Non-perturbative Renormalization and Improvement of Lattice QCD Lecture 3

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- Finite volume schemes and step scaling
- Q Running coupling, quark masses and operators

- Test of perturbation theory at high energies
- Ontinuum limit and lattice artifacts.
- Symanzik's effective theory
- The O(3) model, a sobering example
- Yang-Mills and QCD
- Onclusions

Step Scaling Functions

• Given $\bar{g}(L)$ and $\bar{m}(L)$, the aim is to construct the Step Scaling Functions $\sigma(u)$ and $\sigma_{P}(u)$:

$$\begin{aligned} \sigma(u) &= \bar{g}^2(2L)|_{u=\bar{g}^2(L)}, \\ \sigma_{\rm P}(u) &= \lim_{a \to 0} \left. \frac{Z_{\rm P}(g_0, 2L/a)}{Z_{\rm P}(g_0, L/a)} \right|_{u=\bar{g}^2(L)} \end{aligned}$$

• These are related to the usual RG functions:

$$\int_{\sqrt{\sigma(u)}}^{\sqrt{u}} \frac{\mathrm{d}g}{\beta(g)} = \ln 2 \qquad \sigma_{\mathrm{P}}(u) = \exp \int_{\sqrt{\sigma(u)}}^{\sqrt{u}} \frac{\tau(g)}{\beta(g)} \mathrm{d}g$$

 One thus considers a change of scale by a finite factor s = 2; RG functions β and τ tell us what happens for infinitesimal scale changes.

Lattice approximants $\Sigma(u, a/L)$ for $\sigma(u)$

- choose g_0 and L/a = 4, measure $\bar{g}^2(L) = u$ (this sets the value of u)
- double the lattice and measure

 $\Sigma(u,1/4)=\bar{g}^2(2L)$

- now choose L/a = 6 and tune g'_0 such that $\bar{g}^2(L) = u$ is satisfied
- double the lattice and measure

$$\Sigma(u,1/6)=\bar{g}^2(2L)$$

and so on ...



Continuum extrapolation of the SSF [ALPHA '05]



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The SSF in the continuum limit

[ALPHA coll., Della Morte et al '05]



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Determination of the Λ -parameter

The formula

$$\Lambda = \mu (b_0 \bar{g}^2)^{-b_1/2b_0^2} \exp\left\{-\frac{1}{2b_0 \bar{g}^2}\right\} \\ \times \exp\left\{-\int_0^{\bar{g}} dx \left[\frac{1}{\beta(x)} + \frac{1}{b_0 x^3} - \frac{b_1}{b_0^2 x}\right]\right\}$$

holds for any value of $\mu.$ We may use it at ${\it L}_{\rm min}$ to obtain

 $\Lambda L_{\min} = f(\bar{g}(L_{\min}))$

• The function f(g) can be evaluated at $g = \overline{g}(L_{\min})$ since this is deep in the perturbative region. The integral in the exponent

$$\int_0^{\bar{g}} \mathrm{d}x \left[\frac{b_2 b_0 - b_1^2}{b_0^3} x + \mathcal{O}(x^3) \right] = \frac{b_2 b_0 - b_1^2}{2b_0^3} \bar{g}^2 + \mathcal{O}(\bar{g}^4)$$

may thus be evaluated using the β -function at 3-loop order.

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- Since $L_{\max} = 2^n L_{\min}$ one knows $L_{\max} \Lambda$
- still need $F_{\pi}L_{\max}$

Matching to a low energy scale

Ideally one would like to compute e.g. $F_{\pi}\Lambda$, and take $F_{\pi} = 132 \text{MeV}$ from experiment

 \bullet What is required? The scale ${\it L}_{\rm max}$ is implicitly defined:

 $ar{g}^2(L_{
m max})=4.84 \qquad \Rightarrow \qquad (L_{
m max}/a)(g_0)$

Setting $L_{\text{max}}/a = 6, 8, 10, \ldots$ one then finds corresponding values of the bare coupling (at fixed g_0 some interpolation of L_{max}/a will be necessary instead)

 One must then be able to compute aF_π in a large volume simulation at the very same values of the bare coupling:

 $F_{\pi}\Lambda = \lim_{g_0 \to 0} (L_{\max}/a)(g_0)(aF_{\pi})(g_0)$

- One thus needs a range of g_0 where both can be computed, aF_π and $\bar{g}(L_{\max})$
- Remark: intermediate results are often quoted in terms of Sommer's scale r_0 , rather than F_{π} .

Results for QCD with $N_{\rm f}=0$ and $N_{\rm f}=2$ quark flavours

• The scale r_0 [R. Sommer '93] is obtained from the force F(r) between static quark and antiquark separated by a distance r:

 $r_0^2 F(r_0) = 1.65$

The r.h.s. was chosen so that phenomenological estimates from potential models yield $r_0 = 0.5$ fm.

- Recent result for $N_{\rm f} = 2$ ([ALPHA '12]): $F_{\mathcal{K}} = 155 \,\mathrm{MeV}$ implies $r_0 = 0.503(10) \,\mathrm{fm}$ (at physical pion mass!).
- Results for Λ using $r_0 = 0.5 \text{ fm}$ [ALPHA '99-'12]

$$\begin{array}{lll} \Lambda^{(2)}_{\overline{\mathrm{MS}}} r_0 &=& 0.789(52), & \Lambda^{(2)}_{\overline{\mathrm{MS}}} = 310(20) \, \mathrm{MeV} \\ \Lambda^{(0)}_{\overline{\mathrm{MS}}} r_0 &=& 0.602(48), & \Lambda^{(0)}_{\overline{\mathrm{MS}}} = 238(19) \, \mathrm{MeV} \end{array}$$

The running quark mass

• Coupled evolution of the running mass and the coupling:

 $\overline{m}(2L) = \sigma_m(u)\overline{m}(L), \qquad \sigma_m(u) = 1/\sigma_{\rm P}$ $\overline{g}^2(2L) = \sigma(u)$

• Once the running coupling is known in a range [u₀, u_n],

$$u_0 = \bar{g}^2(L_{\min}), \quad u_k = \bar{g}^2(2^k L_{\min}), k = 1, 2, \dots, n$$

determine $\sigma_m(u)$ for the same range of couplings: evolution of quark mass and coupling recursively

 $\overline{m}(2^k L_{\min})/\overline{m}(2^{k-1}L_{\min}) = \sigma_m(u_k), \qquad k = 1, 2, \dots, n$

- one obtains $\overline{m}(2L_{\max})/\overline{m}(L_{\min})$
- Extract $\overline{m}(L_{\min})/M$ using PT as for A-parameter

Running mass in the SF scheme [ALPHA '05]



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Relation to bare quark masses

• In practice with Wilson type quarks, one avoids the additive renormalisation of the bare quark mass parameter by replacing it by a *measured* bare mass m_{PCAC} from the (bare) PCAC relation:

$$m_{ ext{PCAC}} \stackrel{ ext{def}}{=} rac{\langle \partial_{\mu} A^{a}_{\mu}(x) O
angle}{2 \langle P^{a}(x) O
angle}$$

• The running quark mass is then related to $m_{
m PCAC}$

$$\overline{m}(L) = \underbrace{Z_{\mathrm{P}}^{-1}(g_0, L/a) Z_{\mathrm{A}}(g_0)}_{\mathsf{known factors}} \underbrace{m_{\mathrm{PCAC}}(g_0)}_{\mathsf{measured}},$$

Combine results,

$$M = Z_M(g_0)m_{\rm PCAC}(g_0)$$

and take the continuum limit $g_0 \rightarrow 0$.

 $N_{\rm f}=2$ result for the strange quark mass using this strategy ([ALPHA '12]):

 $M_s = 138(3)(1) \,\mathrm{MeV} \quad \Rightarrow \quad \overline{m}^{\overline{\mathrm{MS}}}(\mu = 2 \,\mathrm{GeV}) = 102(3)(1) \,\mathrm{MeV}$

- Quoted errors are statistical and systematic;
- <u>Note</u>: Except for quenching of the strange quark the ALL systematic errors have been addressed!

Summary step scaling

- The recursive finite volume technique has completely eliminated the problem with large scale differences.
- Physical results require a matching calculation at a low energy scale: it is crucial to have a range in bare couplings where both, the renormalisation conditions and the hadronic input can be computed
- State of the art [ALPHA '17]: QCD with $N_{\rm f}=3$ & technical refinements:
 - gradient flow coupling in finite volume scheme at low energies
 - Global fits to the step-scaling function
 - Improved control of cutoff effects
 - use of the flow time scale t_0 instead of r_0 as intermediate scale
- Many more applications in the literature: all quark bilinear operators, $\Delta F = 2$ 4-quark operators, HQET,...

Renormalized lattice QCD with Wilson quarks

The action $S = S_f + S_g$ is given by

$$S_{\rm f} = a^4 \sum_{x} \overline{\psi}(x) \left(D_W + m_0 \right) \psi(x), \qquad S_{\rm g} = \frac{1}{g_0^2} \sum_{\mu,\nu} \operatorname{tr} \left\{ 1 - P_{\mu\nu}(x) \right\}$$
$$D_W = \frac{1}{2} \left\{ \left(\nabla_{\mu} + \nabla^*_{\mu} \right) \gamma_{\mu} - a \nabla^*_{\mu} \nabla_{\mu} \right\}$$

• Symmetries: $U(N_{\rm f})_{\rm V}$ (mass degenerate quarks), P, C, T and $O(4, {\rm ZZ})$

 \Rightarrow Renormalized parameters:

 $g_{\mathrm{R}}^2 = Z_g g_0^2, \qquad m_{\mathrm{R}} = Z_m \left(m_0 - m_{\mathrm{cr}} \right), \qquad a m_{\mathrm{cr}} = a m_{\mathrm{cr}} (g_0).$

- In general: $Z = Z(g_0^2, a\mu, am_0)$;
- Quark mass independent renormalisation schemes: $Z = Z(g_0^2, a\mu)$
- Simple non-singlet composite fields, e.g. $P^a = \overline{\psi} \gamma_5 \tau^a \psi$ renormalise multiplicatively, $P^a_{\rm R} = Z_{\rm P}(g^2_0, a\mu, am_0)P^a_{\rm P}$

Approach to the continuum limit (1)

Suppose we have renormalised lattice QCD non-perturbatively, how is the continuuum limit approached?

Symanzik's effective continuum theory [Symanzik '79]:

- purpose: render the *a*-dependence of lattice correlation functions explicit. ⇒ structural insight into the nature of cutoff effects
- at scales far below the cutoff a^{-1} , the lattice theory is effectively continuum like; the influence of cutoff effects is expanded in powers of a:

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

 $\mathcal{L}_k(x)$: linear combination of fields

- with canonical dimension 4 + k

Approach to the continuum limit (2)

A complete set of dimension 5 fields for \mathcal{L}_1 is given by:

 $\overline{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi, \qquad \overline{\psi}D_{\mu}D_{\mu}\psi, \qquad m\,\overline{\psi}D\!\!\!/\psi, \qquad m\,\mathrm{tr}\,\{F_{\mu\nu}F_{\mu\nu}\}$

The same procedure applies to composite fields:

 $\phi_{\rm eff}(x) = \phi_0 + a\phi_1 + a^2\phi_2 \dots$

for instance: $\phi(x) = P^a(x)$, basis for ϕ_1 :

$$m \overline{\psi} \gamma_5 \frac{1}{2} \tau^a \psi, \qquad \overline{\psi} \overleftarrow{\mathcal{D}} \gamma_5 \frac{1}{2} \tau^a \psi - \overline{\psi} \gamma_5 \frac{1}{2} \tau^a \mathcal{D} \psi$$

Consider renormalised, connected lattice n-point functions of a multiplicatively renormalisable field ϕ

$$G_n(x_1,\ldots,x_n)=Z_{\phi}^n\langle\phi(x_1)\cdots\phi(x_n)\rangle_{\mathrm{con}}$$

Approach to the continuum limit (3)

Effective field theory description:

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

- $\langle \cdots \rangle$ is defined w.r.t. continuum theory with S_0
- the *a*-dependence is now explicit, up to logarithms, which are hidden in the coefficients.
- In perturbation theory one expects at *I*-loop order:

$$P(a)\sim P(0)+\sum_{n=1}^{\infty}\sum_{k=1}^{l}c_{nk}a^{n}(\ln a)^{k}$$

where e.g. $P(a) = G_n$ at fixed arguments.

Conclusions from Symanzik's analysis:

- Asymptotically, cutoff effects are powers in *a*, modified by logarithms;
- In contrast to Wilson quarks, only even powers of a are expected for
 - bosonic theories (e.g. pure gauge theories, scalar field theories)
 - fermionic theories which retain a remnant axial symmetry (overlap, Domain Wall Quarks, staggered quarks, Wilson quarks with a twisted mass term, etc.)

In QCD simulations a is typically varied by a factor 2

⇒ logarithms vary too slowly to be resolved; linear or quadratic fits (in *a* resp. a^2) are used in practice.

Example 1: quenched hadron spectrum

Linear continuum extrapolation of the quenched hadron spectrum; standard Wilson quarks with Wilson's plaquette action:[CP-PACS coll., Aoki et al. '02] $a = 0.05 - 0.1 \,\text{fm}$, experimental input: m_K , m_π , m_ρ



Example 2: pion mass in $N_{\rm f} = 2 \text{ tmQCD}$

[ETM coll. Baron et al '09]



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Example 3: O(a) improved charm quark mass (quenched)

[ALPHA coll. J. Rolf et al '02]



The 2d O(n) sigma model: a test laboratory for QCD

$$S = \frac{n}{2\gamma} \sum_{\mathbf{x},\mu} (\partial_{\mu} \mathbf{s})^2, \qquad \mathbf{s} = (s_1, \dots, s_n) \qquad \mathbf{s}^2 = 1$$

- like QCD the model has a mass gap and is asymptotically free
- many analytical tools: large *n* expansion, Bethe ansatz, form factor bootstrap, etc.
- efficient numerical simulations due to cluster algorithms.
- \Rightarrow very precise data over a wide range of lattice spacing (a can be varied by 1-2 orders of magnitude).
 - Symanzik: expect $O(a^2)$ effects, up to logarithms
 - Large *n*, at leading [Caracciolo, Pelissetto '98] and next-to-leading [Knechtli, Leder, Wolff '05]:

$$P(a) \sim P(0) + \frac{a^2}{L^2} (c_1 + c_2 \ln(a/L))$$

A sobering result (1):

Numerical study of renormalised finite volume coupling to high precision (n = 3) [Hasenfratz, Niedermayer '00, Hasenbusch et al. '01, Balog et al. '09]



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- Cutoff effects seem to be almost linear in a!
- Is this just an unfortunate case?

A sobering result (2):

[Balog, Niedermayer & Weisz '09]



Fits with a and a ln a terms, lattice sizes $L/a = 10, \ldots, 64$

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[Knechtli, Leder, Wolff '05], plot of cutoff effects vs. a^2/L^2 , various *n*:



Asymptotic behaviour for larger *n* according to expectation, what about n = 3?

A closer look (2)

Continuum limit for mass gap m(L) known analytically [Balog & Hegedus '04]! Subtract & study pure cutoff effect [Balog, Niedermayer, Weisz '09]



A closer look (3)

Continuum limit for mass gap m(L) known analytically [Balog & Hegedus '04]! Subtract & study pure cutoff effect: $\Sigma(2, u_0, a/L) - \sigma(2, u_0)$:



 $c_1 a + c_2 a \ln a + c_3 a^2$ (dashed) vs. $c_1 a^2 + c_2 a^2 \ln a + c_3 a^4$ (solid)

[Balog, Niedermayer & Weisz '09]

- performed two-loop calculation with both effective Symanzik theory and lattice theory (various actions)
- Matching of both sides and subsequent RG considerations
- ⇒ Symanzik theory predicts for O(n) model leading $O(a^2)$ behaviour:

$$\delta(a) \propto a^2 \left(\ln a^2\right)^{n/(n-2)}$$

- compatible with large *n* result since $\lim_{n\to\infty} \{n/(n-2)\} = 1$
- For O(3) model:

$$\delta(a) \propto a^2 \left(\ln^3(a^2) + c_1 \ln^2(a^2) + c_2 \ln(a^2) + c_4 \right) + O(a^4)$$

A closer look (5)

Coefficient of $O(a^2)$ term [Balog, Niedermayer & Weisz '09]:



Not exactly constant! Multiplied with *a*² obtain "fake" linear behaviour in *a*!

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Yang-Mills theory and QCD

Recently, [N. Husung, P. Marquard and R. Sommer, 2020] have obtained the powers of the logs modifying the a^2 -effects for spectral quantities (e.g. glueball masses) in pure SU(3) gauge theory (various lattice regularizations):

- find negative leading exponents of (-7/11, -63/55) of $\ln(a)$!
- \Rightarrow Convergence to continuum is faster than a^2
 - Work for QCD in progress, very interesting, keep tuned!



Summary, approach to the continuum

- Symanzik's analysis is applicable beyond perturbation theory
- Powers of *a* are accompanied by fractional powers of logarithms; these are perturbatively computable due to asymptotic freedom, using Symanzik's effective theory.
- Lesson from O(3) model: logarithmic corrections to powers in a can be large (a² ln³(a));
 However, results by Husung et al. in pure gauge theory and QCD are re-assuring.
- It helps to combine results from different regularisations: renormalised quantities must have the same continuum limit
- Numerical results in QCD: typically lattice spacing varied by a factor 2, logarithms ignored (cannot be resolved).
- \Rightarrow Fitting higher order polynomials in *a* ignoring the logarithms has no theoretical basis and can be dangerous!