Non-perturbative Renormalization and Improvement of Lattice QCD

Lecture 4

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Contents

Continuum vs. lattice symmetries

On the lattice symmetries are typically reduced with respect to the continuum. Examples are

1. Space-Time symmetries: the Euclidean O(4) rotations are reduced to the O(4,$\mathbb{Z}$) group of the hypercubic lattice. Other lattice geometries are possible, even random lattices have been tried.
2. Supersymmetry: only partially realisable on the lattice
3. Chiral and Flavour symmetries:
   - staggered quarks: only a U(1)$\times$U(1) symmetry remains
   - Wilson quarks: an exact $SU(N_{\rm f})_{\rm V}$
   - twisted mass Wilson quarks: various U(1) symmetries (both axial and vector)
   - overlap/Neuberger quarks: complete continuum symmetries!
   - Domain Wall quarks: (negligibly ?) small violations of axial symmetries; consequences are analysed like for Wilson quarks

Case study: chiral and flavour symmetries with Wilson type quarks

Exact lattice Ward identities (1)

Euclidean action $S = S_{\rm f} + S_{\rm g}$:

$$S_{\rm f} = a^4 \sum_x \overline{\psi}(x)\,(D_W + m_0)\,\psi(x), \qquad S_{\rm g} = \frac{1}{g_0^2}\sum_{\mu,\nu} \mathrm{tr}\,\{1 - P_{\mu\nu}(x)\}$$

$$D_W = \tfrac{1}{2}\left\{\left(\nabla_\mu + \nabla^*_\mu\right)\gamma_\mu - a\nabla^*_\mu\nabla_\mu\right\}$$

Isospin transformations ($N_{\rm f} = 2$, $\tau^{1,2,3}$ Pauli matrices):

$$\psi(x) \;\to\; \psi'(x) = \exp\left(i\theta(x)\tfrac{1}{2}\tau^a\right)\psi(x) \approx \left(1 + \delta^a_{\rm V}(\theta)\right)\psi(x),$$

$$\overline{\psi}(x) \;\to\; \overline{\psi}'(x) = \overline{\psi}(x)\exp\left(-i\theta(x)\tfrac{1}{2}\tau^a\right)\psi(x) \approx \left(1 + \delta^a_{\rm V}(\theta)\right)\overline{\psi}(x)$$

Perform change of variables in the functional integral and expand in θ

$$\langle O[\psi,\overline{\psi},U]\rangle = Z^{-1}\int D[\psi,\overline{\psi}]D[U]\mathrm{e}^{-S}\,O[\psi,\overline{\psi},U].$$

Due to $D[\psi,\overline{\psi}] = D[\psi',\overline{\psi}']$ one finds the vector Ward identity

$$\langle \delta^a_{\rm V}(\theta)O\rangle = \langle O\delta^a_{\rm V}(\theta)S\rangle$$

Exact lattice Ward identities (2)

Variation of the action, Noether current:

$$
\begin{aligned}
\delta_{\mathrm{V}}^{a}(\theta)S &= -ia^4\sum_x \theta(x)\partial_\mu^*\widetilde{V}_\mu^a(x) \\
\widetilde{V}_\mu^a(x) &= \overline{\psi}(x)(\gamma_\mu-1)\frac{\tau^a}{4}U(x,\mu)\psi(x+a\hat{\mu}) \\
&\quad +\overline{\psi}(x+a\hat{\mu})(\gamma_\mu+1)\frac{\tau^a}{4}U(x,\mu)^\dagger\psi(x)
\end{aligned}
$$

Choose region R and θ:

$$
R=\{x:\ t_1<x_0\leq t_2\},\qquad \theta(x)=\begin{cases}1 & \text{if } x\in R\\ 0 & \text{otherwise}\end{cases}
$$

Exact lattice Ward identities (3)

if $O = O_{\rm ext}$ is localised outside R:

$$0 = \langle O_{\rm ext}\, i\delta_{\rm V}^{a}(\theta) S\rangle = a^4 \sum_{x_0=t_1+a}^{t_2} \sum_{\mathbf{x}} \langle O_{\rm ext}\, \partial_\mu^* \widetilde{V}_\mu^a(x)\rangle$$
$$= a \sum_{x_0=t_1+a}^{t_2} \partial_0^* \langle O_{\rm ext}\, Q_{\rm V}^a(x_0)\rangle$$
$$= \langle O_{\rm ext}\, Q_{\rm V}^a(t_2)\rangle - \langle O_{\rm ext}\, Q_{\rm V}^a(t_1)\rangle$$

i.e. the vector charge is time-independent;
This expresses the exact vector symmetry on the lattice;
N.B.: These are exact identities between *lattice* correlation functions!

Exact lattice Ward identities (4)

Choosing $O = O_{\rm ext}\,\widetilde{V}^b_\mu(y)$, with $y \in R$:

$$
\begin{aligned}
i\varepsilon^{abc}\left\langle O_{\rm ext}\,\widetilde{V}^c_k(y)\right\rangle &= \left\langle O_{\rm ext}\,\widetilde{V}^b_k(y)\,[Q^a_{\rm V}(t_2) - Q^a_{\rm V}(t_1)]\right\rangle \\
i\varepsilon^{abc}\left\langle O_{\rm ext}\,Q^c_{\rm V}(y_0)\right\rangle &= \left\langle O_{\rm ext}\,Q^b_{\rm V}(y_0)\,[Q^a_{\rm V}(t_2) - Q^a_{\rm V}(t_1)]\right\rangle
\end{aligned}
$$

- N.B. The RHS does not vanish since the time ordering matters: $t_1 < y_0$ and $t_2 > y_0$
- Constitutes Euclidean version of charge algebra!

Exact lattice Ward identities (5)

- implies that the Noether current $\widetilde{V}_\mu^a$ is protected against renormalisation; if we admit a renormalisation constant $Z_{\tilde{\mathrm{V}}}$ it follows that $Z_{\tilde{\mathrm{V}}}^2 = Z_{\tilde{\mathrm{V}}}$ hence $Z_{\tilde{\mathrm{V}}} = 1$; its anomalous dimension vanishes!
- Any other definition of a lattice current, e.g. the local current

$$V_\mu^a(x) = \overline{\psi}(x)\gamma_\mu\gamma_5\psi(x), \qquad (V_{\mathrm{R}})_\mu^a = Z_{\mathrm{V}} V_\mu^a$$

can be renormalised by comparing with the conserved current. Its anomalous dimension must vanish, i.e.

$$Z_{\mathrm{V}} = Z_{\mathrm{V}}(g_0) \quad \stackrel{g_0 \to 0}{\sim} \quad 1 + \sum_{n=1}^{\infty} Z_{\mathrm{V}}^{(n)} g_0^{2n}.$$

Continuum chiral WI's as normalisation conditions

- For chiral symmetry there is no conserved current with Wilson quarks.
- However: expect that chiral symmetry can be restored in the continuum limit!

$\Rightarrow$ [Bochicchio et al '85]: use continuum chiral Ward identities and impose them as normalisation condition at finite lattice spacing a!

Continuum chiral WI's as normalisation conditions

- Define chiral variations:

$$\delta_{\mathrm{A}}^{a}(\theta)\psi(x) = i\gamma_5\tfrac{1}{2}\tau^a\theta(x)\psi(x), \qquad \delta_{\mathrm{A}}^{a}(\theta)\overline{\psi}(x) = \overline{\psi}(x)i\gamma_5\tfrac{1}{2}\tau^a\theta(x)$$

- Derive formal continuum Ward identities assuming that the functional integral can be treated like an ordinary integral:

$$\Rightarrow \qquad \langle\delta_{\mathrm{A}}^{a}(\theta)O\rangle = \langle O\delta_{\mathrm{A}}^{a}(\theta)S\rangle,$$

$$\begin{aligned}
\delta_{\mathrm{A}}^{a}(\theta)S &= -i\int \mathrm{d}^4x\theta(x)\left(\partial_\mu A_\mu^a(x) - 2mP^a(x)\right) \\
A_\mu^a(x) &= \overline{\psi}(x)\gamma_\mu\gamma_5\tfrac{1}{2}\tau^a\psi(x), \qquad P^a(x) = \overline{\psi}(x)\gamma_5\tfrac{1}{2}\tau^a\psi(x)
\end{aligned}$$

Simplest chiral WI: the PCAC relation (1)

- Shrink the region R to a point x:

$$
\begin{aligned}
& \langle O_{\rm ext} \delta_{\rm A}^a(\theta) S \rangle &=& \; 0 \\
\Rightarrow \quad & \left\langle \partial_\mu A_\mu^a(x) O_{\rm ext} \right\rangle &=& \; 2m \, \langle P^a(x) O_{\rm ext} \rangle
\end{aligned}
$$

- The PCAC relation implies that chiral symmetry is restored in the chiral limit.

Simplest chiral WI: the PCAC relation (2)

- Impose PCAC on Wilson quarks at fixed a: define a bare PCAC mass:

$$m = \frac{\langle \partial_\mu A^a_\mu(x) O_{\rm ext} \rangle}{\langle P^a(x) O_{\rm ext} \rangle}$$

- A renormalised quark mass can thus be written in two ways

$$m_{\rm R} = Z_{\rm A} Z_{\rm P}^{-1} m = Z_m (m_0 - m_{\rm cr}) \quad \Rightarrow \quad m = Z_m Z_{\rm P} Z_{\rm A}^{-1} (m_0 - m_{\rm cr})$$

$\Rightarrow$ The critical mass can be determined by measuring the bare PCAC mass m as a function of m_0 and extra/interpolation to $m = 0$.

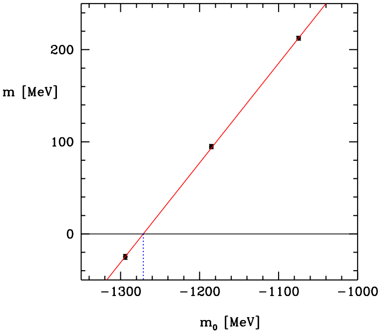
- Note: m is only defined up to O(a); any change in $O_{\rm ext}$ will lead to O(a) differences.

Determination of the critical mass

PCAC quark mass from SF correlation functions:

$$m = \frac{\partial_0 f_{\mathrm{A}}(x_0)}{2 f_{\mathrm{P}}(x_0)}$$

$8^3 \times 16$ lattice, quenched QCD, $a = 0.1\,\mathrm{fm}$



More chiral WI's: axial current normalisation

- At $m = 0$ we can derive the Euclidean current algebra (in finite volume!):

$$i\varepsilon^{abc}\left\langle O_{\rm ext}\, Q_{\rm V}^{c}(y_0)\right\rangle = \left\langle O_{\rm ext}\, Q_{\rm A}^{b}(y_0)\,[Q_{\rm A}^{a}(t_2) - Q_{\rm A}^{a}(t_1)]\right\rangle$$

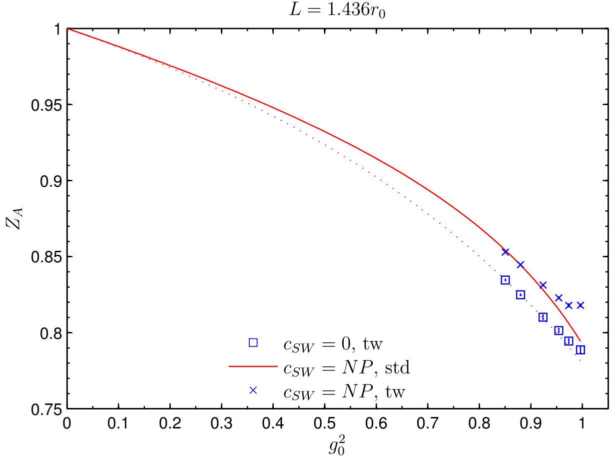
- Imposing this continuum identity on the lattice (at $m = 0$) fixes the normalisation of the axial current

$$(A_{\rm R})_{\mu}^{a} = Z_{\rm A}(g_0)A_{\mu}^{a}, \qquad Z_{\rm A}(g_0) \overset{g_0\to 0}{\sim} 1 + \sum_{n=1}^{\infty} Z_{\rm A}^{(n)} g_0^{2n}.$$

- Note: When changing the external fields $O_{\rm ext}$, the result for $Z_{\rm A}$ will change by terms of $\mathrm{O}(a)$.
- The PCAC relation and the charge algebra become operator identities in Minkowski space. Changing $O_{\rm ext}$ corresponds to looking at different matrix elements of these operator identities. On the lattice these must be equal up to $\mathrm{O}(a)$ terms.

Axial current normalisation with Wilson quarks

Z_{A} in quenched approximation [Lüscher et al. '96, Leder & S '10]



Similar results for $N_{\mathrm{f}} = 2, 3$ by ALPHA collab.

Simplest chiral WI: the PCAC relation

- Shrink the region R to a point x:

$$\begin{aligned} \langle O_{\mathrm{ext}} \delta_{\mathrm{A}}^{a}(\theta) S \rangle &= 0 \\ \Rightarrow \quad \left\langle \partial_{\mu} A_{\mu}^{a}(x) O_{\mathrm{ext}} \right\rangle &= 2m \left\langle P^{a}(x) O_{\mathrm{ext}} \right\rangle \end{aligned}$$

- In the continuum the PCAC quark mass

$$m = \frac{\left\langle \partial_{\mu} A_{\mu}^{a}(x) O_{\mathrm{ext}} \right\rangle}{2 \left\langle P^{a}(x) O_{\mathrm{ext}} \right\rangle}$$

must be independent of the choice for O_{ext}, x, background field,...!

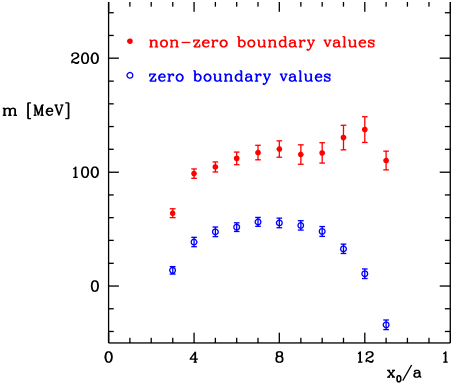
Need for O(a) improvement of Wilson quarks

O(a) artefacts can be quite large with Wilson quarks:

PCAC quark mass from SF correlation functions:

$$m = \frac{\partial_0 f_{\mathrm{A}}(x_0)}{2 f_{\mathrm{P}}(x_0)}$$

$8^3 \times 16$ lattice, quenched QCD, $a = 0.1\,\mathrm{fm}$, 2 different gauge background fields.



On-shell O(a) improvement

Recall Symanzik's effective continuum theory from lecture 1

$$
\begin{aligned}
S_{\mathrm{eff}} &= S_0 + aS_1 + a^2 S_2 + \ldots, \qquad S_0 = S_{\mathrm{QCD}}^{\mathrm{cont}} \\
S_k &= \int \mathrm{d}^4 x \, \mathcal{L}_{\mathrm{k}}(x)
\end{aligned}
$$

where $\mathcal{L}_1$ is a linear combination of the fields:

$$
\overline{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi, \qquad \overline{\psi}D_\mu D_\mu\psi, \qquad m\,\overline{\psi}\not{D}\psi, \quad m^2\overline{\psi}\psi, \qquad m\,\mathrm{tr}\left\{F_{\mu\nu}F_{\mu\nu}\right\}
$$

The action S_1 appears as insertion in correlation functions

$$
\begin{aligned}
G_n(x_1,\ldots,x_n) &= \langle\phi_0(x_1)\ldots\phi_0(x_n)\rangle_{\mathrm{con}} \\
&\quad + a\int \mathrm{d}^4 y \, \langle\phi_0(x_1)\ldots\phi_0(x_n)\mathcal{L}_1(y)\rangle_{\mathrm{con}} \\
&\quad + a\sum_{k=1}^{n}\langle\phi_0(x_1)\ldots\phi_1(x_k)\ldots\phi_0(x_n)\rangle_{\mathrm{con}} + \mathrm{O}(a^2)
\end{aligned}
$$

On-shell O(a) improvement (1)

Basic idea:

- Introduce counterterms to the *lattice* action and composite operators such that S_1 and ϕ_1 are cancelled in the effective theory
- As all physics can be obtained from on-shell quantitities (spectral quantitities like particle energies or correlation function where arguments are kept at non-vanishing distance) one may use the equations of motion to reduce the number of counterterms
- The contact terms which arise from having $y \approx x_i$ can be analysed in the OPE and are found to be of the same structure as the counterterms anyway contained in ϕ_1; this amounts to a redefinition of the counterterms in ϕ_1.
- After using the equations of motion one remains with:

$$\overline{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi, \qquad m^2\overline{\psi}\psi, \qquad m\,\mathrm{tr}\left\{F_{\mu\nu}F_{\mu\nu}\right\}$$

On-shell O(a) improvement (2)

1. On-shell O(a) improved Lattice action
   - The last two terms are equivalent to a rescaling of the bare mass and coupling ($m_\mathrm{q} = m_0 - m_\mathrm{cr}$):

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

   - The first term is the Sheikholeslami-Wohlert or clover term

$$S_{Wilson} \to S_\mathrm{Wilson} + iac_\mathrm{sw}(g_0)a^4 \sum_x \overline{\psi}(x)\sigma_{\mu\nu}\hat{F}_{\mu\nu}(x)\psi(x)$$

2. On-shell O(a) improved axial current and density:

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

On-shell O(a) improvement (3)

- There are 2 counterterms in the massless theory $c_{\rm sw}, c_{\rm A}$, the remaining ones $(b_g, b_{\rm m}, b_{\rm A}, b_{\rm P})$ come with $am_{\rm q}$.
- Note: all counterterms are absent in chirally symmetric regularisations!

$\Rightarrow$ turn this around: impose chiral symmetry to determine $c_{\rm sw}, c_{\rm A}$ non-perturbatively:

- define bare PCAC quark masses from SF correlation functions

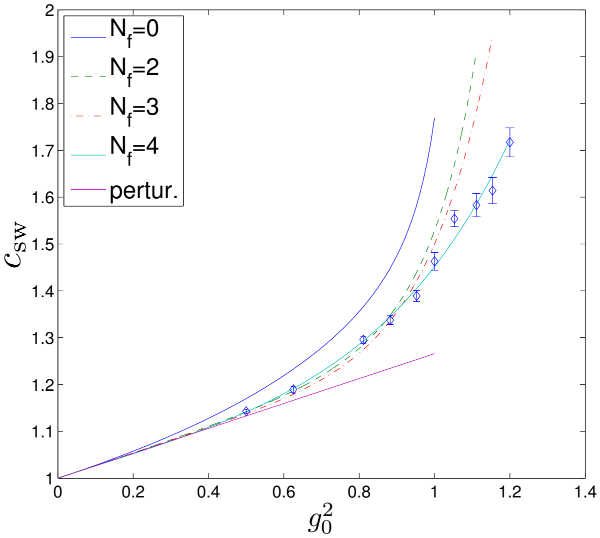
$$m_{\rm R} = \frac{Z_{\rm A}(1 + b_{\rm A}\, am_{\rm q})}{Z_{\rm P}(1 + b_{\rm P}\, am_{\rm q})} m, \qquad m = \frac{\tilde{\partial}_0 f_{\rm A}(x_0) + c_{\rm A}\, a\partial_0^*\partial_0 f_{\rm P}(x_0)}{f_{\rm P}(x_0)}$$

- At fixed g_0 and $am_{\rm q} \approx 0$ define 3 bare PCAC masses $m_{1,2,3}$ (e.g. by varying the gauge boundary conditions) and impose

$$m_1(c_{\rm sw}, c_{\rm A}) = m_2(c_{\rm sw}, c_{\rm A}), \quad m_1(c_{\rm sw}, c_{\rm A}) = m_3(c_{\rm sw}, c_{\rm A}) \Rightarrow c_{\rm sw}, c_{\rm A}$$

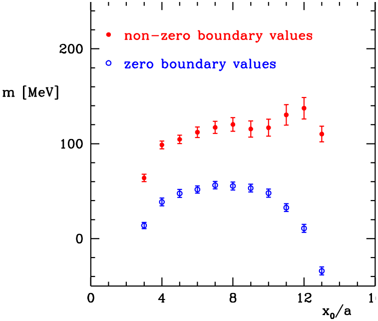
SF b.c.'s $\Rightarrow$ high sensitivity to $c_{\rm sw}$ & simulations near chiral limit

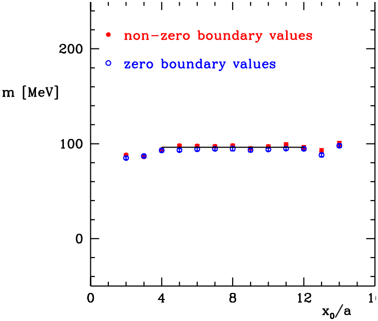
Results for $c_{\rm sw}$, $N_{\rm f} = 4$ [ALPHA '09]



On-shell O(a) improvement (4)

Before and after O(a) improvement (PCAC masses from SF correlation functions, $8^3 \times 16$ lattice)





Quenched result for the charm quark mass [ALPHA '02]

- The RGI charm quark mass can be defined in various ways
  - starting from the subtracted bare quark mass $m_{\mathrm{q,c}} = m_{0,c} - m_{\mathrm{cr}}$
  - starting from the average strange-charm PCAC mass m_{sc}
  - starting from the PCAC mass m_{cc} for a hypothetical mass degenerate doublet of quarks.
- Tune bare charm quark mass to match the D_s meson mass
- Obtain the corresponding O(a) improved RGI masses:

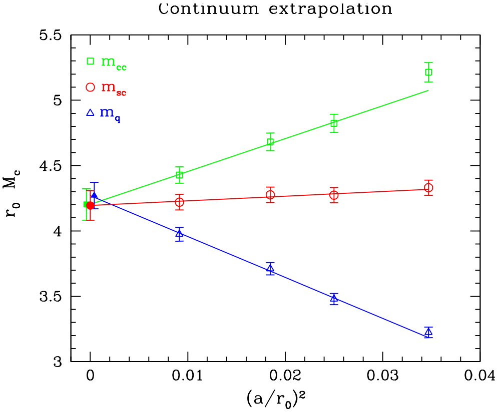
$$
\begin{aligned}
r_0 M_c|_{m_{sc}} &= Z_M r_0 \Big\{ 2m_{sc}\left[1 + (b_{\mathrm{A}} - b_{\mathrm{P}})\tfrac{1}{2}(am_{\mathrm{q,c}} + am_{\mathrm{q,s}})\right] \\
&\qquad\qquad - m_{\mathrm{s}}\left[1 + (b_{\mathrm{A}} - b_{\mathrm{P}})am_{\mathrm{q,s}}\right]\Big\}, \\
r_0 M_c|_{m_{\mathrm{c}}} &= Z_M r_0 m_{\mathrm{c}}\left[1 + (b_{\mathrm{A}} - b_{\mathrm{P}})am_{\mathrm{q,c}}\right], \\
r_0 M_c|_{m_{\mathrm{q,c}}} &= Z_M Z r_0 m_{\mathrm{q,c}}\left[1 + b_{\mathrm{m}} am_{\mathrm{q,c}}\right].
\end{aligned}
$$

- N.B.: all O(a) counterterms are known non-perturbatively in the quenched case!

Continuum extrapolation of the quenched RGI charm quark mass

Continuum extrapolation:

$$
\begin{aligned}
r_0 M_c &= A + B(a^2/r_0^2) \\
r_0 &= 0.5\,\mathrm{fm} \\
M_c &= 1.654(45)\,\mathrm{GeV} \\
\overline{m}_c^{\overline{\mathrm{MS}}}(\overline{m}_c) &= 1.301(34)\,\mathrm{GeV}
\end{aligned}
$$



Summary On-shell O(a) improvement

After O(a) improvement:

- The ambiguity in $m_{\rm cr}$ is reduced to O(a^2)
- Axial current normalisation can be defined up to O(a^2)
- Results exist for $c_{\rm sw}, c_{\rm A}$ for quenched and $N_{\rm f} = 2, 3, 4$ and various gauge actions
- On-shell O(a) improvement seems to work; rather economical for spectral quantities (e.g. hadron masses): just need $c_{\rm sw}$!
- Improvement of quark bilinear operators feasible, four-quark operators difficult
- Non-degenerate quark masses: rather complicated, proliferation of b-coefficients [Bhattacharya et al '99 ff];
- However: for small quark masses and fine lattices $am_{\rm q}$ is small (a few percent at most) and perturbative estimates of improvement coefficients may be good enough!

The Schrödinger functional and O(a) improvement

The presence of the boundaries induces additional O(a) effects:

- counterterms must be local fields of dimension 4 integrated over the boundaries $x_0 = 0, T$:
- pure gauge theory:

$$\int \mathrm{d}^3\mathbf{x}\ \mathrm{tr}\left\{F_{0k}(x)F_{0k}(x)\right\}, \quad \int \mathrm{d}^3\mathbf{x}\ \mathrm{tr}\left\{F_{kl}(x)F_{kl}(x)\right\} = 0\ (\rightarrow \text{b.c.'s})$$

- with fermions:

$$\int \mathrm{d}^3\mathbf{x}\,\overline{\psi}(x)\gamma_0 D_0\psi(x), \quad \int \mathrm{d}^3\mathbf{x}\,\overline{\psi}(x)\gamma_k D_k\psi(x),$$

  eliminate 2nd counterterm by equation of motion

$\Rightarrow$ all boundary O(a) effects can be cancelled by 2 counterterms with coefficients $c_\mathrm{t}, \tilde{c}_\mathrm{t}$!

- In practice use perturbation theory and vary the coefficients in simulations to assess their impact on observables.

Automatic O(a) improvement of massless Wilson quarks [Frezzotti, Rossi '03]

- Assume $m_{\mathrm{PCAC}} = 0$, finite volume without boundaries:

⇒ Symanziks effective continuum action (using eqs. of motion):

$$S_{\mathrm{eff}} = S_0 + aS_1 + \ldots, \quad S_0 = \int \mathrm{d}^4x\, \overline{\psi} \not{D} \psi, \; S_1 = c \int \mathrm{d}^4x\, \overline{\psi} \sigma_{\mu\nu} F_{\mu\nu} \psi$$

- cutoff dependence of lattice correlation functions:

$$\langle O \rangle = \langle O \rangle^{\mathrm{cont}} - a \langle S_1 O \rangle^{\mathrm{cont}} + a \langle \delta O \rangle^{\mathrm{cont}} + O(a^2).$$

δO are O(a) counterterms to the composite fields in O, e.g.

$$\begin{aligned} O &= V_\mu^a(x) A_\nu^b(y) \\ \delta O &= c_{\mathrm{V}}\, i\partial_\nu T_{\mu\nu}^a(x) A_\nu^a(y) + V_\mu^a(x) c_{\mathrm{A}} \partial_\nu P^b(y) \end{aligned}$$

Automatic O(a) improvement of massless Wilson quarks

- Introduce a γ_5-transformation (non-anomalous for even numbers of quarks):

$$\psi \to \gamma_5 \psi, \qquad \overline{\psi} \to -\overline{\psi}\gamma_5$$

- transform Symanzik's effective action and O(a) counterterms

$$S_0 \quad \to \quad S_0, \qquad S_1 \to -S_1$$

- Composite operators can be decomposed in γ_5-even and -odd parts:

$$\begin{aligned} O &= O_+ + O_- \\ O_\pm &\to \pm O \quad \Rightarrow \quad \delta O_\pm \to \mp \delta O_\pm \end{aligned}$$

- Hence for γ_5-even O_+ one finds

$$\begin{aligned}
\langle O_+ \rangle^{\rm cont} &= \langle O_+ \rangle^{\rm cont} \\
\langle O_+ S_1 \rangle^{\rm cont} &= -\langle O_+ S_1 \rangle^{\rm cont} = 0 \\
\langle \delta O_+ \rangle^{\rm cont} &= -\langle \delta O_+ \rangle^{\rm cont} = 0 \\
\Rightarrow \quad \langle O_+ \rangle &= \langle O_+ \rangle^{\rm cont} + O(a^2)
\end{aligned}$$

- while for γ_5-odd O_- one gets

$$\begin{aligned}
\langle O_- \rangle^{\rm cont} &= -\langle O_- \rangle^{\rm cont} = 0 \\
\langle O_- S_1 \rangle^{\rm cont} &= \langle O_- S_1 \rangle^{\rm cont} \\
\langle \delta O_- \rangle^{\rm cont} &= \langle \delta O_- \rangle^{\rm cont} \\
\Rightarrow \quad \langle O_- \rangle &= -a\langle O_- S_1 \rangle^{\rm cont} + a\langle \delta O_- \rangle^{\rm cont} + O(a^2)
\end{aligned}$$

$\Rightarrow$ γ_5-even observables are automatically O(a) improved, while γ_5-odd observables vanish up to O(a) terms.

Remarks:

- The cutoff effects are located in the γ_5-odd components. These can be easily identified and projected out for any lattice field, and the elimination of cutoff effects is then "automatic".
- In fermion regularisation with an exact chiral symmetry (Ginsparg-Wilson quarks) the γ_5-odd fields vanish identically $\Rightarrow$ no need to project out the odd components.
- The automatic O(a) improvement mechanism carries over to the massive theory if the quark mass term is chosen as $\bar{\psi} i \mu_{\rm q} \tau^3 \psi$ (and $m_0 = m_{\rm cr}$)

$\Rightarrow$ twisted mass QCD at "full twist".

Gradient flow & renormalized finite volume coupling

- QCD, gauge field $A_\mu(x)$, Yang-Mills gradient flow equation:

$$\partial_t B_\mu(t,x) \quad = \quad D_\nu G_{\nu\mu}(t,x) \quad \left(= -\tfrac{\delta S_g[B]}{\delta B_\mu(t,x)}\right), \quad B_\mu(0,x) = A_\mu(x)$$

  with field tensor $G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu]$.

- Local gauge invariant composite fields at positive flow time $t > 0$ such as

$$E(t,x) = -\tfrac{1}{2}\mathrm{tr}\{G_{\mu\nu}(x,t)G_{\mu\nu}(x,t)\}$$

  are renormalized; no mixing with other fields of same or lower dimensions! [Lüscher & Weisz '2012];

- Explicit calculations up to 2-loop order (infinite volume, dimensional regularization) [Lüscher 2010; Harlander & Neumann 2016]:

$$\langle E(t,x)\rangle = \frac{3g^2_{\overline{\mathrm{MS}}}(\mu)}{16\pi^2 t^2}\left(1 + \frac{1.0978 + 0.0075\, N_f}{4\pi} g^2_{\overline{\mathrm{MS}}}(\mu) + \ldots\right), \quad \mu = \frac{1}{\sqrt{8t}}$$

  $\Rightarrow$ $E(t,x)$ is, for $t > 0$, a renormalized field; unlike $E(0,x)$ which has a quartic and a logarithmic divergence!

Gradient flow couplings

- Infinite volume: Non-perturbative definition of a renormalized "gradient flow coupling" at scale $\mu = 1/\sqrt{8t}$:

$$g^2_{\mathrm{GF},\infty}(\mu) \stackrel{\mathrm{def}}{=} \frac{16\pi^2}{3} t^2 \langle E(t,x) \rangle$$

- Finite volume: consider $\langle E(t,x) \rangle$ in a finite box of dimension L^4, fix the ratio $c = \sqrt{8t}/L$ and define

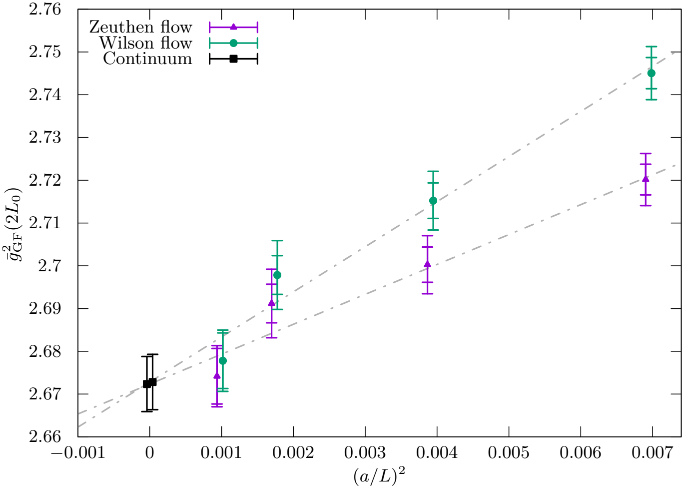
$$\bar{g}^2_{\mathrm{GF}}(L) = \mathcal{N}(c)^{-1} t^2 \langle E(t,x) \rangle, \qquad \lim_{c \to 0} \mathcal{N}(c) = \frac{3}{16\pi^2}$$

- defines family of renormalized couplings, with parameter c.

  (typical range from 0.2 to 0.5);

- $\mathcal{N}(c)$ is calculable in lowest order perturbation theory; depends on b.c's for the gauge field; periodic in space; time direction:
  - periodic b.c.'s [Fodor et al. 2012]
  - $\Rightarrow$ SF (Dirichlet) b.c.'s [Fritzsch & Ramos 2012], used here!
  - twisted periodic b.c.'s [Ramos 2013]
  - open-SF (Neumann-Dirichlet) b.c.'s [Lüscher 2013]

Matching the SF and GF couplings, [ALPHA coll. '17]



$$\bar{g}^2_{\mathrm{SF}}(L_0) = 2.012 \quad \Rightarrow \quad \bar{g}^2_{\mathrm{GF}}(2L_0) = 2.6723(64)$$

Where do we stand?

So far:

$$L_0\Lambda_{\overline{\mathrm{MS}}}^{N_\mathrm{f}=3} = 0.0791(21), \qquad \bar{g}^2_{\mathrm{SF}}(L_0) = 2.012 \quad \Rightarrow \quad \bar{g}^2_{\mathrm{GF}}(2L_0) = 2.6723(64)$$

- A rough estimate indicates that $1/L_0 \approx 4$ GeV
- Need to reach scale $1/L_\mathrm{had}$ around 200 MeV to make safe contact e.g. to $F_K = 160$ MeV
- Define L_had implicitly through

$$\bar{g}^2_{\mathrm{GF}}(L_\mathrm{had}) = 11.31$$

<u>Remaining steps:</u>

1. Scale evolution of $\bar{g}^2_{\mathrm{GF}}(L)$ between $2L_0$ to L_had:

$$\Rightarrow \quad L_\mathrm{had}/L_0$$

2. Determine L_had in $1/\mathrm{MeV}$ e.g. from $L_\mathrm{had}F_K$ ("scale setting")

Determination of $L_{\rm had}/L_0$

Note: ratio $L_{\rm had}/L_0$ not an integer power of 2; how to proceed?

- Determine the step-scaling function in the continuum limit

$$\sigma(u) = \lim_{a/L\to 0} \Sigma(u, a/L), \qquad \Sigma(u, a/L) = \bar{g}^2_{\rm GF}(2L)\Big|_{\bar{g}^2_{\rm GF}(L)=u,\, m(L)=0}$$

- Relation to the β-function:

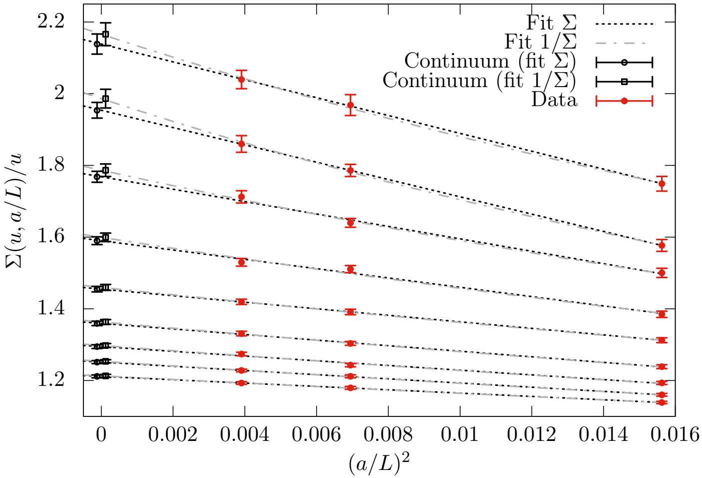
$$\log 2 = -\int_{\sqrt{u}}^{\sqrt{\sigma(u)}} \frac{{\rm d}x}{\beta(x)}, \qquad \beta(\bar{g}_{\rm GF}) = -L\frac{\partial \bar{g}_{\rm GF}(L)}{\partial L}$$

$\Rightarrow$ obtain non-perturbative β-function from the step-scaling function

- Find:

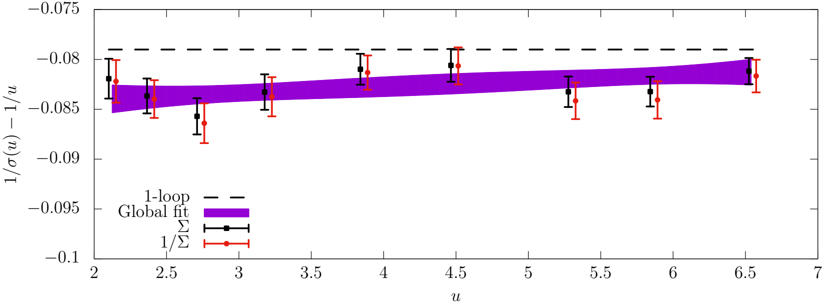
$$\frac{L_{\rm had}}{L_0} = 2 \times \exp\left\{ -\int_{\bar{g}_{\rm GF}(2L_0)}^{\bar{g}_{\rm GF}(L_{\rm had})} \frac{{\rm d}x}{\beta(x)} \right\} = 21.86(42)$$

Obtaining the step-scaling function



- sizable discretization effects → careful extrapolations are needed!
- continuum results are nonetheless very precise!

Continuum extrapolated step-scaling function



Extracting the β-function

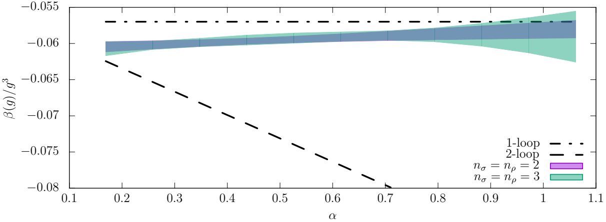
- fit ansatz:

$$\beta(g) = -\frac{g^3}{P(g^2)}\,, \quad P(g^2) = p_0 + p_1 g^2 + p_2 g^4 + \dots\,.$$

- Determine fit coefficients $p_0, p_1, \dots$ from the data for step scaling function $\sigma(u)$

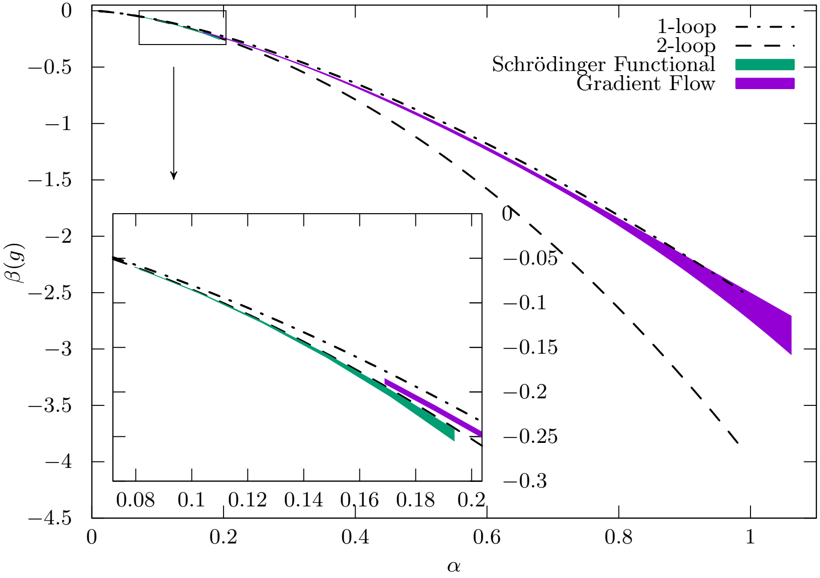
$$\log(2) = -\int_{\sqrt{u}}^{\sqrt{\sigma(u)}} \frac{\mathrm{d}x}{\beta(x)} = \int_{\sqrt{u}}^{\sqrt{\sigma(u)}} \mathrm{d}x\,\frac{P(x^2)}{x^3}$$

$$= -\frac{p_0}{2}\left[\frac{1}{\sigma(u)} - \frac{1}{u}\right] + \frac{p_1}{2}\log\left[\frac{\sigma(u)}{u}\right] + \sum_{n=1}^{n_{\max}} \frac{p_{n+1}}{2n}\left[\sigma^n(u) - u^n\right]\,,$$

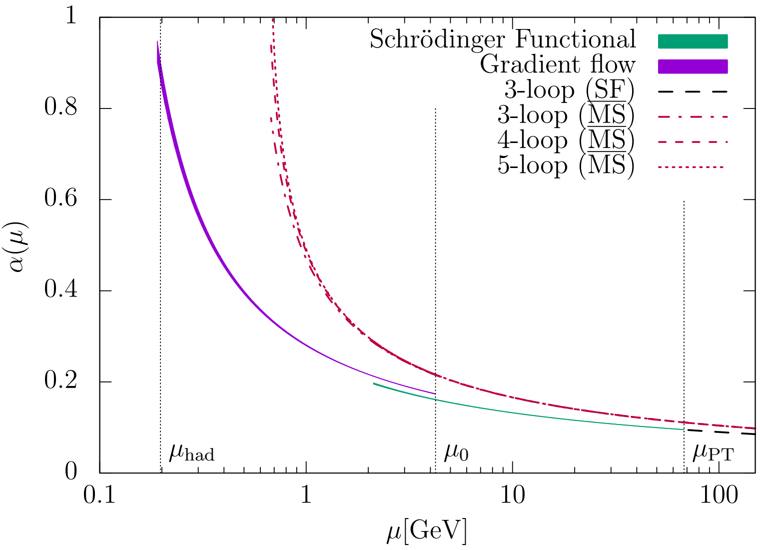


The β-functions, global picture

$\alpha = g^2/(4\pi)$



Non-perturbative running of the SF and GF couplings in $N_f = 3$ QCD



Matching to hadronic physics

So far:

$$\Lambda_{\overline{\rm MS}}^{(N_{\rm f}=3)} = \frac{L_{\rm had}}{L_0} \times L_0 \Lambda_{\overline{\rm MS}}^{(N_{\rm f}=3)} \times \frac{1}{L_{\rm had}} = 1.729(57)/L_{\rm had} \Rightarrow \text{ require } 1/L_{\rm had} \text{ in physical units}$$

The experimental input is

- $m_\pi = 134.8(3)$ MeV, $m_K = 494.2(3)$ MeV [FLAG 2017]
- $f_{\pi K} \equiv \frac{2}{3} f_K + \frac{1}{3} f_\pi = 147.6(5)$ MeV [PDG 2014]

Taking the scale from $f_{\pi K}$ one needs

$$\frac{f_{\pi K}^{\rm PDG}}{f_{\pi K} L_{\rm had}} = \frac{f_{\pi K}^{\rm PDG}}{f_{\pi K}\sqrt{t_0}} \times \frac{\sqrt{t_0}}{L_{\rm had}}$$

where t_0 is an intermediate scale defined with the gradient flow [Lüscher '10]

$$t_0^2 \langle E(t_0, x)\rangle = 0.3$$

One finds, (with t_0^* defined at the flavour SU(3) symmetric point) [Bruno, Korzec, Schaefer 2016]

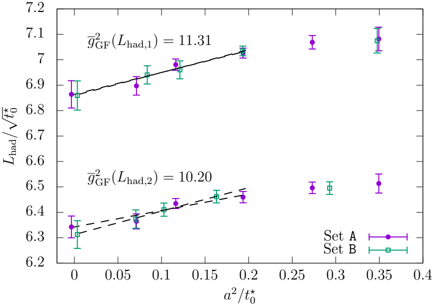
$$\sqrt{8t_0^*} = 0.413(5)(2) \text{ fm}$$

Connecting SF to Large Volume (slide by T. Korzec, Lattice '17)

$$\Lambda_{\overline{\mathrm{MS}}}^{(N_\mathrm{f}=3)} = \underbrace{\frac{f_{\pi K}^{\mathrm{PDG}}}{f_{\pi K}\sqrt{t_0^*}}}_{\text{scale setting}} \times \underbrace{\frac{\sqrt{t_0^*}}{L_{\mathrm{had}}}}_{\text{connection to CLS}} \times \underbrace{\frac{L_{\mathrm{had}}}{2L_0}}_{\text{GF running}} \times \underbrace{\frac{2L_0}{L_0}}_{\text{change of schemes}} \times \underbrace{\Lambda_{\overline{\mathrm{MS}}}^{(N_\mathrm{f}=3)} L_0}_{\text{SF running}}$$

- From large volume simulations
  - t_0^* known in fm
  - t_0^*/a^2 known at $\beta \in \{3.4, 3.46, 3.55, 3.7, 3.85\}$ (massive theory)
  - Corresponds to $\beta \in \{3.3985, 3.4587, 3.549, 3.6992, 3.8494\}$ (massless)
- From gradient flow running
  - L_{had}/a for $\beta \in \{3.3998, 3.5498, 3.6867, 3.8, 3.9791\}$ (massless)
- Interpolate L_{had}/a to large-volume β's (or other way around)
- Continuum extrapolate: $\frac{L_{\mathrm{had}}/a}{\sqrt{t^*/a^2}}$

Connecting L_{had} to infinite volume scale



Final Result

$$\frac{L_{\text{had}}}{\sqrt{t_0^*}} = 6.825(47)$$

Final Result

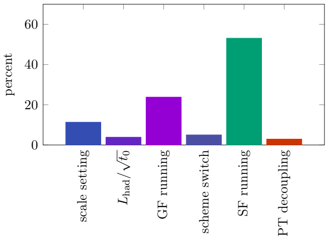
$$\Lambda_{\overline{\mathrm{MS}}}^{(N_\mathrm{f}=3)} = 341(12)\ \mathrm{MeV}$$

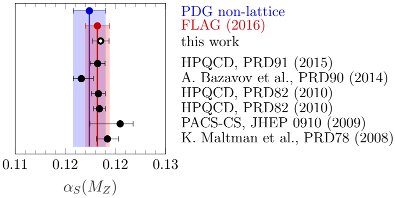
$$\Lambda_{\overline{\mathrm{MS}}}^{(5)} = 215(10)(03)\ \mathrm{MeV} \qquad \text{pert. decoupling}$$

$$\alpha_{\overline{\mathrm{MS}}}(M_Z) = 0.1185(8)(3)$$

$$0.1174(16) \qquad \text{PDG non-lattice}$$

Contribution to relative error squared





Conclusions for $\alpha_s(m_Z)$

- The determination of α_s is well-suited for the lattice approach; in contrast to many other approaches, here the systematics can be controlled by combining technical tools developed over the last 20 years:
    - finite volume renormalization schemes and recursive step-scaling methods
    - gradient flow couplings and scales.
    - non-perturbative Symanzik improvement
    - perturbation theory adapted to finite volume
- The final result $\Lambda_{\overline{\mathrm{MS}}}^{(N_\mathrm{f}=3)} = 341(12)$MeV does not rely on perturbation theory below O(100) GeV!
- $\Rightarrow$ the error is still dominated by statistics!

Final remarks

Gradient flow, many applications:

- Definition of intermediate scales t_0 and w_0, which are easy to measure with high precision
- Definition of renormalized couplings, both in infinite and finite volume
- Access to a wealth of renormalized quantities [Lüscher & Weisz '12, Lüscher '13]
  - gauge invariant composite fields at finite flow time are renormalized!
  - can be generalized to fermion fields; renormalization required but very simple.

  $\Rightarrow$ can use fields at finite flow times as external sources in on-shell renormalization conditions
- Small flow time expansion, $t \to 0$ + PT may yield renormalized matrix elements while bypassing complicated lattice renormalization problems! However, there is a window problem:
$$a^2 \ll t \ll \Lambda^2$$
- Practical problem: lattice artefacts can be large (e.g. SSF for GF coupling)

Some omissions:

- operator renormalization problems including mixing
- strategies to bypass lattice specific renormalization problems (e.g. B_K in tmQCD)
- ...

Thank you!