A chiral twist to the Schrödinger functional

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Topics:

* Schrödinger functional schemes pro's & con's
* Decoupling of heavy quarks
* The Schrödinger functional & O(a) improvement
* Modifying the boundary conditions
* First applications and outlook

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A Schrödinger functional commercial

The Schrödinger functional (SF) provides an attractive scheme for solving renormalization problems:

- finite volume is part of the scheme definition $\mu = L^{-1}$

  $\Rightarrow$ finite size scaling methods to study non-perturbative running over a wide range of scales

- gauge invariance is maintained throughout

- quark mass independence through renormalization in the chiral limit

- simulations can be performed directly at zero mass (no chiral extrapolation is needed)

  $\Rightarrow$ well suited for dynamical fermion simulations!

- good numerical signals due to momentum zero projection of individual quark boundary fields

Disadvantages of SF schemes

- using quark mass dependent SF schemes, the decoupling of heavy quarks is slow ($\propto 1/m$ rather than $\propto 1/m^2$) (S.,Sommer '95)

- cutoff effects are O(a) even in bosonic theories; fermionic O(a) boundary counterterms such as

$$a \int_{x_0=0,T} \mathrm{d}^3\mathbf{x}\ \bar{\psi}\gamma_0\partial_0\psi, \qquad a \int_{x_0=0,T} \mathrm{d}^3\mathbf{x}\ \bar{\psi}\gamma_k\partial_k\psi,$$

  are present with any regularization: (share symmetries with kinetic term)

⇒ problem: the renormalization factors may introduce O(a) effects in otherwise O(a) improved observables!

- in practice: the number of boundary counterterms which may occur can be reduced by equations of motion, and by the choice of correlation functions

⇒ expect typically 2-3 boundary counterterms to contribute;

these can be controlled/monitored/eliminated perturbatively or even non-perturbatively

Decoupling of heavy quarks in the SF coupling

Goal: Match theories with different number of flavours across quark thresholds (in practice the b-quark):

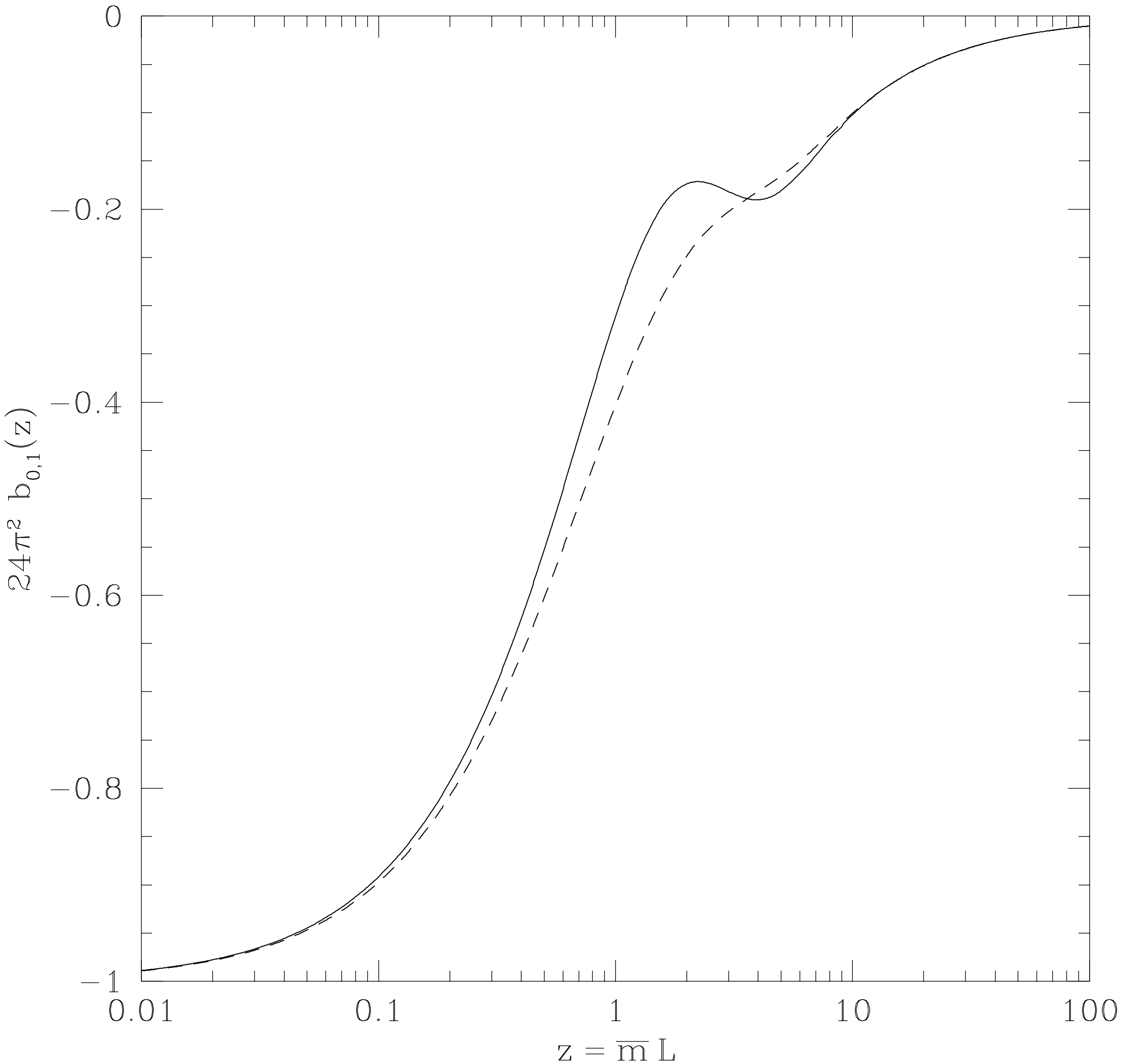
- Match to mass-dependent scheme above the treshold, e.g. SF-coupling defined at finite renormalized quark mass

- Run over the threshold until the heavy quark has decoupled

- Match to mass independent scheme with $N_{\rm f} \to N_{\rm f} - 1$ below the threshold

- Problem with SF coupling: no symmetry under $m \to -m$

$\Rightarrow$ Decoupling is slow, proportional to $1/m$, S.,Sommer '95:



Free quarks with SF boundary conditions

Consider a free quark ψ in the continuum with homogeneous SF boundary conditions

$$P_+\psi(x)|_{x_0=0} = 0, \qquad P_-\psi(x)|_{x_0=T} = 0, \qquad P_\pm = \tfrac{1}{2}(1 \pm \gamma_0)$$

$\gamma_5(\not{\partial} + m)$ is a hermitian operator, with smooth eigenfunctions and no zero modes (S. '93):

$$\begin{aligned} \gamma_5(\not{\partial} + m)\varphi &= \lambda\varphi \\ P_+\gamma_5(\not{\partial} + m)\varphi|_{x_0=0} &= 0 \quad \Rightarrow \quad (\partial_0 - m)P_-\varphi|_{x_0=0} = 0 \\ P_-\gamma_5(\not{\partial} + m)\varphi|_{x_0=T} &= 0 \quad \Rightarrow \quad (\partial_0 + m)P_+\varphi|_{x_0=T} = 0 \end{aligned}$$

complementary components satisfy modified Neumann conditions.

- free eigenvalues are of the form

$$\lambda = \pm\sqrt{p_0^2 + \mathbf{p}^2 + m^2},$$

where p_0 is determined as non-vanishing solution of

$$\tan(p_0 T) = -\frac{p_0}{m}$$

- the spectrum is not symmetric under $m \to -m$, leading to small mass corrections $\propto m$ and large mass corrections of $\propto 1/m$ in the coupling constant and step-scaling functions for renormalization constants

- this is generic: a sign change in the mass can be compensated by a γ_5-transformation of the fields which is not a symmetry of the SF

- possible ways out:

  1. add a twisted mass term and set $m = 0$: $\gamma_5 \tau^1 (\not{\partial} + i\mu_{\mathrm{q}} \gamma_5 \tau^3)$ is hermitian; find Neumann conditions for complementary components
  2. stay with standard mass term but chirally rotate the boundary conditions (see below)

<u>caveat:</u> a priori one can only decouple 2 flavours simultaneously

SF schemes with Wilson quarks and O(a) improvement

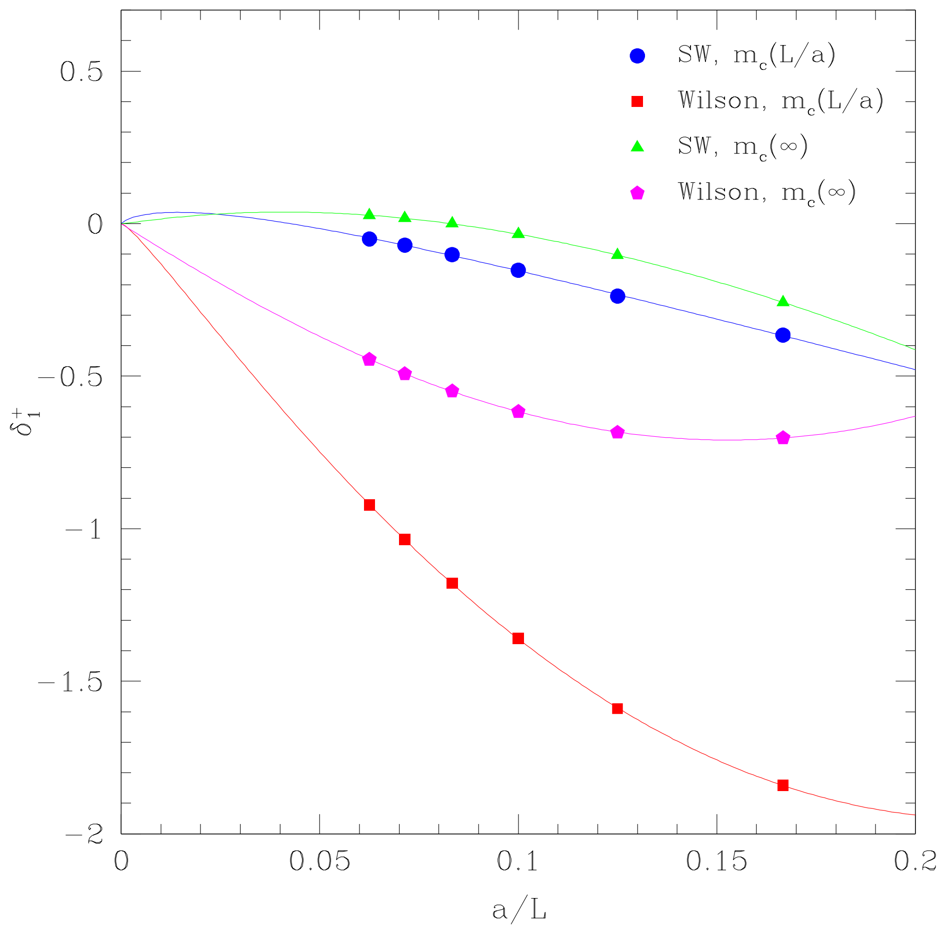
- previous lecture: $\gamma_5\tau^1$-even observables computed with Wilson quarks in a finite volume and with periodic boundary conditions are automatically O(a) improved at zero quark mass

- SF coupling and renormalization factors are computed at zero quark mass.

  distinguish 3 sources for O(a) effects:

  1. O(a) boundary effects (expected in any case!); can be cancelled by inclusion of boundary O(a) counterterms
  2. from the bulk action; can be cancelled by including the SW/clover term
  3. from the composite operators; can be cancelled by including O(a) counterterms determined from chiral Ward identities; difficult for 4-quark operators!

Example: relative cutoff effects in the one-loop coefficient of the step-scaling function for the 4-quark operator needed for B_K (Palombi, Pena, S. '05)



Question: Why do the bulk O(a) counterterms not vanish in the chiral limit?

The Schrödinger functional and O(a) improvement

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

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

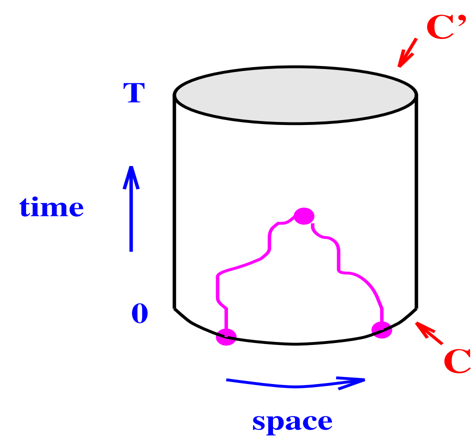
Correlation functions are then defined as usual

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

O may contain quark boundary fields

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

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



- Problem: the $\gamma_5\tau^1$ field transformation switches the projectors of the quark b.c.'s:

$$P_{\pm}\gamma_5\tau^1 = \gamma_5\tau^1 P_{\mp}$$

The boundary conditions, like mass terms, break chiral symmetry and define a direction in chiral flavour space.

$\Rightarrow$ the $\gamma_5\tau^1$ transformation yields inequivalent correlation functions even in the chiral limit,

$$\langle O\rangle_{(m,\mu_{\rm q},P_{\pm})} \rightarrow \langle O\rangle_{(-m,\mu_{\rm q},P_{\mp})}$$

$\Rightarrow$ there are no $\gamma_5\tau^1$-even correlators!

Possible solution:

- change quark boundary projectors, such that they commute with $\gamma_5\tau^1$, e.g.

$$\mathcal{P}_\pm = \tfrac{1}{2}(1 \pm \gamma_0\tau^3), \qquad Q_\pm = \tfrac{1}{2}(1 \pm i\gamma_0\gamma_5\tau^3),$$

- Practical problem: not obvious how to implement such boundary conditions on the lattice!

- Solution for $Q_\pm$ using orbifold techniques; these projectors arise by chirally rotating the standard SF!

SF boundary conditions and chiral rotations

Consider isospin doublets χ' and $\overline{\chi}'$ satisfying homogeneous SF boundary conditions ($P_\pm = \frac{1}{2}(1 \pm \gamma_0)$),

$$P_+\chi'(x)|_{x_0=0} = 0, \qquad P_-\chi'(x)|_{x_0=T} = 0,$$
$$\overline{\chi}'(x)P_-|_{x_0=0} = 0, \qquad \overline{\chi}'(x)P_+|_{x_0=T} = 0.$$

perform a chiral field rotation,

$$\chi' = \exp(i\alpha\gamma_5\tau^3/2)\chi, \qquad \overline{\chi}' = \overline{\chi}\exp(i\alpha\gamma_5\tau^3/2),$$

the rotated fields satisfy chirally rotated boundary conditions

$$P_+(\alpha)\chi(x)|_{x_0=0} = 0, \qquad P_-(\alpha)\chi(x)|_{x_0=T} = 0,$$
$$\overline{\chi}(x)\gamma_0 P_-(\alpha)|_{x_0=0} = 0, \qquad \overline{\chi}(x)\gamma_0 P_+(\alpha)|_{x_0=T} = 0,$$

with the projectors

$$P_\pm(\alpha) = \frac{1}{2}\left[1 \pm \gamma_0\exp(i\alpha\gamma_5\tau^3)\right].$$

Special cases of $\alpha = 0, \pi/2$:

$$P_\pm(0) = P_\pm, \qquad P_\pm(\pi/2) \equiv Q_\pm = \tfrac{1}{2}(1 \pm i\gamma_0\gamma_5\tau^3),$$

Standard SF b.c.'s natural for Wilson quarks due to projector structure

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

but Dirichlet boundary conditions are not always easy to implement:

- what happens with Wilson quarks and Wilson parameter $r \neq 1$?
- how does one implement SF boundary conditions for other lattice regularisations (Ginsparg-Wilson, domain-wall fermions)? (→ Taniguchi '04)
- here: how do we implement the chirally rotated b.c.'s?

Orbifold technique

Orbifold techniques have been used to implemement the standard SF conditions for Ginsparg-Wilson quarks (Taniguchi '04). Here:

- start with standard lattice action for a single quark flavour

$$S_f[\psi, \bar{\psi}, U] = a^4 \sum_x \bar{\psi}(x)\,(D_W + m_0)\,\psi(x)$$

where

$$\psi(x_0 + 2T, \mathbf{x}) = -\psi(x), \qquad \bar{\psi}(x_0 + 2T, \mathbf{x}) = -\bar{\psi}(x)$$

- introduce a reflection ($R^2 = id$)

$$R : \psi(x) \to i\gamma_0\gamma_5\psi(-x_0, \mathbf{x}), \qquad \bar{\psi}(x) \to \bar{\psi}(-x_0, \mathbf{x}) i\gamma_0\gamma_5$$

- the gauge field is extended to $[-T, T]$ and then periodically continued (cp. Taniguchi '04):

$$U_k(-x_0, \mathbf{x}) = U_k(x_0, \mathbf{x}), \qquad U_0(-x_0 - a, \mathbf{x})^\dagger = U_0(x)$$

- Decompose fields into even and odd with respect to R,

$$R\psi_\pm = \pm\psi_\pm, \qquad R\bar{\psi}_\pm = \pm\bar{\psi}_\pm$$

- even/odd fields satisfy the boundary conditions at $x_0 = 0$

$$(1 \mp i\gamma_0\gamma_5)\psi_\pm(0, \mathbf{x}) = 0 \qquad \bar{\psi}_\pm(0, \mathbf{x})(1 \mp i\gamma_0\gamma_5) = 0$$

- and with complementary projectors at $x_0 = T$, due to antiperiodicity:

$$(1 \pm i\gamma_0\gamma_5)\psi_\pm(T, \mathbf{x}) = 0 \qquad \bar{\psi}_\pm(T, \mathbf{x})(1 \pm i\gamma_0\gamma_5) = 0$$

- consistency condition for R:

$$S_f[\psi, \bar{\psi}, U] = S_f[\psi_+ + \psi_-, \bar{\psi}_+ + \bar{\psi}_-, U] = S_f[\psi_+, \bar{\psi}_+, U] + S_f[\psi_-, \bar{\psi}_-, U]$$

is indeed verified; (i.e. R commutes with D_W!)

$\Rightarrow$ the functional integral factorises!

- interpret even and odd fields as quark flavours

$$\chi = \sqrt{2}\begin{pmatrix}\psi_- \\ \psi_+\end{pmatrix}, \qquad \bar{\chi} = \sqrt{2}\begin{pmatrix}\bar{\psi}_- & \bar{\psi}_+\end{pmatrix}$$

- functional integral:

$$\int \prod_{-T\leq x_0<T} \mathrm{d}\psi(x)\mathrm{d}\bar{\psi}(x)\mathrm{e}^{-S_f[\psi,\bar{\psi},U]} \propto \int \prod_{0\leq x_0\leq T} \mathrm{d}\chi(x)\mathrm{d}\bar{\chi}(x)\mathrm{e}^{-\frac{1}{2}S_f[\chi,\bar{\chi},U]}$$

- equivalent to theory in the interval $[0,T]$ with boundary conditions

$$Q_+\chi(x)|_{x_0=0} = 0, \qquad Q_-\chi(x)|_{x_0=T} = 0,$$
$$\bar{\chi}(x)Q_+|_{x_0=0} = 0, \qquad \bar{\chi}(x)Q_-|_{x_0=T} = 0$$

The dynamical field variables are

$$Q_-\chi(0,\mathbf{x}), \qquad \chi(x)|_{0<x_0<T}, \qquad Q_+\chi(T,\mathbf{x})$$

and

$$\bar\chi(0,\mathbf{x})Q_-, \qquad \bar\chi(x)|_{0<x_0<T}, \qquad \bar\chi(T,\mathbf{x})Q_+$$

The Wilson-Dirac operator in the interval is obtained by re-writing

$$S_f[\chi,\bar\chi,U] = a^4 \sum_{-T<x_0\leq T} \bar\chi(x)\,(D_W+m_0)\,\chi(x) = 2a^4 \sum_{0\leq x_0\leq T} \bar\chi(x)\mathcal{D}\chi(x).$$

Properties of $\mathcal{D}$:

- up to modifications near the time boundaries it is just $D_W + m_0$
- hermiticity:

$$\gamma_5\tau^1\mathcal{D}\gamma_5\tau^1 = \mathcal{D}^\dagger$$

  however: not by simple "syntactic extension" of $D_W + m_0$, need to take into account b.c.'s for $\bar\chi$.

- programming: if one wants to avoid using a particular representation where $Q_\pm$ are diagonal, define

$$\phi(0,\mathbf{x}) = Q_-\chi(0,\mathbf{x}) + Q_+\chi(T,\mathbf{x}), \qquad \phi(x)|_{0<x_0<T} = \chi(x),$$

$\Rightarrow$ off-diagonal (in time) matrix elements but no problem in principle.

Alternative set-up (possibly simpler):

- Start with $2(T+a)$ anti-periodic fields ψ, $\bar{\psi}$

$$\psi(x_0 + 2(T+a), \mathbf{x}) = -\psi(x), \qquad \bar{\psi}(x_0 + 2(T+a), \mathbf{x}) = -\bar{\psi}(x),$$

- introduce a reflection ($R^2 = id$)

$$R : \psi(x) \to i\gamma_0\gamma_5\psi(-a - x_0, \mathbf{x}), \qquad \bar{\psi}(x) \to \bar{\psi}(-a - x_0, \mathbf{x})i\gamma_0\gamma_5$$

- the gauge field is extended to $[-T-a, T+a]$ and then periodically continued

$$U_k(-a - x_0, \mathbf{x}) = U_k(x_0, \mathbf{x}), \qquad U_0(-2a - x_0, \mathbf{x})^\dagger = U_0(x)$$

  this implies that the boundary layer is doubled!

- decompose in even/odd fields and define doublets $\chi, \bar{\chi}$ as before

- boundary conditions at "$x_0 \in [-a, 0]$" and "$x_0 \in [T, T+a]$", or at $x_0 = 0, T$ "up to O(a)":

$$Q_+(1 - \tfrac{1}{2}a\partial_0^*)\chi(x)|_{x_0=0} = 0, \qquad Q_-(1 + \tfrac{1}{2}a\partial_0)\chi(x)|_{x_0=T} = 0,$$

$$\bar\chi(x)Q_+(1 - \tfrac{1}{2}a\overleftarrow{\partial}_0^*)|_{x_0=0} = 0, \qquad \bar\chi(x)Q_-(1 + \tfrac{1}{2}a\overleftarrow{\partial}_0)|_{x_0=T} = 0.$$

- orbifold construction ensures that correct boundary conditions are obtained in the continuum limit.

- D_W becomes block diagonal and

$$\det_{-T\le x_0\le T+a}[D_W(N_\mathrm{f}=1)] = \det_{0\le x_0\le T}[2D_W(N_\mathrm{f}=2)]$$

- Defining again $\mathcal{D}$ it is now obtained directly by "syntactic extension" and $\gamma_5\tau^1$ hermitian.

Symmetries and Counterterms

- Symmetries ($C, P \times \tau^1$ etc.) $\Rightarrow$ possible dimension 3 counterterms at the boundaries:

$$K_1 = \overline{\chi} i\gamma_5\tau^3\chi, \qquad K_2 = \overline{\chi}\chi, \qquad K_3 = \overline{\chi} i\gamma_0\gamma_5\tau^3\chi$$

- K_1: multiplicative renormalization of ζ,ζ' and $\bar{\zeta}$,$\bar{\zeta}'$.

- $K_+ = \frac{1}{2}(K_2 + K_3) = \overline{\chi}Q_+\chi$ only refers to Dirichlet components (at $x_0 = 0$)
  $\Rightarrow$ irrelevant for correlation functions used in practice

- $K_- = \frac{1}{2}(K_2 - K_3) = \overline{\chi}Q_-\chi$ only contains non-Dirichlet components (at $x_0 = 0$);
  if chirally rotated back to the standard SF K_- is proportional to $\overline{\chi}' i\gamma_5\tau^3 P_-\chi'$ i.e. it violates parity and flavour symmetries!

- conclude: K_- is a *finite* counterterm which can be fixed by requiring parity restauration!

Mapping of SF correlation functions, continuum consideration:

$$\langle O[\chi,\bar{\chi}]\rangle_{(m,\mu_{\rm q},P_\pm)} = \langle \tilde{O}[\chi,\bar{\chi}]\rangle_{(\tilde{m},\tilde{\mu}_{\rm q},P_\pm(\alpha))}$$

with

$$\begin{aligned} \tilde{O}[\chi,\bar{\chi}] &= O\left[\exp(i\alpha\gamma_5\tau^3/2)\chi, \bar{\chi}\exp(i\alpha\gamma_5\tau^3/2\right] \\ \tilde{m} &= m\cos\alpha - \mu_{\rm q}\sin\alpha \\ \tilde{\mu}_{\rm q} &= m\sin\alpha + \mu_{\rm q}\cos\alpha \end{aligned}$$

boundary quark fields are included by replacing

$$\bar{\zeta}(\mathbf{x}) \leftrightarrow \bar{\chi}(0,\mathbf{x})P_+ \qquad \zeta(\mathbf{x}) \leftrightarrow P_-\chi(0,\mathbf{x})$$

parity/flavour symmetry restoration e.g. by imposing

$$f_{\rm V}^{11}(x_0) = 0, \qquad f_{\rm P}^{12}(x_0) = 0$$

simple example for mapping: SF coupling

$$\bar{g}^{-2}(L) = \langle O[U]\rangle_{(0,0,P_\pm)} = \langle O[U]\rangle_{(0,0,Q_\pm)}$$

A first application: the running coupling to one-loop order

In perturbation the SF coupling can be related to the $\overline{\mathrm{MS}}$-coupling

$$\bar{g}^2(L) = g^2_{\overline{\mathrm{MS}}}(\mu) + k_1(\mu L) g^4_{\overline{\mathrm{MS}}} + O(g^6)$$

here: consider fermionic contribution $\propto N_{\mathrm{f}}$ [Sommer, S. '95]

$$k_1 = k_{1,0} + N_{\mathrm{f}} k_{1,1}, \qquad k_{1,1} = -0.039863(2)/(4\pi)$$

in practice one computes for a sequence of lattices

$$f(L/a) \sim r_0 + (a/L)\left[r_1 + s_1 \ln(a/L)\right] + O(a^2)$$

- the correct continuum limit $r_0 = k_{1,1}$ is reproduced
- r_1 is to be cancelled by boundary O(a) counterterm $\propto c_{\mathrm{t}}$
- observation: s_1 vanishes independently of c_{sw}

Conclusions and Outlook

- Successful implementation of chirally rotated SF boundary conditions for Wilson quarks

- Universality: the additional dimension 3 counterterm needs to be fixed by parity

  $\Rightarrow$ SF coupling should be the same; checked to one-loop order

- Achievement:

  O(a) improvement in the bulk of massless standard or partially improved Wilson quarks

  $\Rightarrow$ Z-factors can be O(a) improved by tuning a couple of boundary O(a) counterterms;

  especially interesting for 4-quark operators

- check universality between maximally twisted mass QCD with standard SF boundary conditions, and standard QCD with twisted boundary projectors. (flavour and parity are just broken by the boundary conditions)