Non-perturbative Renormalization and Improvement of Lattice QCD

Part III/V

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Kolkata, 4 December 2013

Some (more or less) pedagogical references

1. R. Sommer, "Non-perturbative renormalisation of QCD", Schladming Winter School lectures 1997, `hep-ph/9711243v1`; "Non-perturbative QCD: Renormalization, O(a) improvement and matching to heavy quark effective theory" Lectures at Nara, November 2005 `hep-lat/0611020`
2. M. Lüscher: "Advanced lattice QCD", Les Houches Summer School lectures 1997 `hep-lat/9802029`
3. S. Sint "Nonperturbative renormalization in lattice field theory" Nucl. Phys. (Proc. Suppl.) 94 (2001) 79-94, `hep-lat/0011081`
   "Lattice QCD with a chiral twist" Lectures at Nara, November 2005 `hep-lat/0611020`

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1. RI/MOM schemes cont'd, a few examples
2. The problem of large scale differences and how to solve it

$\Rightarrow$ motivates the Schrödinger functional

3. Schrödinger functional (continuum formulation), some properties

RI/MOM Schemes (RI = Regularisation Independent; MOM = Momentum Subtraction)

[Martinelli et al '95]: mimick the procedure in perturbation theory:

- choose Landau gauge

$$\partial_\mu A_\mu = 0$$

  can be implemented on the lattice by a minimisation procedure
- RI/MOM schemes are very popular: many major collaborations use it because
  - it is straightforward to implement on the lattice; many improvements over the years regarding algorithmic questions
  - it can be used on the very same gauge configurations which are produced for hadronic physics
- Regularisation Independence (RI) means: correlation functions of a renormalised operator do not depend on the regularisation used (up to cutoff effects).

RI/MOM schemes, discussion

- Suppose we have calculated a renormalised hadronic matrix element of the multiplicatively renormalisable operator O

$$\mathcal{M}_O(\mu) = \lim_{a\to 0} \langle h | O_{\mathrm{R}}(\mu) | h' \rangle$$

- Provided μ is in the perturbative regime, one may evaluate the MOM scheme in continuum perturbation theory and evolve to a different scale:

$$\begin{aligned} \mathcal{M}_O(\mu') &= U(\mu', \mu) \mathcal{M}_O(\mu), \\ U(\mu', \mu) &= \exp\left\{ \int_{\bar{g}(\mu)}^{\bar{g}(\mu')} \frac{\gamma_O(g)}{\beta(g)} \mathrm{d}g \right\} \end{aligned}$$

- N.B. Continuum perturbation theory is available to 3-loops in some cases!

RI/MOM schemes, what could go wrong?

- The scale μ could be too low; need to hope for a "window"

$$\Lambda_{\mathrm{QCD}} \ll \mu \ll a^{-1}$$

  In practice scales are often too low: non-perturbative effects (e.g. pion poles, condensates) are then eliminated by fitting to expected functional form (from OPE in fixed gauge);

$\Rightarrow$ errors are difficult to quantify!

- Gribov copies: the (Landau) gauge condition does not have a unique solution on the full gauge orbit
- Perturbative calculations are made using
  - infinite volume
  - vanishing quark masses

$\Rightarrow$ difficult for numerical simulations especially in full QCD.

A prominent non-perturbative effect: the pion pole

[Martinelli et al. '95]

- Consider the 3-point correlation function for P^a:

$$\int \mathrm{d}^4 x \int \mathrm{d}^4 y \, \mathrm{e}^{-ipx} \langle \overline{\psi}(0)\gamma_5 \tfrac{1}{2}\tau^b \psi(x) P^a(y) \rangle$$

- For large p^2 it is dominated by short distance contributions either at $x \approx 0$ or $x \approx y$. The contribution for $x \approx 0$ is proportional to the pion propagator

$$\int \mathrm{d}^4 y \langle P^b(0) P^a(y) \rangle \propto \frac{1}{m_\pi^2}$$

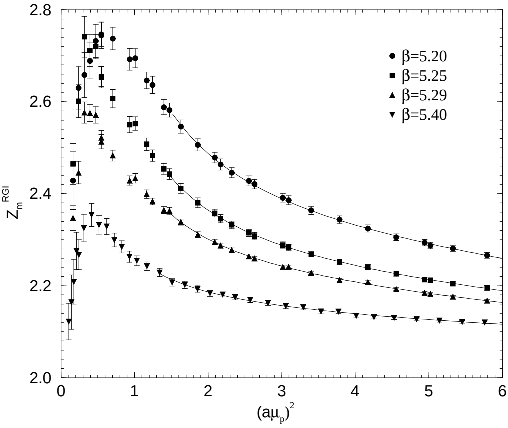
- Dimensional counting: suppression by $1/p^2$ relative to the perturbative term at $x \approx y$:

$$Z_{\mathrm{P}}^{\mathrm{MOM,non-pert}} \sim \frac{A}{\mu^2 m_{\mathrm{q}}} + \ldots$$

$\Rightarrow$ the chiral limit is ill-defined!

RI/MOM scheme, example 1

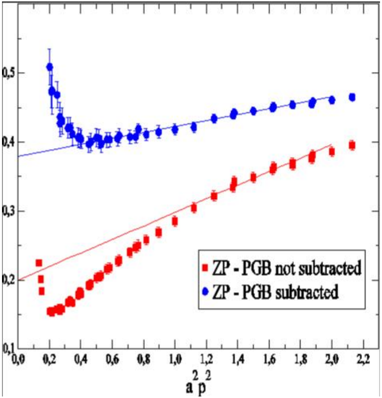
[QCDSF-UKQCD collaboration, Göckeler et al. ’06]

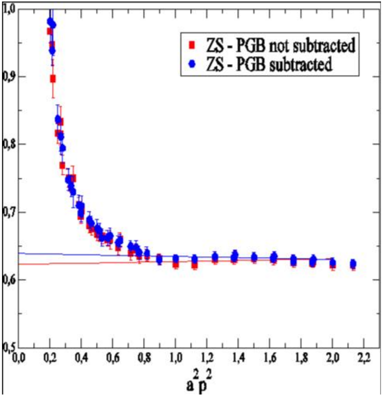


- Z_P^{-1} for the RGI operator after subtraction of the pion pole through a fit. While there is no plateau at fixed β, the situation seems to improve towards higher β, as μ gets larger in physical units.

RI/MOM scheme, example 2

[ETMC collaboration, talk by P. Dimopoulos at Lattice '07]
twisted mass QCD with $N_\mathrm{f} = 2$, subtraction of pion pole à la [Giusti, Vladikas '00]

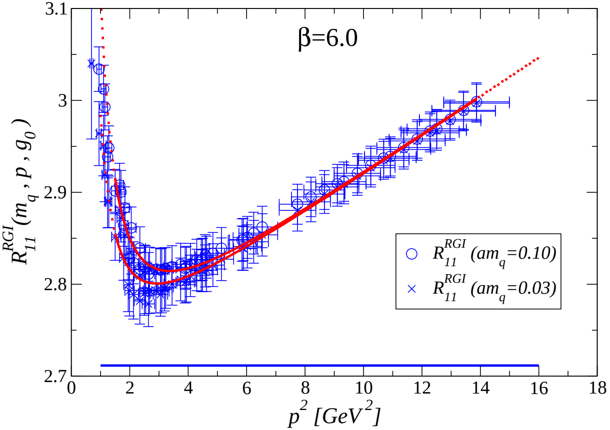




While Z_S shows the expected plateau, Z_P shows some slope even after subtraction of the pion pole (cutoff effects?)

RI/MOM scheme, example 2

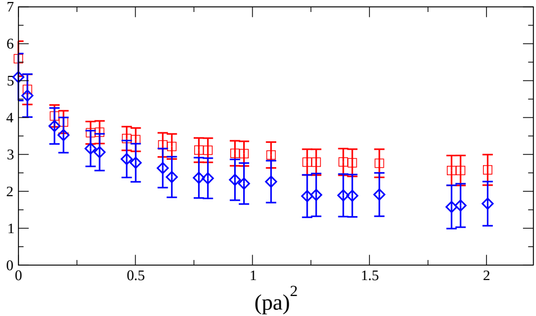
[R. Babich et al. 06] four-quark operator for B_K with overlap quarks (quenched QCD at $\beta = 6.0$):



- non-perturbative effects are eliminated through fit function from OPE including logarithmic terms

RI/MOM scheme, example 3

[Huey-Wen Lin '06] study of quark gluon vertex:



- Comparison of the quark vertex function in Landau gauge, fixed in two different ways on the same ensemble of gauge configurations
- Influence of Gribov copies can be sizable!

RI/MOM schemes; Summary

- There are examples where the method seems to work fine
- Non-perturbative effects like the pion pole are either subtracted or taken into account by fits to the expected p^2-behaviour; but error estimates seem difficult!
- A warning from the quark-gluon vertex: the effect of Gribov copies should be monitored!
- finite volume and quark mass effects often small.
- Since the method can be applied at relatively little cost on the existing configurations (unless charm quark is dynamical!) it can always be tried!
- However, it seems difficult to get reliable errors down to the desired level (say below 1 percent for Z-factors)

Improvement of RI/MOM schemes

Many improvements have been introduced over the last 10–15 years (cf. lattice 2009 review by Y. Aoki): A selection:

- use of non-exceptional momentum configurations (P. Boyle, Lattice 2007):
  reduces the problem with Goldstone poles;
  Continuum perturbation theory needs to be re-done!
- reach higher scales? Small steps may be possible [Arthur & Boyle '10]; in principle need to promote to finite volume scheme: fix μL:
  - need gauge fixing on the torus (complicated)
  - twisted gauge field boundary conditions? link N_c with N_f
  - in any case perturbation theory needs to be re-done from scratch and may be complicated
- use gauge invariant correlation functions $\Rightarrow$ no trouble with Gribov copies; but more demanding in perturbation theory; expect larger cutoff effects on dimensional grounds.
- Perturbative subtraction of cutoff effects
- ...

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!

...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 $m_p L_{\max} = O(1)$
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

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!

$\Rightarrow$ use the Schrödinger functional!

The Schrödinger functional (formal continuum)

The Schrödinger functional appears naturally in the Schrödinger representation of QFT (Symanzik '81), as the time evolution kernel when integrating the functional Schrödinger equation:
Wave functional in Dirac's notation (A, A': field configurations at (Euclidean) times 0, T):

$$\begin{aligned} \psi[A] &\equiv \langle A|\psi\rangle \\ \psi'[A'] &= \int D[A]\langle A'|\mathrm{e}^{-T\mathbb{H}}|A\rangle\langle A|\psi\rangle \end{aligned}$$

The Schrödinger functional is a functional of the initial and final field configuration:

$$\mathcal{Z}[A, A'] = \langle A'|\mathrm{e}^{-T\mathbb{H}}|A\rangle = \int D[\phi]\mathrm{e}^{-S}.$$

The Euclidean field ϕ satisfies Dirichlet boundary conditions

$$\phi(x)|_{x_0=0} = A(\mathbf{x}) \qquad \phi(x)|_{x_0=T} = A'(\mathbf{x})$$

The Schrödinger functional is an example of a field theory defined on a manifold with boundary $\Rightarrow$ problems/questions:

- Translation invariance is broken $\Rightarrow$ momentum is not conserved.
- Conventional proofs of perturbative renormalisability rely on power counting theorems in momentum space: not applicable here!
- Heuristic arguments by Symanzik:

A renormalisable QFT remains renormalisable when considered on a manifold with boundary. Besides the usual parameter and field renormalisations one just needs to add a complete set of local boundary counterterms to the action, i.e. polynomials in the fields and its derivatives of dimension 3 or less, integrated over the boundary.
In the case of scalar ϕ_4^4-theory and boundary at $x_0 = 0$ one finds:

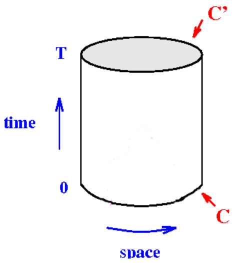
$$\int_{x_0=0} \mathrm{d}^3\mathbf{x}\,\phi^2, \qquad \int_{x_0=0} \mathrm{d}^3\mathbf{x}\,\phi\partial_0\phi$$

The Schrödinger functional in QCD (formal continuum)

The definition for gauge theories and QCD is analogous: The Schrödinger functional is the functional integral on a hyper cylinder,

$$\mathcal{Z} = \int_{\mathrm{fields}} \mathrm{e}^{-S}$$

with periodic boundary conditions in spatial directions and Dirichlet conditions in time.



Boundary conditions for gluon and quark fields:

$P_\pm = \frac{1}{2}(1 \pm \gamma_0)$,

$$\begin{aligned} P_+\psi(x)|_{x_0=0} &= \rho & \qquad P_-\psi(x)|_{x_0=T} &= \rho' \\ \overline{\psi}(x)P_-|_{x_0=0} &= \bar{\rho} & \qquad \overline{\psi}(x)P_+|_{x_0=T} &= \bar{\rho}', \\ A_k(x)|_{x_0=0} &= C_k & \qquad A_k(x)|_{x_0=T} &= C_k' \end{aligned}$$

Correlation functions are then defined as usual

$$\langle O \rangle = \left\{ Z^{-1} \int_{\text{fields}} O\, \mathrm{e}^{-S} \right\}_{\rho=\rho'=0;\, \bar{\rho}=\bar{\rho}'=0}$$

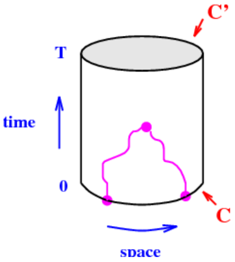
O may contain quark boundary fields

$$\zeta(\mathbf{x}) \equiv P_-\zeta(\mathbf{x}) = \frac{\delta}{\delta\bar{\rho}(\mathbf{x})}$$

$$\bar{\zeta}(\mathbf{x}) \equiv \bar{\zeta}(\mathbf{x})P_+ = -\frac{\delta}{\delta\rho(\mathbf{x})}$$

$$\zeta'(\mathbf{x}) \equiv P_+\zeta'(\mathbf{x}) = \frac{\delta}{\delta\bar{\rho}'(\mathbf{x})}$$

$$\bar{\zeta}'(\mathbf{x}) \equiv \bar{\zeta}'(\mathbf{x})P_+ = -\frac{\delta}{\delta\rho'(\mathbf{x})}$$



$\Rightarrow$ the boundary values of the quark fields are used as external sources

Properties of the QCD Schrödinger functional

- The SF is renormalisable: besides the renormalisation of the coupling and quark masses, the boundary quark fields require a multiplicative renormalisation.
- absence of fermionic zero modes: numerical simulations at zero quark masses are possible!
- For some choices of C_k and C'_k it can be shown that the induced background gauge field is an absolute minimum of the action $\Rightarrow$ perturbation theory is straightforward and seems practical at least to 2-loop order.
- As C_k and C'_k are held fixed only spatially constant gauge transformations are possible at the boundaries!:

$$C_k(\mathbf{x}) \to \Lambda(\mathbf{x})C_k(\mathbf{x})\Lambda^{-1}(\mathbf{x}) + \Lambda(\mathbf{x})\partial_k\Lambda^{-1}(\mathbf{x})$$

  i.e. the allowed $\Lambda(\mathbf{x}) \in \mathrm{SU}(N)$ must be $\mathbf{x}$-independent and commute with C_k.

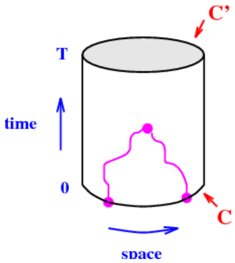
- Therefore, bilinear boundary quark sources such as

$$\mathcal{O}^a = \int \mathrm{d}^3\mathbf{y}\mathrm{d}^3\mathbf{z}\ \bar{\zeta}(\mathbf{y})\gamma_5\tfrac{\tau^a}{2}\zeta(\mathbf{z}), \qquad \mathcal{O}'^a = \int \mathrm{d}^3\mathbf{y}\mathrm{d}^3\mathbf{z}\ \bar{\zeta}'(\mathbf{y})\gamma_5\tfrac{\tau^a}{2}\zeta'(\mathbf{z})$$

  are gauge invariant!

- Typical gauge invariant correlation functions are then

$$f_{\mathrm{P}}(x_0) = -\tfrac{1}{3}\sum_{a=1}^{3}\langle P^a(x)\mathcal{O}^a\rangle, \qquad f_{\mathrm{A}}(x_0) = -\tfrac{1}{3}\sum_{a=1}^{3}\langle A_0^a(x)\mathcal{O}^a\rangle,$$



$\Rightarrow$ convenient in perturbation theory: in contrast to a periodic or infinite volume where gauge invariant fermionic correlation functions lead to one-loop diagrams at lowest order, e.g.

$$g_{\mathrm{PP}}(x_0) = -a^3 \sum_{\mathbf{x}} \sum_{a=1}^{3} \langle P^a(x) P^a(0) \rangle$$

- dimensional analysis $\Rightarrow$ at short distances one finds the asymptotic behaviour (up to logarithms):

$$g_{\mathrm{PP}}(x_0) \sim \frac{\mathrm{const}}{(x_0)^3}, \qquad f_{\mathrm{P}}(x_0) \sim \mathrm{const}$$

- expect
  - small cutoff effects for $f_{\mathrm{P}}(x_0)$ due to mild x_0-dependence
  - good signal in numerical simulations.

More on the renormalisability of the SF

- no gauge invariant dimension ≤ 3 counterterm exists, the pure gauge SF is finite after renormalisation of the coupling constant
- continuum quark action with SF boundary conditions at tree-level:

$$S_{\mathrm{f}} = \int \mathrm{d}^4 x\, \overline{\psi}\left(\tfrac{1}{2}\overleftrightarrow{\not{D}} + m\right)\psi - \tfrac{1}{2}\int_{x_0=0} \mathrm{d}^3\mathbf{x}\, \overline{\psi}\psi - \tfrac{1}{2}\int_{x_0=T} \mathrm{d}^3\mathbf{x}\, \overline{\psi}\psi$$

Exercise:

Show that the boundary terms are necessary if one requires the existence of smooth solutions to the equations of motion with SF boundary conditions

- The counterterms are linear in the boundary fields

$$\begin{aligned} \overline{\psi}(x)\psi(x)|_{x_0=0} &= \bar{\rho}(\mathbf{x})P_-\psi(0,\mathbf{x}) + \overline{\psi}(0,\mathbf{x})P_+\rho(\mathbf{x}), \\ \overline{\psi}(x)\psi(x)|_{x_0=T} &= \bar{\rho}'(\mathbf{x})P_+\psi(T,\mathbf{x}) + \overline{\psi}(T,\mathbf{x})P_-\rho'(\mathbf{x}), \end{aligned}$$

More on the renormalisability of the SF

- The only dimension 3 counterterm with correct symmetries is $\overline{\psi}\psi$
- Time reversal symmetry requires the same coefficient at $x_0 = 0, T$
- This counterterm can thus be absorbed in a multiplicative rescaling of $\rho, \rho', \bar{\rho}, \bar{\rho}'$ by the same renormalization constant:

$$\rho_{\rm R} = Z_\rho \rho, \qquad \bar{\rho}_{\rm R} = Z_\rho \bar{\rho}, \qquad \rho'_{\rm R} = Z_\rho \rho', \qquad \bar{\rho}'_{\rm R} = Z_\rho \bar{\rho}'$$

  Consequently, setting $Z_\zeta = Z_\rho^{-1}$:

$$\zeta_{\rm R} = Z_\zeta \zeta, \qquad \zeta'_{\rm R} = Z_\zeta \zeta', \qquad \overline{\zeta}_{\rm R} = Z_\zeta \overline{\zeta}, \qquad \overline{\zeta}'_{\rm R} = Z_\zeta \overline{\zeta}',$$

- Hence sources like $\mathcal{O}^a$ are multiplicatively renormalised by Z_ζ^2

Definition of the SF coupling [Lüscher et al. '92]

- Choose abelian and spatially constant boundary gauge fields:

$$C_k = \frac{i}{L}\begin{pmatrix}\phi_1 & 0 & 0\\ 0 & \phi_2 & 0\\ 0 & 0 & \phi_3\end{pmatrix}, \qquad C'_k = \frac{i}{L}\begin{pmatrix}\phi'_1 & 0 & 0\\ 0 & \phi'_2 & 0\\ 0 & 0 & \phi'_3\end{pmatrix}, \qquad k = 1,2$$

- with angles taken to be linear functions of a parameter η:

$$\begin{aligned} \phi_1 &= \eta - \tfrac{\pi}{3}, & \phi'_1 &= -\phi_1 - \tfrac{4\pi}{3},\\ \phi_2 &= -\tfrac{1}{2}\eta, & \phi'_2 &= -\phi_3 + \tfrac{2\pi}{3},\\ \phi_3 &= -\tfrac{1}{2}\eta + \tfrac{\pi}{3}, & \phi'_3 &= -\phi_2 + \tfrac{2\pi}{3}. \end{aligned}$$

- The gauge action has an absolute minimum for:

$$B_0 = 0, \qquad B_k = \left[x_0 C'_k + (L - x_0) C_k\right]/L, \quad k = 1,2,3.$$

i.e. other gauge fields with the same action must be gauge equivalent to B_μ

Definition of the SF coupling

- Define the effective action of the induced background field

$$\Gamma[B] = -\ln \mathcal{Z}[C, C']$$

- In perturbation theory the effective action has the expansion

$$\Gamma[B] \quad \sim \quad g_0^{-2}\Gamma_0[B] + \Gamma_1[B] + O(g_0^2)$$

- Definition of the SF coupling:

$$\bar{g}^2(L) = \left.\frac{\partial_\eta \Gamma_0[B]|_{\eta=0}}{\partial_\eta \Gamma[B]|_{\eta=0}}\right|_{m_{\mathrm{q,i}}=0} \qquad \Rightarrow \qquad \bar{g}^2(L) = g_0^2 + \mathrm{O}(g_0^4)$$

- b.c.'s induce a constant colour electric field:

$$G_{0k} = \partial_0 B_k = \frac{C_k - C'_k}{L}$$

$\Rightarrow$ The coupling is defined as "response coefficient" to a variation of a constant colour electric field.