Improving 2+1 flavours of Wilson fermions

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Introduction

General remarks

- In Lattice QCD simulations numerical estimates of expectation value of observables are obtained at a finite value of the lattice spacing.
- Hence, they are affected by cut-off effects.
- In particular, Dirac-Wilson fermions introduce cut-off effects linear in the lattice spacing due to the Wilson term.

$\Rightarrow$ in order to increase the precision of final, continuum extrapolated, results, we would like to construct observables which converge to their continuum limit with a^2.

This can be achieved following Symanzik's improvement program in which higher dimensional operators have to be included in order to cancel the unwanted contributions linear in the lattice spacing.

Introduction

Massive Dirac-Wilson fermions

Symanzik's improvement program

$$S_{\mathrm{QCD}}\big(a(\beta)\big) = S_{\mathrm{continuum}} + aS_1 + a^2 S_2 + \ldots$$

Improvement of the action requires knowledge of the c_{SW} coefficient and of b_g and b_m which are proportional to the quark mass.
Apart of the action itself we want to use improved operators. We usually define

$$A_\mu^{jk,\mathrm{I}}(x) = \bar{\psi}_j(x)\gamma_\mu\gamma_5\psi_k(x) + ac_A\partial_\mu^{\mathrm{sym}} P^{jk}(x)$$

and

$$A_\mu^{jk,\mathrm{R}}(x) = Z_A\big(1 + ab_A m_{jk} + a3\bar{b}_A\overline{m}\big)A_\mu^{jk,\mathrm{I}}(x)$$

$\Rightarrow$ full, non-perturbative improvement of Wilson fermions needs c_{SW}, b_g, c_J, b_J, $\bar{b}_J$, d_J and $\bar{d}_J$.

Introduction

CLS ensembles

The CLS initiative is currently generating ensembles with $N_f = 2 + 1$ flavours of non-perturbatively improved Wilson Fermions and the tree-level Lüscher-Weisz gauge action at $\beta = 3.4, 3.46, 3.55$ and 3.7. This corresponds to lattice spacings of $a \in [0.05, 0.086]$ fm.

Note: some ensembles at $\beta = 3.36$ and $\beta = 3.85$ also available!

Improvement coefficients

- $c_{\mathrm{SW}} \rightarrow$ Bulava, Schaefer, '13
- $c_A \rightarrow$ Bulava, Della Morte, Heitger, Wittemeier '15
- b_Γ, $\tilde{b}_\Gamma \rightarrow$ this talk
- $c_A \rightarrow$ this talk

Traditional way

Schrödinger functional

Improvement condition is based on imposing the PCAC relation, which can be used to define a mass

$$m_{\mathrm{PCAC}} = \frac{\langle \alpha | \partial_\mu A^a_\mu(x) | \beta \rangle}{2\langle \alpha | P^a(x) | \beta \rangle} = r(x,\alpha,\beta) + a c_A s(x,\alpha,\beta)$$

Hence,

$$c_A = -\frac{1}{a} \frac{r(x,\alpha,\beta) - r(x,\gamma,\delta)}{s(x,\alpha,\beta) - s(x,\gamma,\delta)}$$

Pros & cons

- ✓ precise
- ✓ can be estimated directly at $m = 0$
- × needs separate simulations

Plan

Not so new proposal

We use coordinate space method proposed by Martinelli *et al.* '97 to determine b_J and other coefficients.

Outline

- Introduction & Motivations
- b_J coefficients
    - Notation
    - Observables
    - Short and medium distance corrections
    - Examples
    - Assessment of systematic uncertainties
    - Final parametrizations
- $\tilde{b}_J$ coefficients
- c_J coefficients
- Conclusions

Notation

We denote quark mass averages as

$$m_{jk} = \frac{1}{2}(m_j + m_k)\,,$$

where

$$m_j = \frac{1}{2a}\left(\frac{1}{\kappa_j} - \frac{1}{\kappa_{\rm crit}}\right).$$

The mass dependence of physical observables can be parameterized in terms of the average quark mass

$$\overline{m} = \frac{1}{3}\left(m_s + 2m_\ell\right)\,.$$

We define connected Euclidean current-current correlation functions in a continuum renormalization scheme R, e.g., $R = \overline{\rm MS}$, at a scale μ:

$$G^R_{J^{(jk)}}(x, m_\ell, m_s; \mu) = \left\langle \Omega \left| T\, J^{(jk)}(x) \overline{J}^{(jk)}(0) \right| \Omega \right\rangle^R .$$

Method

Two observations

1) The continuum correlation function differs from that of the massless case by mass dependent terms

$$G^R_{J(jk)}(x, m_\ell, m_s; \mu) = G^R_{J(jk)}(x, 0, 0; \mu)$$
$$\times \left[1 + \mathcal{O}\left(m^2x^2, m^2\langle FF\rangle x^6, m\langle\overline{\psi}\psi\rangle x^4, m\langle\overline{\psi}\sigma F\psi\rangle x^6\right)\right] ,$$

2) The continuum Green function G^R above can be related to the corresponding Green function G obtained in the lattice scheme at a lattice spacing $\tilde{a} = a(\tilde{g}^2)$ as follows:

$$G^R_{J(jk)}(x, m_\ell, m_s; \mu) = \left(Z^R_J\right)^2(\tilde{g}^2, \tilde{a}\mu)$$
$$\times \left(1 + 2b_J am_{jk} + 6\bar{b}_J a\overline{m}\right) G_{J(jk),I}(n, \kappa_I, \kappa_s; \beta) .$$

Method

Expanding Z_J around g^2 gives

$$Z_J^R\left[\tilde{g}^2, a(\tilde{g}^2)\mu\right] = Z_J^R\left[g^2, a(g^2)\mu\right] \times$$
$$\times\left[1 + \left(\frac{\partial \ln Z_J^R(g^2, a\mu)}{\partial g^2} + \frac{\mathrm{d}\ln Z_J^R(g^2, a\mu)}{\mathrm{d}\ln a}\frac{\partial \ln a(g^2)}{\partial g^2}\right) g^2 b_g a\overline{m} + \ldots\right] =$$
$$= Z_J^R(g^2, a(g^2)\mu)\left\{1 + \left[\frac{\mathrm{d}\ln Z_J^R(g^2, a\mu)}{\mathrm{d}g^2} - \frac{\gamma_J(g^2)}{4\pi\beta(g^2)}\right] b_g g^2 a\overline{m}\right\},$$

where

$$\beta(g^2) = -\frac{1}{4\pi}\frac{\mathrm{d}g^2}{\mathrm{d}\ln a} = -\frac{g^2}{2\pi}\left[\beta_0\frac{g^2}{16\pi^2} + \cdots\right]$$

is the QCD β-function in the normalization convention $\beta_0 = 11 - \frac{2}{3}N_f$ and

$$\gamma_J(g^2) = \frac{\mathrm{d}\ln Z_J}{\mathrm{d}\ln a}.$$

Method

Previously we had the following relation

$$G^R_{J(jk)}(x, m_\ell, m_s; \mu) = \left(Z^R_J\right)^2(\tilde{g}^2, a(\tilde{g}^2)\mu)$$
$$\times \left(1 + 2b_J am_{jk} + 6\bar{b}_J a\overline{m}\right) G_{J(jk),I}(n, am_{jk}, a\overline{m}; g^2)\,.$$

We can eliminate b_g by redefining

$$\tilde{b}_J(g^2) = \bar{b}_J(g^2) + \frac{b_g(g^2)}{N_f}\left[\frac{\partial \ln Z^R_J(g^2, a\mu)}{\partial g^2} - \frac{\gamma_J(g^2)}{4\pi\beta(g^2)}\right] g^2\,,$$

and get the final equality

$$G^R_{J(jk)}(x, m_\ell, m_s; \mu) = \left(Z^R_J\right)^2(g^2, a(g^2)\mu)$$
$$\times \left(1 + 2b_J am_{jk} + 6\tilde{b}_J a\overline{m}\right) G_{J(jk),I}(n, am_{jk}, a\overline{m}; g^2)\,.$$

Observables

$$\frac{G_{J(jk)}\left(n, am_{jk}^{(\rho)}, a\overline{m}^{(\rho)}; g^2\right)}{G_{J(rs)}\left(n, am_{rs}^{(\sigma)}, a\overline{m}^{(\sigma)}; g^2\right)} = 1 + 2b_J a\left(m_{rs}^{(\sigma)} - m_{jk}^{(\rho)}\right) + 6\tilde{b}_J a\left(\overline{m}^{(\sigma)} - \overline{m}^{(\rho)}\right) + \mathcal{O}\left(a^2, x^2\right),$$

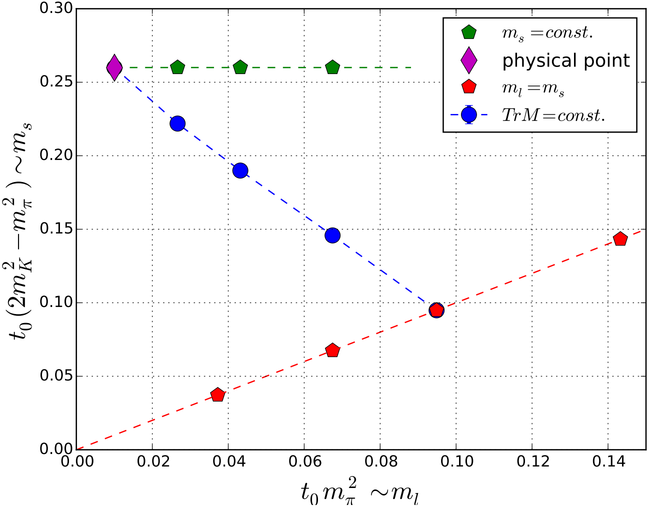
We can construct two useful observables:

$$R_J(x, \delta m) \equiv \frac{G_{J(12)}\left(n, am_{12}^{(\rho)}, a\overline{m}^{(\rho)}; g^2\right)}{G_{J(13)}\left(n, am_{13}^{(\rho)}, a\overline{m}^{(\rho)}; g^2\right)} = 1 + 2b_J a\delta m$$

$$\widetilde{R}_J(x, \delta\overline{m}) \equiv \frac{G_{J(12)}\left(n, a\overline{m}^{(\rho)}, a\overline{m}^{(\rho)}; g^2\right)}{G_{J(12)}\left(n, a\overline{m}^{(\sigma)}, a\overline{m}^{(\sigma)}; g^2\right)} = 1 + (2b_J + 6\tilde{b}_J)a\delta\overline{m}$$

$\Rightarrow$ Let's see how this works in practice!

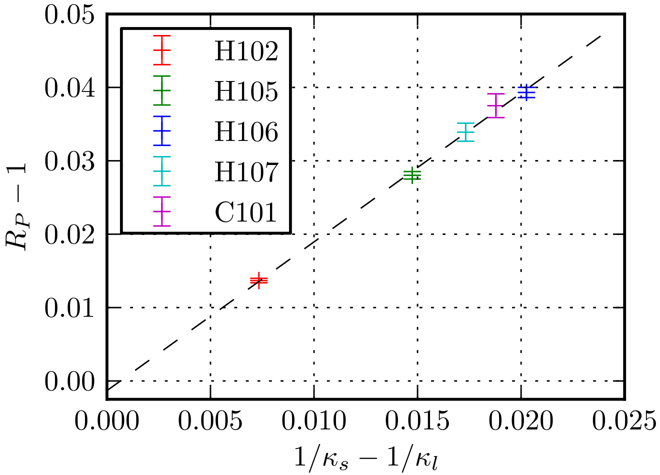
Overview of CLS ensembles at $\beta = 3.4$



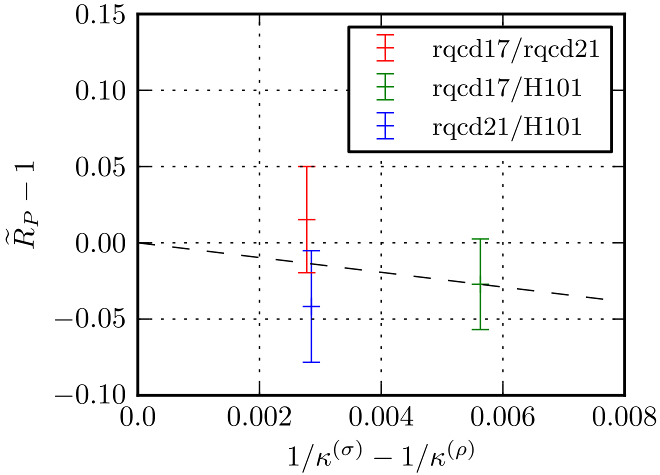
List of ensembles

β	name	κ_l	κ_s	# conf.	step
3.4	H101	0.136759	0.136759	100	10
3.4	H102	0.136865	0.136549339	100	10
3.4	H105	0.136970	0.13634079	103	5
3.4	H106	0.137016	0.136148704	57	5
3.4	H107	0.136946	0.136203165	49	5
3.4	C101	0.137030	0.136222041	59	10
3.4	C102	0.137051	0.136129063	48	10
3.4	rqcd17	0.1368650	0.1368650	150	10
3.4	rqcd19	0.13660	0.13660	50	10
3.46	S400	0.136984	0.136702387	83	10
3.55	N203	0.137080	0.136840284	74	10
3.7	J303	0.137123	0.1367546608	38	10

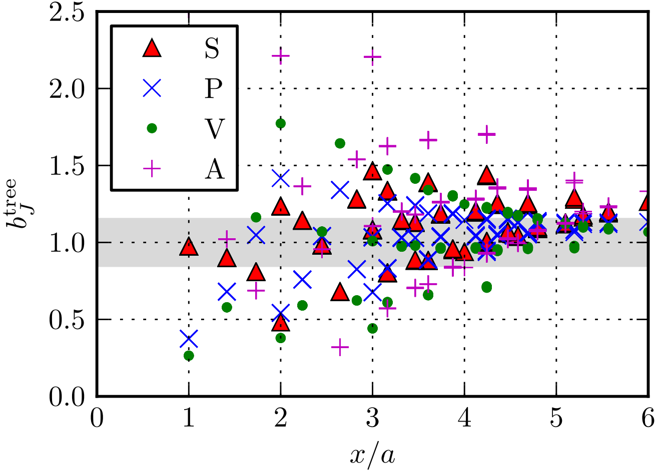
Example: $R_P - 1$ for $n = (0, 1, 1, 1)$



Example: $\widetilde{R}_P - 1$ for $n = (0, 1, 2, 2)$



Corrections at short distances



Applying OPE to the ratio of correlation functions one gets

$$\frac{G_{J(12)}(x)}{G_{J(34)}(x)} = 1 + (A^J_{12} - A^J_{34})x^2 + \left[\left(A^J_{34}\right)^2 - A^J_{12}A^J_{34} + B^J_{12} - B^J_{34} \right] x^4 + \cdots ,$$

with the mass dependent coefficients

$$A^J_{jk} = -\frac{1}{4}\left(m_j^2 + m_k^2 + \frac{m_j m_k}{s_J} \right) ,$$

$$B^J_{jk} = \frac{\pi^2}{32N}\langle FF \rangle + \frac{m_j^2 m_k^2}{16} + \frac{\pi^2}{8N}\frac{2+s_J}{s_J}(m_j + m_k)\langle \overline{\psi}\psi \rangle .$$

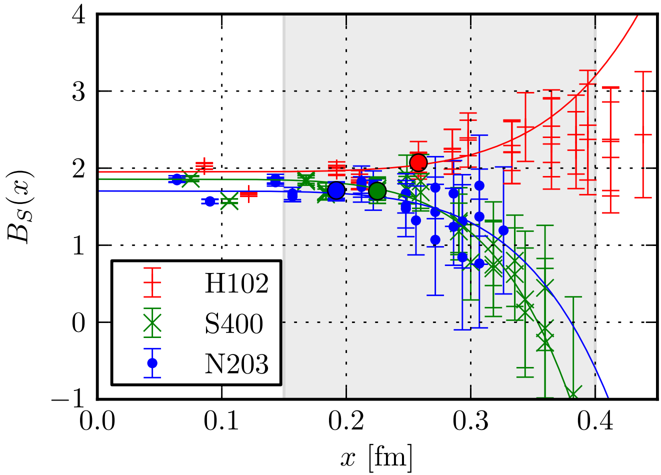
We correct our observables R_J and $\widetilde{R}_J$ by subtracting the leading continuum corrections.

Improved observables

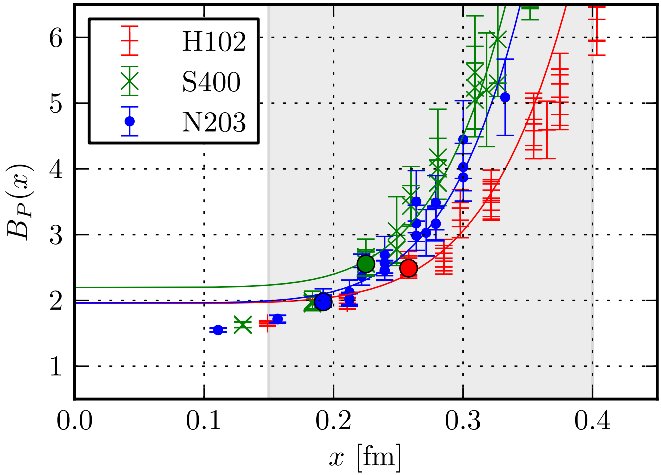
$$B_J(x,\delta m) \equiv \left[R_J(x,\delta m) - R_J^{\text{tree}}(x,\delta m) + \frac{\pi^2}{8N}\frac{2+s_J}{s_J}\left(M_\pi^2 - M_K^2\right) F_0^2 x^4 \right] \times \left(\frac{1}{\kappa_s} - \frac{1}{\kappa_\ell} \right)^{-1} = b_J + \mathcal{O}(x^6) + \mathcal{O}(g^2 a^2) + \cdots ,$$

$$\widetilde{B}_J(x,\delta\overline{m}) \equiv \left[\widetilde{R}_J(x,\delta\overline{m}) - \widetilde{R}_J^{\text{tree}}(x,\delta\overline{m}) + \frac{\pi^2}{8N}\frac{2+s_J}{s_J}\left(\delta {M_\pi}^2\right) F_0^2 x^4 \right] \times \left(\frac{1}{\kappa^{(\sigma)}} - \frac{1}{\kappa^{(\rho)}} \right)^{-1} = b_J + 3\tilde{b}_J + \mathcal{O}(x^6) + \mathcal{O}(g^2 a^2) + \cdots .$$

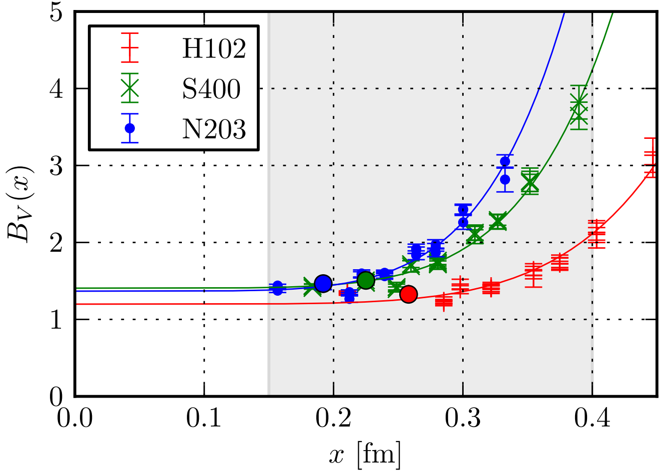
Example of numerical data: scalar channel



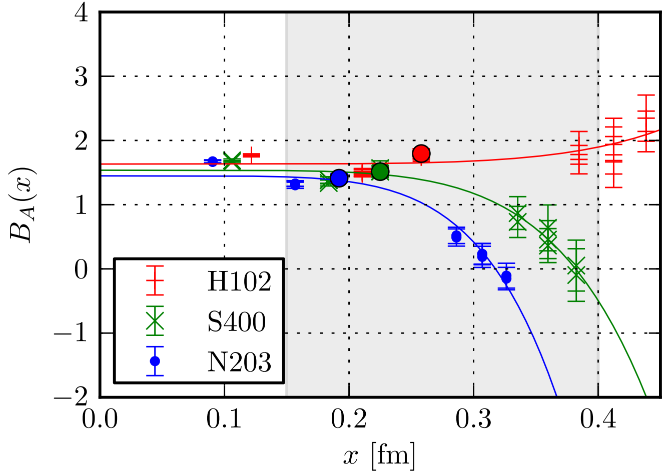
Example of numerical data: pseudoscalar channel

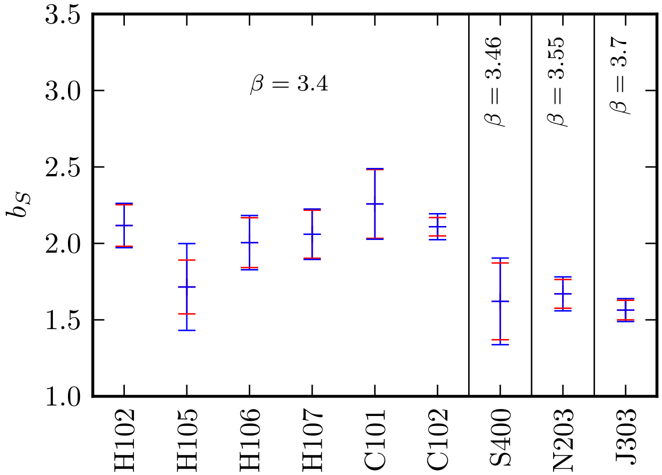


Example of numerical data: vector channel



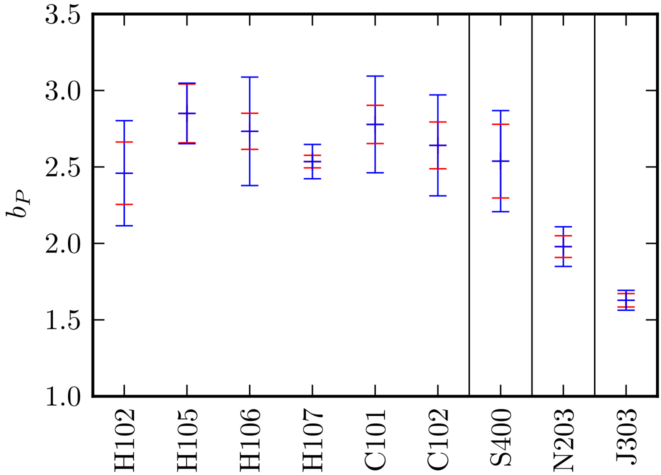
Example of numerical data: axial channel



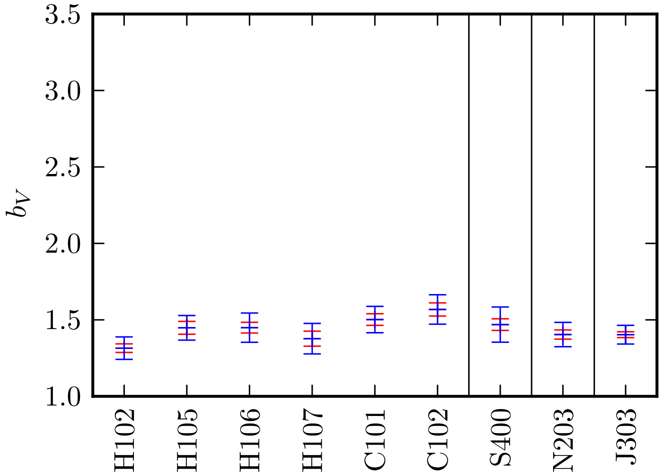


3.5
3.0
2.5
2.0
1.5
1.0
b_S
$\beta = 3.4$
$\beta = 3.46$
$\beta = 3.55$
$\beta = 3.7$
H102
H105
H106
H107
C101
C102
S400
N203
J303

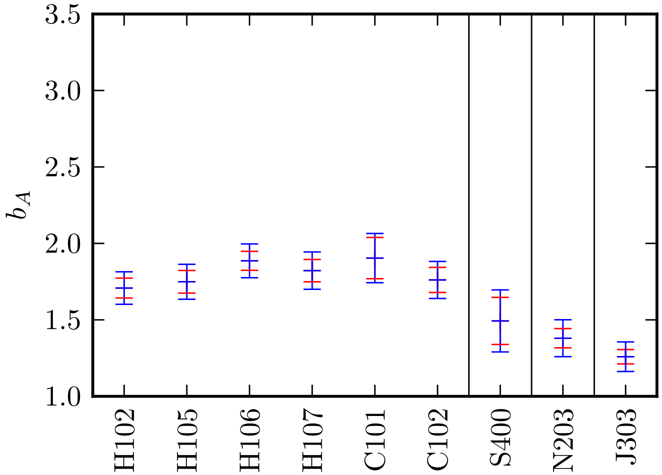
Results in the pseudoscalar channel



Results in the vector channel



Results in the axial channel



Final results: rational parametrizations

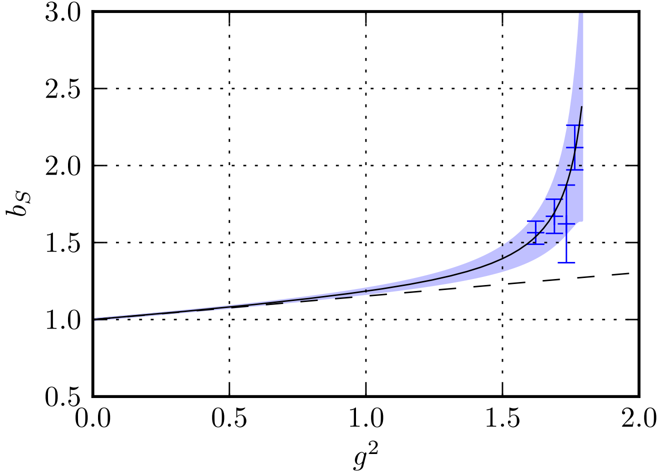
Uncertainties

- statistical error
- Wilson coefficient of the OPE subtraction
- contribution of higher condensates

Final results

$$b_S(g^2) = 1 + 0.11444(1) C_F (1 - 0.439(50) g^2)(1 - 0.535(14) g^2)^{-1}$$
$$b_P(g^2) = 1 + 0.0890(1) C_F (1 - 0.354(54) g^2)(1 - 0.540(11) g^2)^{-1}$$
$$b_V(g^2) = 1 + 0.0886(1) C_F (1 + 0.596(111) g^2)$$
$$b_A(g^2) = 1 + 0.0881(1) C_F (1 - 0.523(33) g^2)(1 - 0.554(10) g^2)^{-1}$$

Final results: rational parametrizations



Final results: discussion

Potential problems

- window problem; need of a sharp hierarchy of scales, whereas $a \approx 0.085$ fm, $x \approx 0.26$ fm and $1/\Lambda = 0.5$ fm.
  As a consequence we work with points $x \approx 3a$ and use perturbation theory at scales $1/x \approx 0.9$ GeV,
- remaining hypercubic artefacts vs. continuum OPE inspired fit ansatz,
- by using x_0/a fixed, we change the physical situation as we go to the continuum limit.

but the consistency of our results seems to indicate that our assumptions are not totally wrong.

Results for $\tilde{b}_J$ coefficients

$\tilde{b}_J$ improvement coefficients at $\beta = 3.4$

$$
\begin{aligned}
\tilde{b}_S &= 2.0 \quad (1.3)_{\mathrm{stat}} \quad (0.3)_{\mathrm{sys}} \\
\tilde{b}_P &= -3.4 \quad (1.3)_{\mathrm{stat}} \quad (0.6)_{\mathrm{sys}} \\
\tilde{b}_V &= -0.1 \quad (0.4)_{\mathrm{stat}} \quad (0.1)_{\mathrm{sys}} \\
\tilde{b}_A &= 1.4 \quad (0.4)_{\mathrm{stat}} \quad (0.9)_{\mathrm{sys}}
\end{aligned}
$$

Work in progress: increasing the precision

Multipoint source

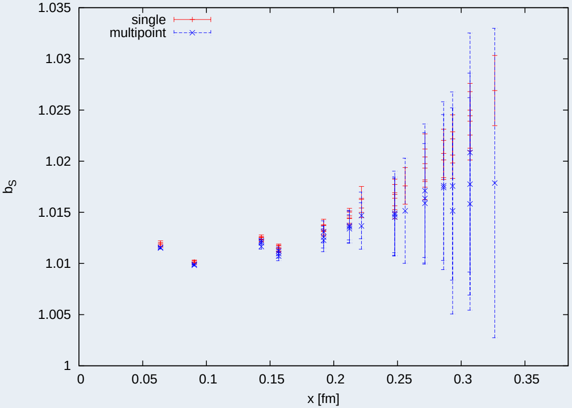


Figure: Comparison of data in the scalar channel obtained at $\beta = 3.55$

Work in progress: increasing the precision

Truncated Solver Method

We factorize the estimated propagator into two parts

$$D^{-1}(x-y) \approx \frac{1}{N_1}\sum_{i=1}^{N_1} D_{n_t}^{-1}(x-y) + \frac{1}{N_2}\sum_{i=1}^{N_2}\left\{D_{\text{exact}}^{-1}(x-y) - D_{n_t}^{-1}(x-y)\right\}$$

where $D_{n_t}^{-1}(x-y)$ is the propagator obtained after n_t iterations of the solver.

In the case of the estimation of the disconnected part of the two-point function with the CG solver the gain is known to be $\mathcal{O}(20)$. We are experimenting with the multigrid solver and currently see an improvement by a factor $\mathcal{O}(2)$.

Work in progress: c_A

Defining condition

We use current-current correlators in position space at short distances to formulate the condition fixing the improvement coefficient c_A. For two vectors x_1 and x_2 such that $(x_1)^2 = (x_2)^2$ we have

$$\sum_\mu \langle \Big[A^I_\mu(x_1) - A^I_\mu(x_2)\Big]\overline{P}(0)\rangle = 0 \quad \text{with} \quad A^I_\mu(x) = A_\mu(x) + a c_A \partial^{\rm sym}_\mu P(x).$$

Hence

$$c_A = -\frac{\sum_\mu \langle \Big[A_\mu(x_1) - A_\mu(x_2)\Big]\overline{P}(0)\rangle}{a\sum_\mu \langle \Big[\partial^{\rm sym}_\mu P(x_1) - \partial^{\rm sym}_\mu P(x_2)\Big]\overline{P}(0)\rangle}$$

$$= -\frac{2\sum_\mu \langle \Big[A_\mu(x_1) - A_\mu(x_2)\Big]\overline{P}(0)\rangle}{\sum_\mu \langle \Big[P(x_1+\hat{\mu}) - P(x_1-\hat{\mu}) - P(x_2+\hat{\mu}) + P(x_2-\hat{\mu})\Big]\overline{P}(0)\rangle}.$$

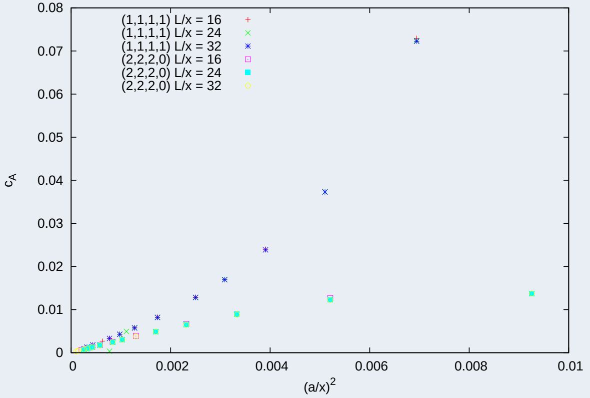
Work in progress: c_A

c_A at tree-level

x_1	x_2	$(x_1)^2 = (x_2)^2$
1 1 1 1	2 0 0 0	4
2 2 1 0	3 0 0 0	9
2 2 1 1	3 1 0 0	10
2 2 2 0	3 1 1 1	12
2 2 2 1	3 2 0 0	13
2 2 2 2	4 0 0 0	16

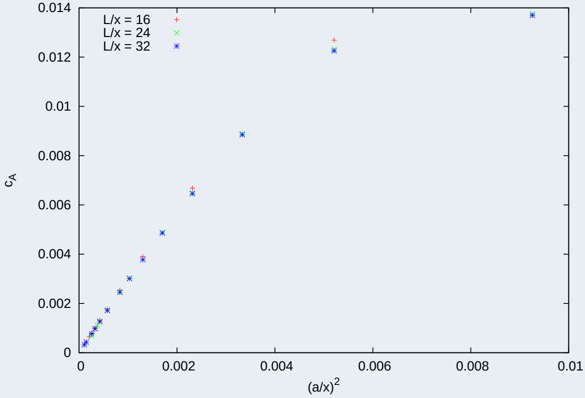
Work in progress: c_A

c_A at tree-level



Work in progress: c_A

c_A at tree-level



Conclusions

Conclusions

- We implemented a coordinate space method to determine improvement coefficients
- b_J improvement coefficients are accessible
- With a negligible numerical effort we can achieve a 5% - 10% precision on b_J
- $\tilde{b}_J$ more demanding, practical solution using Truncated Solver Method implemented and under investigation
- Straigthforward extension to d_J: implementation under way
- c_J improvement coefficients may be also accessible
- $\Rightarrow$ all improvement coefficients at hand from current-current correlators