

Testing universality and automatic $O(a)$ improvement in massless lattice QCD with Wilson quarks



Stefan Sint, in collaboration with Björn Leder



- * $O(a)$ effects in the Schrödinger functional
- * The chirally rotated Schrödinger functional
- * Lattice implementation
- * Relations from universality
- * Lattice set-up and simulation results

CERN Theory Institute “Future directions in lattice gauge theory”, 21 July 2010

Motivation: a typical renormalisation problem

A typical calculation of a hadronic matrix element such as B_K can be split in 4 independent parts:

$$\langle h_f | O^{\overline{\text{MS}}}(\mu = 1/L_{\min}) | h_i \rangle =$$

$$\underbrace{Z_{\overline{\text{MS}},\text{SF}}(\bar{g}^2(L_{\min}))}_{\text{1-loop PT}} \times \underbrace{U(L_{\min}, L_{\max})}_{\text{scale evolution in CL}} \times \lim_{a \rightarrow 0} \underbrace{\left\{ Z(g_0^2, a/L_{\max}) \underbrace{\langle h_f | O(a) | h_i \rangle}_{\text{bare matrix element}} \right\}}_{\text{renormalized matrix element at scale } 1/L_{\max}}$$

The factor

$$U(L_{\min}, L_{\max}) = \lim_{a \rightarrow 0} \frac{Z(g_0^2, a/L_{\min})}{Z(g_0^2, a/L_{\max})}$$

is constructed in the continuum limit from the step-scaling functions;

- may use different regularisation from calculation of bare matrix element;
- use Wilson quarks or staggered quarks (computationally cheap).

$O(a)$ effects in SF schemes

- The time boundaries induce $O(a)$ effects; can be cancelled by 2 boundary counterterms:

$$a \int_{x_0=0,T} d^3\mathbf{x} \operatorname{tr} \{F_{0k}F_{0k}\}, \quad a \int_{x_0=0,T} d^3\mathbf{x} \bar{\psi} \gamma_0 D_0 \psi.$$

- Wilson fermions: additional $O(a)$ effects are cancelled by bulk $O(a)$ counterterms $\propto c_{\text{SW}}, c_A, \dots$
- \Rightarrow these are needed despite automatic $O(a)$ improvement of massless Wilson quarks (Frezzotti & Rossi '03)!
- The boundary $O(a)$ terms can be monitored/controlled; it would be nice if the mechanism of automatic $O(a)$ improvement in the bulk could be made compatible with the SF!

Mechanism of automatic $O(a)$ improvement (Frezzotti & Rossi '03)

In the absence of boundaries, automatic $O(a)$ improvement follows from chiral symmetry of the massless continuum action:

$$\psi \rightarrow \gamma_5 \psi \quad \bar{\psi} \rightarrow -\bar{\psi} \gamma_5,$$

Observables can be decomposed

$$O = O_+ + O_-, \quad O_{\pm}[\psi, \bar{\psi}] \rightarrow O_{\pm}[\gamma_5 \psi, -\bar{\psi} \gamma_5] = \pm O_{\pm}[\psi, \bar{\psi}]$$

One then shows that

$$\langle O_+ \rangle = \langle O_+ \rangle^{\text{cont}} + O(a^2), \quad \langle O_- \rangle = O(a),$$

Thus $O(a)$ effects are localised in γ_5 -odd observables/correlation functions & can be avoided!

- With SF boundary conditions: standard argument of automatic $O(a)$ improvement fails:

$$\gamma_5 P_{\pm} = P_{\mp} \gamma_5, \quad P_{\pm} = \frac{1}{2}(1 \pm \gamma_0)$$

\Rightarrow no way to define γ_5 -even or γ_5 -odd correlation functions!

- Possible solution: Give a flavour structure to the γ_5 -transformation, for $N_f = 2$:

$$\psi \rightarrow \gamma_5 \tau^1 \psi, \quad \bar{\psi} \rightarrow -\bar{\psi} \gamma_5 \tau^1,$$

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

$$\mathcal{P}_{\pm} = \frac{1}{2}(1 \pm \gamma_0 \tau^3), \quad \tilde{Q}_{\pm} = \frac{1}{2}(1 \pm i \gamma_0 \gamma_5 \tau^3)$$

$$\Rightarrow [\mathcal{P}_{\pm}, \gamma_5 \tau^1] = 0 = [\tilde{Q}_{\pm}, \gamma_5 \tau^1]$$

- Here: focus on projectors \tilde{Q}_{\pm} ; these arise naturally when chirally rotating the standard SF b.c.'s!

The Schrödinger functional and chiral rotations

In correlation functions derived from the Schrödinger functional,

$$\langle O[\psi, \bar{\psi}] \rangle_{(P_+)} = \mathcal{Z}^{-1} \int D[\psi, \bar{\psi}, A] O[\psi, \bar{\psi}] e^{-S}$$

the fermion fields ψ and $\bar{\psi}$ satisfy homogeneous Dirichlet boundary conditions with projectors $P_{\pm} = \frac{1}{2}(1 \pm \gamma_0)$,

$$\begin{aligned} P_+ \psi(x)|_{x_0=0} &= 0, & P_- \psi(x)|_{x_0=T} &= 0, \\ \bar{\psi}(x) P_-|_{x_0=0} &= 0, & \bar{\psi}(x) P_+|_{x_0=T} &= 0. \end{aligned}$$

Perform a chiral field rotation,

$$\psi \rightarrow \exp(i\alpha\gamma_5\tau^3/2)\psi, \quad \bar{\psi} \rightarrow \bar{\psi} \exp(i\alpha\gamma_5\tau^3/2),$$

the rotated fields satisfy chirally rotated boundary conditions

$$\begin{aligned} P_+(\alpha)\psi(x)|_{x_0=0} &= 0, & P_-(\alpha)\psi(x)|_{x_0=T} &= 0, \\ \bar{\psi}(x)\gamma_0 P_-(\alpha)|_{x_0=0} &= 0, & \bar{\psi}(x)\gamma_0 P_+(\alpha)|_{x_0=T} &= 0, \end{aligned}$$

with the projectors

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

Setting $\alpha = \pi/2$:

$$P_{\pm}(\pi/2) \equiv \tilde{Q}_{\pm} = \frac{1}{2}(1 \pm i\gamma_0\gamma_5\tau^3) = \text{diag}(Q_+, Q_-), \quad Q_{\pm} = \frac{1}{2}(1 \pm i\gamma_0\gamma_5)$$

A change of variables in the functional integral leads to:

$$\langle O[\psi, \bar{\psi}] \rangle_{(P_{\pm})} = \langle \tilde{O}[\psi, \bar{\psi}] \rangle_{(P_{\pm}(\alpha))}$$

with

$$\tilde{O}[\psi, \bar{\psi}] = O [\exp(i\alpha\gamma_5\tau^3/2)\psi, \bar{\psi} \exp(i\alpha\gamma_5\tau^3/2)]$$

NB: All mass terms are set to zero, otherwise one also needs to rotate masses covariantly (\rightarrow twisted mass QCD)

A note on symmetries

- In QCD the flavour vector transformation are identified as those leaving the quark mass term invariant. In massless QCD we are free to pick a convention.
 - Convention used here: standard SF boundary conditions are parity & isospin invariant, this defines our “physical basis”
- ⇒ Symmetries take a non-standard form in the chirally rotated SF (χ SF), as illustrated by the Ward identities:

$$\langle \delta_A^a O \rangle_{(P_\pm)} = \frac{1}{2} \int d^3z \langle [\bar{\zeta}(\mathbf{z}) \gamma_5 \tau^a \zeta(\mathbf{z}) + \bar{\zeta}'(\mathbf{z}) \gamma_5 \tau^a \zeta'(\mathbf{z})] O \rangle_{(P_\pm)}$$

$$\langle \delta_V^a O \rangle_{(P_\pm)} = 0$$

$$\langle \delta_A^a O \rangle_{(\tilde{Q}_\pm)} = \frac{i}{2} \delta^{3a} \int d^3z \langle [\bar{\zeta}(\mathbf{z}) \zeta(\mathbf{z}) + \bar{\zeta}'(\mathbf{z}) \zeta'(\mathbf{z})] O \rangle_{(\tilde{Q}_\pm)}$$

$$\langle \delta_V^a O \rangle_{(\tilde{Q}_\pm)} = \frac{i}{2} \varepsilon^{3ab} \int d^3z \langle [\bar{\zeta}(\mathbf{z}) \gamma_5 \tau^b \zeta(\mathbf{z}) - \bar{\zeta}'(\mathbf{z}) \gamma_5 \tau^b \zeta'(\mathbf{z})] O \rangle_{(\tilde{Q}_\pm)}$$

Lattice implementation of rotated SF boundary conditions

An orbifold procedure yields the structure of the lattice Dirac operator in the free theory:

$$\begin{aligned}
 S_f[U, \psi, \bar{\psi}] &= a^4 \sum_x \bar{\psi}(x) (\mathcal{D}_W + m_0) \psi(x) \\
 a\mathcal{D}_W \psi(x) &= -U(x, 0) P_- \psi(x + a\hat{\mathbf{0}}) + K \psi(x) - U(x - a\hat{\mathbf{0}})^\dagger P_+ \psi(x - a\hat{\mathbf{0}}). \\
 K \psi(x) &= \left(1 + am_0 + \frac{1}{2} \sum_{k=1}^3 \{ a(\nabla_k + \nabla_k^*) \gamma_k - a^2 \nabla_k^* \nabla_k \} \right) \psi(x) \\
 &\quad + \delta_{x_0, 0} i \gamma_5 \tau^3 P_- \psi(x) + \delta_{x_0, T} i \gamma_5 \tau^3 P_+ \psi(x).
 \end{aligned}$$

The lattice symmetries imply a list of possible $d = 3$ counterterms:

$$\begin{aligned}
 O_1 &= \bar{\psi} \gamma_0 Q_+ \psi - \bar{\psi} \gamma_0 Q_- \psi = \bar{\psi} i \gamma_5 \tau^3 \psi, \\
 O_2 &= \bar{\psi} \tilde{Q}_+ \psi, \\
 O_3 &= \bar{\psi} \tilde{Q}_- \psi,
 \end{aligned}$$

List of dimension-4 counterterms:

$$\begin{aligned}
O_4 &= \bar{\psi} \tilde{Q}_+ \gamma_k D_k \psi - \bar{\psi} \overleftarrow{D}_k \gamma_k \tilde{Q}_+ \psi, \\
O_5 &= \bar{\psi} \tilde{Q}_- \gamma_k D_k \psi - \bar{\psi} \overleftarrow{D}_k \gamma_k \tilde{Q}_- \psi, \\
O_6 &= \bar{\psi} \tilde{Q}_+ \gamma_0 D_0 \psi - \bar{\psi} \overleftarrow{D}_0 \gamma_0 \tilde{Q}_+ \psi, \\
O_7 &= \bar{\psi} \tilde{Q}_- \gamma_0 D_0 \psi - \bar{\psi} \overleftarrow{D}_0 \gamma_0 \tilde{Q}_- \psi, \\
O_8 &= \bar{\psi} \tilde{Q}_+ D_0 \psi + \bar{\psi} \overleftarrow{D}_0 \tilde{Q}_+ \psi, \\
O_9 &= \bar{\psi} \tilde{Q}_- D_0 \psi + \bar{\psi} \overleftarrow{D}_0 \tilde{Q}_- \psi, \\
O_{10} &= \bar{\psi} \tilde{Q}_+ \gamma_0 \gamma_k D_k \psi + \bar{\psi} \overleftarrow{D}_k \gamma_k \gamma_0 \tilde{Q}_+ \psi, \\
O_{11} &= \bar{\psi} \tilde{Q}_- \gamma_0 \gamma_k D_k \psi + \bar{\psi} \overleftarrow{D}_k \gamma_k \gamma_0 \tilde{Q}_- \psi,
\end{aligned}$$

Equations of motion:

$$O_4 + O_6 = 0, \quad O_5 + O_7 = 0, \quad O_8 + O_{10} = 0, \quad O_9 + O_{11} = 0.$$

Total derivative:

$$O_{10} - O_{11} = \partial_k (\bar{\psi} \gamma_k i \gamma_5 \tau^3 \psi),$$

So there are 11 operators and 5 relations \Rightarrow 6 counterterms!

Implementation of counterterms

- Replace $\mathcal{D}_W \rightarrow \mathcal{D}_W + \delta\mathcal{D}_W$,

$$\delta\mathcal{D}_W\psi(x) = (\delta_{x_0,0} + \delta_{x_0,T}) \left[(z_f - 1) + (d_s - 1) a\mathbf{D}_s \right] \psi(x).$$

$$\mathbf{D}_s = \frac{1}{2}(\nabla_k + \nabla_k^*)\gamma_k.$$

- Parameterize the basic fermionic 2-point functions, e.g.

$$[\psi(x)\bar{\zeta}(\mathbf{y})]_F = S(x; a, \mathbf{y})U_0(0, \mathbf{y})^\dagger (1 - \bar{d}_s a\bar{\mathbf{D}}_s) \tilde{Q}_-,$$

$$[\zeta(\mathbf{x})\bar{\zeta}(\mathbf{y})]_F = \tilde{Q}_- (1 + \bar{d}_s a\mathbf{D}_s) \left[\bar{S}(0, \mathbf{x}; 0, \mathbf{y}) - (\tilde{z}_f + \tilde{d}_s a\mathbf{D}_s)\delta(\mathbf{x} - \mathbf{y}) \right] (1 - \bar{d}_s a\bar{\mathbf{D}}_s) \tilde{Q}_-$$

$$[\zeta(\mathbf{x})\bar{\zeta}'(\mathbf{y})]_F = \tilde{Q}_- (1 + \bar{d}_s a\mathbf{D}_s) \bar{S}(0, \mathbf{x}; T, \mathbf{y}) (1 - \bar{d}_s a\bar{\mathbf{D}}_s) \tilde{Q}_+,$$

- Renormalize the quark boundary fields:

$$\zeta_R = Z_\zeta \zeta, \quad \bar{\zeta}_R = Z_\zeta \bar{\zeta}, \quad \zeta'_R = Z_\zeta \zeta', \quad \bar{\zeta}'_R = Z_\zeta \bar{\zeta}'.$$

Some observations

- The constants z_f, \tilde{z}_f are finite (scale independent) and must be tuned to restore parity & flavour symmetry
- The constant \bar{d}_s parametrizes the $\gamma_5\tau^1$ -odd counterterm O_{10} and can usually be ignored.
- The constants \tilde{z}_f and \tilde{d}_s only occur in correlation functions where disconnected diagrams contribute; can be avoided by appropriate flavour assignments.
- Comparison to standard SF: in practice,

$$\{Z_\zeta, c_t, \tilde{c}_t, c_{\text{sw}}, c_A, \dots\} \longleftrightarrow \{Z_\zeta, c_t, d_s, z_f\}$$

i.e. automatic $O(a)$ improvement is obtained by tuning z_f .

- Tree level values: $Z_\zeta = 1, z_f = 1, d_s = \frac{1}{2}, \tilde{d}_s = 1, \bar{d}_s = 0,$

SF correlation functions

Standard SF correlators: use pseudo-scalar and vector boundary sources

$$\mathcal{O}_5^{f_1 f_2} = a^6 \sum_{\mathbf{y}, \mathbf{z}} \bar{\zeta}_{f_1}(\mathbf{y}) \gamma_5 P_- \zeta_{f_2}(\mathbf{z}) \quad \mathcal{O}_k^{f_1 f_2} = a^6 \sum_{\mathbf{y}, \mathbf{z}} \bar{\zeta}_{f_1}(\mathbf{y}) \gamma_k P_- \zeta_{f_2}(\mathbf{z})$$

consider all possible 2-point functions with quark bilinear operators $X^{f_1 f_2}(x)$ ($X = A_0, P, V_0, S$) and $Y_k^{f_1 f_2}(x)$ ($Y_k = V_k, T_{0k}, A_k, \tilde{T}_{0k}$):

$$f_X(x_0) = -\frac{1}{2} \langle X^{f_1 f_2}(x) \mathcal{O}_5^{f_2 f_1} \rangle_{(P_{\pm})}, \quad k_Y(x_0) = -\frac{1}{6} \sum_{k=1}^3 \langle Y_k^{f_1 f_2}(x) \mathcal{O}_k^{f_2 f_1} \rangle_{(P_{\pm})},$$

Boundary-to-boundary correlators:

$$f_1 = -\frac{1}{2} \langle \mathcal{O}_5^{f_1 f_2} \mathcal{O}_5^{\prime f_2 f_1} \rangle_{(P_{\pm})}, \quad k_1 = -\frac{1}{6} \sum_{k=1}^3 \langle \mathcal{O}_k^{f_1 f_2} \mathcal{O}_k^{\prime f_2 f_1} \rangle_{(P_{\pm})}$$

χ SF correlation functions

Main difference: two-point functions now depend on the flavour indices:

$$g_X^{f_1 f_2}(x_0)_\pm = -\frac{1}{2} \langle X^{f_1 f_2}(x) Q_{5,\pm}^{f_2 f_1} \rangle_{(\tilde{Q}_\pm)} \quad l_Y^{f_1 f_2}(x_0)_\pm = -\frac{1}{6} \sum_{k=1}^3 \langle Y_k^{f_1 f_2}(x) Q_k^{f_2 f_1} \rangle_{(\tilde{Q}_\pm)}$$

Boundary-to-boundary correlators:

$$g_1^{f_1 f_2} = -\frac{1}{2} \langle Q_5^{f_1 f_2} Q_5'^{f_2 f_1} \rangle_{(\tilde{Q}_\pm)}, \quad l_1^{f_1 f_2} = -\frac{1}{6} \sum_{k=1}^3 \langle Q_k^{f_1 f_2} Q_k'^{f_2 f_1} \rangle_{(\tilde{Q}_\pm)}$$

Boundary sources:

$$Q_5^{uu'} = a^6 \sum_{y,z} \bar{\zeta}_u(\mathbf{y}) \gamma_0 \gamma_5 Q_- \zeta_{u'}(\mathbf{z}), \quad Q_5^{ud} = a^6 \sum_{y,z} \bar{\zeta}_u(\mathbf{y}) \gamma_5 Q_+ \zeta_d(\mathbf{z})$$

$$Q_k^{uu'} = a^6 \sum_{y,z} \bar{\zeta}_u(\mathbf{y}) \gamma_k Q_- \zeta_{u'}(\mathbf{z}), \quad Q_k^{ud} = a^6 \sum_{y,z} \bar{\zeta}_u(\mathbf{y}) \gamma_0 \gamma_k Q_+ \zeta_d(\mathbf{z})$$

Notation: $\zeta(\mathbf{x}) \leftrightarrow \psi(x)|_{x_0=0}$ and $\bar{\zeta}(\mathbf{x}) \leftrightarrow \bar{\psi}(x)|_{x_0=0}$ (translated to the lattice)

Dictionary: standard \leftrightarrow rotated SF correlation functions

- Perform a chiral rotation by $\alpha = \pi/2$; 4 possibilities: $f_1 f_2 = uu', dd', ud, du$; assume existence of a second doublet (u', d') \Rightarrow no disconnected diagrams
- Non-vanishing correlations functions with pseudo-scalar source

$$f_A = g_A^{uu'} = -ig_V^{ud}, \quad f_P = ig_S^{uu'} = g_P^{ud}, \quad f_1 = g_1^{uu'} = g_1^{ud}$$

- Non-vanishing correlations functions with vector source

$$k_V = l_V^{uu'} = -il_A^{ud} \quad k_T = il_{\tilde{T}}^{uu'} = l_T^{ud} \quad k_1 = l_1^{uu'} = l_1^{ud}$$

- All other correlation functions vanish by parity or flavour symmetries!

$$f_S = ig_P^{uu'} = g_S^{ud} = 0 = f_V = g_V^{uu'} = -ig_A^{ud},$$

$$k_A = l_A^{uu'} = -il_V^{ud} = 0 = k_{\tilde{T}} = il_{\tilde{T}}^{uu'} = l_{\tilde{T}}^{ud}$$

Rôle of z_f and boundary conditions

- Counterterm $\propto z_f$: renormalisation of α in the boundary projectors $P_{\pm}(\alpha)$ away from $P_{\pm}(\pi/2) \equiv \tilde{Q}_{\pm}$.
 - Tuning of z_f restores the $\gamma_5\tau^1$ -symmetry which is necessary for automatic $O(a)$ improvement. This symmetry is a flavour symmetry in our conventions.
- \Rightarrow Tuning conditions for z_f : require any $\gamma_5\tau^1$ -odd quantity (e.g. g_A^{ud} , $l_T^{uu'}$, ...) to vanish exactly; different tuning conditions: expect $O(a)$ differences in tuned values z_f^*
- Boundary quark fields are defined as in the standard SF:

$$\zeta(\mathbf{x}) \leftrightarrow U(0, \mathbf{x}; 0)\tilde{Q}_-\psi(a, \mathbf{x}), \quad \bar{\zeta}(\mathbf{x}) \leftrightarrow \bar{\psi}(a, \mathbf{x})\tilde{Q}_-U(x, 0)^\dagger,$$

To test the Dirichlet boundary conditions we reverse the projectors $\tilde{Q}_- \rightarrow \tilde{Q}_+$. For comparison we do the same in the standard SF.

Non-perturbative quenched study

- Quenched simulations with Wilson quarks with and without $O(a)$ improvement à la Sheikholeslami-Wohlert
- DDHMC code + SF boundary conditions, both standard and rotated
- Lattice sizes $(L/a)^3 \times (T/a)$ with $T = L$ and

$$L/a = 8, 12, 16, 24, 32$$

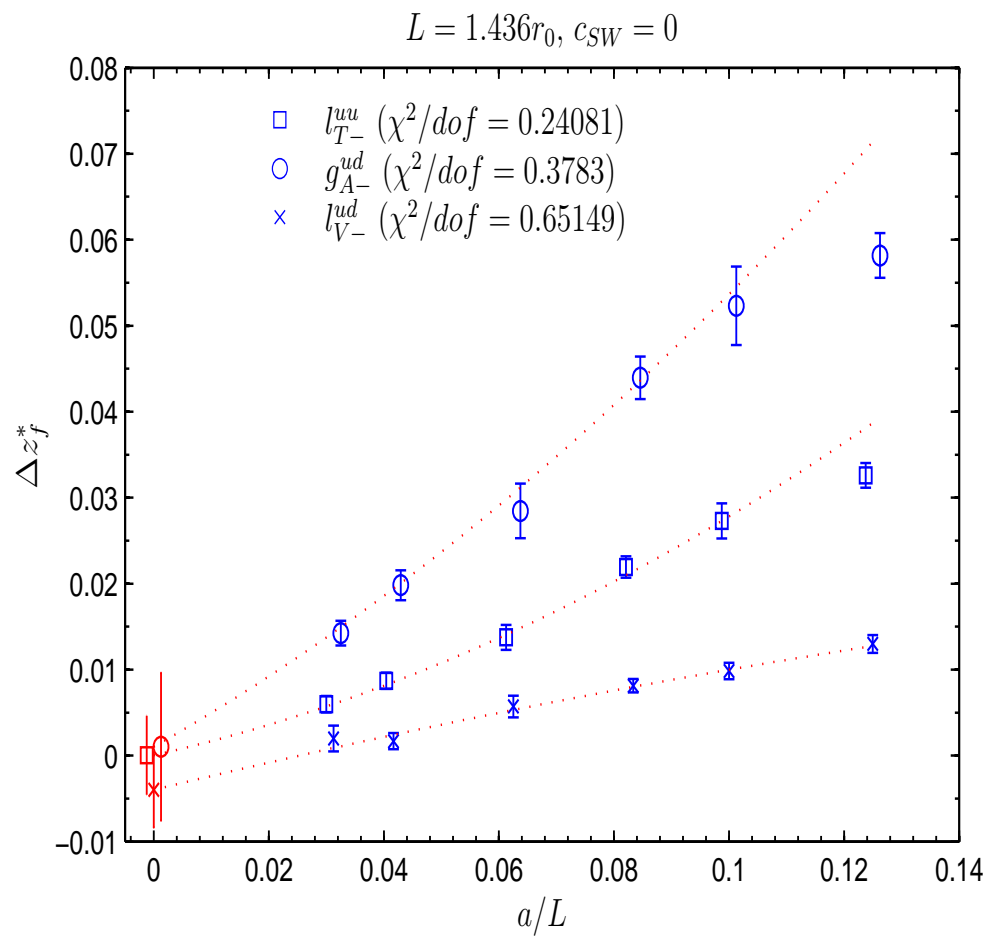
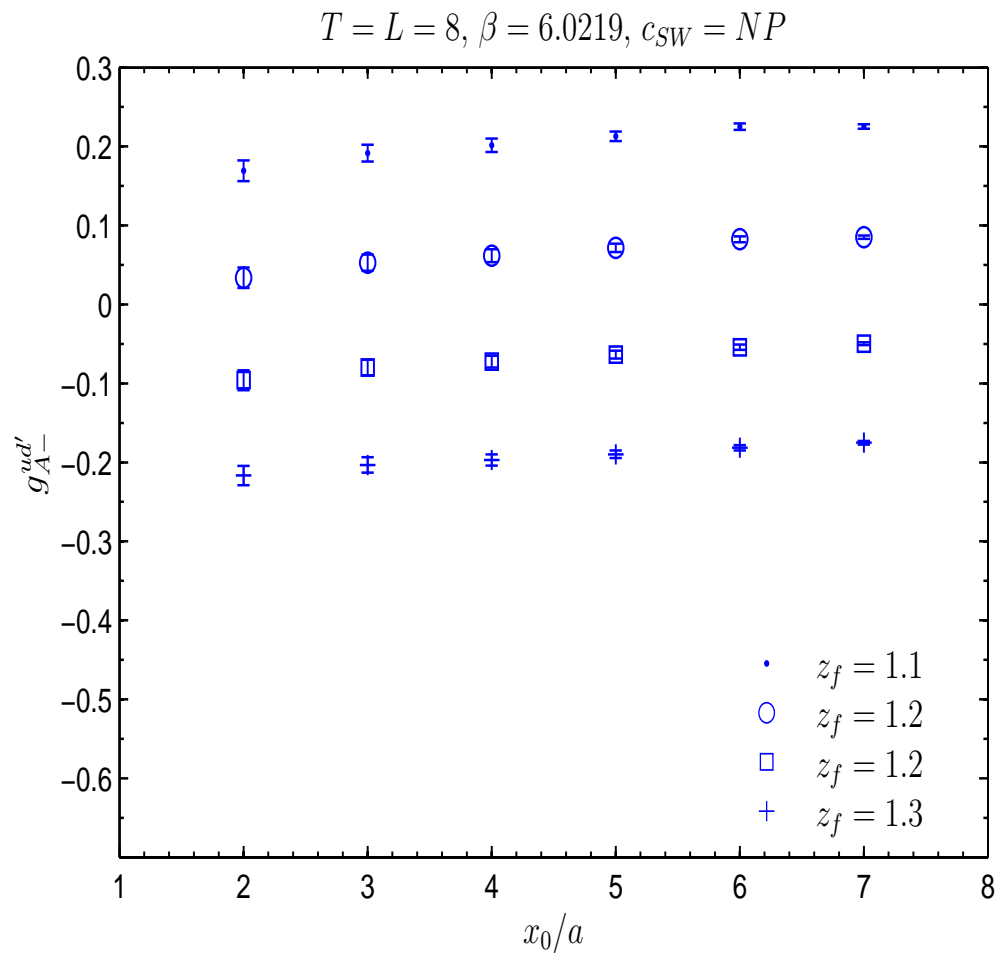
keeping L/r_0 constant $\Rightarrow a = 0.025 - 0.1$ fm

- m_{critical} is taken from the PCAC relation in the standard SF

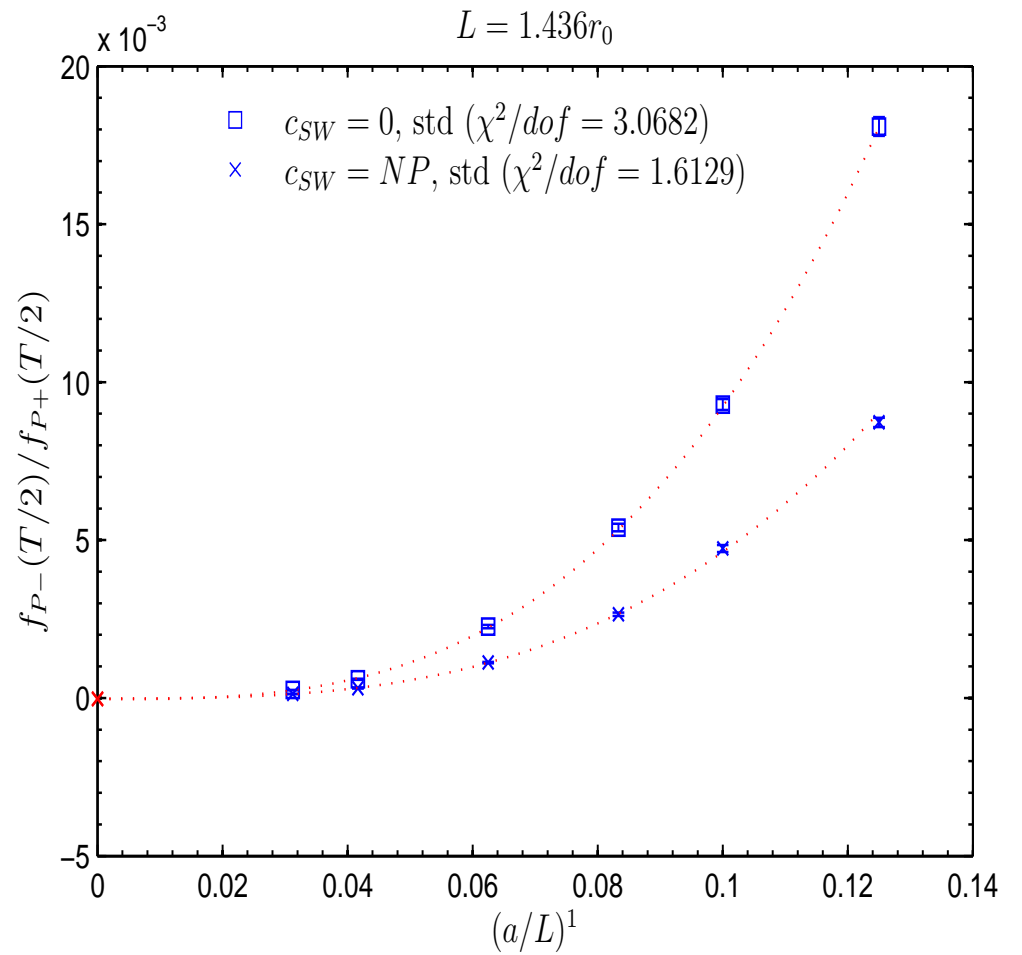
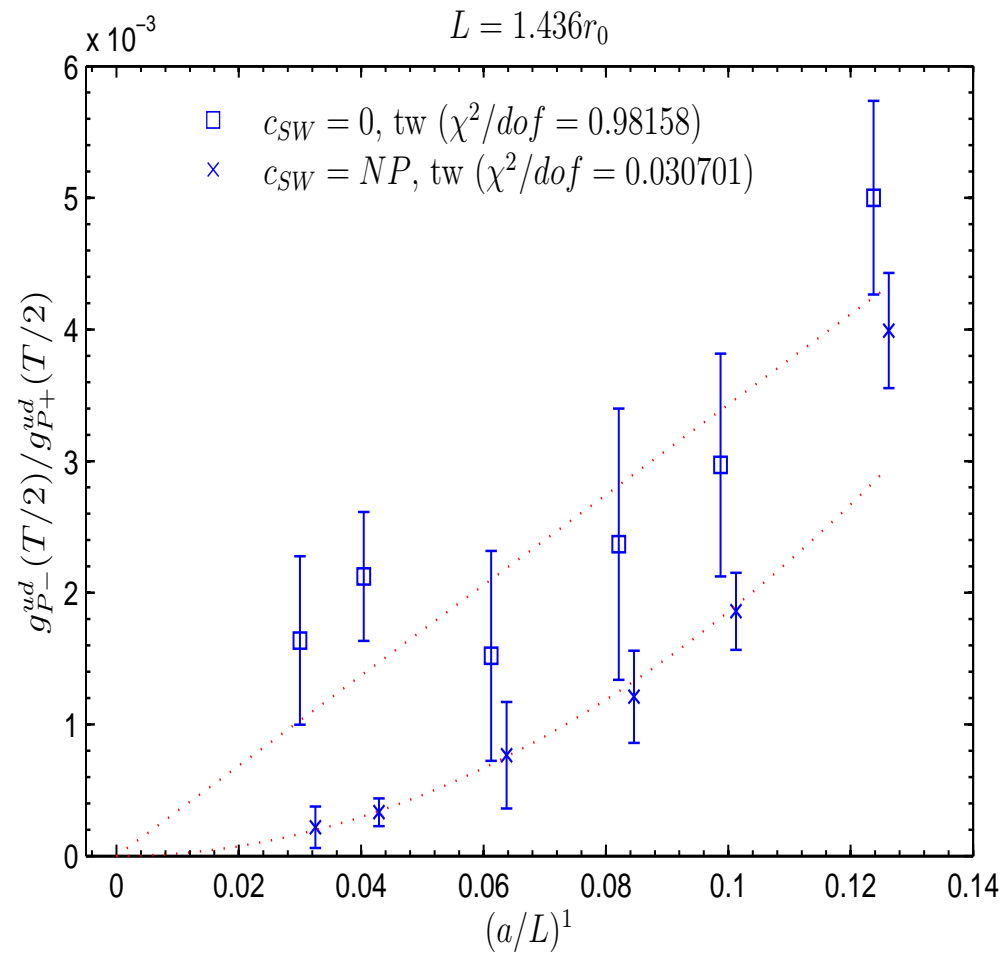
A laundry list

- How difficult is the tuning of z_f ?
- check that the Dirichlet boundary conditions are indeed obtained as expected.
- check universality between rotated and standard SF correlation functions
- check that automatic $O(a)$ improvement works out as expected: $\gamma_5\tau^1$ -odd correlators should be of $O(a)$.
- Use universality to determine finite ratios of renormalization constants

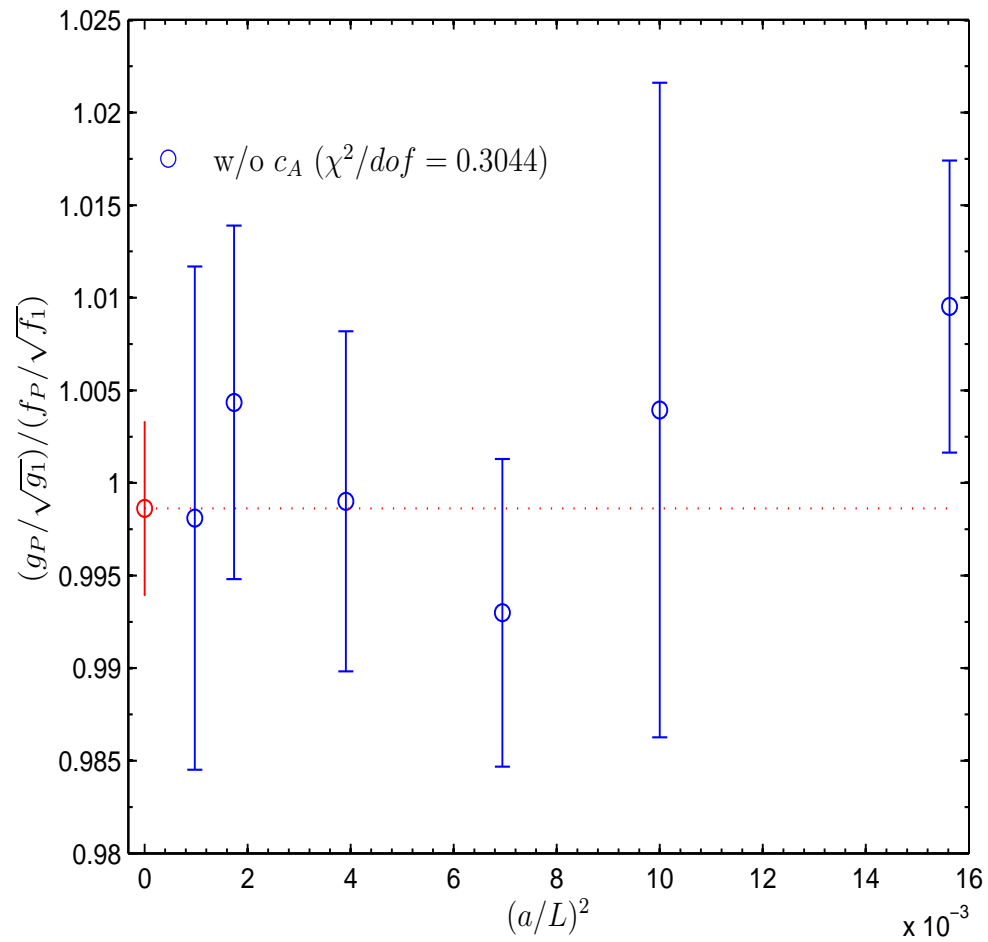
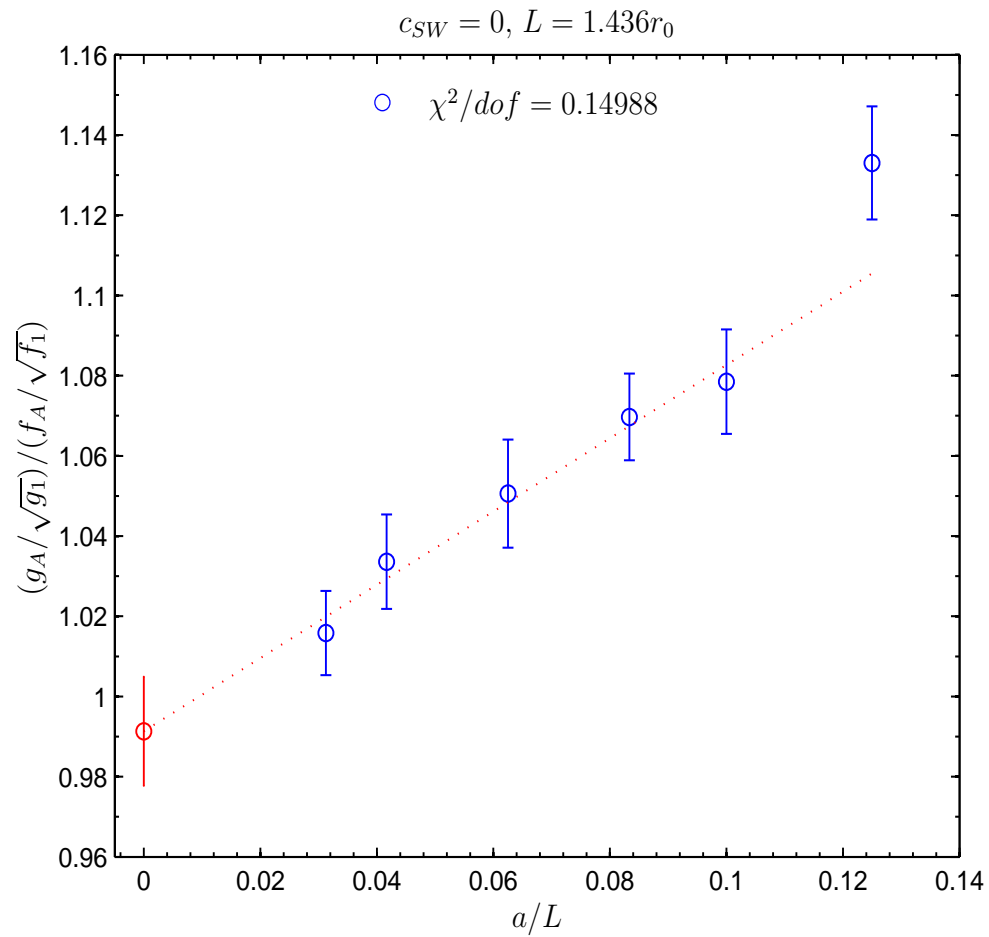
Tuning of z_f (see also ETMC (J. Gonzalez-Lopez et al), 09)



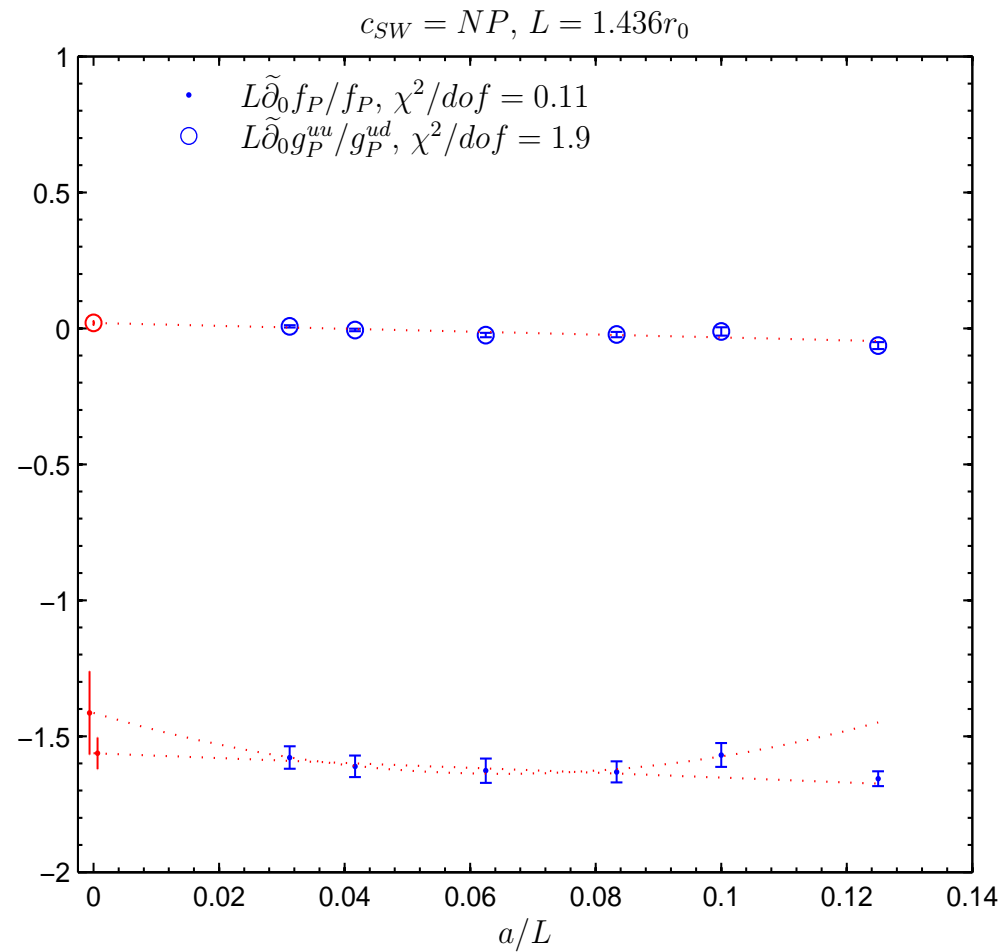
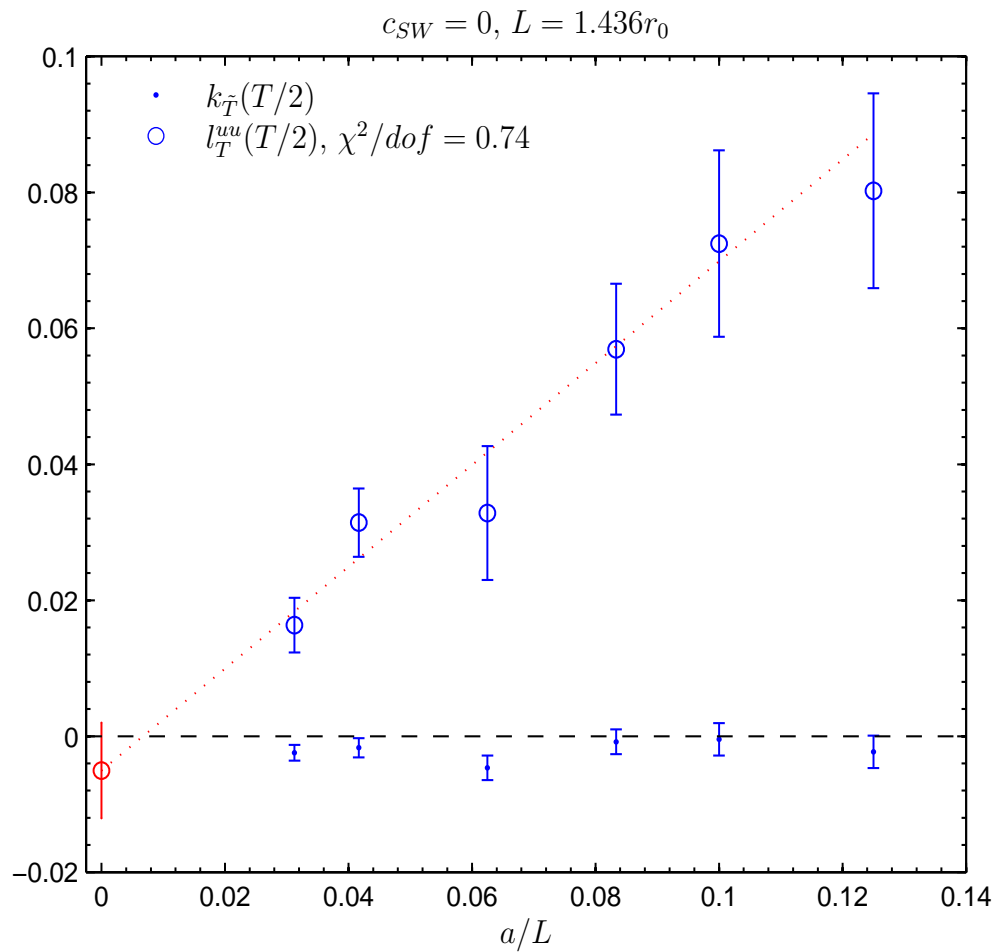
Check of Dirichlet boundary conditions



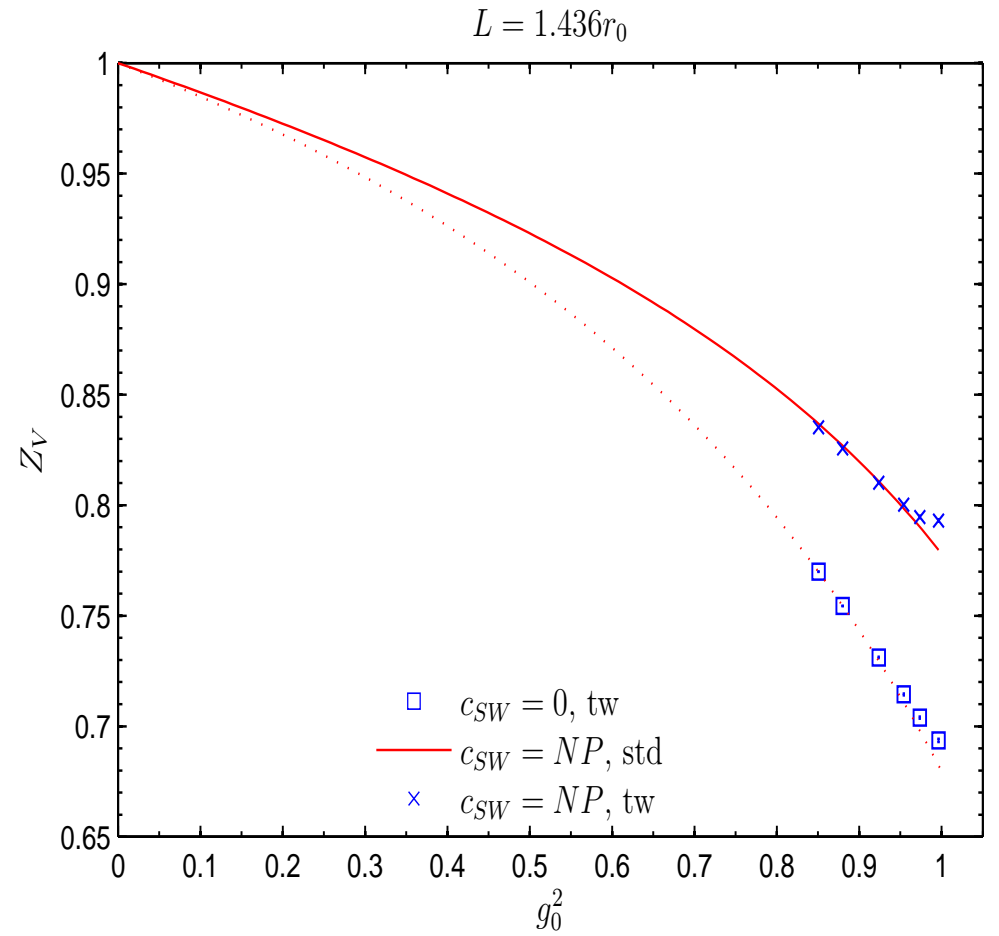
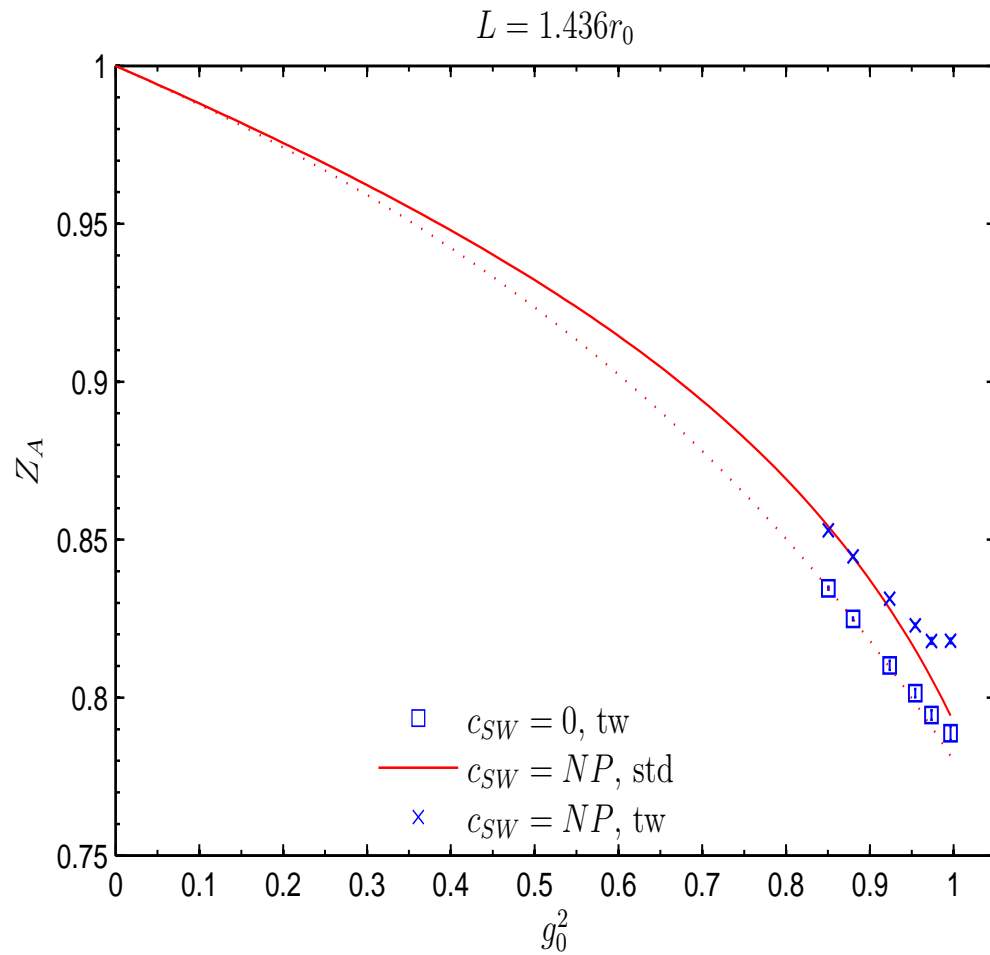
Universality checks



Check of automatic $O(a)$ improvement



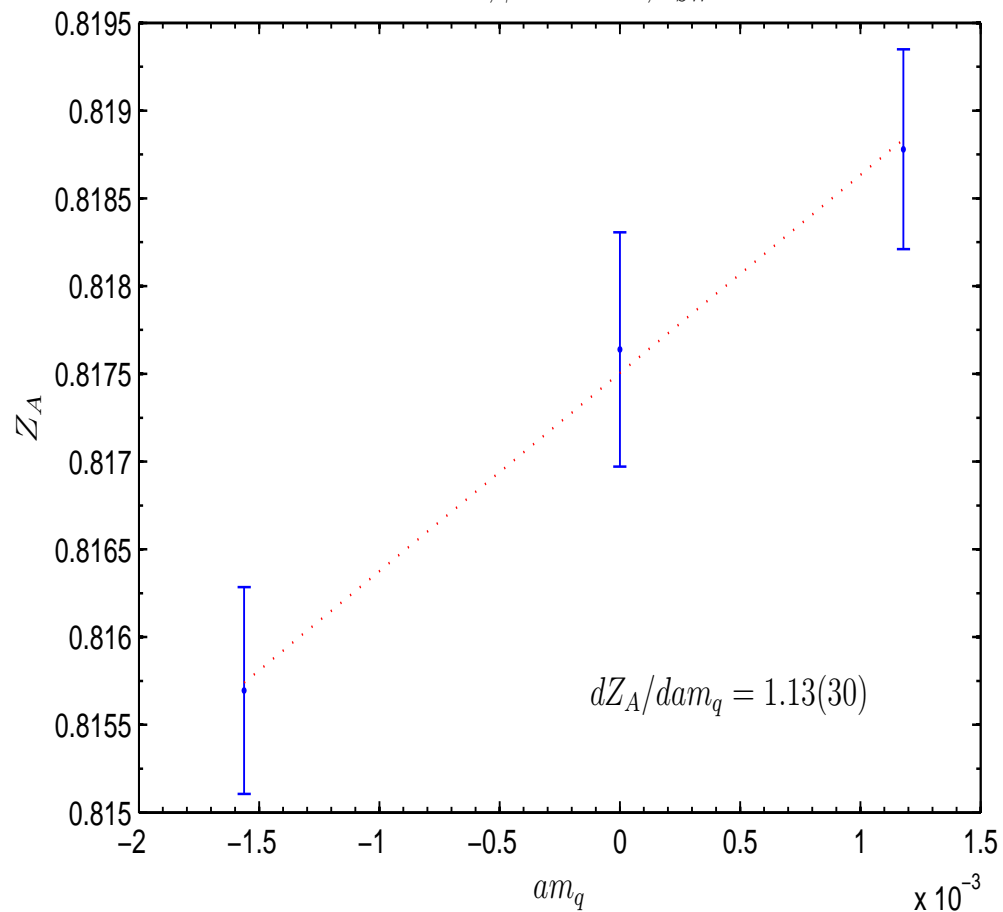
Determination of $Z_{A,V}$



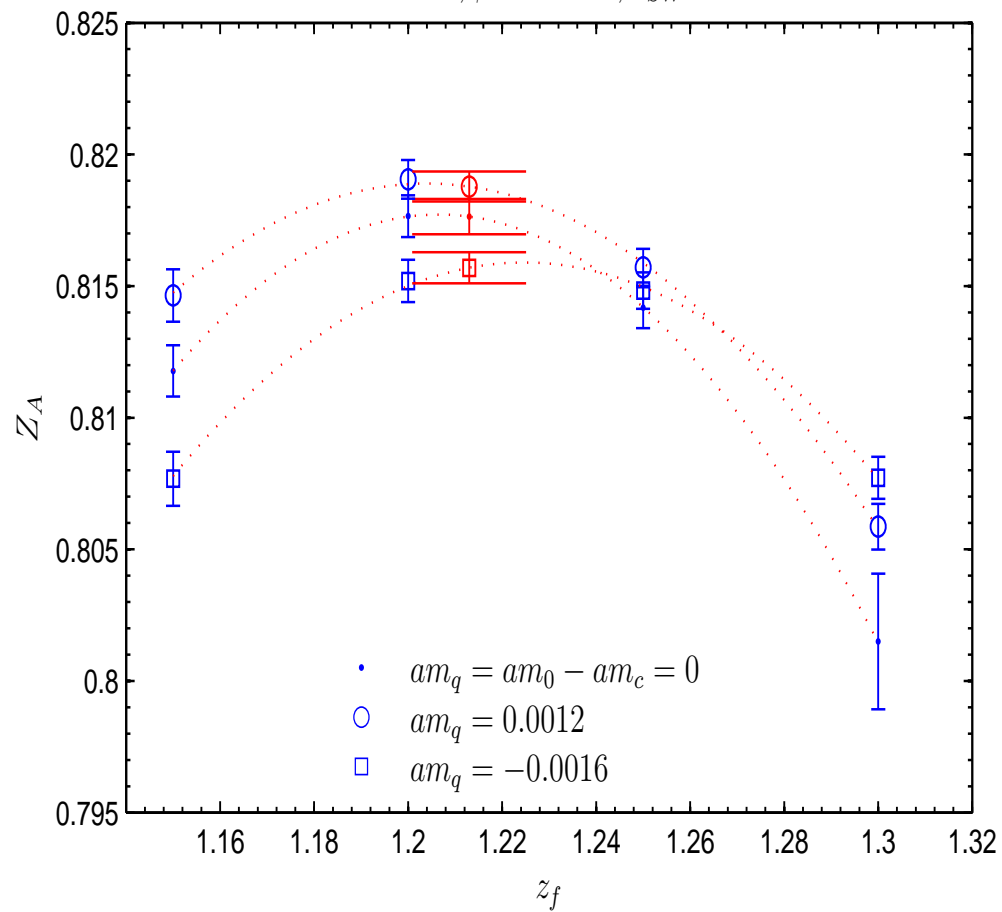
$$Z_A = ig_{\tilde{V}}(T/2)/g_A(T/2) \text{ and } Z_V = g_{\tilde{V}}(T/2)/g_V(T/2)$$

m_0 - and z_f -dependence of Z_A

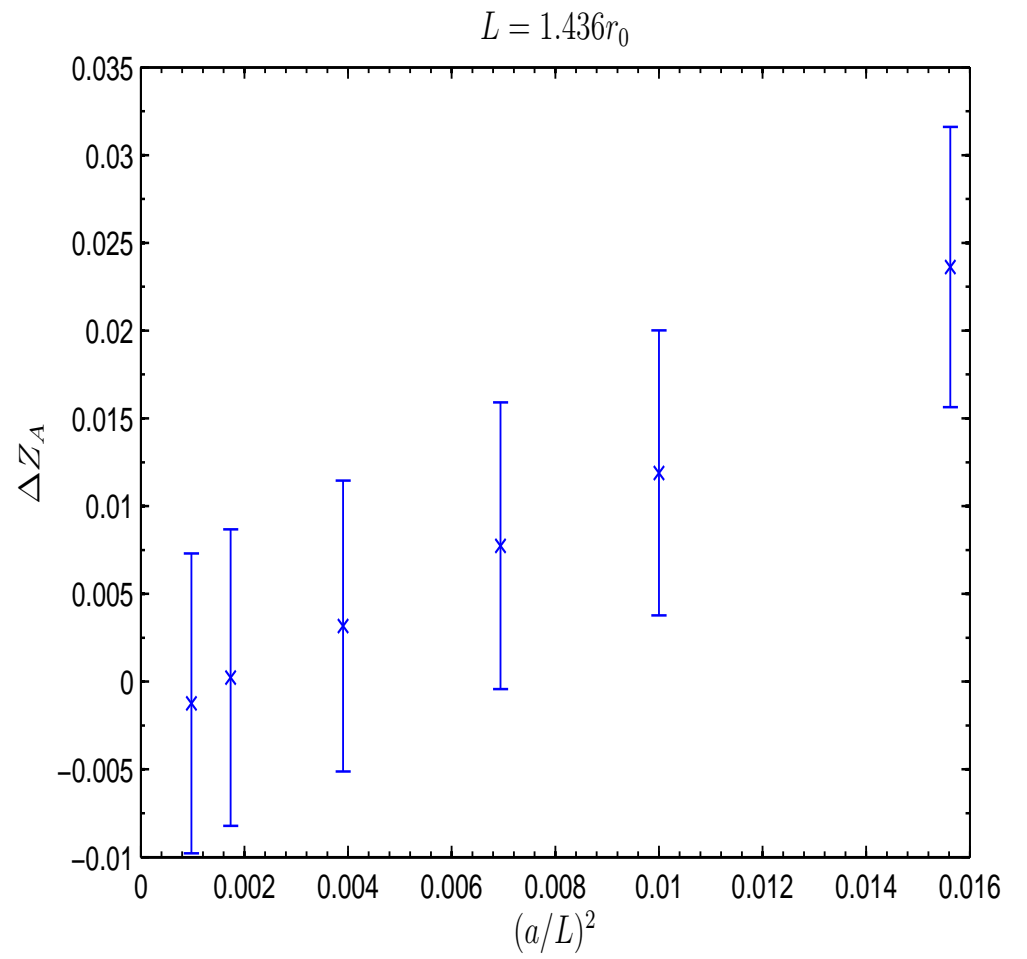
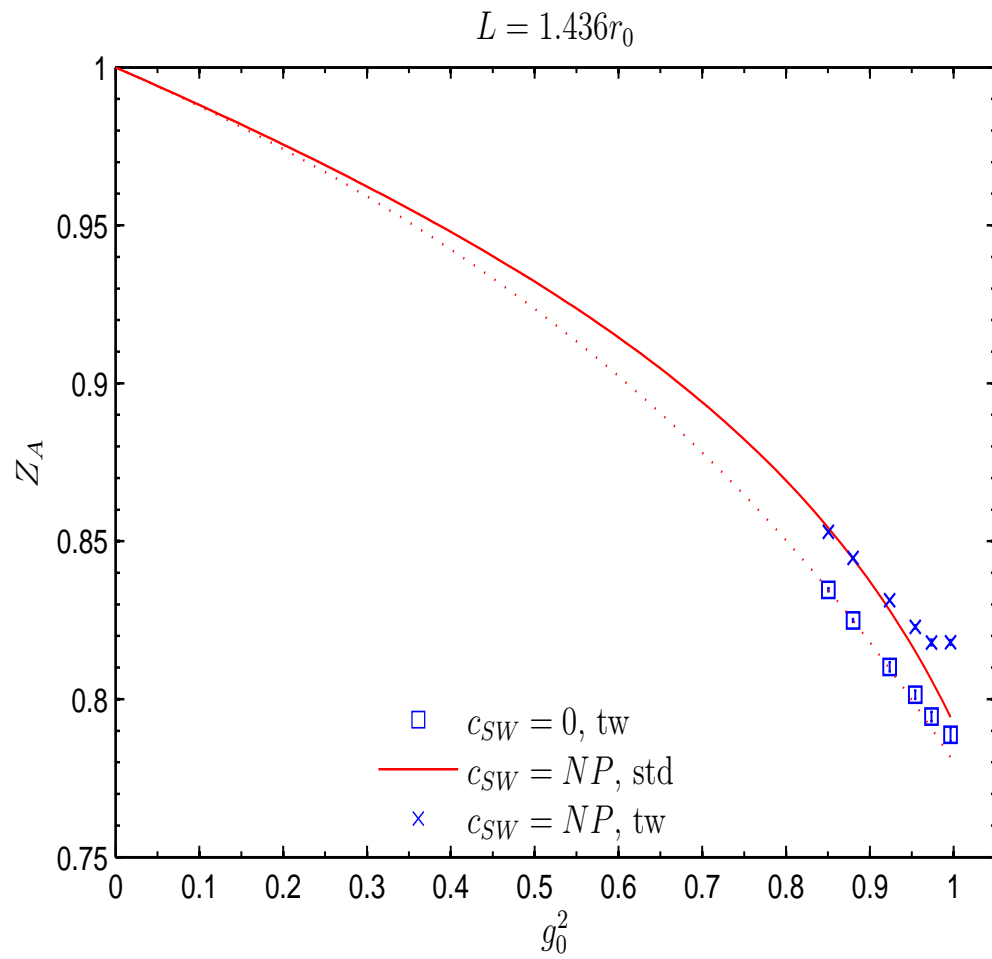
$T = L = 8, \beta = 6.0219, c_{SW} = NP$



$T = L = 8, \beta = 6.0219, c_{SW} = NP$



$O(a^2)$ uncertainty in Z_A



Conclusions and Outlook

- Successful implementation of chirally rotated SF b.c.'s for Wilson quarks
- Tuning of the dimension-3 counterterm coefficient z_f straightforward and almost orthogonal to the tuning of m_0 .
- Achievement: bulk $O(a)$ improvement of massless standard or partially improved Wilson quarks
 - ⇒ Z -factors in SF schemes are $O(a)$ improved by tuning the boundary $O(a)$ counterterms (c_t and $d_s \Leftrightarrow \tilde{c}_t$;
interesting for 4-quark operators, higher twist operators, . . .
- Applications to Technicolor-inspired models, avoids determination of c_{SW} .
- New methods to determine finite renormalisation constants $Z_A, Z_V, Z_P/Z_S, \dots$ and improvement coefficients $c_A, c_V, c_{\text{SW}}, \dots$).