Simulations of $N_f = 3 + 1$ QCD and first physical results

Roman Höllwieser, Francesco Knechtli, Tomasz Korzec

ALPHA Collaboration

- Introduction
- Massive O(a) renormalization and improvement scheme for dynamical charm
- Tuning and scale setting
- Sytematics: Lattice artifacts, finite volume, decoupling
- Charmonium spectrum
- Conclusions & Outlook

based on `2002.02866`, Eur.Phys.J.C 80 (2020)

Lattice Seminar, Humboldt-Universität zu Berlin & NIC, DESY Zeuthen,
June 8, 2020

Part I

Introduction

Dymamical charm on the lattice

Dynamical charm: why?

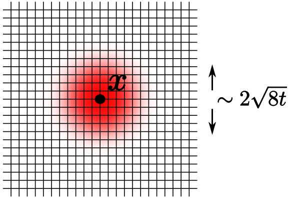
- Appelquist-Carazzone decoupling theorem : heavy quarks decouple from low energy physics [T. Appelquist, J. Carazzone, Phys.Rev.D 11 (1975)]
- Effective theory [S. Weinberg, Phys.Lett.B 91 (1980)], $1/M^2$ corrections make only 2 permille effects for charm [FK, T. Korzec, B. Leder, G. Moir, Phys.Lett.B 774 (2017)]
- But dynamical charm is essential for example to compute charm-annihilation effects in charmonium or the four-flavour Λ-parameter without perturbation theory for charm or string breaking

Dynamical charm: issues on the lattice

- Large lattice artifacts of order $(am_c)^2$ with improved or even am_c with unimproved Wilson fermions
- Cost and tuning of the simulations

Gradient Flow

[M. Lüscher, JHEP 08, 071 (2010); R. Narayanan, H. Neuberger, JHEP 03, 064 (2006)]



[M. Lüscher, `1308.5598`]

Flow equation

$$\partial_t B_\mu = D_\nu G_{\nu\mu}\,, \qquad B_\mu\big|_{t=0} = A_\mu$$

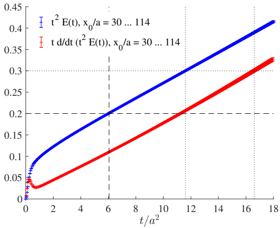
Correlators of B_μ at $t > 0$ are renormalized quantities [M. Lüscher, P. Weisz, JHEP 1102, 051 (2011)]

Physical scales $\sqrt{t_0}$, $\sqrt{t_c}$ and w_0

Based on $\mathcal{E}(t) = t^2 \left\langle \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu} \right\rangle$, together with

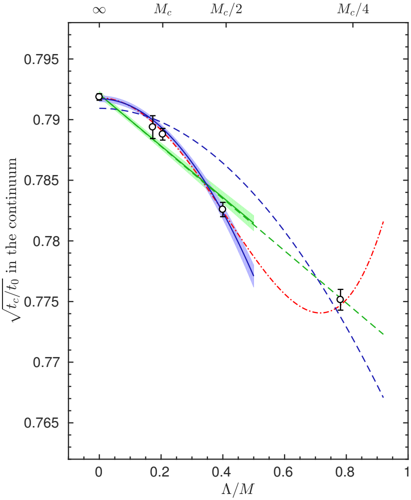
$$\begin{aligned} \mathcal{E}(t_0) &= 0.3\,, \\ \mathcal{E}(t_c) &= 0.2\,, \\ w_0^2 \mathcal{E}'(w_0^2) &= 0.3\,. \end{aligned}$$

[M. Lüscher, JHEP 08, 071 (2010); S. Borsanyi et al., JHEP 1209, 010 (2012)]



Ensemble B

Decoupling $N_f = 2 \rightarrow N_f = 0$

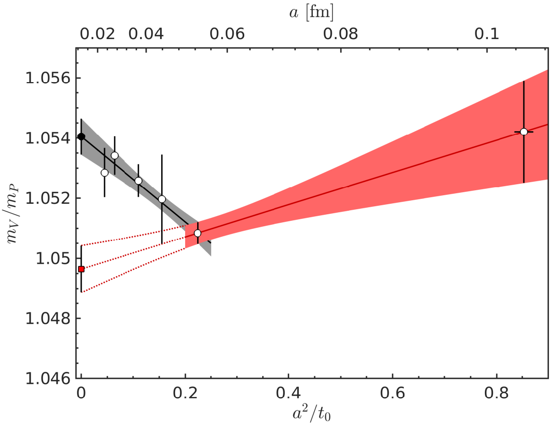


Effective theory prediction $R(M) = R(\infty) + k\Lambda^2/M^2$ with fit parameter k

[FK, T. Korzec, B. Leder, G. Moir, Phys.Lett.B 774 (2017)]

Lattice artifacts

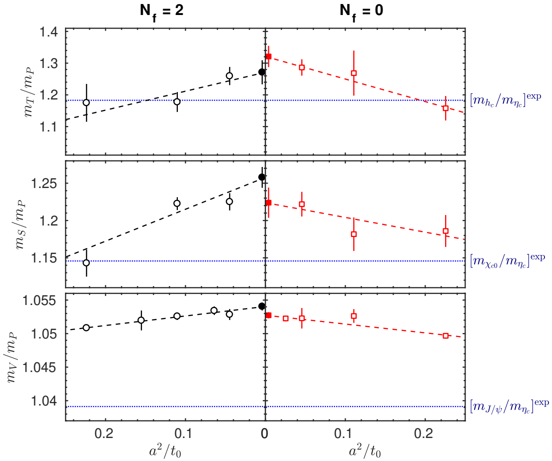
$N_f = 2$ twisted mass fermions at maximal twist, O($(a\mu)^2$) lattice artifacts



Isovector charmonium masses, continuum extrap. of $m_{Vector}/m_{Pseudoscalar}$
$\sqrt{t_0}m_P = 1.807463$ fixed (≈ charm mass) ⇒ $(am_P)^2 = 3.3a^2/t_0$
Continuum extrap. reliably starts at lattice spacings presently achievable in large-volume simulations with light quarks

Decoupling in charmonium

Comparison $N_f = 2$ charm quarks with pure gauge



Sea effects $([m_V/m_P]^{N_f=2} - [m_V/m_P]^{N_f=0})/[m_V/m_P]^{N_f=2} = 0.12(7)\%$

Difference with exp: no light quarks, charm annihilation, electromagnetism; one charm quark too many [S. Calì, FK, T. Korzec, Eur.Phys.J.C 79 (2019)]

Part II

Massive O(a) renormalization and improvement scheme for dynamical charm

Symanzik improved 3+1 scheme for Wilson quarks

Mass-independent scheme

- Symanzik improvement for Wilson fermions: $\mathcal{O}(a) \longrightarrow \mathcal{O}(a^2)$
- Mass-independent renormalization scheme: renormalization and improvement factors do not depend on quark masses
- Improvement terms $\propto am_q$ M. Lüscher, S. Sint, R. Sommer, P. Weisz, Nucl.Phys.B 478 (1996); T. Bhattacharya, R. Gupta, W. Lee, S. R. Sharpe, J. M. S. Wu, Phys.Rev. D73 (2006)

$$
\begin{aligned}
\overline{g}^2 &= Z_g(\tilde{g}_0^2, a\mu)\tilde{g}_0^2\,, \quad \tilde{g}_0^2 = g_0^2(1 + ab_g(g_0)\mathrm{tr}\,[M_q]/N_\mathrm{f}) \\
\overline{m}_i &= Z_m(\tilde{g}_0^2, a\mu)\Big[m_{q,i} + (r_m(\tilde{g}_0^2) - 1)\frac{\mathrm{tr}\,[M_q]}{N_\mathrm{f}} + a\Big\{b_m(g_0^2)m_{q,i}^2 + \overline{b}_m(g_0^2)\mathrm{tr}\,[M_q]m_{q,i} \\
&\quad + (r_m(g_0^2)d_m(g_0^2) - b_m(g_0^2))\frac{\mathrm{tr}\,[M_q^2]}{N_\mathrm{f}} + (r_m(g_0^2)\overline{d}_m(g_0^2) - \overline{b}_m(g_0^2))\frac{(\mathrm{tr}\,[M_q])^2}{N_\mathrm{f}}\Big\}\Big]
\end{aligned}
$$

bare subtracted quark masses of flavor i: $m_{q,i} = m_i - m_\mathrm{crit}(g_0^2)$, $M_q = \mathrm{diag}(m_{q,1}, \ldots, m_{q,N_\mathrm{f}})$

- Pratically almost impossible to determine all b coefficients non-perturbatively, usually low order perturbation theory is OK for light quarks but charm gives an order of magnitude larger contribution

Symanzik improved 3+1 scheme for Wilson quarks contd

Alternative: massive scheme

- Massive renormalization scheme with close to realistic charm mass m_c and $m_{uds} = \sum_{i=uds} m_i^{\mathrm{phys}}/3$ P. Fritzsch, R. Sommer, F. Stollenwerk, U. Wolff, JHEP 06 (2018)
- mass-dependent renormalization and improvement factors

$$\begin{aligned} \overline{g}^2 &= \tilde{Z}_g(g_0^2, a\mu, aM) g_0^2 \\ \overline{m}_i &= \tilde{Z}_m^i(g_0^2, a\mu, aM)[m_i - \tilde{m}_{\mathrm{crit}}(g_0^2, a\mathrm{tr}\,[M_{\mathrm{q}}])] \end{aligned}$$

  b- and d-terms are absorbed into $\tilde{Z}$; $(r_m - 1)$-term into $\tilde{m}_{\mathrm{crit}} = m_{\mathrm{crit}} - (r_m - 1)\mathrm{tr}\,[M_{\mathrm{q}}]/N_{\mathrm{f}}$
- clover action term Sheikholeslami and Wohlert (SW), Nucl.Phys.B 259 (1985)
  $S_{\mathrm{SW}} = a^5 \tilde{c}_{\mathrm{sw}}(g_0^2, aM) \sum_x \bar{\psi}(x) \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu}(x) \psi(x)$
- non-perturbatively determined clover coefficient $\tilde{c}_{\mathrm{sw}}(g_0^2, aM)$
- reduce the number of mass parameters via $M_{\mathrm{q}} = \mathrm{diag}(m_{\mathrm{q},l}, m_{\mathrm{q},l}, m_{\mathrm{q},l}, m_{\mathrm{q},c})$

Part III

Tuning and scale setting

Action

$S = S_{\mathrm{g}} + S_{\mathrm{f}}$, open boundaries in time

Gauge action

Lüscher–Weisz M. Lüscher, P. Weisz Commun.Math.Phys. 97 (1985) and Phys.Lett.B 158 (1985)

$$S_{\mathrm{g}}[U] = \frac{1}{g_0^2}\left\{\frac{5}{3}\sum_p w(p)\mathrm{tr}\left[1 - U_p(x)\right] - \frac{1}{12}\sum_r w(r)\mathrm{tr}\left[1 - U_r(x)\right]\right\}$$

oriented plaquettes p and rectangles r; weights $w(p) = w(r) = 1$ except for spatial boundaries, there $w(p) = w(r) = 1/2 \leftrightarrow$ boundary improvement term $c_G = 1.0$

Fermion action

$\mathcal{O}(a)$ improved Wilson fermions

$$S_{\mathrm{f}}[U, \overline{\psi}, \psi] = a^4 \sum_{f=1}^4 \sum_x \overline{\psi}_f(x)\left[D_{\mathrm{W}} + m_f\right]\psi_f(x) + S_{\mathrm{SW}}$$

with clover coefficient $\tilde{c}_{\mathrm{sw}}(g_0^2, aM) = \frac{1+Ag_0^2+Bg_0^4}{1+(A-0.196)g_0^2}$, $A = -0.257$, $B = -0.050$ P. Fritzsch, R. Sommer, F. Stollenwerk, U. Wolff, JHEP 06 (2018) and boundary improvement term $c_F = 1.0$

Preliminary work

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

- relation between bare coupling g_0 and lattice spacing in fm
- dimensionless quantity $\sqrt{t_0^\star} m_\mathrm{had}$ in the continuum limit
- m_had experimentally accessible quantity of mass dimension 1
- $t_0^\star$ (mass dimension -2) flow scale M. Lüscher, JHEP 08 (2010) at the symmetric mass point
- $\sqrt{8t_0^\star} = 0.413(5)(2)$fm M. Bruno et al., Phys.Rev.Lett. 119 (2017); M. Bruno, T. Korzec, S. Schaefer, Phys.Rev.D 95 (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 $O(1/m_\mathrm{charm}^2)$
- study of non-perturbative decoupling of the charm quark
  Bruno et al., Phys.Rev.Lett. 114 (2015); Knechtli et al., Phys.Lett.B 774 (2017); Athenodorou et al., Nucl.Phys.B 943 (2019); Calì et al., Eur.Phys.J.C 79 (2019)

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

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

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

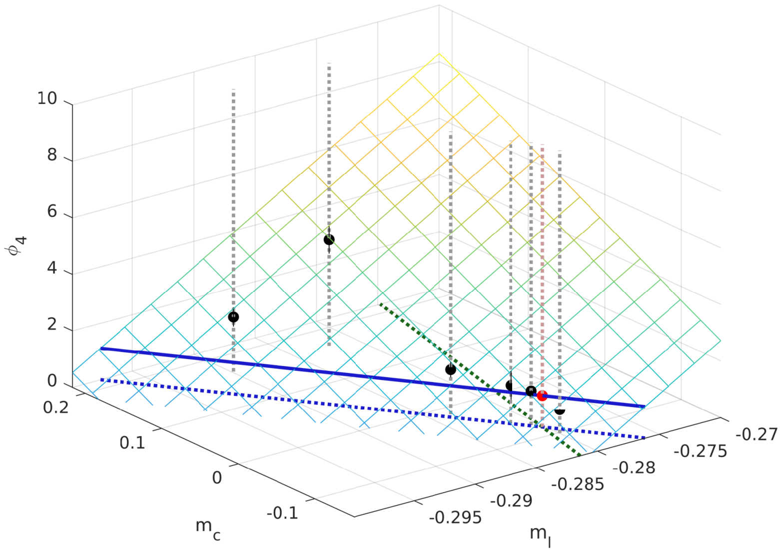
- we use first tuning results from P. Fritzsch, R. Sommer, F. Stollenwerk, U. Wolff, JHEP 06 (2018)

$$\begin{aligned} \beta &= 3.24 \text{ (bare coupling)} \\ \kappa_\mathrm{uds} &= 0.134484 \text{ (light quark mass)} \\ \kappa_c &= 0.12 \text{ (charm quark mass)} \\ c_\mathrm{sw} &= 2.188591 \text{ (bulk improvement)} \end{aligned}$$

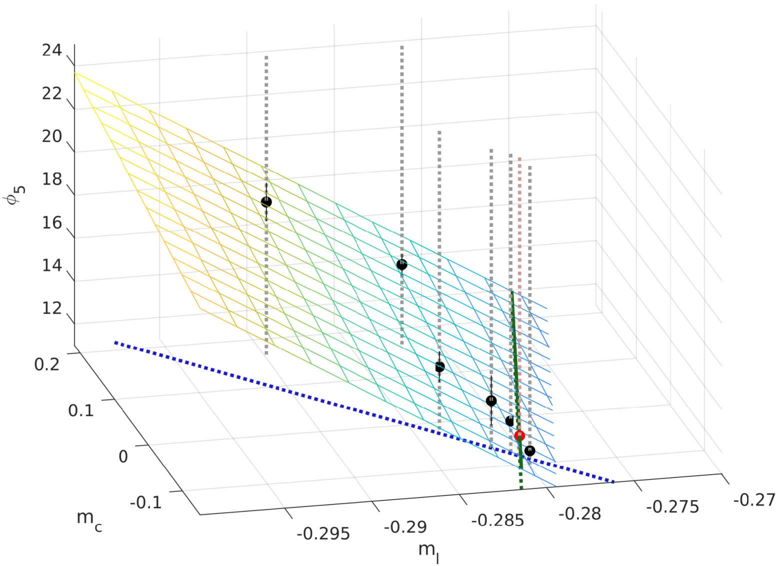
Simulations using openQCD-1.6 Lüscher, Schaefer

- start with algorithmic setup of CLS's H400 simulation Bruno et al., JHEP 02 (2015) and Bruno, Korzec, Schaefer, Phys.Rev.D 95 (2017) and add a charm quark
- u/d quark doublet in terms of even-odd prec. $\hat{D}$ with weight $\propto \det[D^\dagger D] \to \det[(D_{oo})^2]\det\frac{\hat{D}^\dagger\hat{D}+\mu_0^2}{\hat{D}^\dagger\hat{D}+2\mu_0^2}\det[\hat{D}^\dagger\hat{D}+\mu_0^2]$ (twisted mass reweighting type 2 Lüscher,Palombi `0810.0946`) and further factorization $\det[\hat{D}^\dagger\hat{D}+\mu_0^2] = \det[\hat{D}^\dagger\hat{D}+\mu_N^2] \times \frac{\det[\hat{D}^\dagger\hat{D}+\mu_0^2]}{\det[\hat{D}^\dagger\hat{D}+\mu_1^2]} \times \ldots \times \frac{\det[\hat{D}^\dagger\hat{D}+\mu_{N-1}^2]}{\det[\hat{D}^\dagger\hat{D}+\mu_N^2]}$ with $a\mu_i$ given by $\{0.0005, 0.005, 0.05, 0.5\}$ Hasenbusch, Phys.Lett.B 519 (2001)
- strange and charm quarks are simulated with RHMC, Zolotarev rational functions have degrees 12 and 10
- rational function of the strange is further decomposed (partial fraction decomposition)
- both, doublet and rational parts need reweighting
- 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, Comp.Phys.Comm. 151 (2003) integrators
- SAP preconditioning and low-mode-deflation based on local coherence Lüscher, Comp.Phys.Comm. 156 (2004), JHEP 07 (2007); Frommer et al. SIAMJ.Sci.Comp. 36 (2014)

Tuning of $\phi_4 = 1.11$ (A1)



Tuning of $\phi_5 = 11.94$ (A1)



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

ens.	$\frac{T}{a} \times \frac{L^3}{a^3}$	$Lm_\pi^\star$	N_{ms}	t_0/a^2	$am_{\pi,K}$	am_{D,D_s}	ϕ_4	ϕ_5
A0	96×16^3	1.7	700	8.8(2)	0.310(6)	0.614(17)	10.2(9)	15.5(4)
A1	96×32^3	3.5	1954	7.43(4)	0.1138(8)	0.5251(7)	1.16(2)	12.17(4)
A2	128×48^3	5.3	1934	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.
- 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.

Tuning of ensemble B and mis-tuning corrections

ens.	$\frac{T}{a} \times \frac{L^3}{a^3}$	β	a[fm]	$Lm_\pi^\star$	N_{ms} [4 MDU]	τ_{exp}
A2	128×48^3	3.24	0.0536(11)	5.354(13)	1934	25
B	144×48^3	3.43	0.0428(7)	4.282(14)	2000	40

$$\frac{d\langle\mathcal{O}_i\rangle_{QCD}}{dm} = \left\langle \frac{\partial \mathcal{O}_i}{\partial m} \right\rangle_{QCD} - \left\langle \mathcal{O}_i \frac{\partial S}{\partial m} \right\rangle_{QCD} + \langle\mathcal{O}_i\rangle_{QCD} \left\langle \frac{\partial S}{\partial m} \right\rangle_{QCD}$$

$$1.11 = \phi_4 + \left(\frac{d\phi_4}{dm_u} + \frac{d\phi_4}{dm_d} + \frac{d\phi_4}{dm_s} \right) \Delta m_l + \frac{d\phi_4}{dm_c} \Delta m_c$$

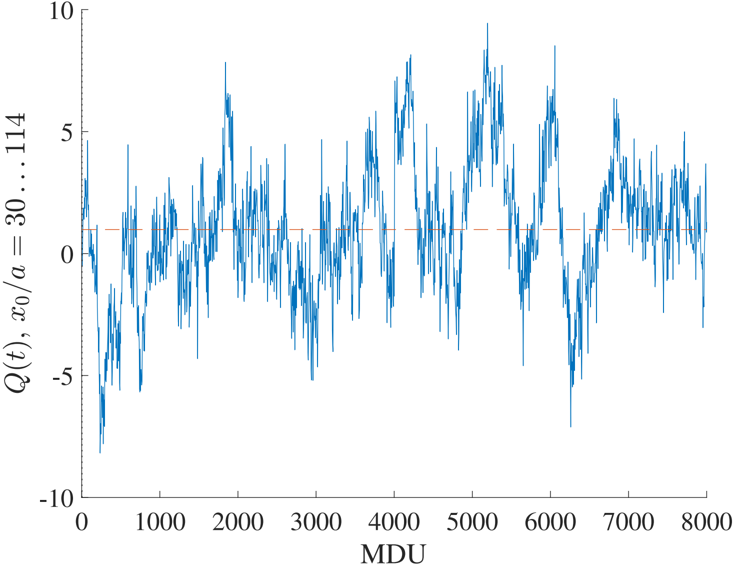
$$11.94 = \phi_5 + \left(\frac{d\phi_5}{dm_u} + \frac{d\phi_5}{dm_d} + \frac{d\phi_5}{dm_s} \right) \Delta m_l + \frac{d\phi_5}{dm_c} \Delta m_c$$

$$f = f(\langle\mathcal{O}_1\rangle_{QCD}, \ldots, \langle\mathcal{O}_N\rangle_{QCD}, m)$$

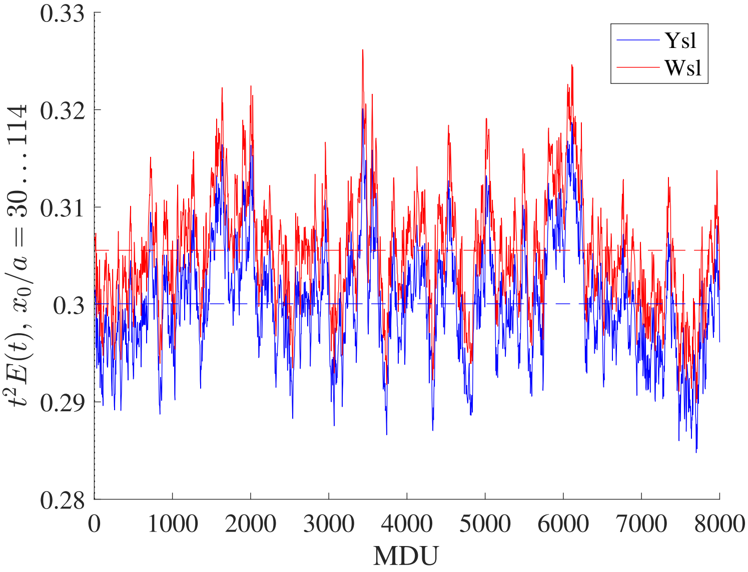
$$f_{\rm corrected} = f + \left(\frac{df}{dm_u} + \frac{df}{dm_d} + \frac{df}{dm_s} \right) \Delta m_l + \frac{df}{dm_c} \Delta m_c$$

ens.	$a\Delta m_l$	$a\Delta m_c$
A2	0.00031(6)	-0.0043(9)
B	-0.00001(5)	-0.0004(12)

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



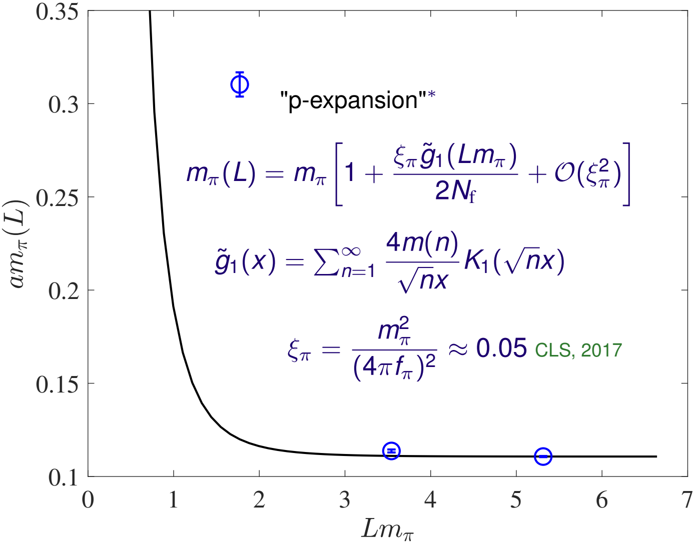
History of $t^2 E(t)$ where $E(t) = \frac{1}{4} G^a_{\mu\nu}(t) G^a_{\mu\nu}(t)$ (ens. B)



Part IV

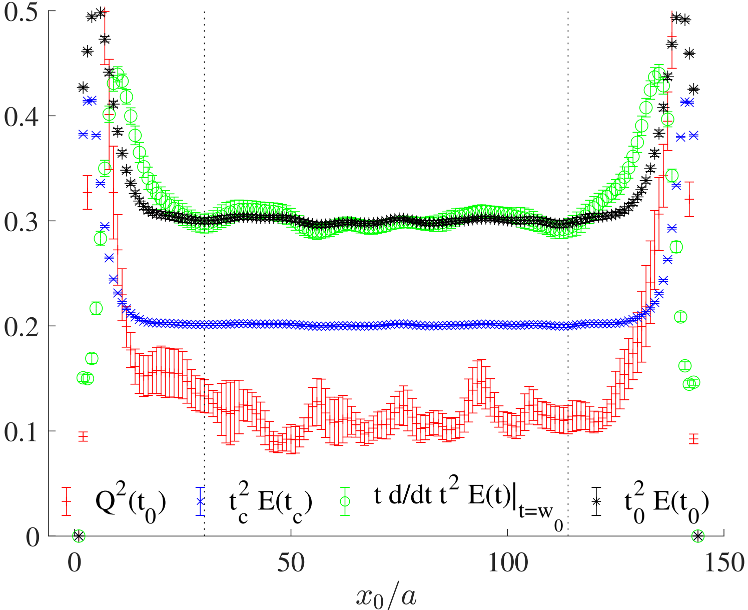
Sytematics: Lattice artifacts, finite volume, decoupling

Finite volume scaling effect of am_π

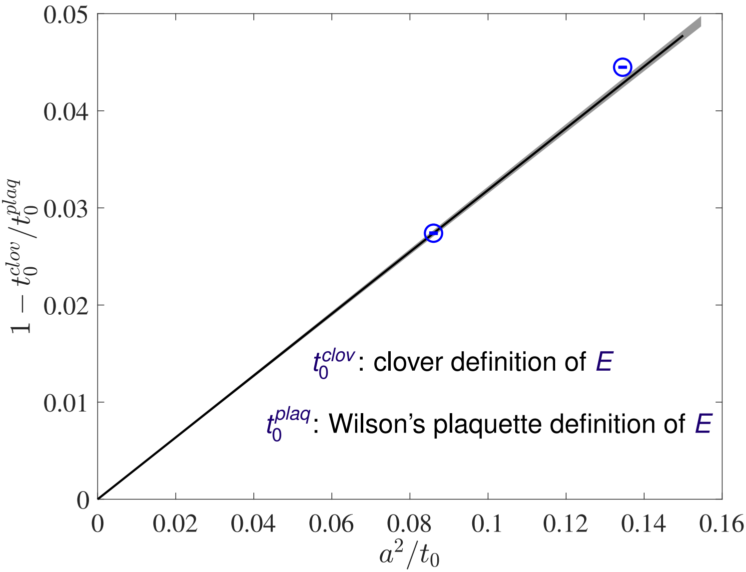


*: Gasser and Leutwyler, Phys.Lett.B 184 (1987); Colangelo, Dürr, Haefeli, Nucl.Phys.B 721 (2005)

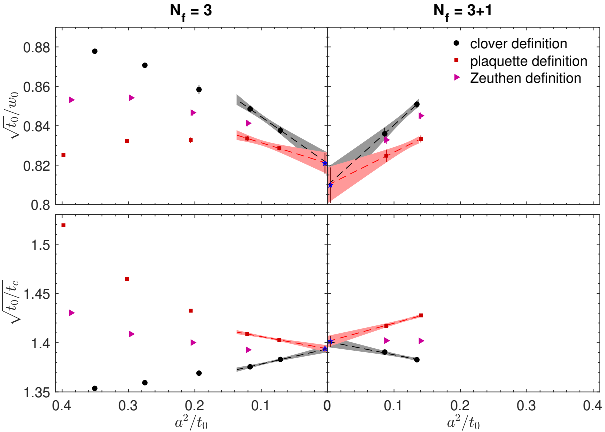
Effects of open boundaries (ens. B)



Continuum limit, 1.7 permille non-a^2 lattice artifacts



Test of decoupling $N_f = 3 + 1 \to N_f = 3$ CLS



Charm sea effects far below 1%

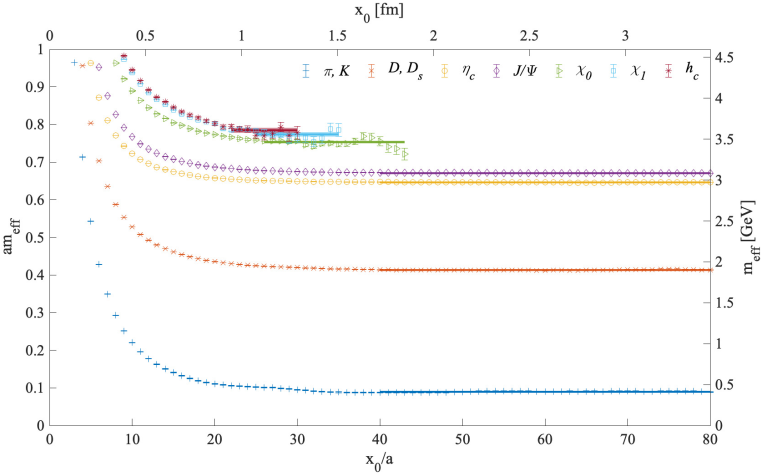
Continuum extrapolations by constrained linear fits to plaq and clov definitions

Zeuthen: Symanzik-improved flow and observable A. Ramos, S. Sint, Eur.Phys.J.C 76

Part V

Charmonium spectrum

Meson spectrum (ens. B)



$f_{\mathcal{O}\mathcal{O}}(x_0, y_0) = a^6 \sum_{\mathbf{x},\mathbf{y}} \langle \mathcal{O}(x) \mathcal{O}^\dagger(y) \rangle$, $\mathcal{O} = \bar{q}_1 \Gamma q_2$

Charmonium Spectrum

	η_c (0^{-+})	J/ψ (1^{--})	χ_{c0} (0^{++})	χ_{c_1} (1^{++})	h_c (1^{+-})
m_{eff} A2 [GeV]	2.990(4)	3.104(4)	3.445(91)	3.605(13)	3.683(12)
m_{eff} B [GeV]	2.973(4)	3.086(5)	3.458(22)	3.538(37)	3.650(41)
PDG [GeV]	2.9834(5)	3.096900(6)	3.4148(3)	3.51066(7)	3.52538(11)

	A2	B	cont.	PDG
hyperfine splitting $\frac{m_{J/\Psi}-m_{\eta c}}{m_{\eta c}}$	0.0382(3)	0.0380(3)	0.0376(11)	0.038

Chiral trajectories for charmonia X

- choice ϕ_4, ϕ_5 $\leftrightarrow$ sum of light quark masses and charm mass physical
- chiral trajectories: lines ϕ_4 =const. ($\leftrightarrow$ constant $\mathrm{tr}\,(\bar{m})$ M. Bruno, T. Korzec, S. Schaefer, Phys.Rev.D 95 (2017)), ϕ_5 =const.
- approach the physical point by decreasing $\bar{m}_u = \bar{m}_d$ and increasing $\bar{m}_s$
- no light quarks in the valence sector, hence the derivatives $dm_x/d\bar{m}_u = dm_x/d\bar{m}_d = dm_x/d\bar{m}_s$ at the symmetric point
- $m_x^{\mathrm{phys}} = m_x + (\Delta\bar{m}_u + \Delta\bar{m}_d + \Delta\bar{m}_s)\frac{dm_x}{d\bar{m}_u} + O(\Delta^2)$
- linear term vanishes along trajectories with $\mathrm{tr}\,(\bar{m}) = const.$

Part VI

Conclusions & Outlook

Conclusions & Outlook

Conclusions

- scale setting and tuning of $N_{\mathrm{f}} = 3 + 1$ QCD
- massive renormalization and improvement scheme with a non-perturbatively determined clover coefficient
- two ensembles with $a = 0.054\,\mathrm{fm}$ and $a = 0.043\,\mathrm{fm}$
- ratios of flow scales and test of decoupling
- charmonium spectrum and hyperfine splitting

Outlook

- further states, smearing, distillation, charm-annihilation, string breaking
- continuum limit
- $N_{\mathrm{f}} = 2 + 1 + 1$
- 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	0.043	4.3
C ?	192×64^3	0.032	4.2