Finite volume schemes based on the Schrödinger functional (lecture III)

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- Definition & properties of the Schrödinger functional
- Definition of the running SF coupling
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The Schrödinger functional (formal continuum)

The Schödinger 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):

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

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:

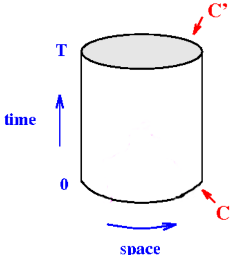
$$\int_{x_0=0} \mathrm{d}^3\mathbf{x}\,\phi^2, \qquad \int_{x_0=0} \mathrm{d}^3\mathbf{x}\,\phi\partial_0\phi$$

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,

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

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



Boundary conditions for gluon and quark fields:

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

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

Correlation functions are then defined as usual

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

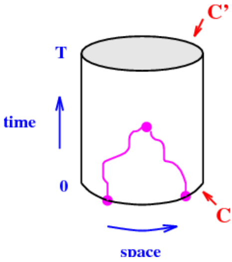
O may contain quark boundary fields

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

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

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

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



$\Rightarrow$ 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!:

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

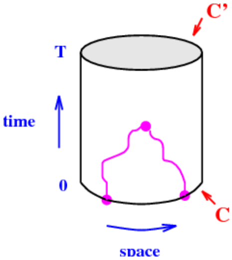
i.e. the allowed $\Lambda(\mathbf{x}) \in \mathrm{SU}(N)$ must be **x**-independent and commute with C_k.

- Therefore, bilinear boundary quark sources such as

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

  are gauge invariant!
- Typical gauge invariant correlation functions are then

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



$\Rightarrow$ 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.

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

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

$$g_{\rm PP}(x_0) \sim \frac{1}{(x_0)^3}, \qquad f_{\rm P}(x_0) \sim \text{const}$$

- expect
  - small cutoff effects for $f_{\rm P}(x_0)$ 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:

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

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:

$$C_k = \frac{i}{L}\begin{pmatrix}\phi_1 & 0 & 0\\ 0 & \phi_2 & 0\\ 0 & 0 & \phi_3\end{pmatrix}, \qquad C'_k = \frac{i}{L}\begin{pmatrix}\phi'_1 & 0 & 0\\ 0 & \phi'_2 & 0\\ 0 & 0 & \phi'_3\end{pmatrix}, \qquad k=1,2,3,$$

- 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:

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

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

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

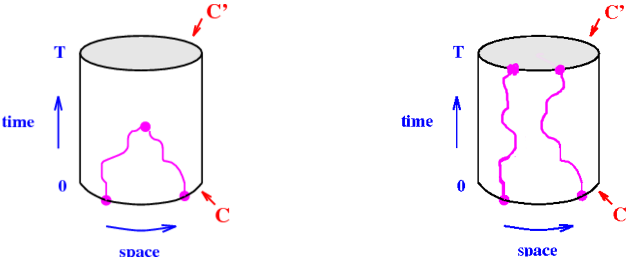
$\Rightarrow$ The coupling is defined as "response coefficient" to a variation of a constant colour electric field.

Renormalisation of operators in the SF scheme (1)

Example: renormalisation of $P^a = \overline{\psi}\gamma_5 \frac{\tau^a}{2}\psi$:

- In this case we set $C_k = C'_k = 0$, i.e. trivial background field $B = 0$
- Define correlation functions

$$f_{\mathrm{P}}(x_0) = \langle \mathcal{O}^a P^a(x) \rangle, \qquad f_1 = L^{-6} \langle \mathcal{O}^a \mathcal{O}'^a \rangle$$



Renormalisation of operators in the SF scheme (2)

- Renormalised correlation functions:

$$f_{\mathrm{P,R}}(x_0) = Z_\zeta^2 Z_P f_{\mathrm{P}}(x_0), \qquad f_{1,R} = Z_\zeta^4 f_1,$$

  set $T = L$, $m = 0$, $x_0 = L/2$, and impose

$$Z_{\mathrm{P}}(g_0, L/a) \frac{f_{\mathrm{P}}(L/2)}{\sqrt{f_1}} = \left. \frac{f_{\mathrm{P}}(L/2)}{\sqrt{f_1}} \right|_{g_0=0}$$

- similarity with MOM schemes: the renormalised amplitude at $\mu = L^{-1}$ equals its tree-level expression
- The ratio is formed to cancel any Z_ζ.
- definition of running quark mass: $\overline{m}(L) = Z_{\mathrm{P}}^{-1}(L)m$.

Step Scaling Functions

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

$$\sigma(u) = \bar{g}^2(2L)\big|_{u=\bar{g}^2(L)},$$
$$\sigma_{\mathrm{P}}(u) = \lim_{a\to 0} \frac{Z_{\mathrm{P}}(g_0, 2L/a)}{Z_{\mathrm{P}}(g_0, L/a)}\bigg|_{u=\bar{g}^2(L)}$$

- 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.

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

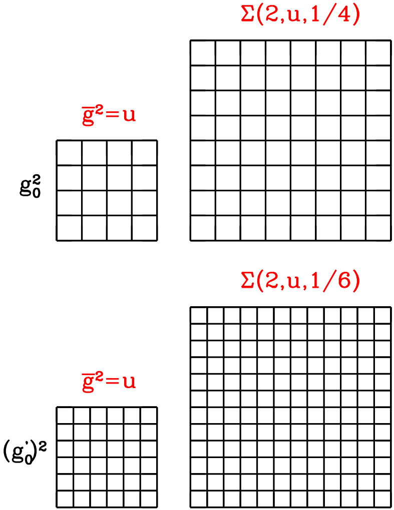
- choose g_0 and $L/a = 4$, measure $\bar{g}^2(L) = u$ (this sets the value of u)
- double the lattice and measure

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

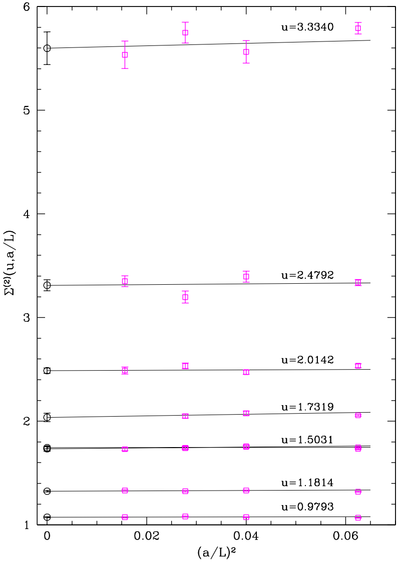
- now choose $L/a = 6$ and tune g_0' such that $\bar{g}^2(L) = u$ is satisfied
- double the lattice and measure

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

- and so on ...

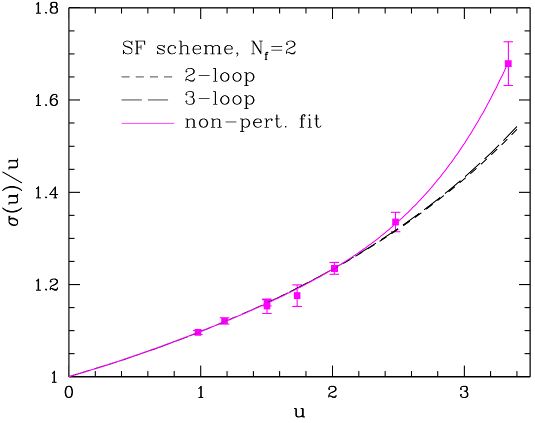


Continuum extrapolation of the SSF [ALPHA '05]



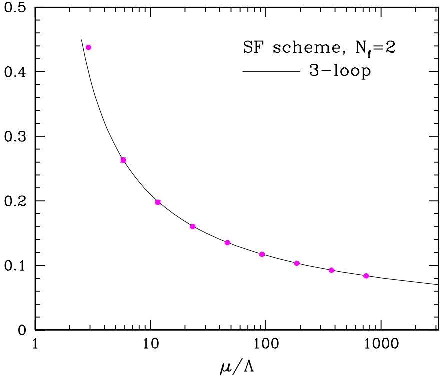
The SSF in the continuum limit

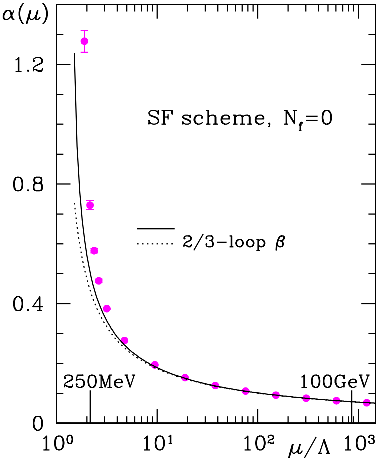
[ALPHA coll., Della Morte et al ’05]



The running of the SF coupling

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





Determination of the Λ-parameter

- The formula

$$\Lambda = \mu\,(b_0\bar{g}^2)^{-b_1/2b_0^2}\,\exp\left\{-\frac{1}{2b_0\bar{g}^2}\right\} \times \exp\left\{-\int_0^{\bar{g}} \mathrm{d}x\left[\frac{1}{\beta(x)}+\frac{1}{b_0x^3}-\frac{b_1}{b_0^2x}\right]\right\}$$

  holds for any value of μ. We may use it at $L_{\rm min}$ to obtain

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

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

$$\int_0^{\bar{g}} \mathrm{d}x\left[\frac{b_2b_0-b_1^2}{b_0^3}x+\mathrm{O}(x^3)\right] = \frac{b_2b_0-b_1^2}{2b_0^3}\bar{g}^2+\mathrm{O}(\bar{g}^4)$$

  may thus be evaluated using the β-function at 3-loop order.
- Since $L{\rm max} = 2^nL_{\rm min}$ one knows $L_{\rm max}\Lambda$
- still need $F_\pi L_{\rm max}$

Matching to a low energy scale

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

- What is required? The scale $L_{\max}$ is implicitly defined:

$$\bar{g}^2(L_{\max}) = 4.61 \qquad \Rightarrow \qquad (L_{\max}/a)(g_0)$$

  For example, setting $L_{\max}/a = 6, 8, 10, \ldots$ one then finds corresponding values of the bare coupling

- 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 $\bar{g}L_{\max}$
- This has not yet been accomplished with a hadronic scale, but only using the scale r_0; expect this to change in the near future

Results

- 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 $r_0 = 0.5\,\mathrm{fm}$.
- Note: recent simulations (QCDSF coll., ETM coll.) indicate $r_0 \approx 0.47\,\mathrm{fm}$ when matching to hadronic quantities
- Published results for Λ using $r_0 = 0.5\,\mathrm{fm}$ [ALPHA '05]

$$\begin{aligned} \Lambda^{(2)}_{\overline{\mathrm{MS}}} r_0 &= 0.62(4)(4), \qquad \Lambda_{\overline{\mathrm{MS}}} = 245(16)(16)\,\mathrm{MeV} \\ \Lambda^{(0)}_{\overline{\mathrm{MS}}} r_0 &= 0.602(48), \qquad \Lambda_{\overline{\mathrm{MS}}} = 238(19)\,\mathrm{MeV} \end{aligned}$$

The running quark mass

- Coupled evolution of the running mass and the coupling:

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

- Once the running coupling is known in a range $[u_0, u_n]$,

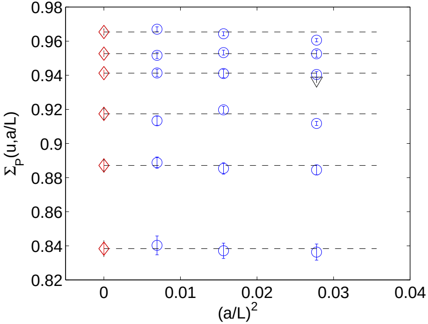
$$u_0 = \bar{g}^2(L_{\rm min}), \quad u_k = \bar{g}^2(2^k L_{\rm min}), k = 1, 2, \ldots, n$$

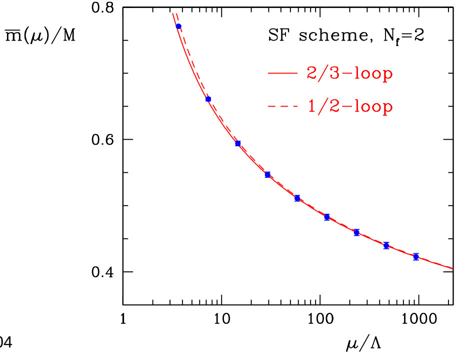
  determine $\sigma_m(u)$ for the same range of couplings: evolution of quark mass and coupling recursively

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

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

Running mass in the SF scheme [ALPHA '05]





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 $m_{\rm PCAC}$ from the (bare) PCAC relation:

$$m_{\rm PCAC} \stackrel{\rm def}{=} \frac{\langle \partial_\mu A_\mu^a(x) O\rangle}{2\langle P^a(x) O\rangle}$$

- The running quark mass is then related to $m_{\rm PCAC}$

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

- Combine results,

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

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

Concluding remarks

- The recursive finite volume technology has completely eliminated the problem with large scale differences. The RG running is determined in the continuum limit and universal (i.e. regularisation independent)
- To obtain physical results one needs to perform 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
- Whether perturbation theory for the running operator is working well or not down to low scales is not so important; you would not know this beforehand! What error estimate would you have given?!
- Many operator renormalisation problems have been treated already; the technique can be generalised to operators containing static quarks (cf. R. Sommer's Nara lectures) and works fine with dynamical quarks!