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

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* The chirally rotated Schödinger functional

* Relations from universality

* Automatic O(a) improvement

* Lattice set-up and simulations

* Some results

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The Schrödinger functional and chiral rotations

In correlation functions derived from the Schrödinger functional,

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

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

$$P_+\psi(x)|_{x_0=0} = 0, \qquad P_-\psi(x)|_{x_0=T} = 0,$$

$$\overline{\psi}(x)P_-|_{x_0=0} = 0, \qquad \overline{\psi}(x)P_+|_{x_0=T} = 0.$$

Perform a chiral field rotation,

$$\psi \to \exp(i\alpha\gamma_5\tau^3/2)\psi, \qquad \overline{\psi} \to \overline{\psi}\exp(i\alpha\gamma_5\tau^3/2),$$

the rotated fields satisfy chirally rotated boundary conditions

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

with the projectors

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

Setting $\alpha = \pi/2$:

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

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

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 (χSF), as illustrated by the Ward identities:

$$\begin{aligned}
\langle \delta_{\mathrm{A}}^a O \rangle_{(P_\pm)} &= \tfrac{1}{2} \int \mathrm{d}^3 z \, \langle \left[\bar{\zeta}(\mathbf{z}) \gamma_5 \tau^a \zeta(\mathbf{z}) + \bar{\zeta}'(\mathbf{z}) \gamma_5 \tau^a \zeta'(\mathbf{z}) \right] O \rangle_{(P_\pm)} \\
\langle \delta_{\mathrm{V}}^a O \rangle_{(P_\pm)} &= 0
\end{aligned}$$

$$\begin{aligned}
\langle \delta_{\mathrm{A}}^a O \rangle_{(\tilde{Q}_\pm)} &= \tfrac{i}{2} \delta^{3a} \int \mathrm{d}^3 z \, \langle \left[\bar{\zeta}(\mathbf{z}) \zeta(\mathbf{z}) + \bar{\zeta}'(\mathbf{z}) \zeta'(\mathbf{z}) \right] O \rangle_{(\tilde{Q}_\pm)} \\
\langle \delta_{\mathrm{V}}^a O \rangle_{(\tilde{Q}_\pm)} &= \tfrac{i}{2} \varepsilon^{3ab} \int \mathrm{d}^3 z \, \langle \left[\bar{\zeta}(\mathbf{z}) \gamma_5 \tau^b \zeta(\mathbf{z}) - \bar{\zeta}'(\mathbf{z}) \gamma_5 \tau^b \zeta'(\mathbf{z}) \right] O \rangle_{(\tilde{Q}_\pm)}
\end{aligned}$$

SF correlation functions

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

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

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

$$f_{\mathrm{X}}(x_0) = -\tfrac{1}{2} \langle X^{f_1 f_2}(x) \mathcal{O}_5^{f_2 f_1} \rangle_{(P_\pm)}, \qquad k_{\mathrm{Y}}(x_0) = -\tfrac{1}{6} \sum_{k=1}^{3} \langle Y_k^{f_1 f_2}(x) \mathcal{O}_k^{f_2 f_1} \rangle_{(P_\pm)},$$

Boundary-to-boundary correlators:

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

χSF correlation functions

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

$$g_{\mathrm{X}}^{f_1 f_2}(x_0)_\pm = -\tfrac{1}{2}\langle X^{f_1 f_2}(x)\mathcal{Q}_{5,\pm}^{f_2 f_1}\rangle_{(\tilde{Q}_\pm)} \qquad l_{\mathrm{Y}}^{f_1 f_2}(x_0)_\pm = -\tfrac{1}{6}\sum_{k=1}^{3}\langle Y_k^{f_1 f_2}(x)\mathcal{Q}_k^{f_2 f_1}\rangle_{(\tilde{Q}_\pm)}$$

Boundary-to-boundary correlators:

$$g_1^{f_1 f_2} = -\tfrac{1}{2}\langle \mathcal{Q}_5^{f_1 f_2}\mathcal{Q}_5^{\prime\, f_2 f_1}\rangle_{(\tilde{Q}_\pm)}, \qquad l_1^{f_1 f_2} = -\tfrac{1}{6}\sum_{k=1}^{3}\langle \mathcal{Q}_k^{f_1 f_2}\mathcal{Q}_k^{\prime\, f_2 f_1}\rangle_{(\tilde{Q}_\pm)}$$

Boundary sources:

$$\mathcal{Q}_5^{uu'} = a^6\sum_{\mathbf{y},\mathbf{z}}\bar{\zeta}_u(\mathbf{y})\gamma_0\gamma_5 Q_-\zeta_{u'}(\mathbf{z}), \qquad \mathcal{Q}_5^{ud} = a^6\sum_{\mathbf{y},\mathbf{z}}\bar{\zeta}_u(\mathbf{y})\gamma_5 Q_+\zeta_d(\mathbf{z})$$

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

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

$$f_{\rm A} = g_{\rm A}^{uu'} = -i g_{\rm V}^{ud}, \qquad f_{\rm P} = i g_{\rm S}^{uu'} = g_{\rm P}^{ud}, \qquad f_1 = g_1^{uu'} = g_1^{ud}$$

- Non-vanishing correlations functions with vector source

$$k_{\rm V} = l_{\rm V}^{uu'} = -i l_{\rm A}^{ud} \qquad k_{\rm T} = i l_{\tilde{\rm T}}^{uu'} = l_{\rm T}^{ud} \qquad k_1 = l_1^{uu'} = l_1^{ud}$$

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

$$\begin{aligned} f_{\rm S} = i g_{\rm P}^{uu'} = g_{\rm S}^{ud} = \quad & 0 \quad = f_{\rm V} = g_{\rm V}^{uu'} = -i g_{\rm A}^{ud}, \\ k_{\rm A} = l_{\rm A}^{uu'} = -i l_{\rm V}^{ud} = \quad & 0 \quad = k_{\tilde{\rm T}} = i l_{\rm T}^{uu'} = l_{\tilde{\rm T}}^{ud} \end{aligned}$$

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

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

$$\gamma_5 P_\pm = P_\mp \gamma_5$$

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

- χSF boundary conditions: can define $\gamma_5\tau^1$-even/odd correlation functions:

$$\gamma_5\tau^1\tilde{Q}_\pm = \tilde{Q}_\pm\gamma_5\tau^1$$

- The $\gamma_5\tau^1$-transformation is a flavour symmetry in our convention!

- Analogous argument using parity (Shindler '05)

The lattice action

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

Implement counterterms by replacing $\mathcal{D}_W \to \mathcal{D}_W + \delta\mathcal{D}_W$,

$$
\begin{aligned}
\delta\mathcal{D}_W\psi(x) &= (\delta_{x_0,0} + \delta_{x_0,T})\Big[(z_f - 1)\,\psi(x) \\
&\quad + (d_s - 1)\,\tfrac{1}{2}\sum_{k=1}^{3}\left\{a(\nabla_k + \nabla_k^*)\gamma_k - a^2\nabla_k^*\nabla_k\right\}\psi(x)\Big].
\end{aligned}
$$

with $d_s = 1/2 + \mathrm{O}(g_0^2)$ and $z_f = 1 + \mathrm{O}(g_0^2)$

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 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:

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

Test the Dirichlet boundary conditions: 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 $\Rightarrow a = 0.025 - 0.1\,\mathrm{fm}$

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

A laundry list

- How difficult is the tuning of z_f?

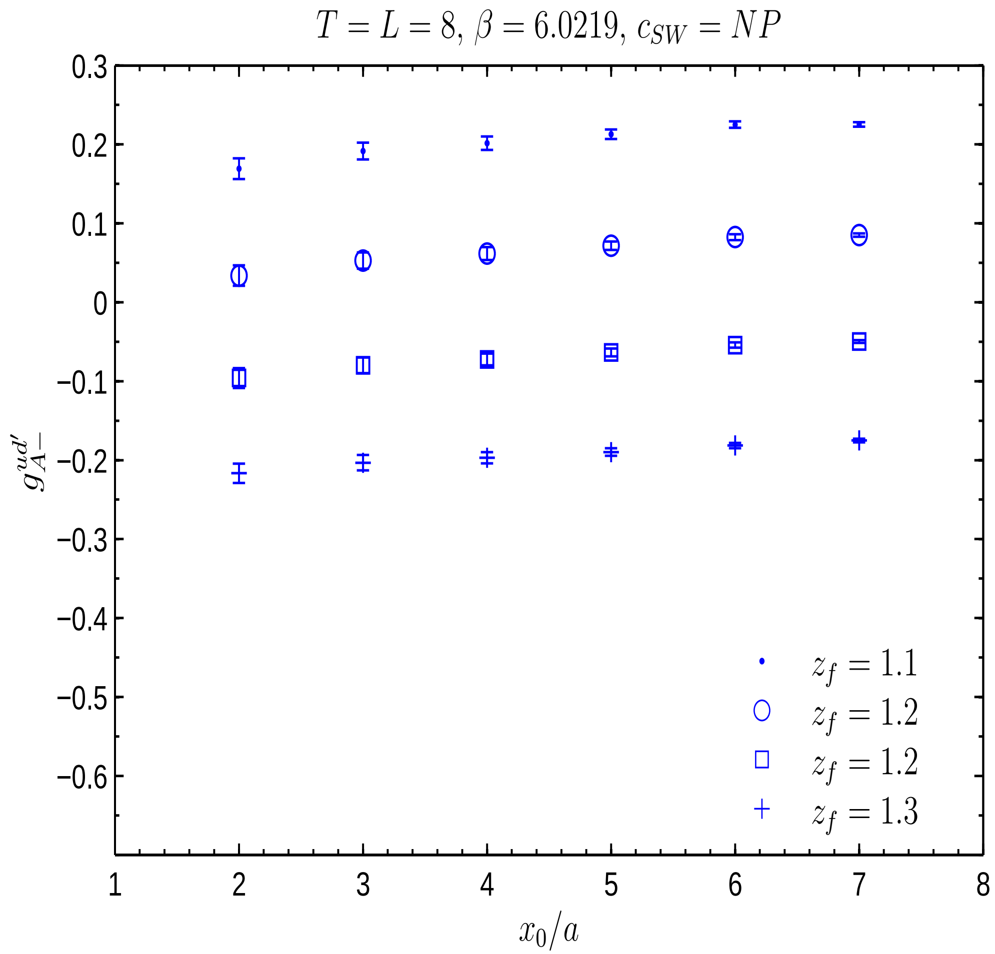
- check that the Dirichlet boundary conditions are indeed obtained as expected.

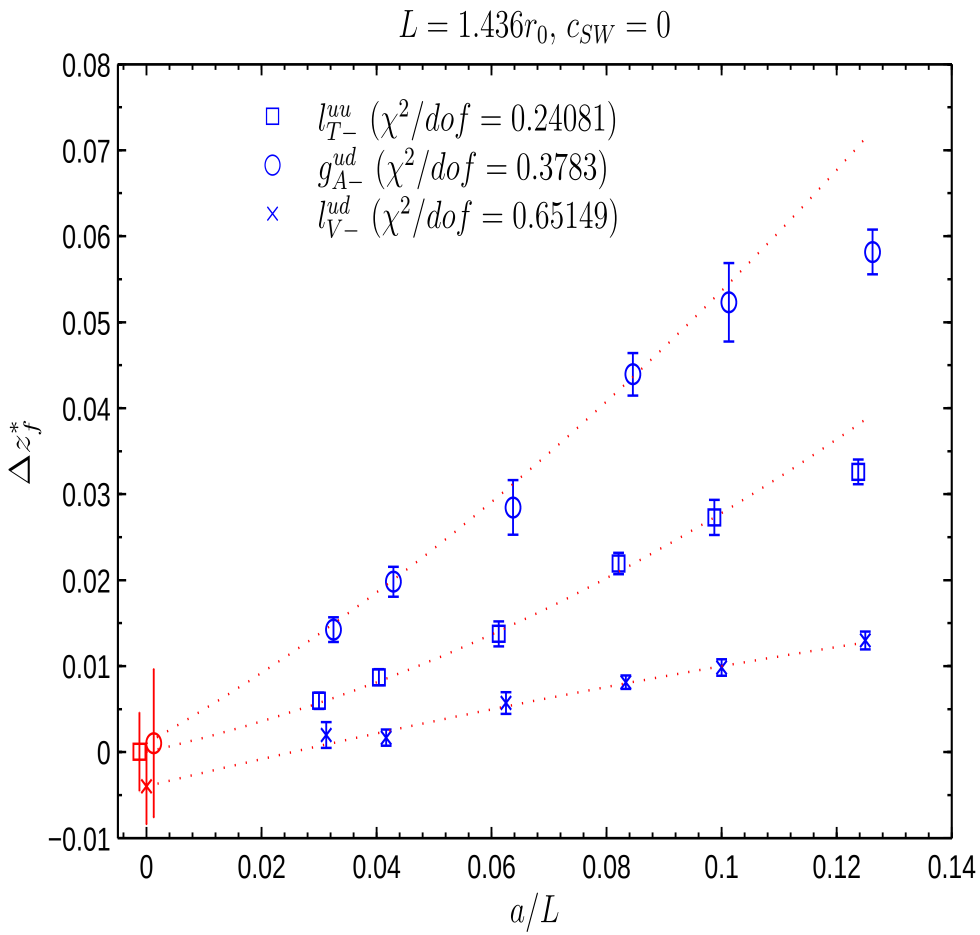
- check universality between rotated and standard SF correlation functions

- check that automatic O(a) improvement works out as expected: $\gamma_5\tau^1$-odd correlators should be of O(a).

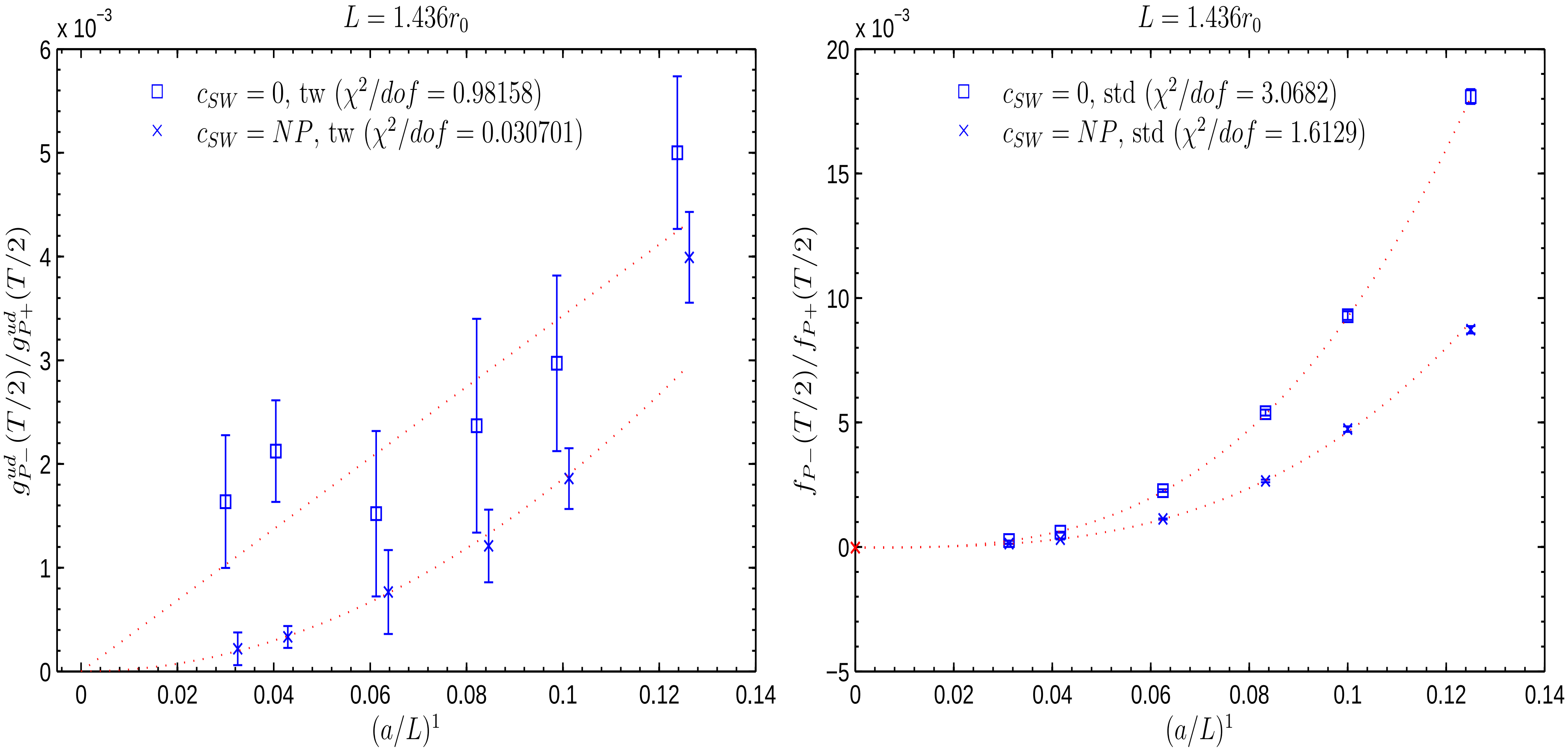
- Use universality to determine finite ratios of renormalization constants

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

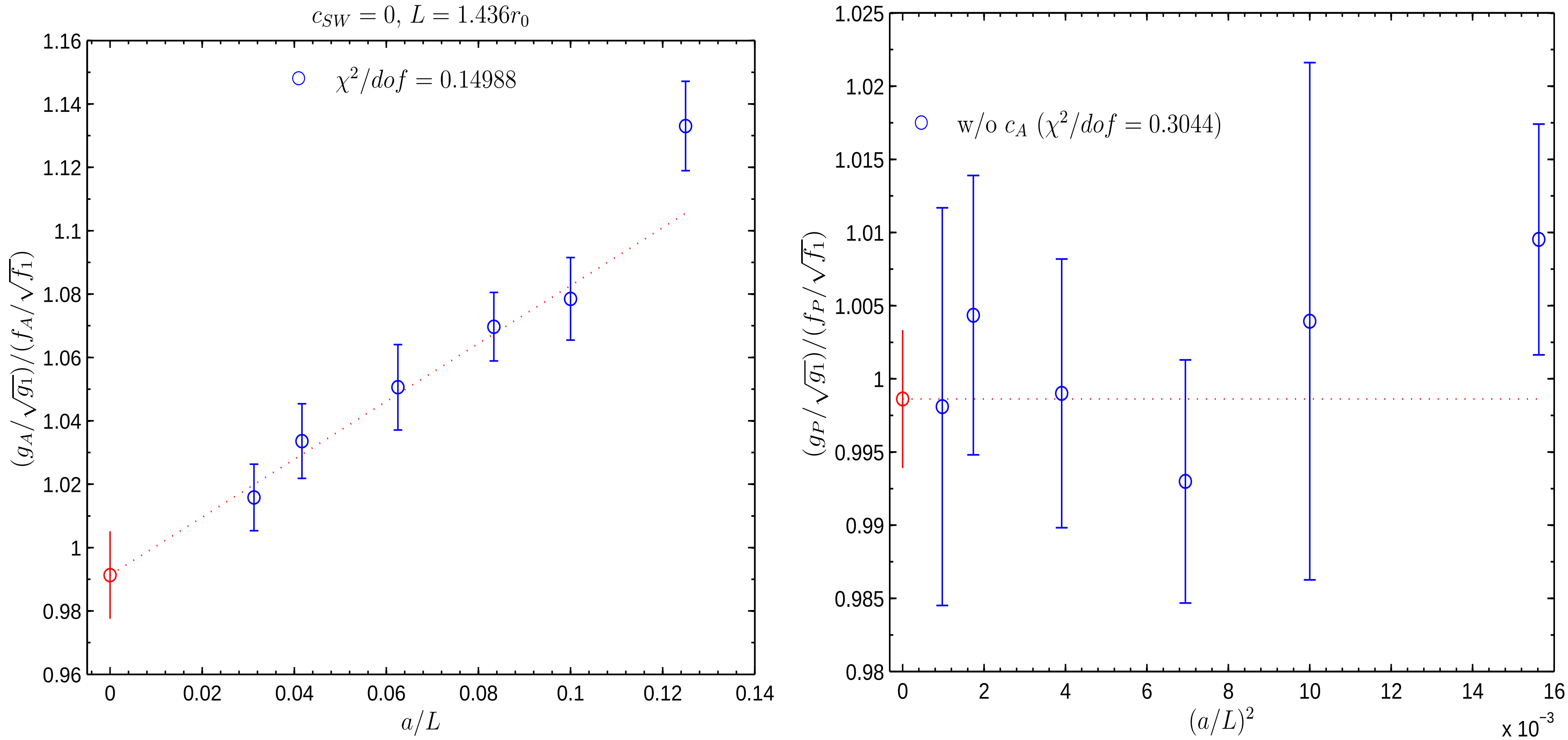




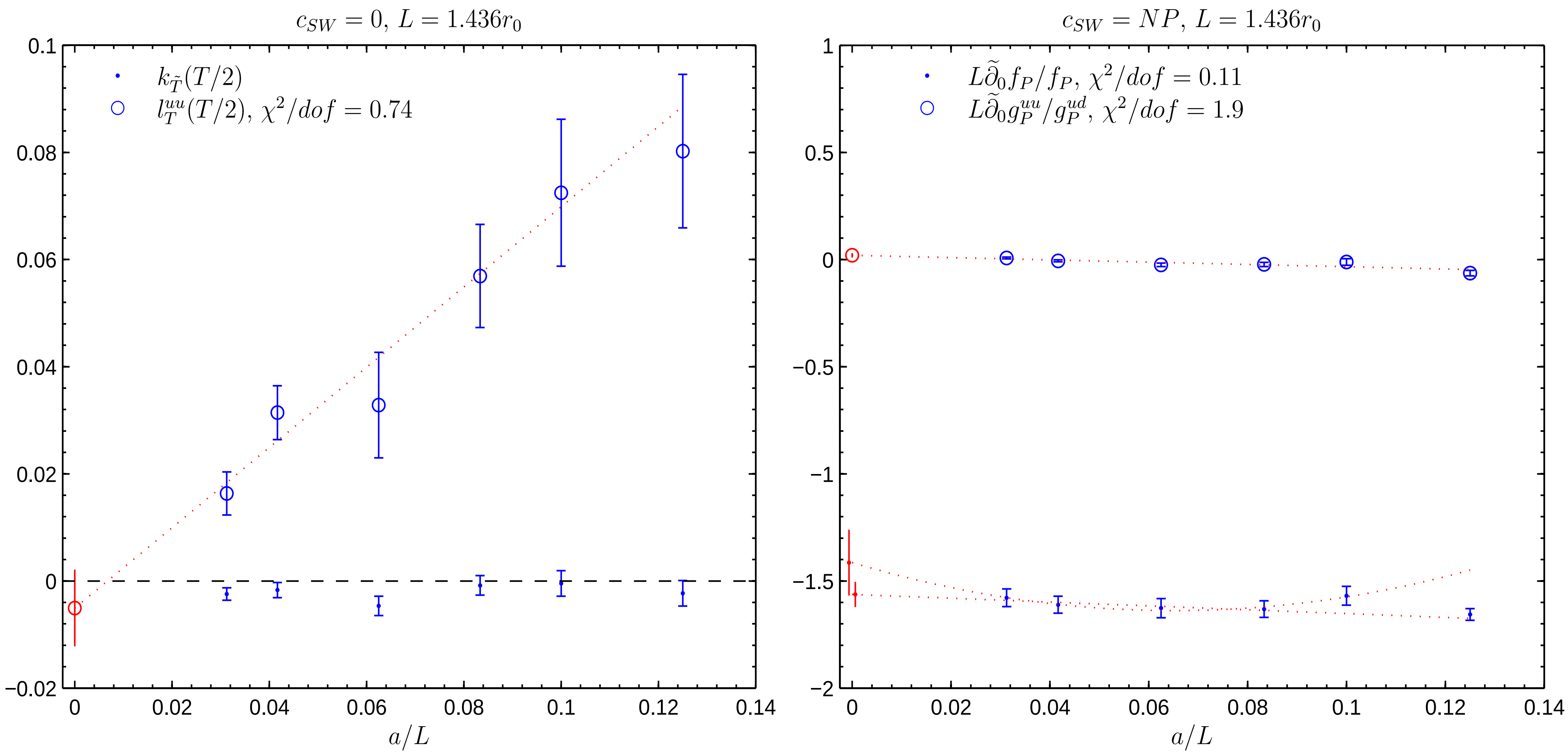
Check of Dirichlet boundary conditions



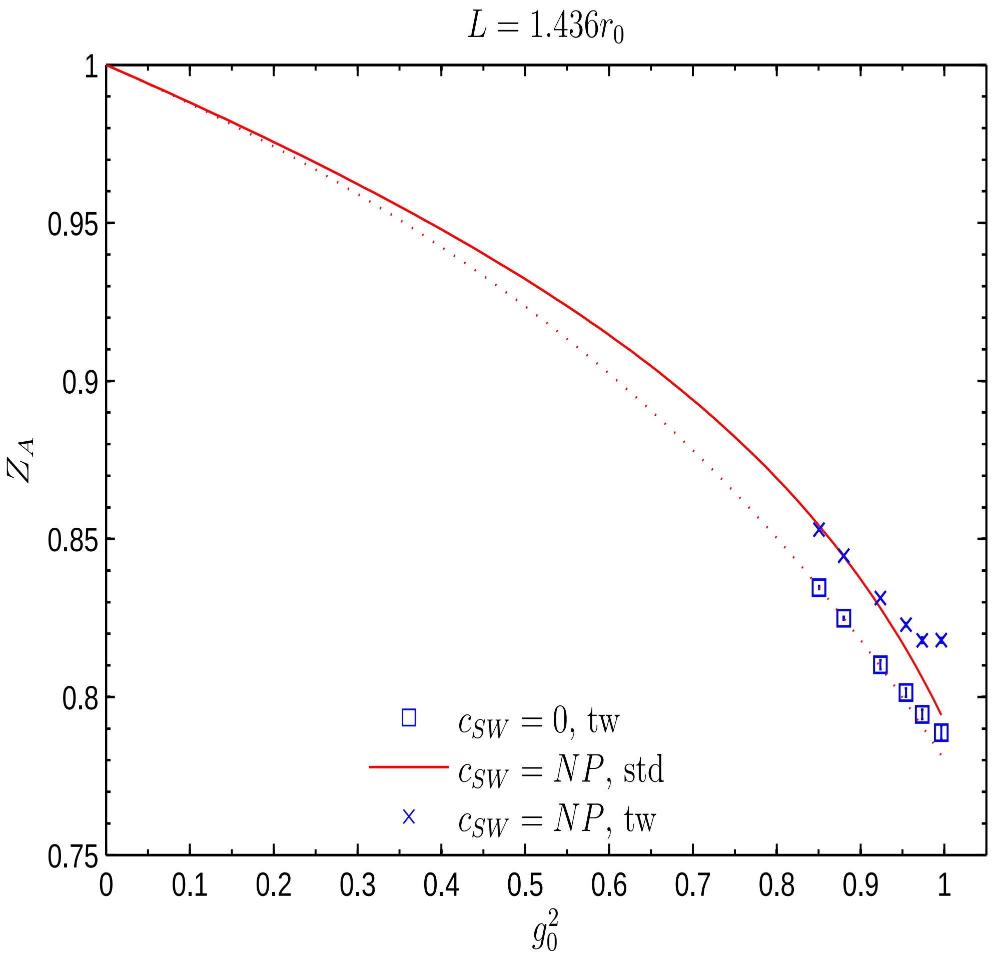
Universality checks

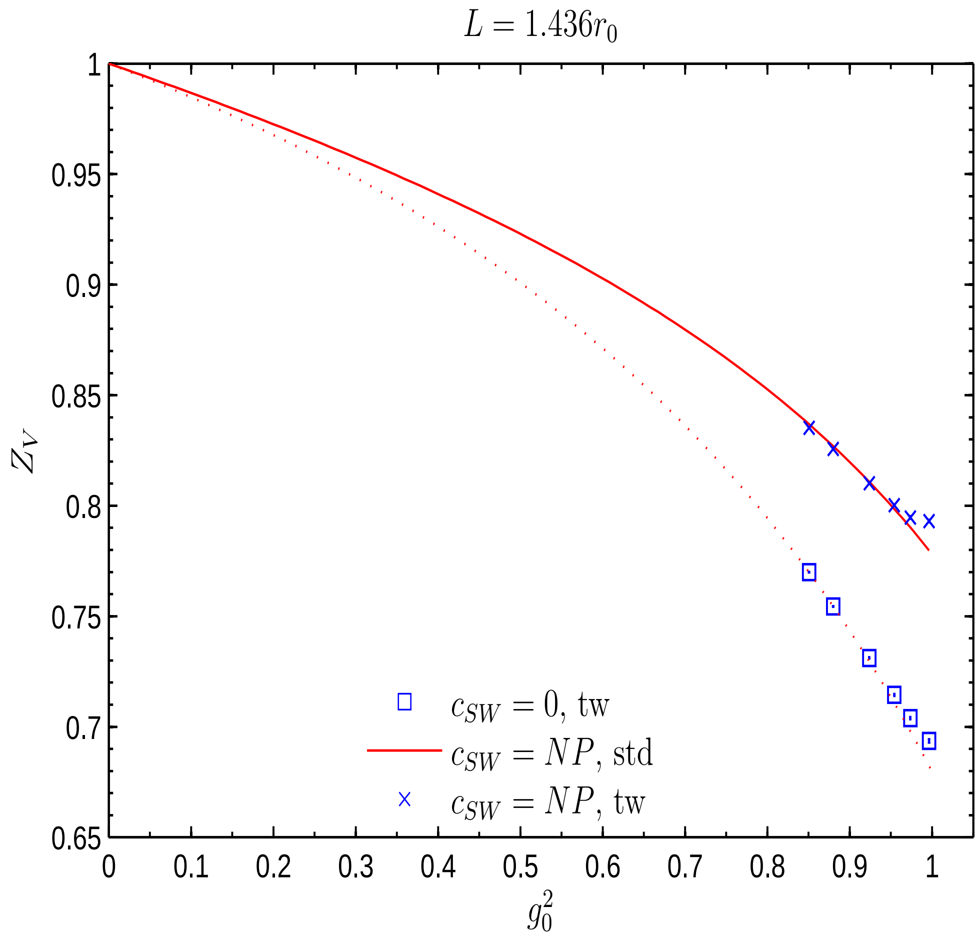


Check of automatic O(a) improvement



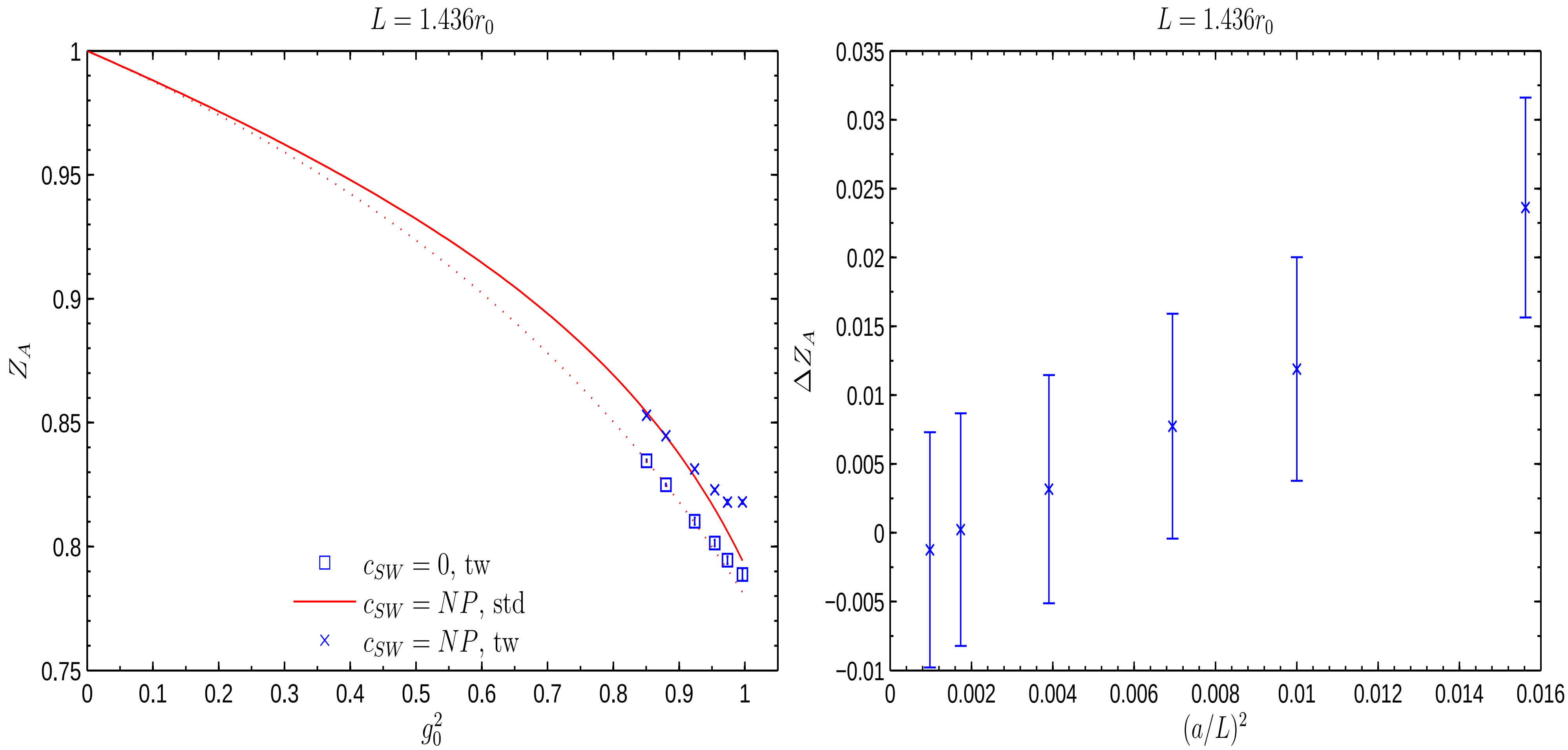
Determination of $Z_{\mathrm{A,V}}$





$Z_{\mathrm{A}} = i g_{\tilde{V}}(T/2)/g_A(T/2)$ and $Z_{\mathrm{V}} = g_{\tilde{V}}(T/2)/g_V(T/2)$

O(a^2) uncertainty in $Z_{\rm A}$



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

  $\Rightarrow$ Z-factors in SF schemes are O(a) improved by tuning the boundary O(a) counterterms ($c_{\rm t}$ and $d_s \Leftrightarrow \tilde{c}_{\rm t}$;

  interesting for 4-quark operators, higher twist operators,. . .
- Applications to Technicolor-inspired models, avoids determination of $c_{\rm sw}$.
- New methods to determine finite renormalisation constants $Z_{\rm A}$, $Z_{\rm V}$, $Z_{\rm P}/Z_{\rm S}, \ldots$ and improvement coefficients $c_{\rm A}$, $c_{\rm V}$, $c_{\rm sw}, \ldots$).