Non-perturbative Renormalization and Improvement of Lattice QCD

Lecture 1

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Some references

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2. A. Vladikas, "Three Topics in Renormalization and Improvement" Les Houches Summer School 2009, `arXiv:1103.1323[hep-lat]`;
3. R. Sommer, "Non-perturbative renormalisation of QCD", Schladming Winter School lectures 1997, `hep-ph/9711243v1`;
4. M. Lüscher: "Advanced lattice QCD", Les Houches Summer School lectures 1997 `hep-lat/9802029`
5. S. Capitani, "Lattice perturbation theory" Phys. Rept. 382 (2003) 113-302 `hep-lat/0211036`

Contents

QCD and the Standard Model of particle physics

The Standard Model (SM):

- describes strong, weak and electromagnetic interactions; gauge theory SU(3)×SU(2)×U(1)
- large scale differences, for instance:

$$m_t, m_H, m_Z, m_W = \mathrm{O}(100\,\mathrm{GeV}) \qquad m_b, m_c = \mathrm{O}(1\mathrm{GeV})$$

  with light quark masses still much lighter.

$\Rightarrow$ SM for energies $\ll m_W$ reduces to QCD + QED + tower of effective weak interaction vertices (4-quark-operators, 6-quark operators ...).

$\Rightarrow$ the structure of this effective "weak hamiltonian" is obtained perturbatively e.g in $\overline{\mathrm{MS}}$ scheme.

$\Rightarrow$ QCD + effective 4-quark operators a priori defined in perturbative framework at high energies.

Non-perturbative definition of QCD (1)

To define QCD as a QFT beyond perturbation theory it is not enough to write down its classical Lagrangian:

$$\mathcal{L}_{\mathrm{QCD}}(x) = \frac{1}{2g^2}\,\mathrm{tr}\left\{F_{\mu\nu}(x)F_{\mu\nu}(x)\right\} + \sum_{i=1}^{N_\mathrm{f}} \overline{\psi}_i(x)\left(\not{D} + m_i\right)\psi_i(x)$$

One needs to define the functional integral:

- Introduce a Euclidean space-time lattice and discretise the continuum action such that the doubling problem is solved
- Consider a finite space-time volume $\Rightarrow$ the functional integral becomes a finite dimensional ordinary or Grassmann integral, i.e. mathematically well defined!
- Take the infinite volume limit $L \to \infty$
- Take the continuum limit $a \to 0$

Non-perturbative definition of QCD (2)

- The infinite volume limit is reached with exponential corrections $\Rightarrow$ usually not a major problem.
- Continuum limit: existence only established order by order in perturbation theory; only for selected lattice regularisations:
  - lattice QCD with Wilson quarks [Reisz '89]
  - lattice QCD with overlap/Neuberger quarks [Reisz, Rothe '99]
  - but not (yet?) for lattice QCD with staggered quarks [cf. Giedt '06]
- From asymptotic freedom we expect

$$g_0^2 = g_0^2(a) \quad \overset{a \to 0}{\sim} \quad \frac{-1}{2b_0 \ln a}, \qquad b_0 = \tfrac{11N}{3} - \tfrac{2}{3} N_{\mathrm{f}}$$

"lat" - scheme = minimal subtraction of logarithms $\ln(a\cdot\mu)$

(analogous to MS scheme in $D=4-2\varepsilon$)

$$\bar{g}^2_{lat}(\mu) \quad \text{s.t.} \quad \bar{g}^2_{lat}\left(\mu=\tfrac{1}{a}\right) = g_0^2$$

scheme independent

$$\mu\frac{\partial}{\partial\mu}\bar{g}_{lat}(\mu) = \beta(\bar{g}_{lat}) \overset{\bar{g}_{lat}\to 0}{=} -b_0\,\bar{g}^3_{lat} + \ldots$$

$$b_0 = \left(\frac{11N}{3} - \frac{2}{3}N_f\right)/16\pi^2 > 0$$

integrate
$$\frac{1}{\bar{g}^2_{lat}(\mu_2)} = \frac{1}{\bar{g}^2_{lat}(\mu_1)} + 2b_0\ln\frac{\mu_2}{\mu_1}$$

$\mu_2=\frac{1}{a}$, $\mu_1=\mu$
$$\frac{1}{g_0^2} = \frac{1}{\bar{g}^2_{lat}(\mu)} - 2b_0\ln a\mu \xrightarrow[(\mu\text{ fixed})]{a\to 0} \infty$$

Non-perturbative definition of QCD (3)

Working hypothesis: the perturbative picture is essentially correct:

- The continuum limit of lattice QCD exists and is obtained by taking $g_0 \to 0$
- Hence, QCD is asymptotically free, anomalous dimensions are small & naive dimensional analysis applies:

$\Rightarrow$ Non-perturbative renormalisation of QCD is based on the very same counterterm structure as in perturbation theory! *

- Absence of analytical methods: try to take the continuum limit numerically, i.e. by numerical simulations of lattice QCD at decreasing values of g_0.

* PT with a physical cutoff, not $\overline{MS}$ scheme

Renormalisation of QCD

- The basic parameters of QCD are g_0 and $m_i, \quad i = u, d, \ldots.$
- To renormalise QCD one must impose a corresponding number of renormalisation conditions
- If we only consider gauge invariant observables

$\Rightarrow$ no need to renormalize quark, gluon, ghost field and gauge parameter.

- All physical information (particle masses and energies, particle interactions) is contained in the (Euclidean) correlation functions of gauge invariant composite, local fields $\phi_i(x)$

$$\langle \phi_1(x_1) \cdots \phi_n(x_n) \rangle$$

- a priori each ϕ_i requires renormalisation, and thus further renormalisation conditions.

What would we like to achieve?

Natural question to ask:

What are the values of the fundamental parameters of QCD (and thus of the Standard Model!),

$$\alpha_s, \; m_u \approx m_d, \; m_s, \ldots \qquad \alpha \approx \frac{g}{4\pi}$$

if we renormalise QCD in a hadronic renormalization scheme, i.e. by choosing the same number of experimentally well-measured hadron properties: $F_\pi, \; m_\pi, m_K, ...$?

- QCD is regarded as a low energy approximation to the Standard Model; e.m. effects/isospin breaking effects are small $(\alpha_{e.m.} = 1/137)$ and must be subtracted from experimental results.
- conceptually clean, natural question for lattice QCD
- alternative: combination of perturbation theory + assumptions ("quark hadron duality", sum rules, hadronisation Monte-Carlo, ...).

Renormalization of QCD in hadronic scheme

Sketch of the procedure, using e.g. hadronic observables F_π, m_π, m_K, m_D:

1. Choose a value of the bare coupling $g_0^2 = 6/\beta$; this determines the lattice spacing (i.e. mass independent scheme); choose some intial values for the bare quark mass parameters and a spatial lattice volume $(L/a)^3$ that is large enough to contain the hadrons ($\Rightarrow$ constraint for choice of g_0 or β in 1.);
2. tune the bare quark mass parameters such that m_π/F_π, m_K/F_π, m_D/F_π take their desired values (e.g. experimental ones, but not necessarily!)
3. The lattice spacing is obtained from $a(\beta) = (aF_\pi)(\beta)/F_\pi|_{\rm exp.}$
4. Reduce the value of g_0^2 (i.e. increase β) and increase L/a accordingly.
5. Repeat steps 1 – 4 until you run out of resources...

Auxiliary scale parameters r_0, t_0, w_0

For technical reasons one often introduces an auxiliary scale parameter:

- serves as a yardstick for precise tuning or scaling studies;
- should be easily computable (in any case easier than say F_π);
- should have a mild dependence on the quark masses;
- Example: Sommer's scale r_0 obtained from the force $F(r)$ between static quarks:

$$r_0^2 F(r_0) = 1.65 \qquad \Rightarrow r_0 \approx 0.5\,\mathrm{fm}$$

- Idea: at finite a use r_0/a rather than aF_π but also determine $r_0 F_\pi(\beta)$; Conversion to physical units from F_π is then postponed to the continuum limit.
- Advantage: constant physics conditions can be satisfied more precisely.

Present ~~Future~~: a very convenient scale t_0 is based on the gradient flow [M. Lüscher '10]; (later also a variant w_0 by the BMW coll.)

From bare to renormalised parameters

- For g_0^2 (or β) in some interval one obtains:

$$F_\pi, m_\pi, m_K, m_D \quad \Rightarrow \quad g_0, am_{0,l}(g_0), am_{0,s}(g_0), am_{0,c}(g_0)$$

- These are bare parameters, their continuum limit vanishes!
- N.B.: due to quark confinement there is no natural definition of "physical" quark masses or the coupling constant from particle masses or interactions
- At high energy scales, $\mu \gg m_p$, one may use perturbative schemes to define renormalised parameters (e.g. dimensional regularisation and minimal subtraction)
- How can we relate the bare lattice parameters to the renormalised ones in, say, the $\overline{\mathrm{MS}}$ scheme?
- basic idea: introduce an intermediate renormalisation scheme which can be evaluated both perturbatively and non-perturbatively.

Why not use perturbation theory directly?

Shortcut: try to relate the bare parameters directly to $\overline{\mathrm{MS}}$ scheme, e.g. coupling: Allowing for a constant $d = \mathrm{O}(1)$,

$$
\begin{aligned}
\alpha_{\overline{\mathrm{MS}}}(d/a) &= \alpha_0(a) + c_1\alpha_0^2(a) + c_2\alpha_0^3(a) + \ldots, \qquad \alpha_0 = \frac{g_0^2}{4\pi} \\
\overline{m}_{\overline{\mathrm{MS}}}(d/a) &= m(a)\left(1 + Z_m^{(1)}\alpha_0(a) + Z_m^{(2)}\alpha_0^2(a) + \ldots\right\}
\end{aligned}
$$

Main difficulties:

- Setting $\mu \propto a^{-1}$ means that cutoff effects and renormalisation effects cannot be disentangled; any change in the scale is at the same time a change in the cutoff.
- One needs to assume that the cutoff scale d/a is in the perturbative region, higher order effects negligible.
- One furthermore assumes that cutoff effects are negligible

$\Rightarrow$ how reliable are the error estimates?

Consider the force $F(r)$ between static quarks at a distance r, and *define*

$$\alpha_{\mathrm{qq}}(r) = r^2 F(r)|_{m_{\mathrm{q},i}=0}$$

- at short distances:

$$\alpha_{\mathrm{qq}}(r) = \alpha_{\overline{\mathrm{MS}}}(\mu) + c_1(r\mu)\alpha^2_{\overline{\mathrm{MS}}}(\mu) + \ldots$$

- at large distances:

$$\lim_{r\to\infty} \alpha_{\mathrm{qq}}(r) = \begin{cases} \infty & \text{for } N_\mathrm{f} = 0 \\ 0 & \text{for } N_\mathrm{f} > 0 \end{cases}$$

- NB: renormalization condition is imposed in the chiral limit $\Rightarrow$ $\alpha_{\mathrm{qq}}(r)$ and its β-function are quark mass independent.

Example for a renormalised quark mass

Use PCAC relation as starting point:

$$\partial_\mu (A_\mathrm{R})^a_\mu = 2 m_\mathrm{R} (P_\mathrm{R})^a$$

- A^a_μ, P^a: isotriplet axial current & density
- The normalization of the axial current is fixed by current algebra (i.e. axial Ward identities) and scale independent!

$\Rightarrow$ Quark mass renormalization is inverse to the renormalization of the axial density:

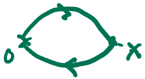
$$(P_\mathrm{R})^a = Z_\mathrm{P} P^a, \qquad m_\mathrm{R} = Z_\mathrm{P}^{-1} m_\mathrm{q}.$$

$\Rightarrow$ Impose renormalization condition for the axial density rather than for the quark mass

Renormalization condition for axial density

Define $\langle P_{\mathrm{R}}^{a}(x) P_{\mathrm{R}}^{b}(y)\rangle = \delta^{ab} G_{\mathrm{PP}}(x-y)$, and impose the condition

$$G_{\mathrm{PP}}(x)\Big|_{\mu^2 x^2=1,\, m_{\mathrm{q},i}=0} = -\frac{1}{2\pi^4 (x^2)^3}$$



$G_{\mathrm{PP}}(x)$ is defined at all distances:

$$G_{\mathrm{PP}}(x) \overset{x^2\to 0}{\sim} -\frac{1}{2\pi^4 (x^2)^3} + \mathrm{O}(g^2), \qquad G_{\mathrm{PP}}(x) \overset{x^2\to \infty}{\sim} -\frac{1}{4\pi^2 x^2} G_\pi^2 + \ldots$$

$\Rightarrow Z_{\mathrm{P}}$ is defined at all scales μ:

- at large μ (but $\mu \ll 1/a$):

$$Z_P(g_0, a\mu) = 1 + g_0^2 d_0 \ln(a\mu) + \ldots,$$

- at low scales μ:

$$Z_{\mathrm{P}}(g_0, a\mu) \propto \mu^2$$

Renormalization group functions

The renormalized coupling and quark mass are defined non-perturbatively at all scales

$\Rightarrow$ Renormalization group functions are defined non-perturbatively, too:

- β-function

$$\beta(\bar{g}) = \mu \frac{\partial \bar{g}(\mu)}{\partial \mu}, \qquad \bar{g}^2(\mu) = 4\pi \alpha_{\mathrm{qq}}(1/\mu)$$

- quark mass anomalous dimension:

$$\tau(\bar{g}) = \frac{\partial \ln \overline{m}(\mu)}{\partial \ln \mu} = -\lim_{a \to 0} \left. \frac{\partial \ln Z_{\mathrm{P}}(g_0, a\mu)}{\partial \ln a\mu} \right|_{\bar{g}(\mu)}$$

Asymptotic expansion for weak couplings:

$$\begin{aligned} \beta(g) &\sim -g^3 b_0 - g^5 b_1 \ldots, \qquad & b_0 &= \left\{\tfrac{11}{3} N - \tfrac{2}{3} N_{\mathrm{f}}\right\}(4\pi)^{-2}, \ldots \\ \tau(g) &\sim -g^2 d_0 - g^4 d_1 \ldots, \qquad & d_0 &= 3(N - N^{-1})(4\pi)^{-2}, \ldots \end{aligned}$$

The Callan-Symanzik equation

Physical quantities P (e.g. hadron masses & energies,...) are independent of μ, and thus satisfy the CS-equation:

$$\left\{\mu\frac{\partial}{\partial\mu}+\beta(\bar{g})\frac{\partial}{\partial\bar{g}}+\tau(\bar{g})\overline{m}\frac{\partial}{\partial\overline{m}}\right\}P=0$$

Λ and M_i are special solutions:

$$\begin{aligned}\Lambda &= \mu\,(b_0\bar{g}^2)^{-b_1/2b_0^2}\,\exp\left\{-\frac{1}{2b_0\bar{g}^2}\right\}\\ &\quad\times\exp\left\{-\int_0^{\bar{g}}\mathrm{d}x\left[\frac{1}{\beta(x)}+\frac{1}{b_0x^3}-\frac{b_1}{b_0^2x}\right]\right\}\\ M_i &= \overline{m}_i\,(2b_0\bar{g}^2)^{-d_0/2b_0}\exp\left\{-\int_0^{\bar{g}}\mathrm{d}x\left[\frac{\tau(x)}{\beta(x)}-\frac{d_0}{b_0x}\right]\right\}\end{aligned}$$

N.B. no approximations involved!

Λ and M_i as fundamental parameters of QCD

- defined beyond perturbation theory
- scale independent
- scheme dependence? Consider finite renormalization:

$$g'_{\mathrm{R}} = g_{\mathrm{R}} c_g(g_{\mathrm{R}}), \qquad m'_{\mathrm{R},i} = m_{\mathrm{R},i} c_m(g_{\mathrm{R}})$$

with asymptotic behaviour $c(g) \sim 1 + c^{(1)} g^2 + \dots$
$\Rightarrow$ find the exact relations

$$M'_i = M_i, \qquad \Lambda' = \Lambda \exp(c_g^{(1)}/b_0).$$

$\Rightarrow$ $\Lambda_{\overline{\mathrm{MS}}}$ can be defined indirectly beyond PT; to obtain Λ in any other scheme requires the one-loop matching of the respective coupling constants.

Strategy to compute Λ and M_i

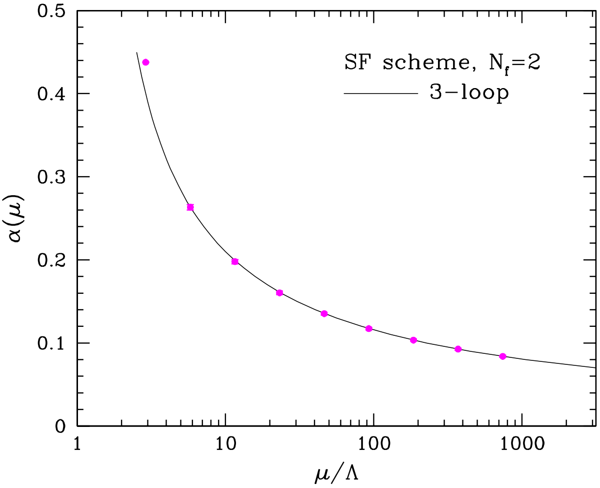
- At fixed g_0 determine the bare parameters corresponding to the experimental input.
- Determine $\alpha_{\mathrm{qq}}(1/\mu)$ and $Z_{\mathrm{P}}(g_0, a\mu)$ at the same g_0 in the chiral limit
- use Z_{P} to pass from bare to renormalised quark masses
- do this for a range of μ-values
- repeat the same for a range of g_0-values and take the continuum limit

$$\lim_{a\to 0} Z_{\mathrm{P}}^{-1}(g_0, a\mu) m_i(g_0), \qquad \lim_{a\to 0} \alpha_{\mathrm{qq}}(1/\mu)$$

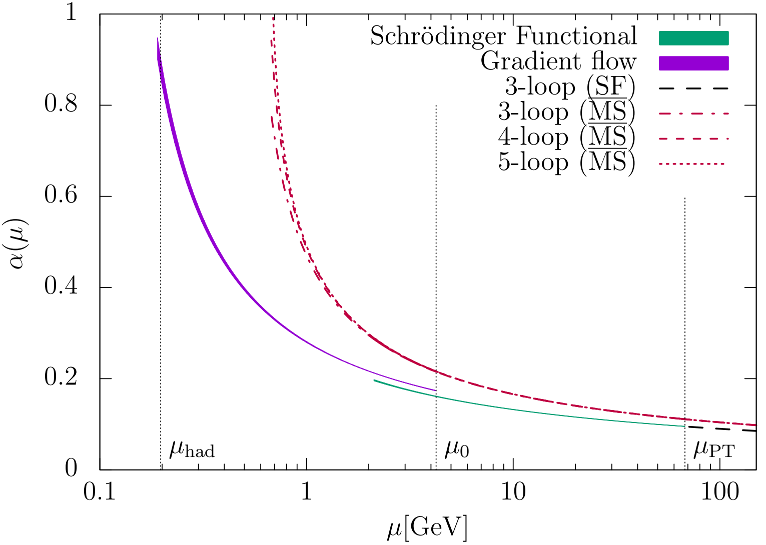
- check wether perturbative scales μ have been reached
- if this is the case, use the perturbative β- and τ-function to extrapolate to $\mu = \infty$; extract Λ and M_i (equivalently convert to $\overline{\mathrm{MS}}$ scheme deep in perturbative region).

Example: running of the coupling (SF scheme, $N_f = 2$)

[ALPHA, M. Della Morte et al. 2005]



Non-perturbative running of the SF and GF couplings in $N_\mathrm{f} = 3$ QCD [ALPHA coll. 2017]



The problem of large scale differences

Λ and M_i refer to the high energy limit of QCD

- The scale μ must reach the perturbative regime: $\mu \gg \Lambda_{\mathrm{QCD}}$
- The lattice cutoff must still be larger: $\mu \ll a^{-1}$
- The volume must be large enough to contain pions: $L \gg 1/m_\pi$
- Taken together a naive estimate gives

$$L/a \gg \mu L \gg m_\pi L \gg 1 \quad \Rightarrow L/a \simeq \mathrm{O}(10^3)$$

$\Rightarrow$ widely different scales cannot be resolved simultaneously on a finite lattice!

In practice ...

This estimate may be a little too pessimistic:

- $Lm_\pi \approx 3 - 4$ often sufficient
- if cutoff effects are quadratic one only needs $a^2\mu^2 \ll 1$.
- when working in momentum space one may argue that the cutoff really is π/a;
- in any case, one must satisfy the requirement $\mu \gg \Lambda_{\mathrm{QCD}}$

Heavy quark thresholds

Λ and M_i implicitly depend on N_f the number of active flavours! If computed for $N_\mathrm{f} = 2, 3$ one needs to perform a matching across the charm and bottom thresholds to match the real world at high energies.

...and its solution

- widely different scales cannot be resolved simultaneously on a *single* finite lattice

$\Rightarrow$ break-up in smaller steps [Lüscher, Weisz, Wolff '91; Jansen et al. '95]:

1. define renormalized parameters that run with the space-time volume, i.e. $\mu = 1/L$
2. match to the chosen hadronic input at a hadronic scale $m_p L_{\mathrm{max}} = \mathrm{O}(1)$
3. Non-perturbative renormalization group: recursively connect scales $L = 1/\mu$ and $2L = 1/(\mu/2)$,

$$L \to 2L \to 4L \to 8L \ldots$$

4. once arrived in the perturbative regime (to be checked) convert perturbatively e.g. to the $\overline{\mathrm{MS}}$ scheme

Step Scaling Functions

- The aim is to construct the Step Scaling Functions $\sigma(u)$ and $\sigma_{\mathrm{P}}(u)$:

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

- 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 tell us what happens for infinitesimal scale changes.

Requirements

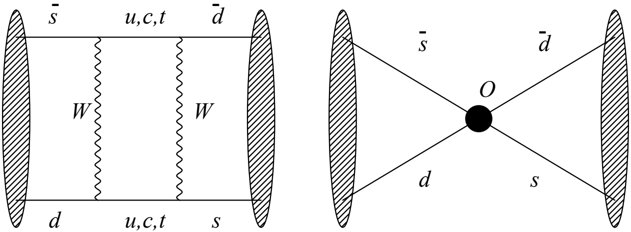
Wanted: renormalization scheme which

- is defined in a finite space-time volume
- is non-perturbatively defined;
- can be expanded in perturbation theory (up to 2-loop) with reasonable effort;
- is gauge invariant;
- is quark mass-independent.
- can be evaluated by numerical simulation!

$\Rightarrow$ motivates the Schrödinger functional (s. later)

QCD & composite operators (1)

Apart from the fundamental parameters of QCD one is interested in hadronic matrix elements of composite operators:
Example: $K^0 - \bar{K}^0$ mixing amplitude in the Standard Model:



A local interaction arises by integrating out W-bosons and t, b, c quarks, corresponding to a composite 4-quark operator

QCD & composite operators (2)

- The mixing amplitude reduces to the hadronic matrix element:

$$\begin{aligned} \langle \bar{K}^0 | O^{\Delta S=2} | K^0 \rangle &= \frac{8}{3} m_K^2 F_K^2 B_K \\ O^{\Delta S=2} &= \sum_\mu [\bar{s}\gamma_\mu(1-\gamma_5)d][\bar{s}\gamma_\mu(1-\gamma_5)d] \end{aligned}$$

  $O^{\Delta S=2}$ requires a multiplicative renormalization; it is initially defined in continuum scheme used for the Operator Product Expansion (OPE)
- Other composite operators arise by applying the OPE with respect to some hard scale, such as the photon momentum in Deep Inelastic Scattering (DIS)
- We thus need to discuss renormalisation of composite operators (cf. quark mass renormalisation for a first example)

RGI operators (1)

- Consider renormalized n-point function of multiplicatively renormalizable operators O_i:

$$G_{\mathrm{R}}(x_1, \cdots, x_n; m_{\mathrm{R}}, g_{\mathrm{R}}) = \prod_{i=1}^{n} Z_{O_i}(g_0, a\mu) G(x_1, \cdots, x_n; m_0, g_0)$$

- Callan-Symanzik equation:

$$\left\{ \mu \frac{\partial}{\partial \mu} + \beta(\bar{g}) \frac{\partial}{\partial \bar{g}} + \tau(\bar{g}) \overline{m} \frac{\partial}{\partial \overline{m}} + \sum_{i=1}^{n} \gamma_{O_i}(\bar{g}) \right\} G_R = 0$$

where

$$\gamma_{O_i}(\bar{g}(\mu)) = \left. \frac{\partial \ln Z_O(g_0, a\mu)}{\partial \ln(a\mu)} \right|_{\bar{g}(\mu)}$$

- Asymptotic behaviour for small couplings:

$$\gamma_O(g) \sim -g^2 \gamma_O^{(0)} - g^4 \gamma_O^{(1)} + \ldots$$

RGI operators (2)

RGI operators can be defined as solutions to the CS equation:

$$\left(\beta(\bar{g}) \frac{\partial}{\partial \bar{g}} + \gamma_O \right) O_{\mathrm{RGI}} = 0$$

where

$$O_{\mathrm{RGI}} = O_{\mathrm{R}}(\mu) \left(\frac{\bar{g}^2(\mu)}{4\pi} \right)^{-\gamma_O^{(0)}/2b_0} \exp \left\{ - \int_0^{\bar{g}} \mathrm{d}x \left[\frac{\gamma_O(x)}{\beta(x)} - \frac{\gamma_O^{(0)}}{b_0 x} \right] \right\}$$

- Its name derives from the fact that O_{RGI} is renormalisation scheme independent (analogous to M_i, verify it!)!
- Beware: the overall normalisation for O_{RGI} here follows the standard convention used for B_K, which differs from the one used for M.

Concluding remarks

- Renormalization and the continuum limit of lattice QCD are closely connected.
- Renormalized QCD parameters (quark masses, coupling) not accessible experimentally due to confinement
- Asymptotic freedom $\Rightarrow$ universal definitions available in the perturbative regime.
- Keeping hadronic input constant defines the bare quark mass parameters as functions of g_0 at relatively low scales (hadronic regime)
- Challenge: connect bare parameters to the $\overline{\mathrm{MS}}$ renormalized ones defined in perturbative regime;
  Alternatively: connect to RGI invariants, Λ and M_i (conceptually nicer but technically equivalent)
- Analogous challenges for hadronic matrix elements of composite operators;
- Problem of large scale differences: define finite volume renormalization scheme and take recursive steps in energy.