Scale setting for QCD with $N_f = 3 + 1$

dynamical quarks

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Motivation

Reasons for dynamical charm quarks

- investigate decoupling with light quarks, high precision charm physics, $\alpha_S$ in 4 flavor theory, ...

Difficulties/Solutions

- lattice artefacts due to cutoff effects $\propto O(am_c \approx 0.5)$
- [ 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 $m_{uds} = \sum_{i=uds} m_i^{phys} / 3$
- 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

\[
g_R^2 = \tilde{Z}_g(g_0^2, a\mu, aM)g_0^2, \quad m_{R,i} = \tilde{Z}_m^i(g_0^2, a\mu, aM)m_{q,i}
\]

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

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

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

- non-perturbative fit formula for the clover coefficient $c_{SW}(g_0^2)$ from LCP, cf. [Fritzsch et al., 2018]

- reduce the number of mass parameters via

\[
M_q = \text{diag}(m_{q,l}, m_{q,l}, m_{q,l}, m_{q,c})
\]
## Preliminary Work

### Scale setting in CLS $N_f = 2 + 1$ QCD

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

### Non-perturbative decoupling of the charm quark

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

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

  and

  $$\phi_4 \equiv 8t_0 \left( m_K^2 + \frac{m_\pi^2}{2} \right) = 12t_0 m_\pi^2 = 1.11$$

  $$\phi_5 \equiv \sqrt{8t_0 (m_{D_s} + 2m_D)} = \sqrt{72t_0 m_D} = 11.94$$

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

  $\beta = 3.24$ (bare coupling)

  $\kappa_{uds} = 0.134484$ (light quark mass)

  $\kappa_c = 0.12$ (charm quark mass)

  $c_0 = 5/3$ (Lüscher–Weisz action)

  $c_{SW} = 2.188591$ (bulk improvement)

  $c_F = c_G = 1.0$ (boundary improvements)
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 $\propto \det[(D_{oo})^2]\det[\hat{D}^\dagger\hat{D} + \mu^2]^2\det[\hat{D}^\dagger\hat{D} + 2\mu^2]^{-1}$
- 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]
  \[
  \det[D^2] = \frac{\det[D^\dagger D + \mu_0^2]}{\det[D^\dagger D + \mu_N^2]} \times \frac{\det[D^\dagger D + \mu_1^2]}{\det[D^\dagger D + \mu_N^2]} \times \ldots \times \frac{\det[D^\dagger D]}{\det[D^\dagger D + \mu_N^2]}
  \]
- 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
Tuning of $\phi_4 = 1.11$
Tuning of $\phi_5 = 11.94$
Tuning Results: \( \kappa_l = 0.13440733, \kappa_c = 0.12784 \)

<table>
<thead>
<tr>
<th>( \frac{T}{a} \times \frac{L^3}{a^3} )</th>
<th>( L \mu^* )</th>
<th>( N_{\text{tra}} )</th>
<th>( t_0/a^2 )</th>
<th>( a m_{\pi,K} )</th>
<th>( a m_{D,D_s} )</th>
<th>( \phi_4 )</th>
<th>( \phi_5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>96 \times 16^3</td>
<td>1.7</td>
<td>1000</td>
<td>8.8(2)</td>
<td>0.310(6)</td>
<td>0.614(17)</td>
<td>10.2(9)</td>
<td>15.5(4)</td>
</tr>
<tr>
<td>96 \times 32^3</td>
<td>3.5</td>
<td>3908</td>
<td>7.43(4)</td>
<td>0.1138(8)</td>
<td>0.5251(7)</td>
<td>1.16(2)</td>
<td>12.17(4)</td>
</tr>
<tr>
<td>128 \times 48^3</td>
<td>5.3</td>
<td>3868</td>
<td>7.36(3)</td>
<td>0.1108(4)</td>
<td>0.5236(4)</td>
<td>1.087(6)</td>
<td>12.06(2)</td>
</tr>
</tbody>
</table>

- The integrated autocorrelation time of \( t_0 \) is \( \tau_{\text{int},t_0} \approx 20 \pm 10 \) [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 \( \phi_4 \) and \( \phi_5 \) 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 $Q(t \approx t_0)$

$n_{f31}H100, \ t/a^2 \approx 7.45$

$n_{f31}H100p000, n_{f31}H100p001$

$Q(t), x_0/a = 22 \ldots 72$
History of $t^2 E(t)$ where $E(t) = \frac{1}{4} G_{\mu\nu}^a(t) G_{\mu\nu}^a(t)$

nf31H100, $t/a^2 \approx 7.45$

R. Höllwieser, Scale setting for QCD with $N_f = 3 + 1$ dynamical quarks
Meson spectrum

R. Höllwieser, Scale setting for QCD with $N_f = 3 + 1$ dynamical quarks
Charmonium Spectrum

<table>
<thead>
<tr>
<th></th>
<th>$\eta_c$</th>
<th>$J/\psi$</th>
<th>$\chi_{c0}$</th>
<th>$\chi_{c1}$</th>
<th>$h_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$am_{eff}$</td>
<td>0.8180(2)</td>
<td>0.8489(2)</td>
<td>0.9398(86)</td>
<td>0.9833(72)</td>
<td>0.9902(81)</td>
</tr>
<tr>
<td>$m_{eff}$ [GeV]</td>
<td>2.9890(7)</td>
<td>3.1019(7)</td>
<td>3.434(31)</td>
<td>3.593(26)</td>
<td>3.618(30)</td>
</tr>
<tr>
<td>PDG [GeV]</td>
<td>2.9834(5)</td>
<td>3.096900(6)</td>
<td>3.4148(3)</td>
<td>3.51066(7)</td>
<td>3.52538(11)</td>
</tr>
</tbody>
</table>

- sum of the light quark masses has physical value
- no light quarks in the valence sector, hence the derivatives $dm_x/dm_{up} = dm_x/dm_{down} = dm_x/dm_{strange}$
- $m_{x phys} = m_x + (\Delta_{up} + \Delta_{down} + \Delta_{strange}) \frac{dm_{nc}}{dm_u} + O(\Delta^2)$
- linear term vanishes, because $\phi_4$ is chosen such that $\Delta_{up} = \Delta_{down} = -0.5\Delta_{strange}$ ($m_{uds} = \sum_{i=uds} m_{i phys}/3$)
- derivatives of correlation functions with respect to bare quark masses allow us to correct (small) mistunings in $\phi_4$ and $\phi_5$
Finite volume scaling effects for $a m_\pi$ [Colangelo, Dürr, Haefeli, 2005]

"p-expansion"

$$m_\pi(L) = m_\pi(\infty) \left[ 1 + \frac{\xi_\pi \tilde{g}_1(L m_\pi)}{2 N_f} + \mathcal{O}(\xi^2_\pi) \right]$$

$$\tilde{g}_1(x) = \sum_{n=1}^{\infty} \frac{4m(n)}{\sqrt{n}x K_1(\sqrt{n}x)}$$

$$\xi_\pi = \frac{m^2_\pi}{(4\pi f_\pi)^2} \approx 0.05 \ [\text{CLS, 2017}]$$
Conclusions & Outlook

Conclusions

- Scale setting and tuning of $N_f = 3 + 1$ 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
  \[ \frac{d m_{\text{had}}}{d m_q}, \frac{d t_0}{d m_q}, \frac{d S}{d m_q} \]
- continuum limit
- $\Lambda, \alpha_S$ in $N_f = 4$

\[
\begin{array}{cccc}
\text{ens.} & \frac{T_a}{a} \times \frac{L^3}{a^3} & a \text{ [fm]} & L m_{\pi}^* \\
A1 & 96 \times 32^3 & 0.054 & 3.5 \\
A2 & 128 \times 48^3 & 0.054 & 5.3 \\
B & 144 \times 48^3 & 0.041 & 4.0 \\
C ? & 192 \times 64^3 & 0.032 & 4.2 \\
\end{array}
\]
THANK YOU

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