O(a) improved Wilson quarks and the O(am) rescaling of g_0^2

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Outline

- O(a) improved Wilson quarks
- The rôle of b_{g}
- Strategies to determine b_{g} non-perturbatively
- A perturbative test
- Conclusions

N_f mass-degenerate O(a) improved Wilson quarks

- O(a) improved lattice action, bare parameters m_0 and g_0^2:

$$S = a^4 \sum_x \overline{\psi}(x)(D_\mathrm{W} + m_0)\psi(x) + \frac{1}{g_0^2} \underbrace{\left(g_0^2 \times S_\mathrm{g}\right)}_{g_0\text{-indep.}}$$

$$D_\mathrm{W} = \sum_\mu \left\{ \tfrac{1}{2}(\nabla_\mu + \nabla_\mu^*)\gamma_\mu - a\nabla_\mu^*\nabla_\mu \right\} + ia\, c_\mathrm{sw}(g_0^2) \sum_{\mu,\nu} \sigma_{\mu\nu}\hat{F}_{\mu\nu}(x)$$

- O(a) improvement at non-vanishing masses requires the rescaling of the bare mass and coupling ($m_\mathrm{q} = m_0 - m_\mathrm{cr}(g_0)$):

$$\tilde{g}_0^2 = g_0^2(1 + b_\mathrm{g}(g_0^2)am_\mathrm{q}), \qquad \widetilde{m}_\mathrm{q} = m_\mathrm{q}(1 + b_\mathrm{m}(g_0^2)am_\mathrm{q})$$

- Renormalized & on-shell O(a) improved composite operators, e.g. axial current and density:

$$(A_\mathrm{R})_\mu^a = Z_\mathrm{A}(\tilde{g}_0^2)(1 + b_\mathrm{A}(g_0^2)am_\mathrm{q}) \left\{ A_\mu^a + c_\mathrm{A}(g_0^2)\tilde{\partial}_\mu P^a \right\}$$

$$(P_\mathrm{R})^a = Z_\mathrm{P}(\tilde{g}_0^2, a\mu)(1 + b_\mathrm{P}(g_0^2)am_\mathrm{q})P^a$$

$\Rightarrow$ On-shell O(a) improvement requires c_sw, b_g, b_m, c_A, b_A, b_P, ...

Relevance of $b_{\rm g}$, Decoupling strategy [ALPHA 2019-22]

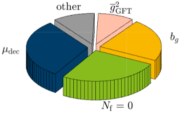
- Simulations at fixed a as $m_{\rm q}$ is varied $\Leftrightarrow$ fix $\tilde{g}_0^2$, requires $b_{\rm g}$!
- $b_{\rm g}$ is known to 1-loop order [Sommer, S. '95]: $b_{\rm g} = 0.0120 \times N_{\rm f} g_0^2 + {\rm O}(g_0^4)$; sufficient for light & strange quark masses, for which e.g. $am_{\rm q} < 0.03$.
- Non-perturbative estimates needed for heavier quarks!

Decoupling strategy: Relate Λ-parameters of $N_{\rm f} = 3$ and $N_{\rm f} = 0$ QCD by simultaneously decoupling $N_{\rm f} = 3$ heavy quarks:

- Trace a (finite volume) GF coupling as function of M, up to $M = {\rm O}(10)\,{\rm GeV}$;
- Lattice spacings such that $aM < 0.4 - 0.5$; ($am_{\rm q}$ smaller by factor $\approx 1.5 - 2$)
- Result [ALPHA '22] (compatible with [ALPHA '17], error of same size but **largely independent**!)

$$\Lambda_{\overline{\rm MS}}^{(3)} = 336(10)(6)_{b_{\rm g}}(3)_{\hat{\Gamma}_m}{\rm MeV} = 336(12){\rm MeV} \quad \Rightarrow \quad \alpha_s(m_Z) = 0.11823(84)$$

$\Rightarrow$ $b_{\rm g}$-error estimated assuming a 100% uncertainty on 1-loop value.



contributions to error^2

Strategies to determine $b_{\rm g}$ non-perturbatively; Chiral Ward identities

$b_{\rm g}$ can be related to the O(a) improvement of the flavour singlet scalar density $S^0 = \overline{\psi}\psi$: [Bhattacharya et al, '05]

$$S^0_{\rm R} = Z_{S^0}\left(1 + b_{\rm S^0}\, a m_{\rm q}\right)\left[S^0 + c_S a^{-3} + d_S\, a\, \mathrm{tr}\,\{F_{\mu\nu}F_{\mu\nu}\}\right]$$

Basic argument:

- Differentiating a gradient flow observable with respect to the renormalized O(a) improved quark mass and coupling generates insertion of an O(a) improved scalar and action density, respectively.
- Changing variables to unimproved quark mass and coupling allows to identify the counterterms such that
$$b_{\rm g} = -2 g_0^2 d_S,$$
- provided the O(a) counterterm takes the particular form dictated by the lattice action:
$$\mathrm{tr}(F_{\mu\nu}F_{\mu\nu}) \to -2g_0^2\left(\mathcal{L}_g - g_0^2 \times \frac{ia}{4} c'_{\rm sw}(g_0^2)\overline{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi\right),$$
- $\mathcal{L}_g$ denotes the gauge action density and the SW-term contribution was missing in earlier papers.
- Chiral Ward identities can now be applied to massless (connected) correlation functions, e.g. in the SF [S.'98, Münster coll. '22].

Alternative: Physical vs. cutoff m_{q}-dependence

Consider QCD in a finite space-time volume, no boundaries, gradient flow observable (e.g. GF coupling):

- Absence of spontaneous symmetry breaking; functional integral well defined with exact chiral symmetry in GW regularization

$\Rightarrow$ N_{f} even: functional integral is even function of m; physical quark mass effects are function of m^2!

$\Rightarrow$ N_{f} odd: no definite m-parity, however no first order terms in m, since [Dalla Brida, Giusti, Pepe, '20]

$$\psi \to \exp(i\pi\gamma_5/N_{\mathrm{f}})\psi, \quad \overline{\psi} \to \overline{\psi}\exp(i\pi\gamma_5/N_{\mathrm{f}})$$

has unit Jacobian and transforms the mass term $\overline{\psi}\psi \to \overline{\psi}\exp(2i\pi/N_{\mathrm{f}}\gamma_5)\psi$ with parity-conserving part $\cos(2\pi/N_{\mathrm{f}}) \times \overline{\psi}\psi$

- Expanding in powers of m shows that the linear term in m must vanish.

Conclusion: For small masses, physical quark mass effects are O(m^2), while the b_{g} term muliplies a term linear in m!

Explicit condition for $b_{\rm g}$

We consider a gradient flow observable $\langle O_{\rm gf}\rangle$ in a finite volume, as a function of the renormalized quark mass m.

- In the continuum limit:

$$\langle O_{\rm gf}\rangle = A + O(m^2) \qquad \Rightarrow \qquad \left.\frac{\partial\langle O_{\rm gf}\rangle}{\partial m}\right|_{m=0} = 0$$

- On the lattice m is proportional to $\widetilde{m}_{\rm q}$;
- Reformulate in terms of bare parameters;

$$\left.\frac{\partial S}{\partial \widetilde{m}_{\rm q}}\right|_{\tilde{g}_0^2} = (1-2b_{\rm m}am_{\rm q})\left(\left.\frac{\partial S}{\partial m_{\rm q}}\right|_{g_0^2} - ag_0^2 b_{\rm g}\left.\frac{\partial S}{\partial g_0^2}\right|_{m_{\rm q}}\right) + {\rm O}(a^2)$$

- Setting $m_{\rm q} = 0$ this translates to

$$\left.\frac{\partial\langle O_{\rm gf}\rangle}{\partial \widetilde{m}_{\rm q}}\right|_{\tilde{g}_0^2} = \left.\frac{\partial\langle O_{\rm gf}\rangle}{\partial m_{\rm q}}\right|_{g_0^2} - ag_0^2 b_{\rm g}\left.\frac{\partial\langle O_{\rm gf}\rangle}{\partial g_0^2}\right|_{m_{\rm q}} + {\rm O}(a^2)$$

- Requiring this to vanish, up to ${\rm O}(a^2)$:

$$b_{\rm g} = \left.\frac{\partial\langle O_{\rm gf}\rangle}{\partial am_{\rm q}}\right|_{g_0;m_{\rm q}=0}\left\{g_0^2\left.\frac{\partial\langle O_{\rm gf}\rangle}{\partial g_0^2}\right|_{m_{\rm q}=0}\right\}^{-1}$$

A perturbative test

Consider $\langle O_{\rm gf}\rangle \to \bar{g}^2$, the SF coupling with χSF b.c's

- Presence of boundary & absence of gradient flow: no problem in this case.
- define $z = m_{\rm R} L$ and expand perturbatively

$$\bar{g}^2(L,z) = g_0^2 + p_1(L/a,z) g_0^4 + {\rm O}(g_0^6) = \tilde{g}_0^2 + \left(p_1(L/a,z) - am_{\rm q} b_{\rm g}^{(1)}\right) \tilde{g}_0^4 + {\rm O}(\tilde{g}_0^6)$$

- To this order $m_{\rm R} = \widetilde{m}_{\rm q} = m_{\rm q} + {\rm O}(m_{\rm q}^2)$:
- Asymptotic expansion for small a/L:

$$p_1 \sim r_0(z) + s_0 \ln(L/a) + \frac{a}{L} r_1(z) + {\rm O}(a^2);$$

- Expect $r_0(z) = r_0(0) + {\rm O}(z^2)$

$$\left.\frac{\partial \bar{g}^2}{\partial z}\right|_{z=0} = \frac{a}{L}\left(r_1'(0) - b_{\rm g}^{(1)}\right) \tilde{g}_0^2 + {\rm O}(a^2, \tilde{g}_0^4) \quad \Rightarrow \quad b_{\rm g}^{(1)} = r_1'(0)$$

- Result from asymptotic analyis reproduces the known 1-loop result $b_{\rm g}^{(1)} = 0.0120 N_{\rm f}$
- The old result was obtained with SF b.c.'s but then $r_0(z) = r_0(0) + {\rm O}(z)$, $\Rightarrow$ extra term from physical quark mass dependence!

A perturbative test cont'd

Test formula for dependence on bare parameters:

$$\left.\frac{\partial \bar{g}^2}{\partial a m_{\mathrm{q}}}\right|_{g_0^2, m_{\mathrm{q}}=0} = g_0^4 \left.\frac{\partial p_1}{\partial a m_{\mathrm{q}}}\right|_{m_{\mathrm{q}}=0} + \ldots, \qquad \left.\frac{\partial \bar{g}^2}{\partial g_0^2}\right|_{m_{\mathrm{q}}=0} = 1 + 2 p_1 g_0^2 + \ldots$$

$$\Rightarrow \qquad b_{\mathrm{g}} = b_{\mathrm{g}}^{(1)} g_0^2 + \mathrm{O}(g_0^4), \qquad b_{\mathrm{g}}^{(1)} = \left.\frac{\partial p_1}{\partial a m_{\mathrm{q}}}\right|_{m_{\mathrm{q}}=0} = \left.\frac{L}{a} r_0'(z)\right|_{z=0} + r_1'(0)$$

Numerical results, using the standard SF coupling with χSF b.c.'s, $m_0 = 0$, $\theta = \pi/2$

$$\left.\frac{b_{\mathrm{g}}^{(1),\mathrm{est}}}{0.0120 N_{\mathrm{f}}}\right|_{L/a} = 0.8992,\ 0.9125,\ 0.9213,\ 0.9405,\ 0.9477, \quad \text{for} \quad L/a = 16, 24, 30, 48, 60$$

- Corrections are O(a); relative effects seem large but b_{g} is numerically small!
- $L/a \times r_0'(z) \propto z \times L/a$: requires to control $z = 0$ up to effects $\mathrm{O}(a^2)$ (requires c_{A} in O(a) improved PCAC mass)
- χSF b.c.'s only available for N_{f} even; setup with periodic or twisted periodic ($N_{\mathrm{f}} = 3$) boundary conditions preferred.

Conclusions

- At quark mass values that are not very small in lattice units, a non-perturbative determination of b_{g} becomes important
- Decoupling project by the ALPHA collaboration: physical M_{RGI}-values up to O$(10\,\mathrm{GeV})$ data used for continuum extrapolation has $aM < 0.5$
- The O(am) improvement coefficient b_{g} can be determined either
    1. by chiral WI's for the flavour singlet scalar density (albeit with lattice action density including SW-term!) or
    2. by separating the physical mass dependence (quadradic in m) from the cutoff dependence (linear in m)
- ALPHA collaboration: determination of b_{g} at β-values used in ALPHA decoupling project
    - periodic/anti-periodic boundary condition in all directions for gauge/fermion fields

  $\Rightarrow$ for preliminary results cf. poster by Mattia Dalla Brida this evening

Thank you!