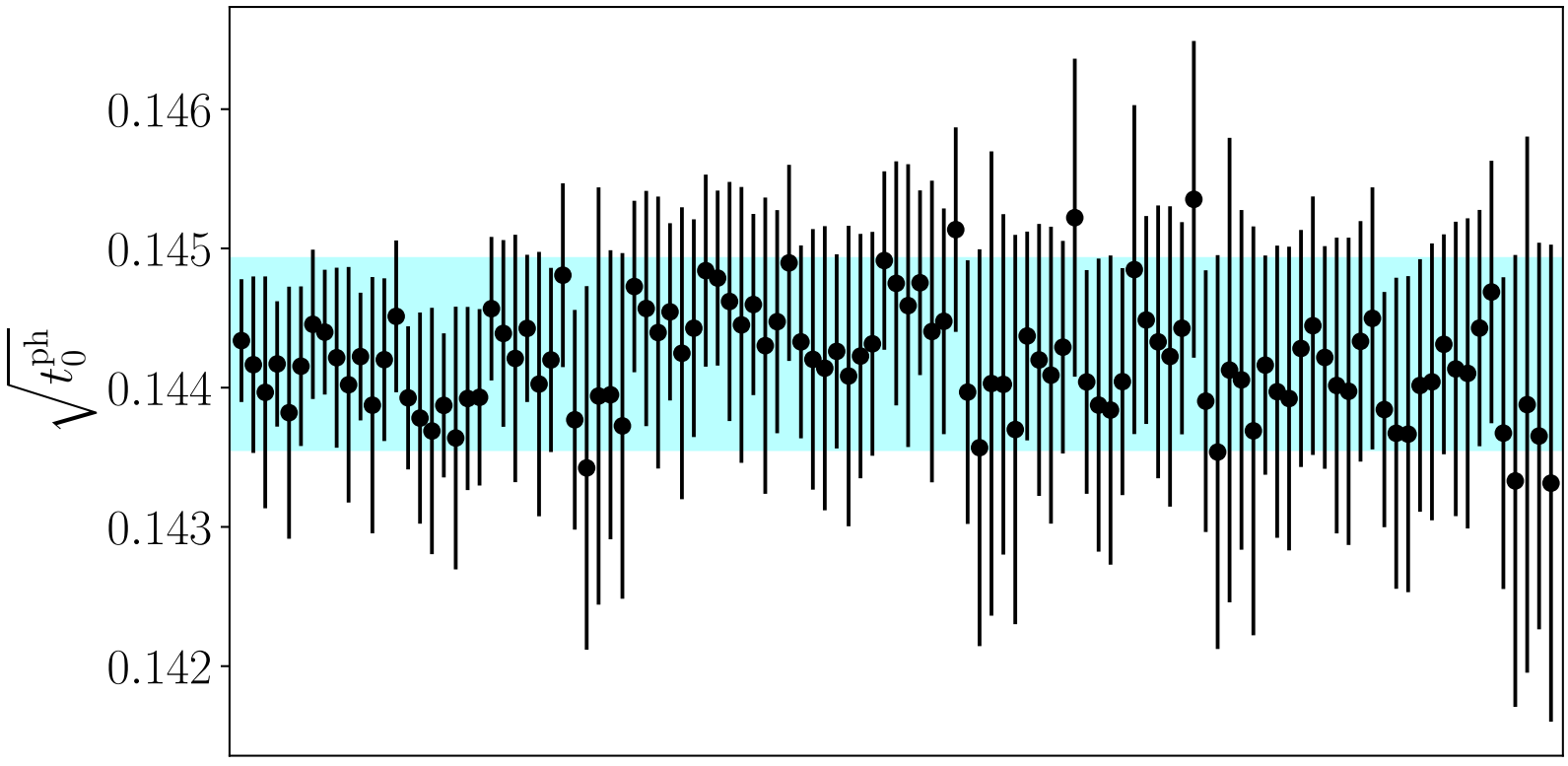
$\mathrm{AIC} = \chi^2 + 2n_{\mathrm{param}}$, Combined



Scale setting: IC variations



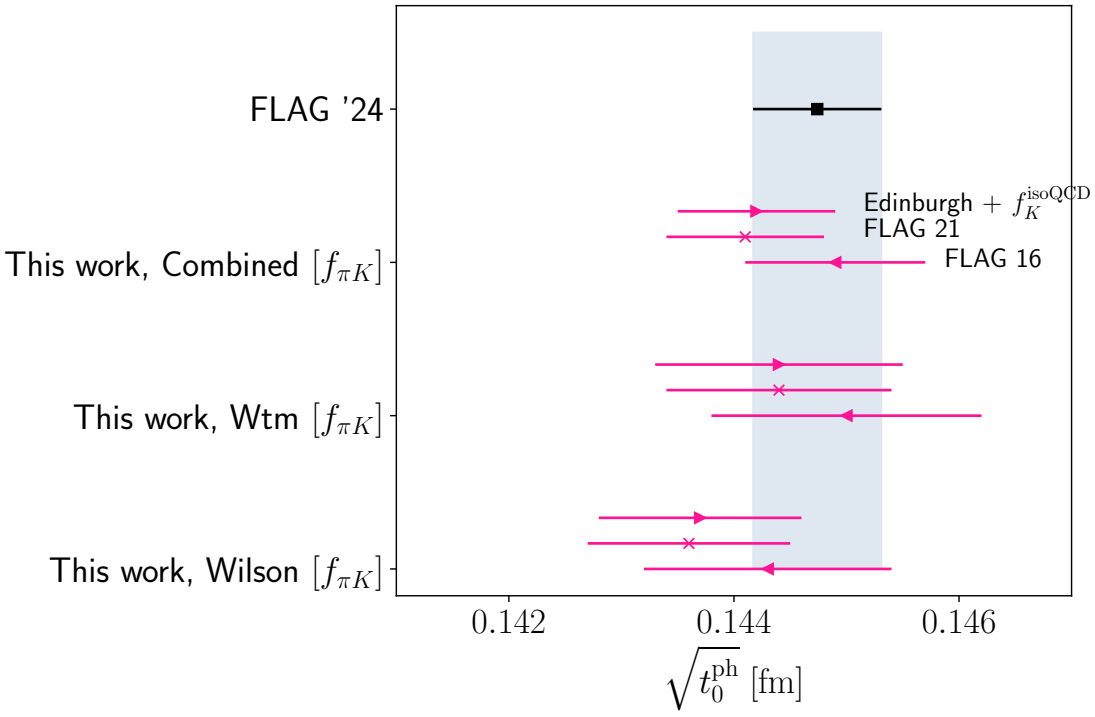
Average: "maximum spread"



$$\sqrt{t_0^{\rm ph}} = 0.1442(6)_{\rm stat}(4)_{\rm syst}[7]_{\rm tot} \text{ fm [model average, TIC]}$$

$$\sqrt{t_0^{\rm ph}} = 0.1442(10)_{\rm tot} \text{ fm [à la ALPHA]}$$

Scale setting: physical input variations

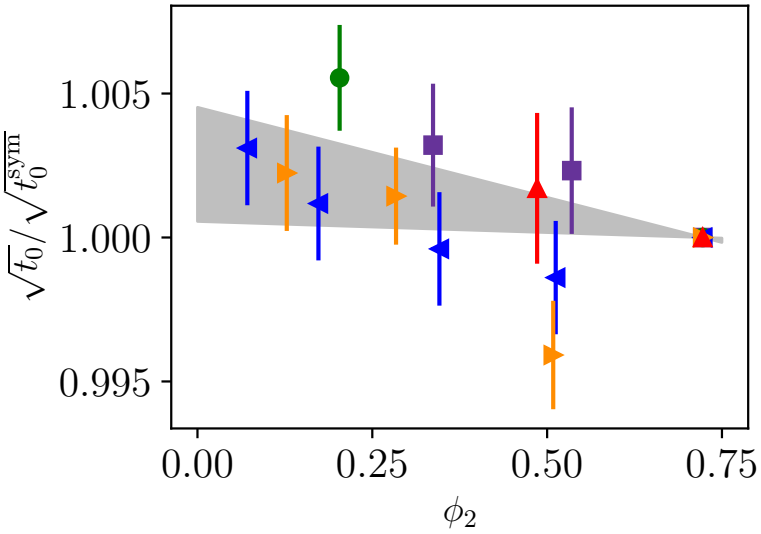


	Edinburgh $+f_K^{\rm isoQCD}$	FLAG21	FLAG16
m_π [MeV]	135.0	134.9768(5)	134.8(3)
m_K [MeV]	494.6	497.611(13)	494.2(3)
f_π [MeV]	130.5	130.56(3)	130.4(2)
f_K [MeV]	157.1(5)	157.2(5)	156.2(7)

[PRELIMINARY]

- $\phi_4 = 1.11,\ \phi_2 = \phi_2^{\rm sym} = \frac{2}{3}\phi_4$
- Compute t_0 mass shifting to $\phi_4 = 1.11$
- Fit $\dfrac{\sqrt{t_0/a^2}}{\sqrt{t_0^{\rm sym}/a^2}} = \sqrt{1 + p_1(\phi_2 - \phi_2^{\rm sym})}$

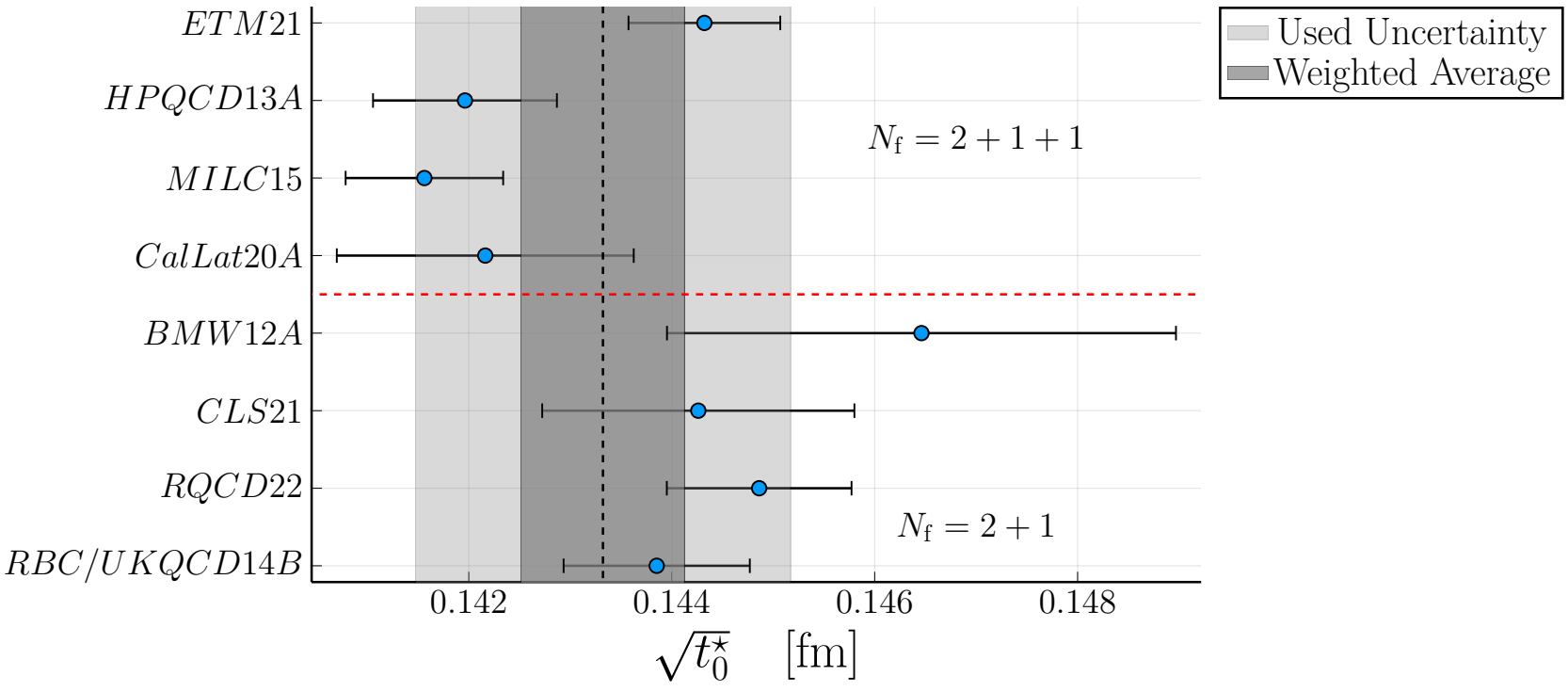
[Strassberger et al., 2112.06696]



⇝ Ours: $\dfrac{\sqrt{t_0^{\rm ph}}}{\sqrt{t_0^*}} = 1.0016(18)$

⇝ Quoted in [M. Dalla Brida et al. [ALPHA], 2501.06633]: $\dfrac{\sqrt{t_0^{\rm ph}}}{\sqrt{t_0^*}} = 1.0003(30)$

[PRELIMINARY]



Plot from [M. Dalla Brida et al. [ALPHA], 2501.06633]

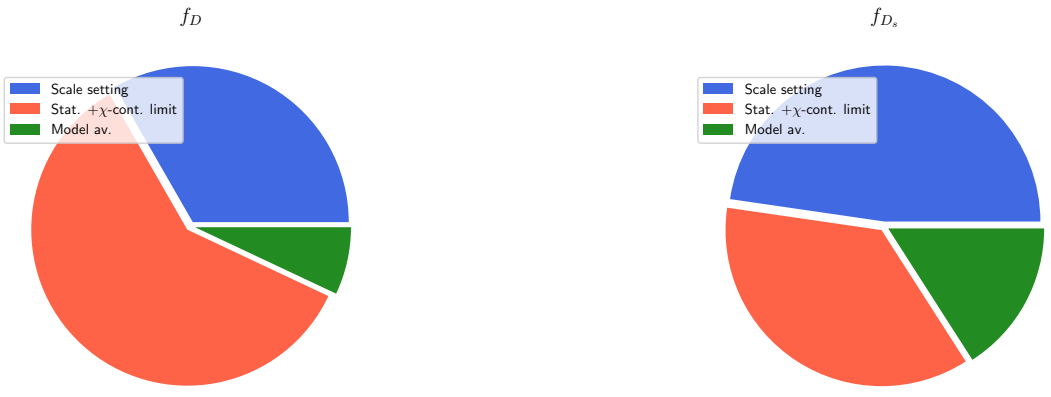
↝ Ours: $\sqrt{t_0^*} = 0.1439(7)_{\text{stat}}(4)_{\text{syst}}[8]_{\text{tot}}$ fm

↝ Quoted in [M. Dalla Brida et al. [ALPHA], 2501.06633]: $\sqrt{t_0^*} = 0.1434(19)$ fm

Conclusions

Conclusions

- Combining Wilson unitary and Mixed action regularizations:
  - ⇝ Controlled continuum limit
  - ⇝ Increased statistics



[A. Bussone et al., [ALPHA], 2309.14154]

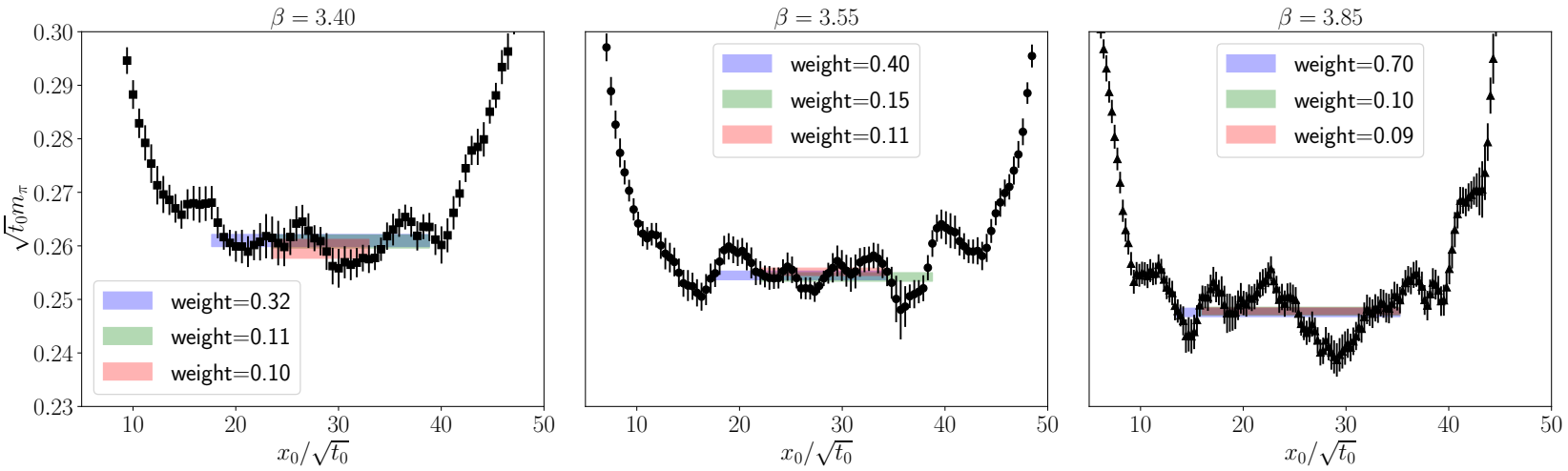
- Current effort: set the scale only with f_π

Backup

Wilson unitary setup

- OBC in time for gauge fields: avoid topology freezing

[Lüscher, Schaefer, 1105.4749] $m_\pi \approx 360$ MeV

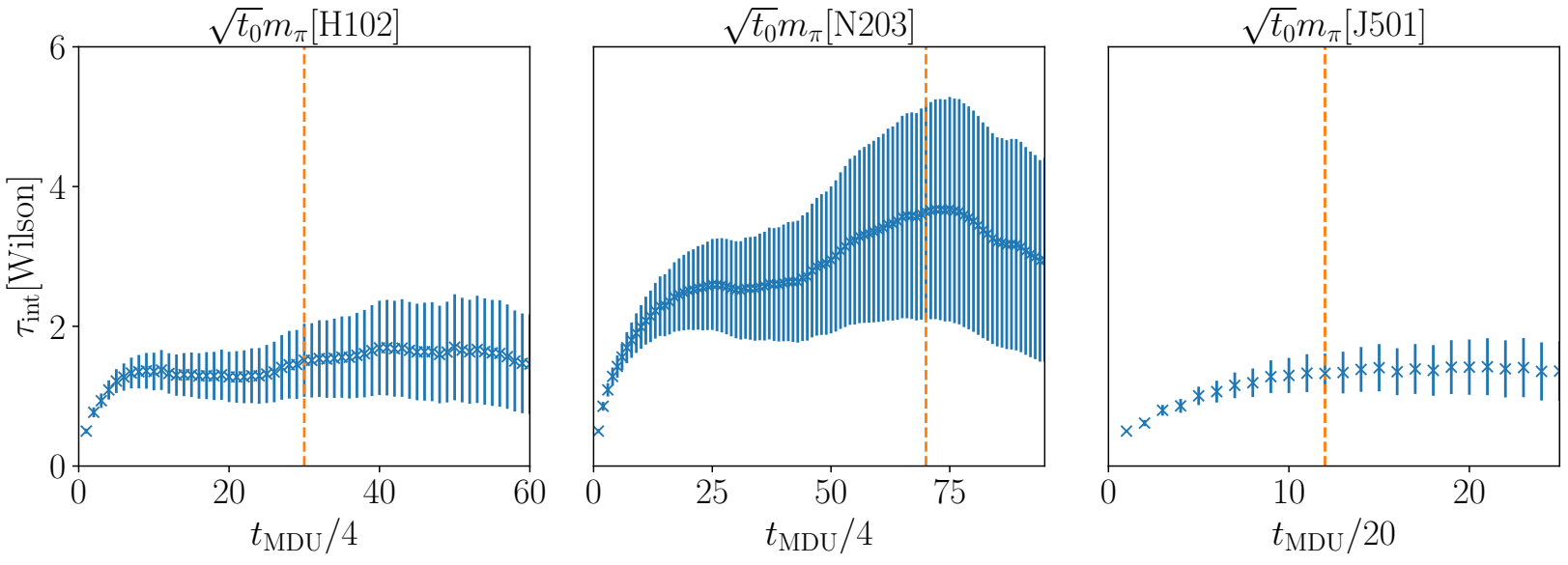


- Plateau extraction through model average
  1. Fit to a constant
  2. Vary fit/plateau range
  3. $\mathrm{TIC} = \chi^2 - 2\langle\chi^2\rangle \to \mathrm{W} \propto \exp(-0.5 \times \mathrm{TIC})$ [Frison, 2302.06550], [Bruno,Sommer, 2209.14188]
  4. $m_\pi = \sum_i m_\pi^{(i)} W^{(i)}$, $\sigma^2_{\mathrm{syst}}[m_\pi] = \left(\sum_i m_\pi^{(i)} W^{(i)}\right)^2 - \sum_i m_\pi^{2,(i)} W^{(i)}$

Wilson unitary setup

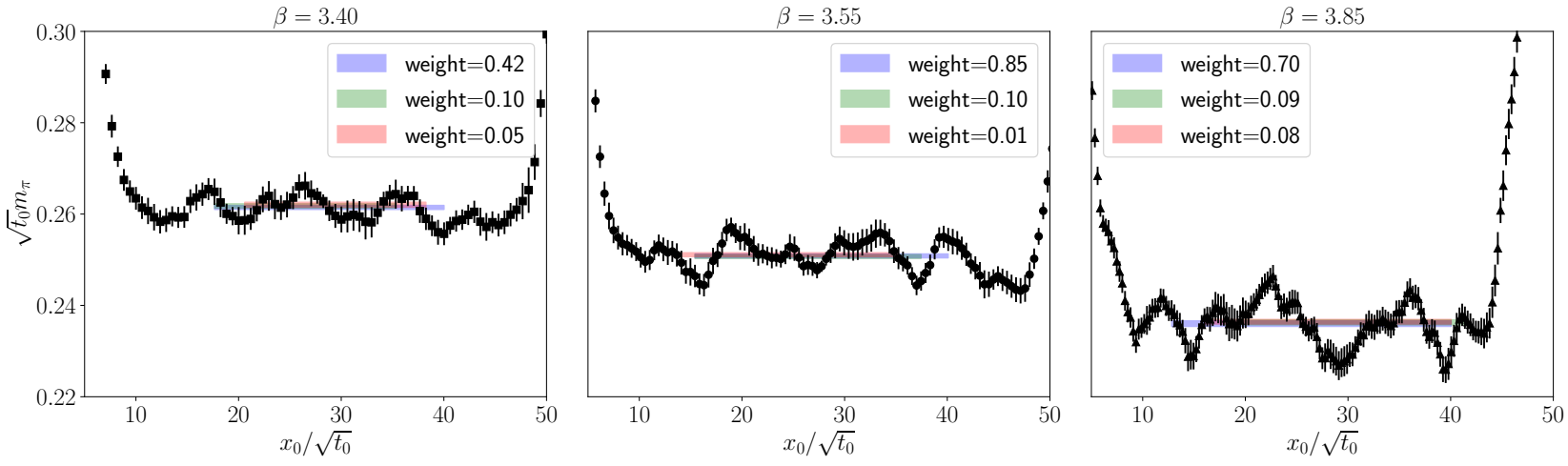
- OBC in time for gauge fields: avoid topology freezing

  [Lüscher, Schaefer, 1105.4749]



#config = 997, MDUs = 3988 [H102r001],
#config = 1543, MDUs = 6172 [N203],
#config = 787, MDUs = 15380 [J501]

OBC: boundary effects, Wtm

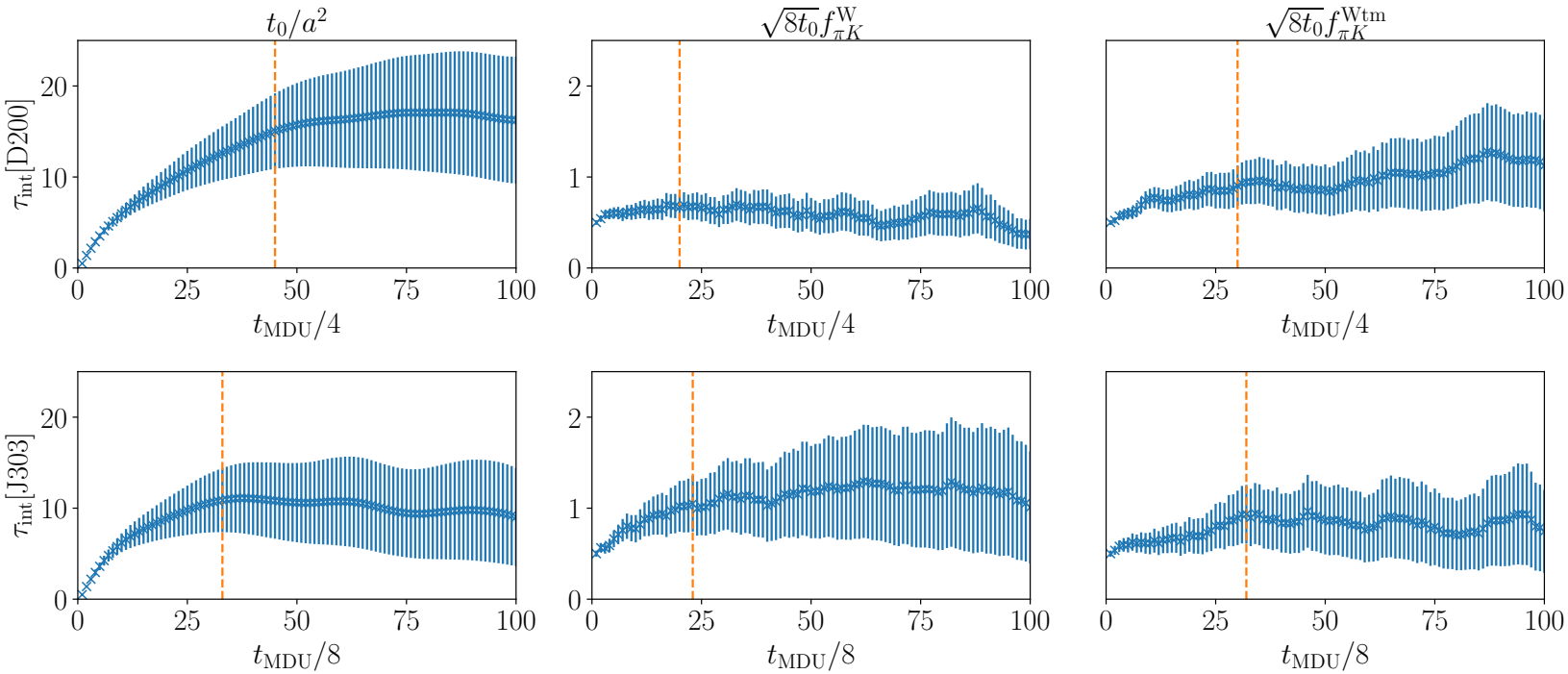


$m_\pi \approx 360$ MeV

Autocorrelation times

$$F = f(P_i), \quad \sigma_F^2 = \sum_\alpha 2\tau_{\mathrm{int}}(F)\frac{\Gamma_F(0)}{N}, \quad \tau_{\mathrm{int}}(F) = \frac{1}{2} + \sum_{t=1}^{\infty}\frac{\Gamma_F(t)}{\Gamma_F(0)},$$

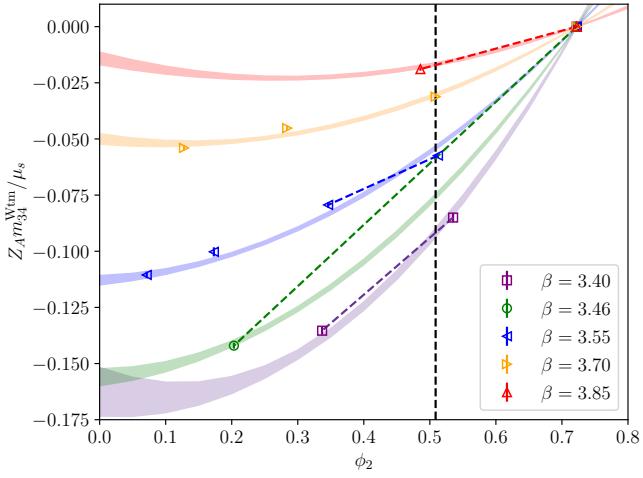
$$\Gamma_F(t) = \sum_{ij}\bar{f}_i\bar{f}_j\frac{1}{N-t}\sum_{t'=1}^{N-t}\delta_i(t+t')\delta_j(t'), \quad \bar{f}_i = \frac{\partial f}{\partial P_i}\Big|_{\bar{p}_i}.$$

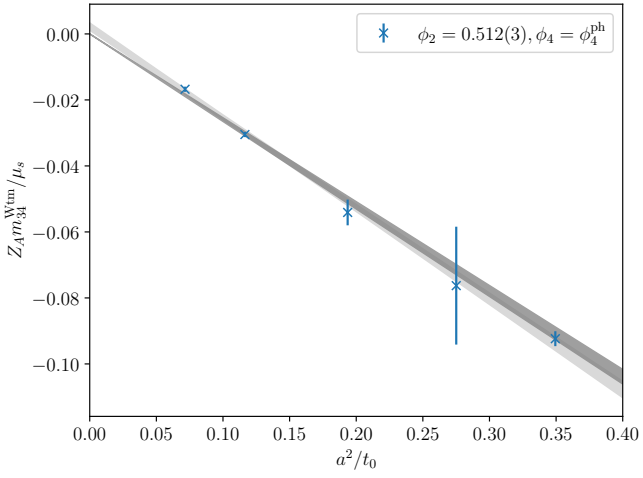


Twist angles

- Maximal twist condition through light PCAC quark mass

$$am_{12}^{\mathrm{Wtm}} = 0$$





- Continuum limit not constrained:

$$\rightsquigarrow \quad \mathrm{p-value} = 0.3,\ \mathrm{acot}\left(Z_A m_{34}^{\mathrm{Wtm}}/\mu_s\right) = 89.87(6)^\circ$$

- Continuum limit constrained to $Z_A m_{34}^{\mathrm{Wtm}}/\mu_s = 0$:

$$\rightsquigarrow \quad \mathrm{p-value} = 0.08$$

Chiral-continuum extrapolation: χ^2 definition

[M. Dalla Brida et al., 1607.06423]

$$\chi^2 = (y_i - f(x_i, p))W_{ij}(y_j - f(x_j, p)),$$

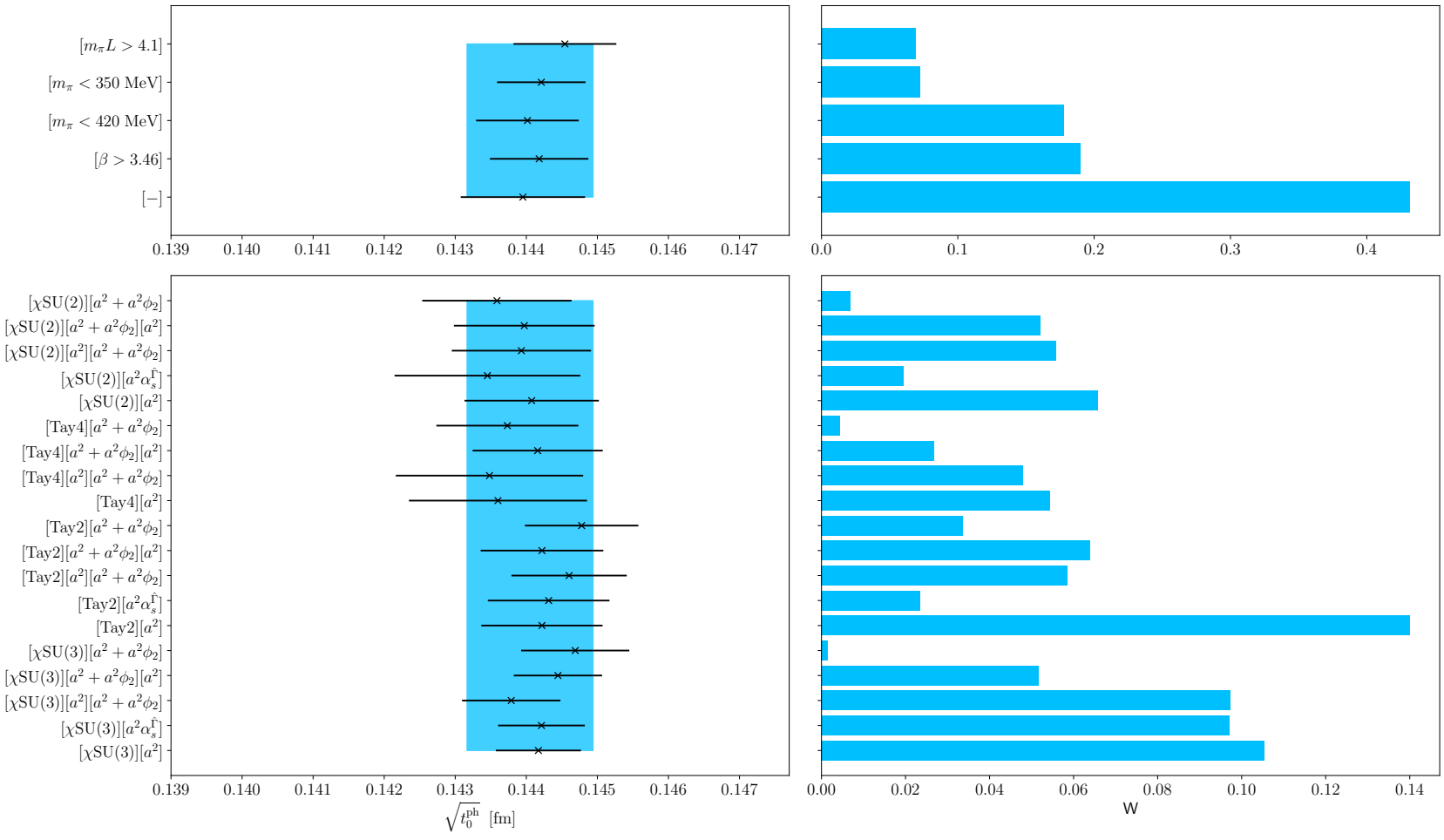
$$C \to \tilde{C}_{ij} = C_{ij} \times \sqrt{1 + z_i/C_{ii}}\sqrt{1 + z_j/C_{jj}},$$

$$z_i = \Theta(3.40 - \beta)p_\beta^2 \left(\frac{a^2}{t_0}\right)^4 + \Theta(0.77 - \phi_2)p_{\phi_2}^2 \phi_2^4,$$

$$W = \tilde{C}^{-1}$$

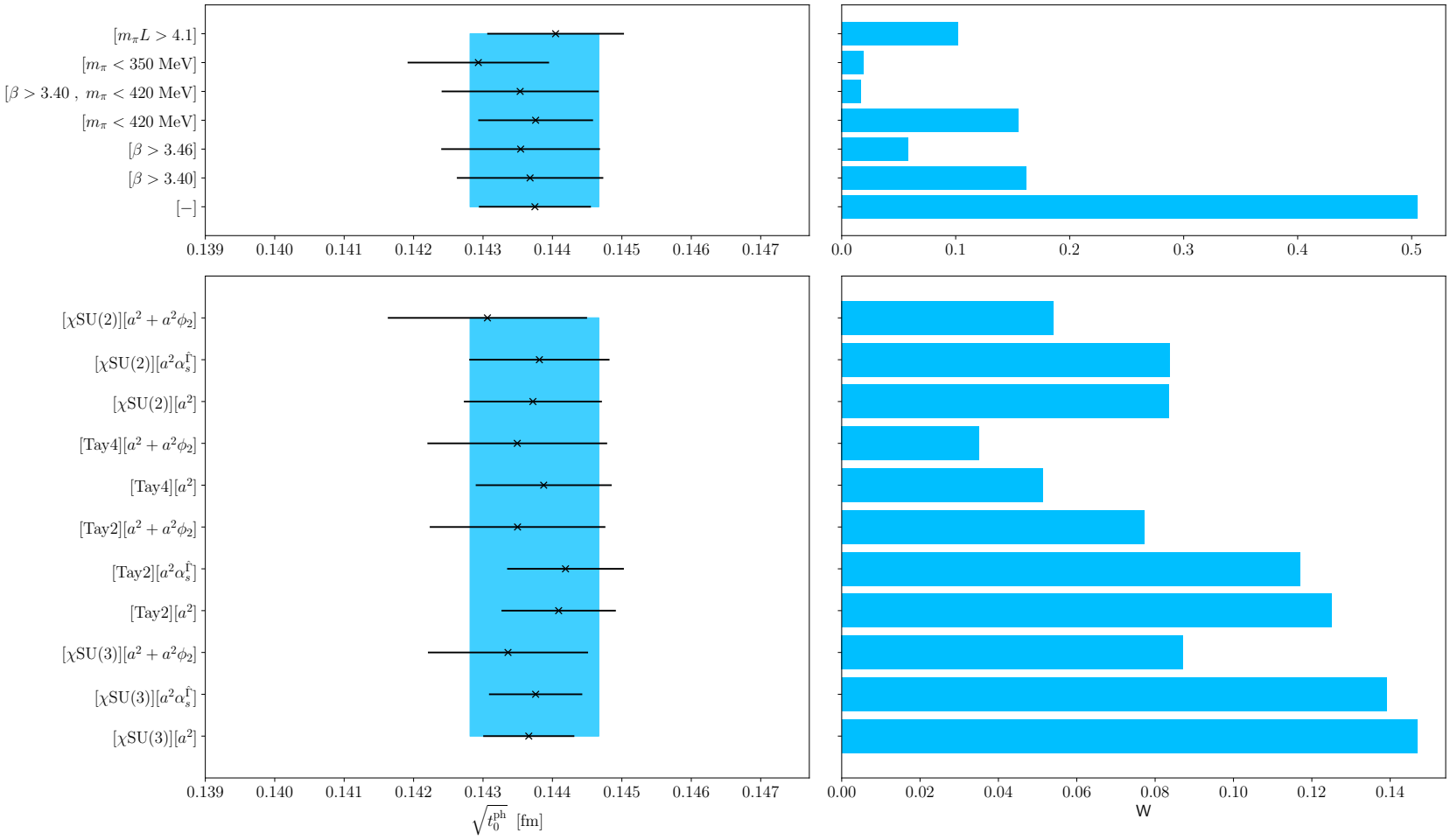
Remove $\beta = 3.40$

Remove $\beta = 3.40 \rightarrow 22\%$ increase in total error



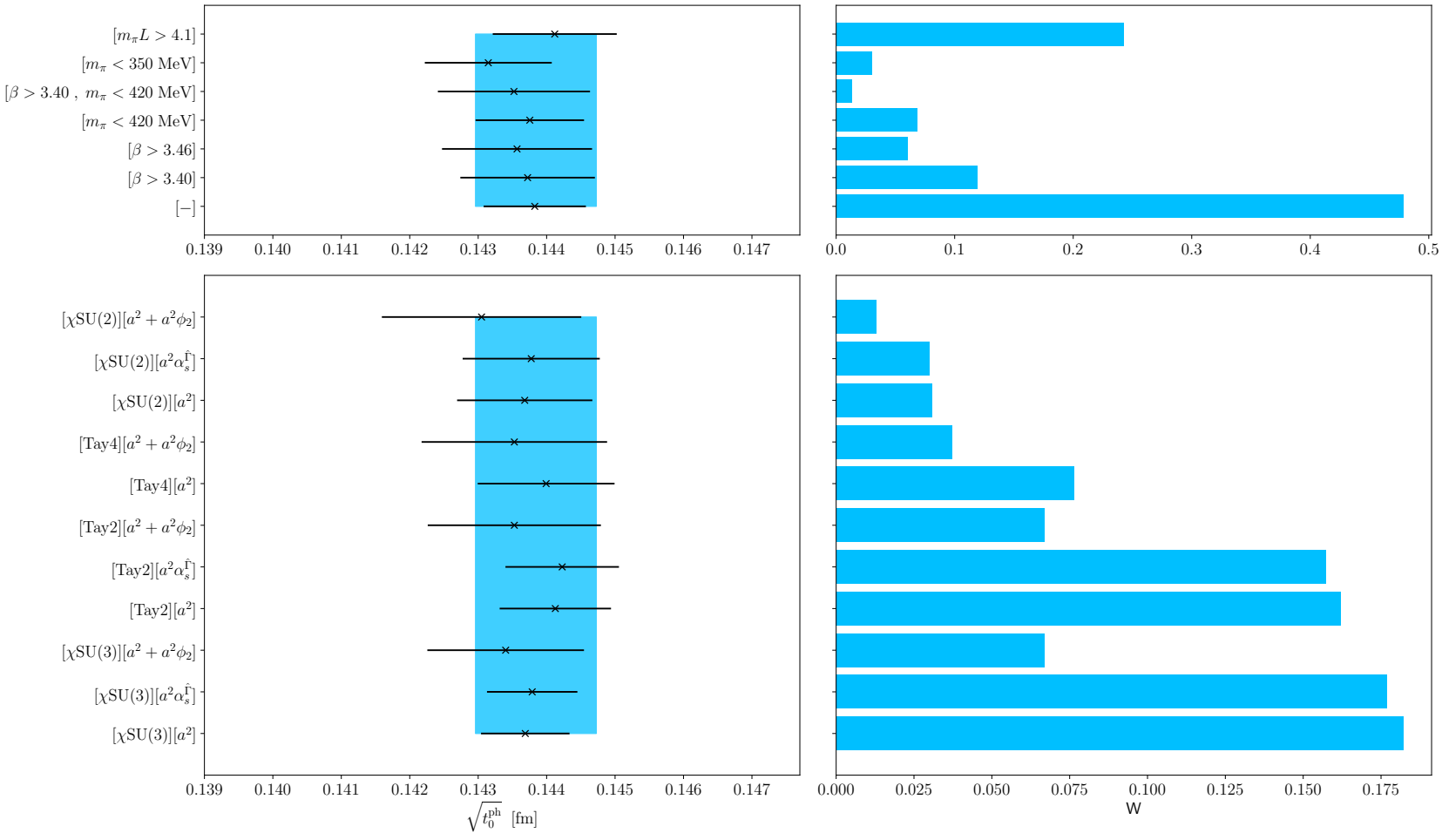
IC variations: TIC, Wilson

$$\mathrm{TIC} = \chi^2 - 2\left\langle \chi^2 \right\rangle, \text{ Wilson}$$



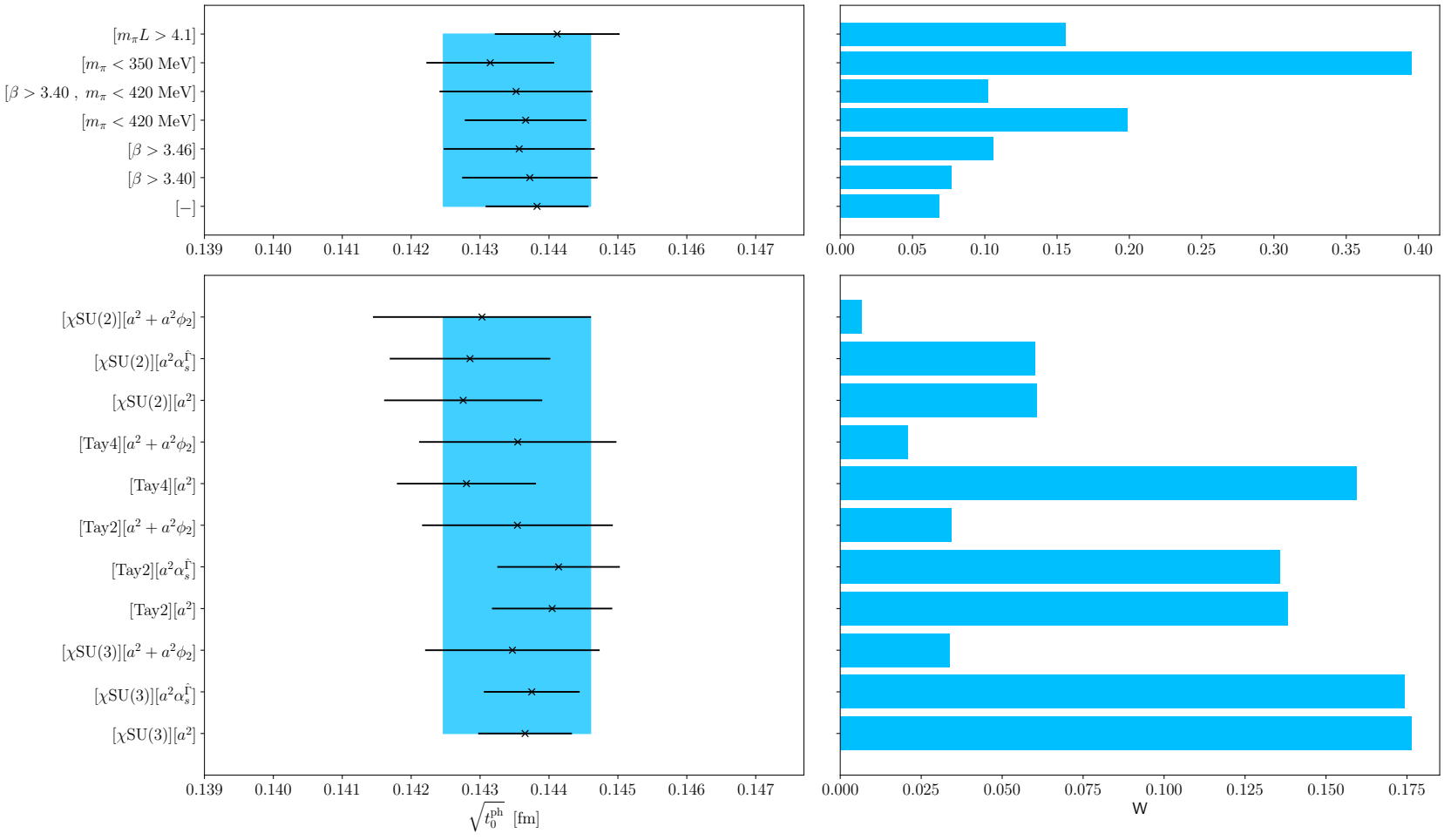
IC variations: $\mathrm{AIC}^{\mathrm{sub}}$, Wilson

$$\mathrm{AIC}^{\mathrm{sub}} = \chi^2 + 2n_{\mathrm{param}} + n_{\mathrm{cut}}, \text{ Wilson}$$



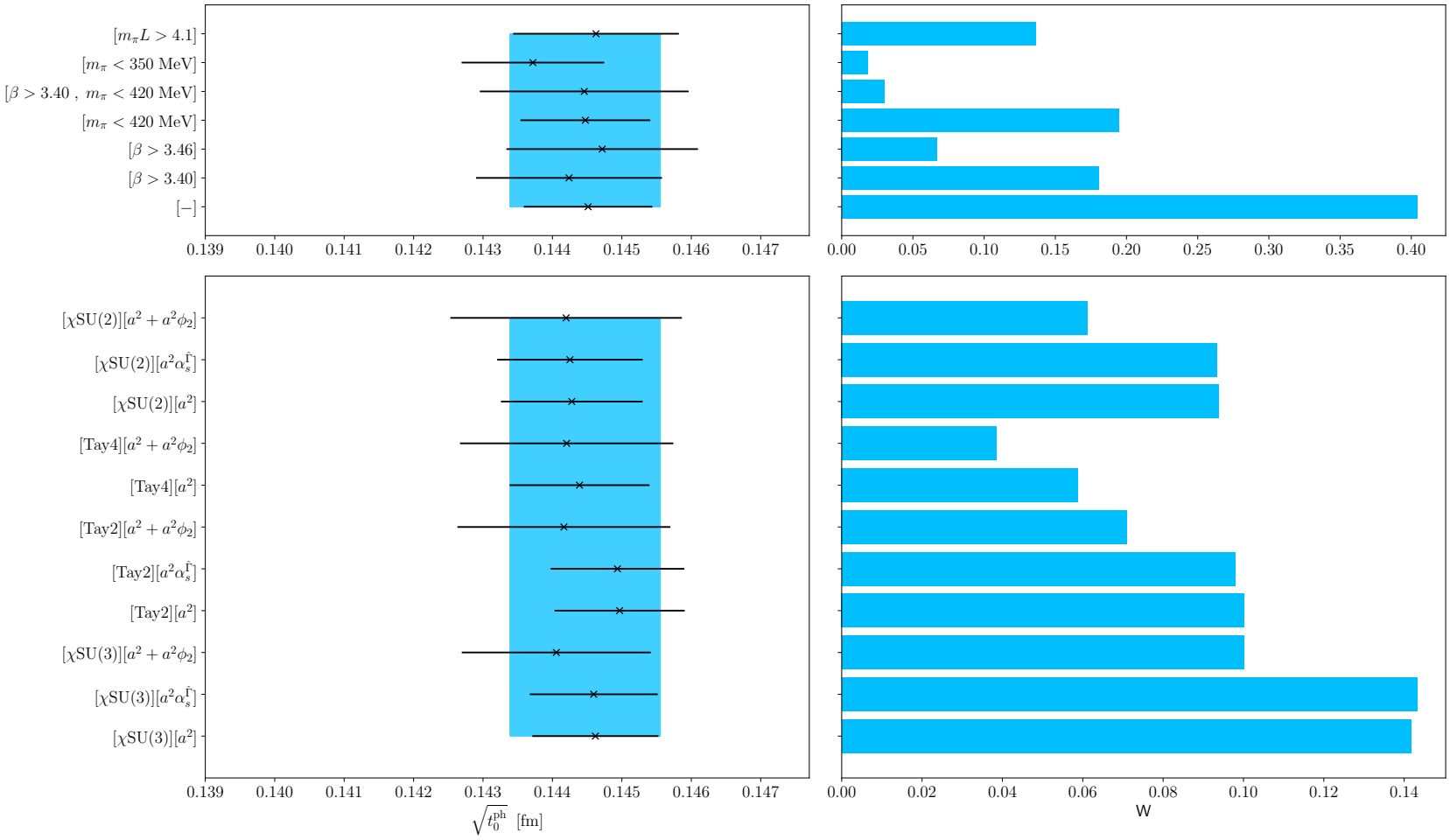
IC variations: AIC, Wilson

$$\mathrm{AIC} = \chi^2 + 2n_{\mathrm{param}}\text{, Wilson}$$



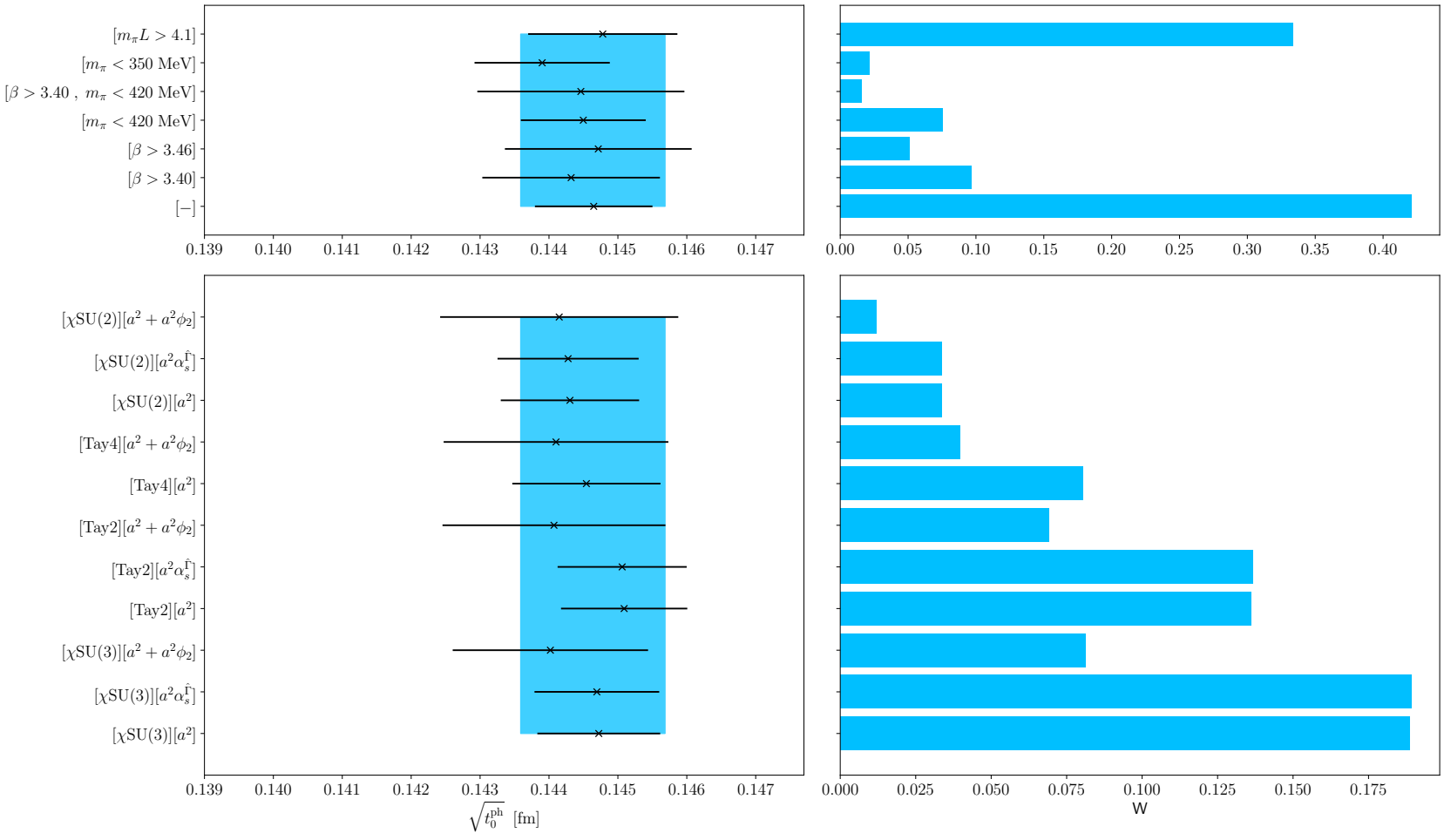
IC variations: TIC, Wtm

$$\mathrm{TIC} = \chi^2 - 2\left\langle \chi^2 \right\rangle, \text{ Wtm}$$



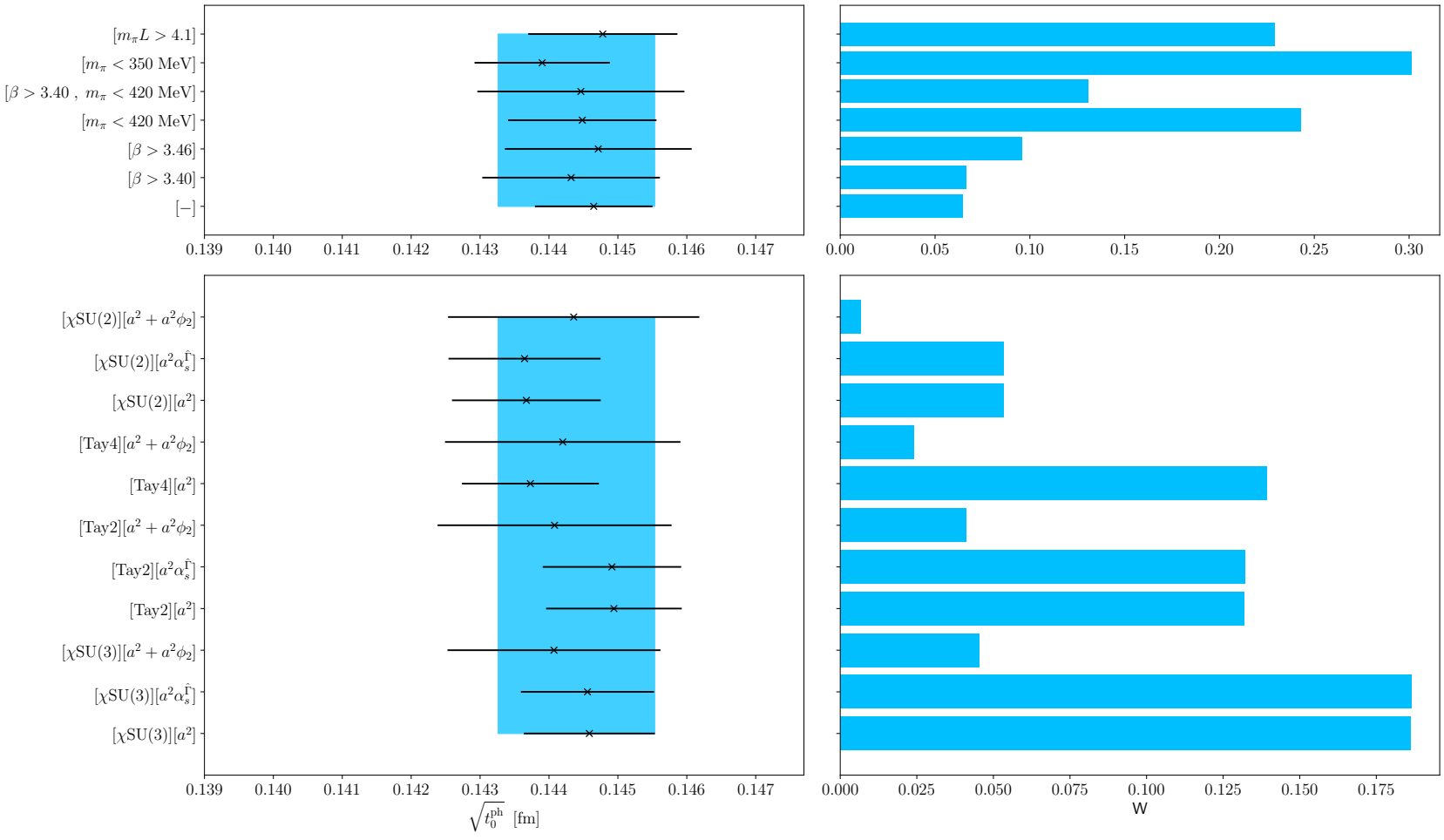
IC variations: $\mathrm{AIC}^{\mathrm{sub}}$, Wtm

$$\mathrm{AIC}^{\mathrm{sub}} = \chi^2 + 2n_{\mathrm{param}} + n_{\mathrm{cut}}, \text{ Wtm}$$

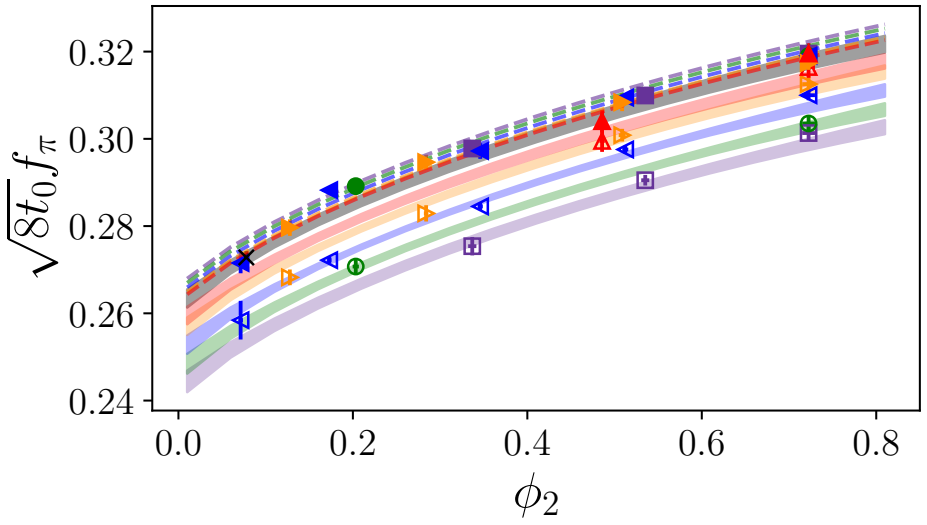


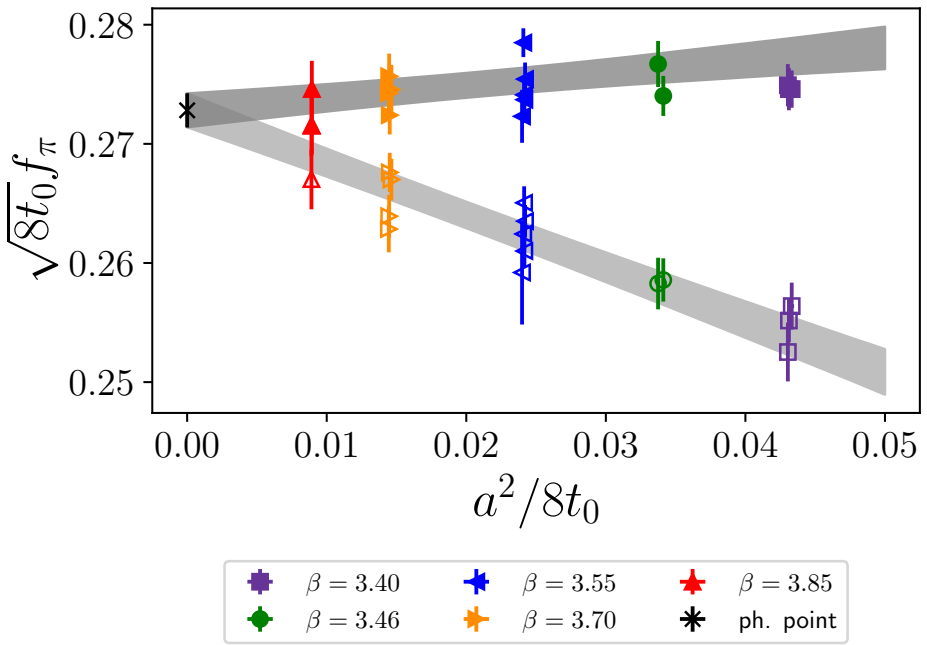
IC variations: AIC, Wtm

$$\mathrm{AIC} = \chi^2 + 2n_{\mathrm{param}}, \text{ Wtm}$$



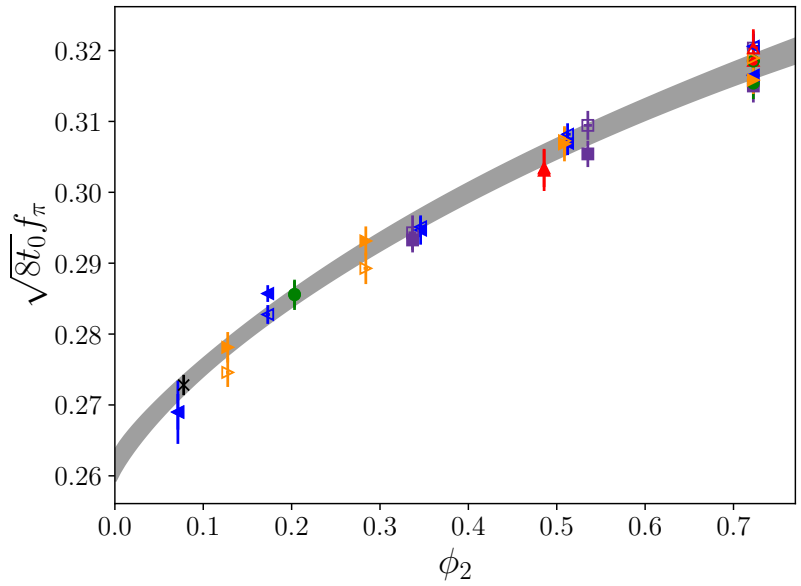
Setting the scale with f_π: test model [PRELIMINARY]



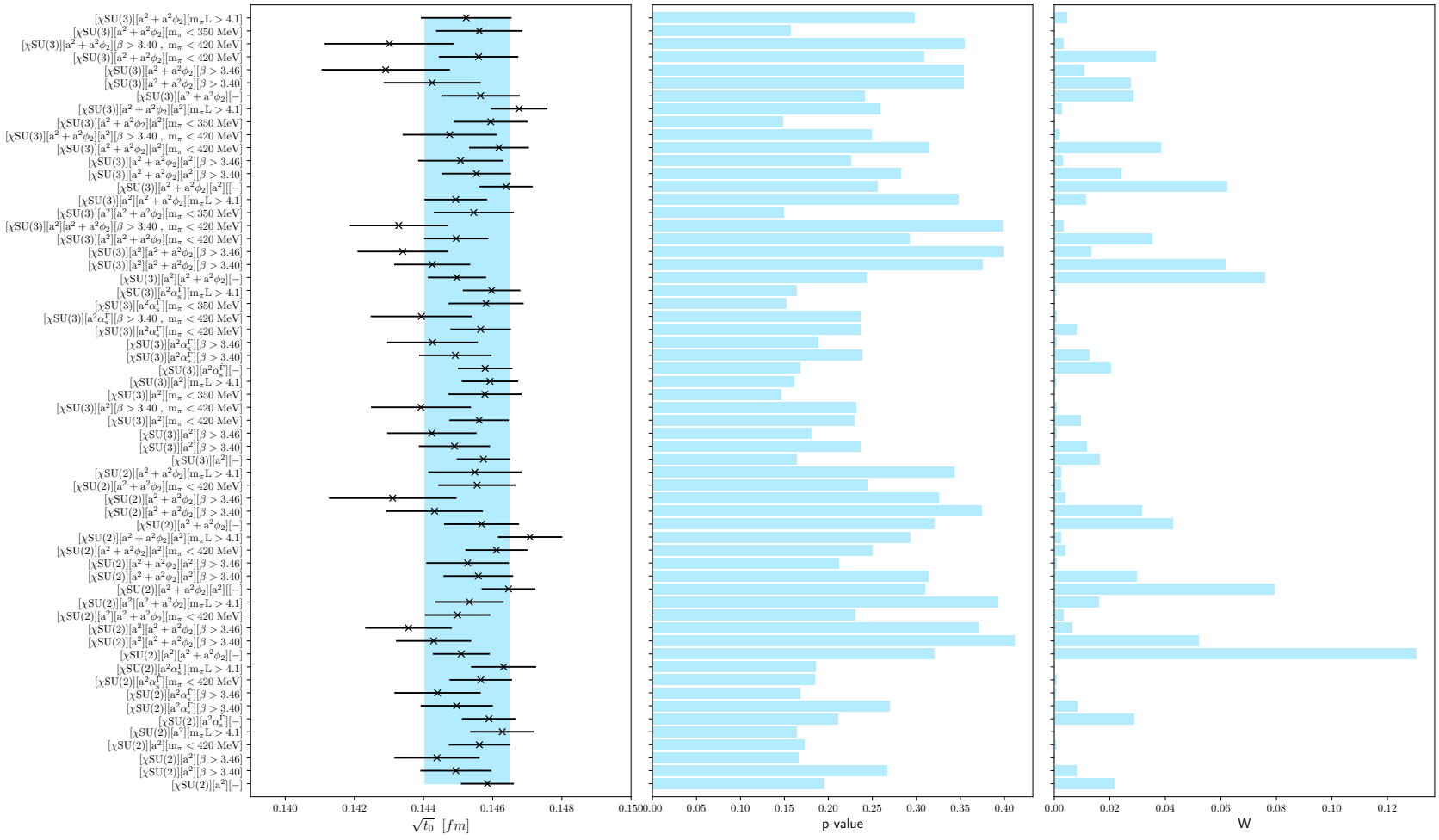


- SU(2) χPT
- $\mathcal{O}(a^2)$ cutoff effects
- All data included

  ⇝ $\mathrm{p-value} = 0.2$



Setting the scale with f_π [PRELIMINARY]



Uncertainty $\sqrt{t_0^{\rm ph}}$ $[f_\pi]$ grows $\sim 60\%$ w.r.t. that of $\sqrt{t_0^{\rm ph}}$ $[f_{\pi K}]$

⇝ Not only bigger systematic, also statistical

Setting the scale with f_π

[PRELIMINARY]

