Scale setting for QCD with $N_{\mathrm{f}} = 3 + 1$ dynamical quarks

R. Höllwieser, F. Knechtli and T. Korzec

Bergische Universität Wuppertal

SFB/TR55, Project B5

Lattice Symposium, Wuhan, China, 6/18/2019

Motivation

Reasons for dynamical charm quarks

- investigate decoupling with light quarks, high precision charm physics, α_S in 4 flavor theory,...
- c.f. [Tomasz Korzec], [Cali, Knechtli and Korzec, arXiv:1905.12971]

Difficulties/Solutions

- lattice artefacts due to cutoff effects $\propto \mathcal{O}(am_c \approx 0.5)$
- [Fritzsch, Sommer, Stollenwerk and Wolff, arXiv:1805.01661]
- physical charm quark in a mass independent scheme gives improvement terms about an order of magnitude larger than strange contributions
- massive renormalization scheme with close to realistic charm mass m_c and $m_{uds} = \sum_{i=uds} m_i^{\rm phys}/3$
- Symanzik improved 3+1 scheme for Wilson quarks

Symanzik improved 3+1 scheme for Wilson quarks

massive renormalization scheme and improvement

- massive renormalization and finite size scheme to maintain $\mathcal{O}(a)$ improvement

$$g_{\mathrm{R}}^2 = \tilde{Z}_g(g_0^2, a\mu, aM) g_0^2, \; m_{\mathrm{R},i} = \tilde{Z}_m^i(g_0^2, a\mu, aM) m_{\mathrm{q},i}$$

$$m_{\mathrm{q},i} = m_i - \tilde{m}_{\mathrm{crit}}(g_0^2, a\mathrm{tr}\,[M_{\mathrm{q}}])$$

- clover action term [Sheikholeslami and Wohlert (SW), 1985]

$$S_{\mathrm{SW}} = a^5 \tilde{c}_{\mathrm{sw}}(g_0^2, aM) \sum_x \bar{\psi}(x) \tfrac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu}(x) \psi(x)$$

- non-perturbative fit formula for the clover coefficient $c_{\mathrm{sw}}(g_0^2)$ from LCP, cf. [Fritzsch et al., 2018]
- reduce the number of mass parameters via

$$M_{\mathrm{q}} = \mathrm{diag}(m_{\mathrm{q},l}, m_{\mathrm{q},l}, m_{\mathrm{q},l}, m_{\mathrm{q},c})$$

Preliminary Work

scale setting in CLS $N_\mathrm{f} = 2 + 1$ QCD

- relation betw. bare coupling and lattice spacing in fm
- dimensionless quantity $\sqrt{t_0^\star} m_\mathrm{had}$ in the continuum limit
- m_had experimentally accessible quantity
- $t_0^\star$ (mass dimension -2) flow scale [Lüscher, 2010]
- $\sqrt{8t_0^\star} = 0.413(5)(2)$fm [Bruno, Korzec, Schaefer, 2017]

non-perturbative decoupling of the charm quark

- scale $t_0^\star$ is the same in $N_\mathrm{f} = 3$ and $N_\mathrm{f} = 3 + 1$ theories, up to small corrections $O(1/m_\mathrm{charm}^2)$
- detailed study of non-perturbative decoupling of the charm quark [Knechtli et al. 2017, Athenodorou et al. 2018]

Scale setting and tuning of $N_\mathrm{f} = 3 + 1$ QCD

- computation of $t_0^\star/a^2$ at the mass point $m_\text{up} = m_\text{down} = m_\text{strange}$ and

$$\begin{aligned} \phi_4 &\equiv 8t_0\left(m_\mathrm{K}^2 + \frac{m_\pi^2}{2}\right) = 12t_0 m_\pi^2 = 1.11 \\ \phi_5 &\equiv \sqrt{8t_0}\,(m_{\mathrm{D_s}} + 2m_\mathrm{D}) = \sqrt{72t_0}\,m_\mathrm{D} = 11.94 \end{aligned}$$

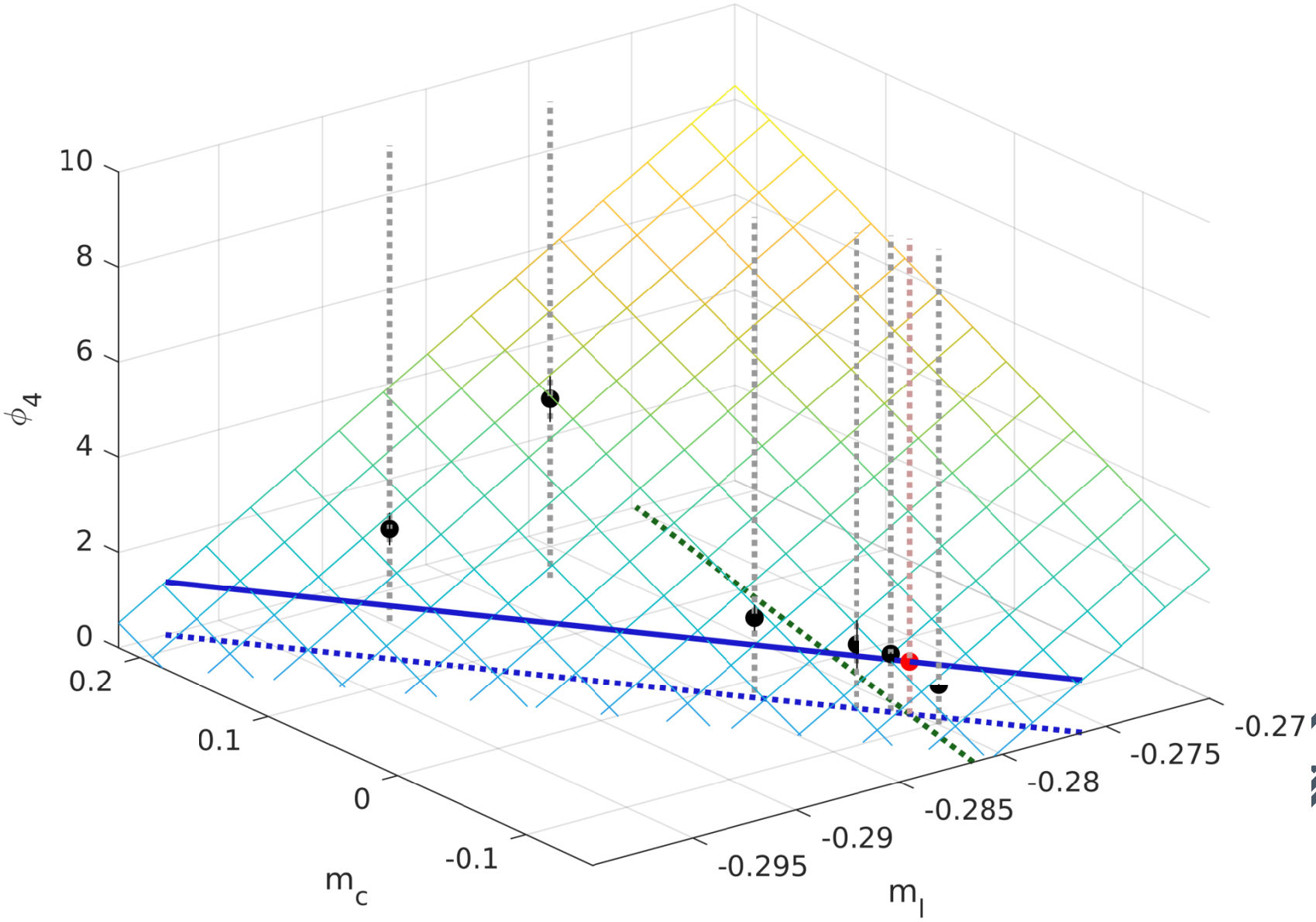
- we use first tuning results from [Fritzsch et al., 2018]

$$\begin{aligned} \beta &= 3.24 \text{ (bare coupling)} \\ \kappa_\mathrm{uds} &= 0.134484 \text{ (light quark mass)} \\ \kappa_c &= 0.12 \text{ (charm quark mass)} \\ c_0 &= 5/3 \text{ (Lüscher–Weisz action)} \\ c_\mathrm{sw} &= 2.188591 \text{ (bulk improvement)} \\ c_F &= c_G = 1.0 \text{ (boundary improvements)} \end{aligned}$$

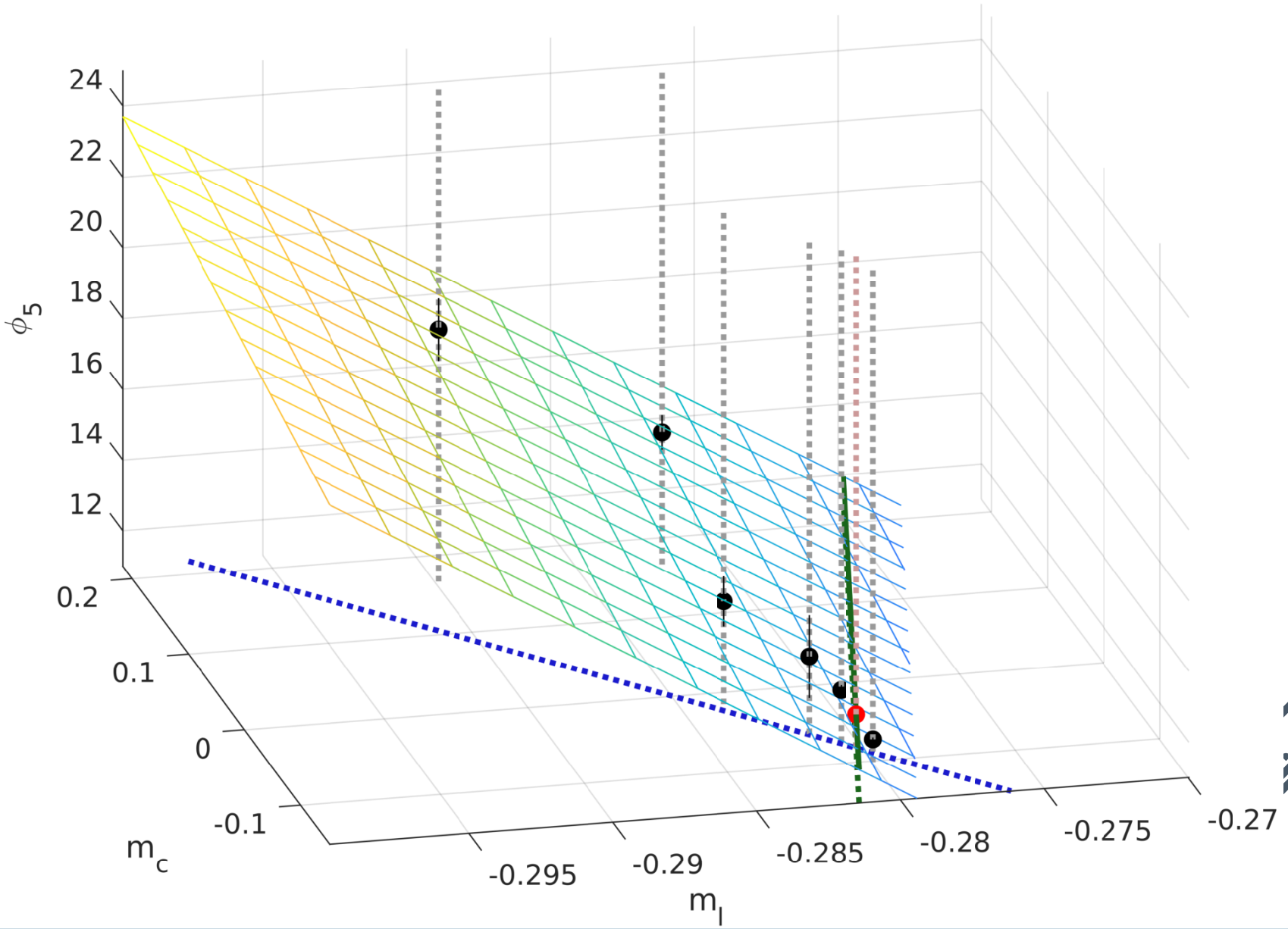
Simulations using openQCD-1.6 [Lüscher, Schaefer]

- start with algorithmic setup of CLS's H400 simulation [Bruno et al., 2015] and add a charm quark
- u/d quark doublet in terms of even-odd prec. $\hat{D}$ with weight $\propto \det[(\mathrm{D_{oo}})^2]\det[\hat{\mathrm{D}}^\dagger\hat{\mathrm{D}}+\mu^2]^2\det[\hat{\mathrm{D}}^\dagger\hat{\mathrm{D}}+2\mu^2]^{-1}$
- strange and charm quarks are simulated with RHMC, Zolotarev rational functions have degrees 12 and 10
- both, doublet and rational parts need reweighting and are further factorized [Hasenbusch, 2001]
  $\det[D^2] = \det[D^\dagger D+\mu_0^2] \times \frac{\det[D^\dagger D+\mu_1^2]}{\det[D^\dagger D+\mu_0^2]} \times \ldots \times \frac{\det[D^\dagger D]}{\det[D^\dagger D+\mu_N^2]}$
- gauge + 13 pseudo-fermion fields on 3 different time scale integration levels: $N_0 = 2, N_1 = 1, N_2 = 8$
- 2nd and 4th order [Omelyan, Mryglod, Folk, 2003] integrators
- SAP preconditioning and low-mode-deflation based on local coherence [Lüscher, 2004, 2007, Frommer et al. 2013]

Tuning of $\phi_4 = 1.11$



Tuning of $\phi_5 = 11.94$

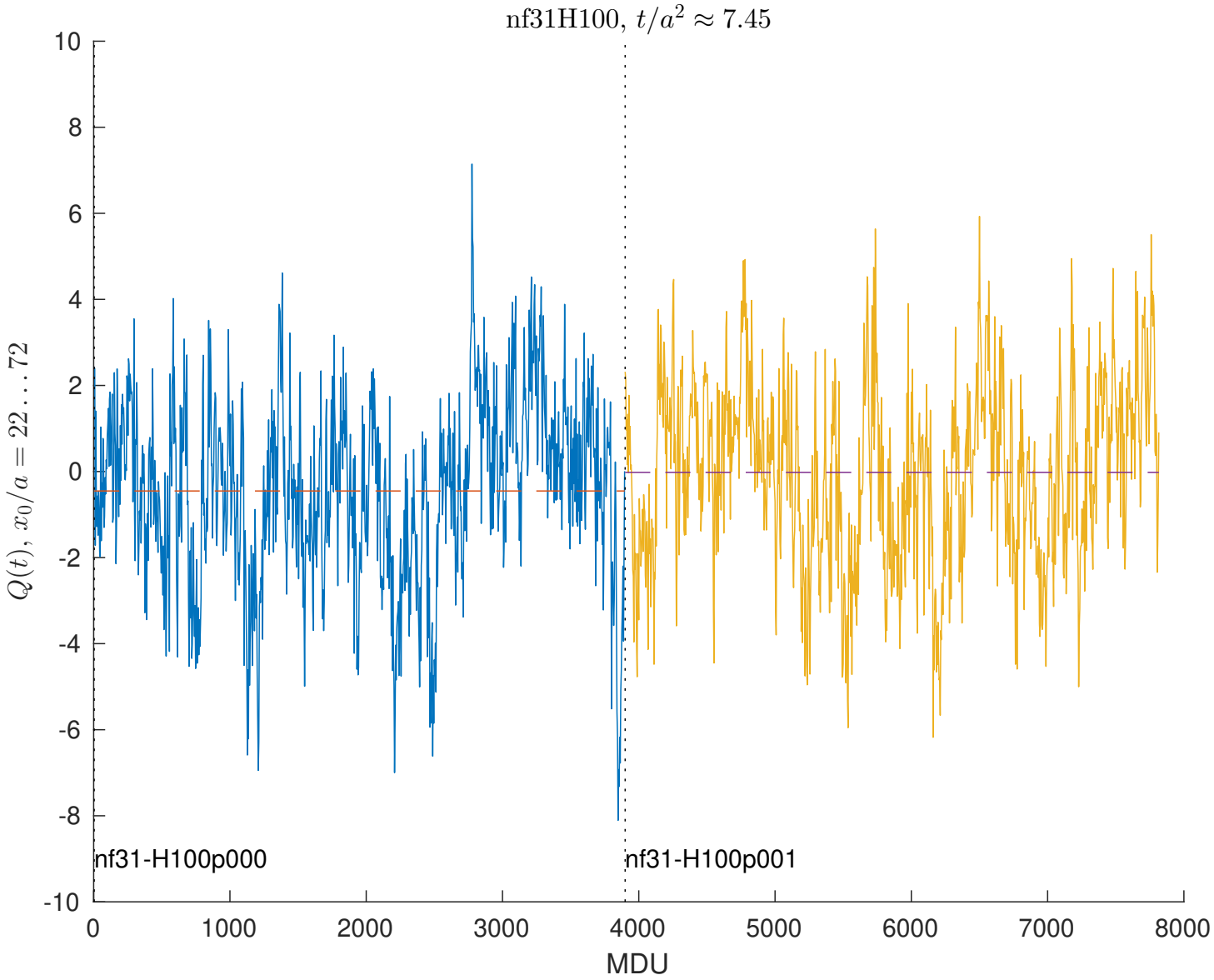


Tuning Results: $\kappa_l = 0.13440733$, $\kappa_c = 0.12784$

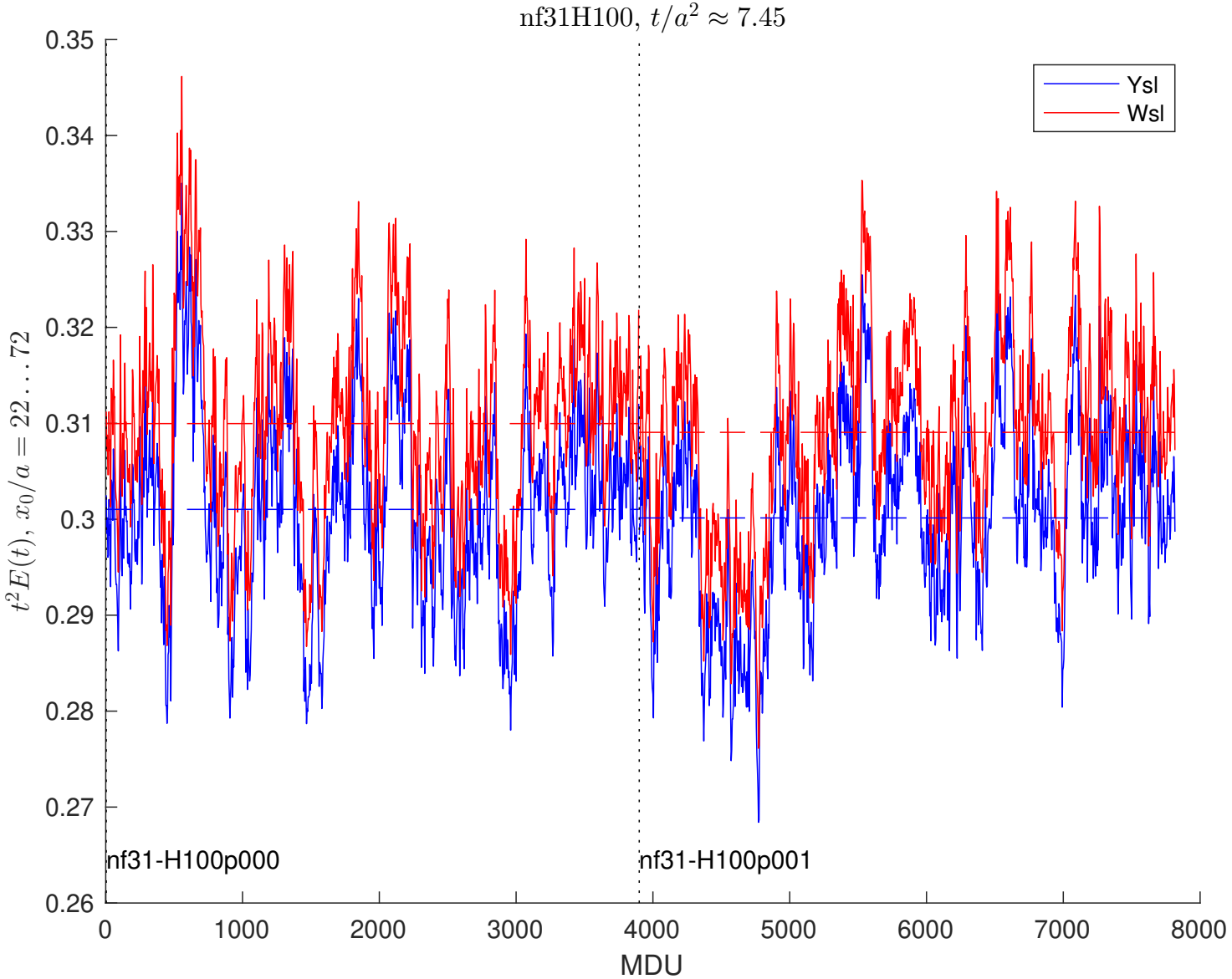
$\frac{T}{a} \times \frac{L^3}{a^3}$	$Lm_\pi^\star$	N_{traj}	t_0/a^2	$am_{\pi,K}$	am_{D,D_s}	ϕ_4	ϕ_5
96×16^3	1.7	1000	8.8(2)	0.310(6)	0.614(17)	10.2(9)	15.5(4)
96×32^3	3.5	3908	7.43(4)	0.1138(8)	0.5251(7)	1.16(2)	12.17(4)
128×48^3	5.3	3868	7.36(3)	0.1108(4)	0.5236(4)	1.087(6)	12.06(2)

- The integrated autocorrelation time of t_0 is $\tau_{\mathrm{int},t_0} \approx 20 \pm 10$ [4 MDU].
- Assuming decoupling, our value of $t_0/a^2 \approx 7.4$ corresponds to a lattice spacing $a \approx 0.054$ fm.
- The ratio of PCAC masses $m_{ud}/m_{cc'} \approx 0.026$ is very close to the experimental ratio $\frac{m_s/3}{m_c}$.
- In ϕ_4 and ϕ_5 the mass dependence of t_0 and the masses go in opposite directions.
- The sampling of the topology is sufficient.

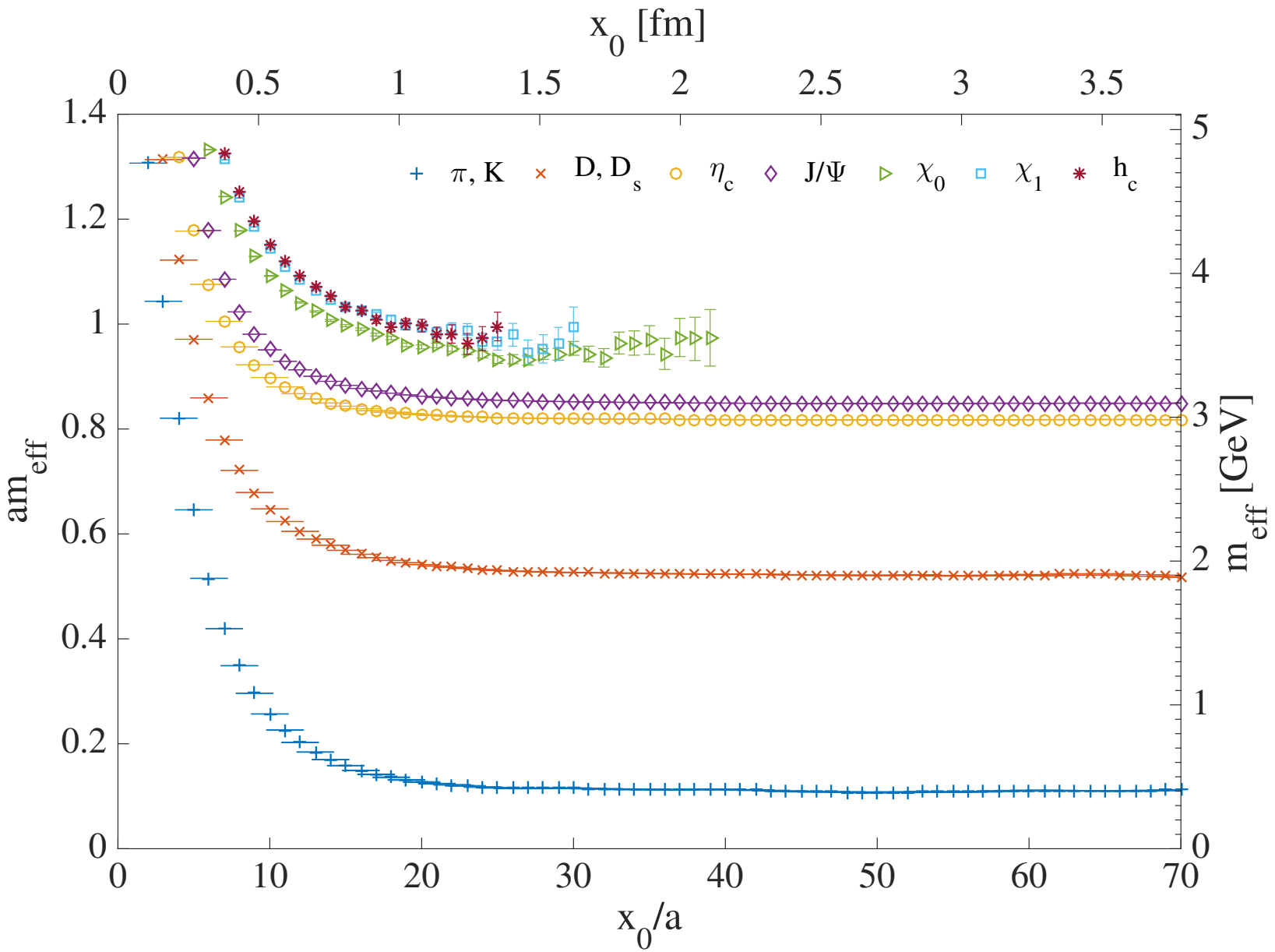
History of the topological charge $Q(t \approx t_0)$



History of $t^2E(t)$ where $E(t) = \frac{1}{4}G^a_{\mu\nu}(t)G^a_{\mu\nu}(t)$



Meson spectrum

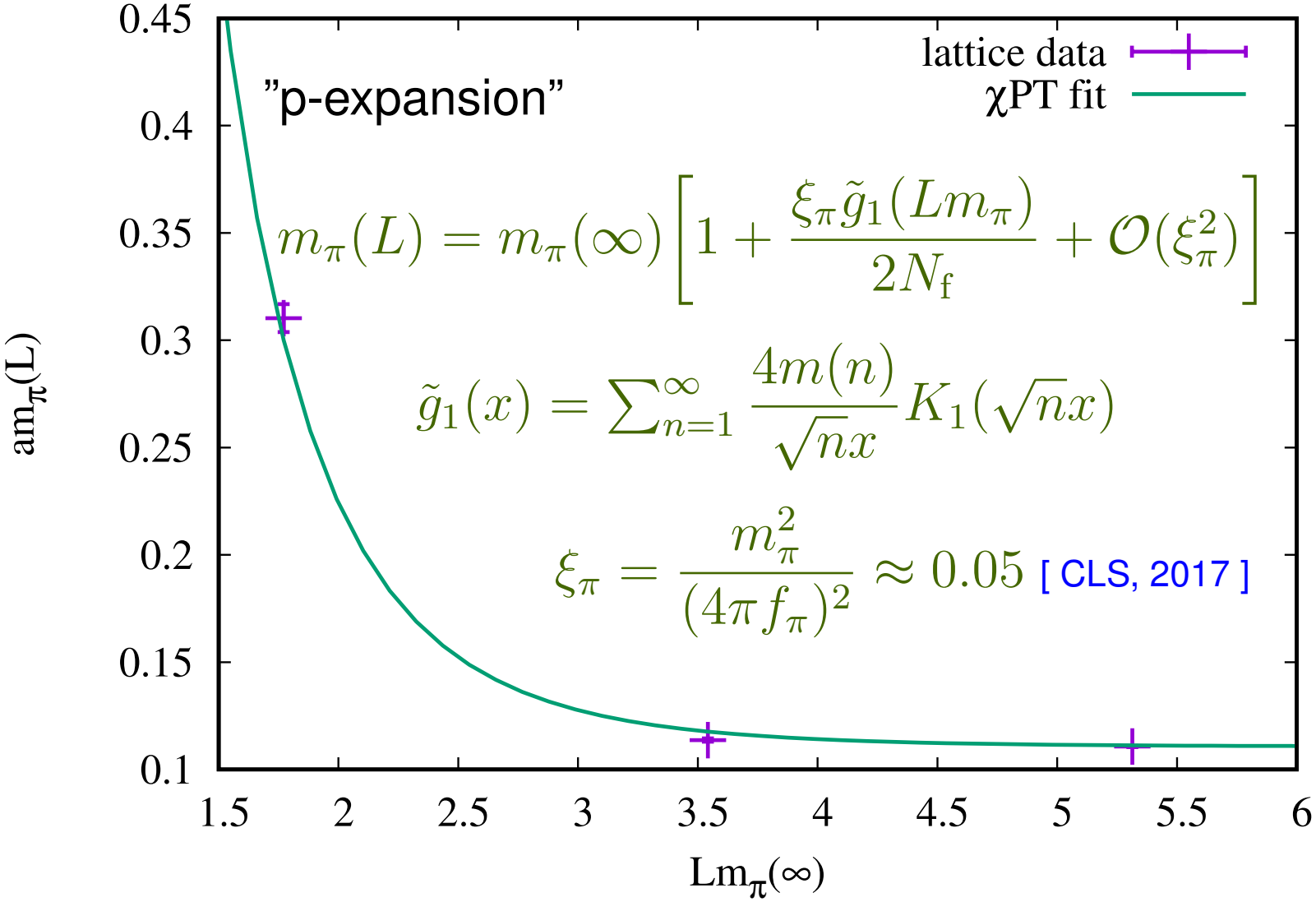


Charmonium Spectrum

	η_c	J/ψ	χ_{c_0}	χ_{c_1}	h_c
am_{eff}	0.8180(2)	0.8489(2)	0.9398(86)	0.9833(72)	0.9902(81)
m_{eff} [GeV]	2.9890(7)	3.1019(7)	3.434(31)	3.593(26)	3.618(30)
PDG [GeV]	2.9834(5)	3.096900(6)	3.4148(3)	3.51066(7)	3.52538(11)

- sum of the light quark masses has physical value
- no light quarks in the valence sector, hence the derivatives $dm_x/dm_{\rm up} = dm_x/dm_{\rm down} = dm_x/dm_{\rm strange}$
- $m_x^{\rm phys} = m_x + (\Delta_{\rm up} + \Delta_{\rm down} + \Delta_{\rm strange})\frac{dm_{\eta_c}}{dm_u} + O(\Delta^2)$
- linear term vanishes, because ϕ_4 is chosen such that $\Delta_{\rm up} = \Delta_{\rm down} = -0.5\Delta_{\rm strange}$ ($m_{uds} = \sum_{i=uds} m_i^{\rm phys}/3$)
- derivatives of correlation functions with respect to bare quark masses allow us to correct (small) mistunings in ϕ_4 and ϕ_5

Finite volume scaling effects for am_π [Colangelo, Dürr, Haefeli, 2005]



Conclusions & Outlook

Conclusions

- Scale setting and tuning of $N_\mathrm{f} = 3 + 1$ QCD
- massive renormalization scheme with a non-perturbatively determined clover coefficient
- Production of two ensembles with $a = 0.054$ fm
- Reasonable charmonium spectrum

Outlook

- further analysis $\frac{dm_\mathrm{had}}{dm_q}, \frac{dt_0}{dm_q}, \frac{dS}{dm_q}$
- continuum limit
- Λ, α_S in $N_\mathrm{f} = 4$

ens.	$\frac{T}{a} \times \frac{L^3}{a^3}$	a [fm]	$Lm_\pi^\star$
A1	96×32^3	0.054	3.5
A2	128×48^3	0.054	5.3
B	144×48^3	0.041	4.0
C ?	192×64^3	0.032	4.2

Acknowledgements

THANK YOU

R. Sommer

F. Knechtli and T. Korzec

Bergische Universität Wuppertal

SFB/TR55, Project B5