Non perturbative determination of improvement b–coefficients in $N_f = 3$

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RG flow

- Renormalized couplings satisfy the RG flow equations in mass-independent scheme

$$\begin{cases} \mu \frac{\partial}{\partial \mu} g_{\mathrm{R}}(\mu) & = \beta(g_{\mathrm{R}}(\mu), \cancel{m_{\mathrm{R}}(\mu)}) \\ \mu \frac{\partial}{\partial \mu} m_{\mathrm{R}}(\mu) & = \tau(g_{\mathrm{R}}(\mu), \cancel{m_{\mathrm{R}}(\mu)})\, m_{\mathrm{R}}(\mu) \end{cases}$$

- Velocities β and τ have perturbative expansion

$$\begin{cases} \beta(g_{\mathrm{R}}) & \overset{g_{\mathrm{R}} \to 0}{\sim} -{g_{\mathrm{R}}}^3(b_0 + b_1 {g_{\mathrm{R}}}^2 + b_2 {g_{\mathrm{R}}}^4 + \mathcal{O}({g_{\mathrm{R}}}^6)) \\ \tau(g_{\mathrm{R}}) & \overset{g_{\mathrm{R}} \to 0}{\sim} -{g_{\mathrm{R}}}^2(d_0 + d_1 {g_{\mathrm{R}}}^2 + d_2 {g_{\mathrm{R}}}^4 + \mathcal{O}({g_{\mathrm{R}}}^6)) \end{cases}$$

with universal coefficients b_0, b_1, d_0.

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RGI quantities

- Integration of the equations yields to dimensionful finite constants, the renormalization group invariants (RGI)

$$\Lambda = \mu \left[b_0 {g_\mathrm{R}}^2(\mu)\right]^{-\frac{b_1}{2b_0^2}} \exp\left\{ -\int_0^{g_\mathrm{R}(\mu)} dg \left[\frac{1}{\beta(g)} + \frac{1}{b_0 g^3} - \frac{b_1}{b_0^2 g}\right] - \frac{1}{2b_0 {g_\mathrm{R}}^2(\mu)} \right\}$$

$$M = m_\mathrm{R}(\mu) \left[2b_0 {g_\mathrm{R}}^2(\mu)\right]^{-\frac{d_0}{2b_0}} \exp\left\{ -\int_0^{g_\mathrm{R}(\mu)} dg \left[\frac{\tau(g)}{\beta(g)} - \frac{d_0}{b_0 g}\right] \right\}$$

- In the adimensional ratio, the function f depends only on $g_\mathrm{R}^2(\mu)$

$$\frac{M}{\Lambda} = m_\mathrm{R}(\mu)\, 1/\mu \;\; f({g_\mathrm{R}}^2(\mu))$$

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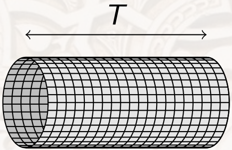
Finite volume & mass independent renormalization scheme

- Finite size scaling approach to run between high energy and low energy scales:

$$\mu = 1/L \qquad\qquad \frac{M}{\Lambda} = m_{\mathrm{R}}(1/L)\,L \;\; f(g_{\mathrm{R}}{}^2(L))$$

- Finite volume requires boundary conditions:



Schrödinger functional (SF) cylinder $L^3 \times T$
periodic bc in spatial directions,
Dirichlet bc in temporal direction

- Physical extent of the box and masses fixed by working at constant values of the renormalized couplings

$$\left(\mu,\ \frac{M}{\Lambda}\right) = \text{fixed} \quad \Longleftrightarrow \quad \boxed{\left(g_{\mathrm{R}}{}^2(L),\ m_{\mathrm{R}}(1/L)\,L\right) = \text{constant}}$$

Improved & mass-independent

- In $O(a)$ improved & mass-independent schemes bare quantities must be renormalized with mass-dependent terms

$$g_{\mathrm{R}}^2 = Z_{\mathrm{g}}(\tilde{g}_0^2, a\mu)\,\tilde{g}_0^2 \qquad \tilde{g}_0^2 = (1 + b_{\mathrm{g}}(g_0^2)am_q)\,g_0^2$$

$$m_{\mathrm{R}} = Z_{\mathrm{m}}(\tilde{g}_0^2, a\mu)\,\tilde{m} \qquad \tilde{m} = (1 + b_{\mathrm{m}}(g_0^2)am_q)\,m_q$$

$$X_{\mathrm{R}} = Z_{\mathrm{X}}(\tilde{g}_0^2, a\mu)\,\tilde{X} \qquad \tilde{X} = (1 + b_{\mathrm{X}}(g_0^2)am_q)\,X_I$$

- Improvement parameters depend on the choice of the improvement conditions $\equiv$ NP ambiguity of $O(a)$
- ALPHA Collaboration: improvement conditions at *constant physics*

  $\Longrightarrow$ improvement coefficients smooth functions of g_0^2

$$\boxed{\left(g_{\mathrm{R}}{}^2(L),\ m_{\mathrm{R}}(1/L)\,L\right) = \text{constant}}$$

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History of non–perturbative *b* coefficients

- 1997 Quenched

[GMdD and R Petronzio, [hep-lat/9710071],Phys. Lett. B **419** (1998) 311]

- 2000 Quenched

[M Guagnelli *et al.* [ALPHA], [hep-lat/0009021], Nucl. Phys. B **595** (2001) 44]

- 2000 Quenched

[T Bhattacharya, *et al.*, [hep-lat/0009038], Phys. Rev. D **63** (2001) 074505]

- 2003 Quenched

[J Heitger *et al.* [ALPHA], [hep-lat/0312016], JHEP **0402** (2004) 064]

- 2010 Unquenched $N_f = 2$

[P Fritzsch, et al. [ALPHA], [arXiv:1004.3978 [hep-lat]], JHEP **1008** (2010) 074]

- 2016 Unquenched $N_f = 2 + 1$

[G S Bali *et al.* [RQCD Collaboration], [arXiv:1606.09039 [hep-lat]], Phys. Rev. D **94** (2016) no.7, 074501]

[P Korcyl and G S Bali, [arXiv:1607.07090 [hep-lat]], Phys. Rev. D **95** (2017) no.1, 014505]

- 2017(?) Unquenched $N_f = 3$

[GMdD, M Firrotta, J Heitger, C C Köster, A Vladikas [ALPHA], this work]

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Improvement condition

- (non–singlet) PCAC relation free of $O(a)$ violations

$$\boxed{\tilde{\partial}_\mu \left\langle A_R{}_\mu^{ij}(x)\, \mathcal{O}^{ji} \right\rangle = (m_{\mathrm{R},i} + m_{\mathrm{R},j})\ \left\langle P_R{}^{ij}(x)\, \mathcal{O}^{ji} \right\rangle + O(a^2)}$$

- Standard renormalization pattern of improved lattice operators (for $\hat{m}^{(\mathrm{sea})} \sim 0$)

$$A_R{}_\mu^{ij} = Z_\mathrm{A}\,(1 + b_\mathrm{A}\, a m_{q,ij} + \cancel{\bar{b}_\mathrm{A}\, a\, \mathrm{tr}\, \hat{m}^{(\mathrm{sea})}})\,\{A_\mu^{ij} + c_\mathrm{A}\, a\, \tilde{\partial}_\mu P^{ij}\}$$

$$P_R{}_\mu^{ij} = Z_\mathrm{P}\,(1 + b_\mathrm{P}\, a m_{q,ij} + \cancel{\bar{b}_\mathrm{P}\, a\, \mathrm{tr}\, \hat{m}^{(\mathrm{sea})}})\, P^{ij}$$

$$m_{\mathrm{R},i} = Z_\mathrm{m}\Big\{ m_{q,i}(1 + b_\mathrm{m}\, a m_{q,i} + \cancel{\bar{b}_\mathrm{m}\, a\, \mathrm{tr}\, \hat{m}^{(\mathrm{sea})}}) + \cancel{x\, \mathrm{tr}\, \hat{m}^{(\mathrm{sea})}} + \cancel{y\, a\, \mathrm{tr}\, \hat{m}^{2(\mathrm{sea})}} + \cancel{z\, a\, (\mathrm{tr}\, \hat{m}^{(\mathrm{sea})})^2} \Big\}$$

$$x = (r_\mathrm{m} - 1)/N_f, \quad y = (r_\mathrm{m} d_\mathrm{m} - b_\mathrm{m})/N_f \quad z = (r_\mathrm{m} \bar{d}_\mathrm{m} - \bar{b}_\mathrm{m})/N_f$$

$$A_\mu^{ij} = \bar{\psi}_i \gamma_\mu \gamma_5 \psi_j\,, \quad P^{ij} = \bar{\psi}_i \gamma_5 \psi_j$$

$$m_{q,ij} = \tfrac{1}{2}(m_{q,i} + m_{q,j}), \quad m_{q,i} = m_{0,i} - m_c = \tfrac{1}{2a}\left(\tfrac{1}{\kappa_i} - \tfrac{1}{\kappa_c}\right)$$

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SF Correlation functions

$$m_{ij}(x_0) = \frac{\tilde{\partial}_0 f_{\mathrm{A}}^{ij}(x_0) + a c_{\mathrm{A}} \partial_0^* \partial_0 f_{\mathrm{P}}^{ij}(x_0)}{2\, f_{\mathrm{P}}^{ij}(x_0)}$$

$$= \frac{Z_{\mathrm{m}} Z_{\mathrm{P}}}{Z_{\mathrm{A}}} \Big(x \,\mathrm{tr}\, \hat{m}^{(\mathrm{sea})} + (z + x\,(\bar{b}_{\mathrm{P}} - \bar{b}_{\mathrm{A}}))\, a\, (\mathrm{tr}\, \hat{m}^{(\mathrm{sea})})^2 + y\, a\, \mathrm{tr}\, \hat{m}^{2(\mathrm{sea})} \Big\}$$

$$+ m_{q,ij}\, (1 + (x\,(b_{\mathrm{P}} - b_{\mathrm{A}}) + \bar{b}_{\mathrm{P}} - \bar{b}_{\mathrm{A}} + \bar{b}_{\mathrm{m}})\, a\, \mathrm{tr}\, \hat{m}^{(\mathrm{sea})})$$

$$+ a m_{q,ij}^2\, (b_{\mathrm{P}} - b_{\mathrm{A}}) + \frac{1}{2} a (m_{q,i}^2 + m_{q,j}^2)\, b_{\mathrm{m}} \Big)$$

$$f_{\mathrm{A}}^{ij}(x_0) = -\frac{a^3}{3L^3} \sum_{\mathbf{x}} \left\langle A_0^{ij}(x)\, \mathcal{O}^{ji} \right\rangle$$

$$f_{\mathrm{P}}^{ij}(x_0) = -\frac{a^3}{3L^3} \sum_{\mathbf{x}} \left\langle P^{ij}(x)\, \mathcal{O}^{ji} \right\rangle$$

$$\mathcal{O}^{ji} = a^6 \sum_{\mathbf{u},\mathbf{v}} \bar{\zeta}_j(\mathbf{u})\, \gamma_5 \zeta_i(\mathbf{v})$$

$$g_{\mathrm{A}}^{ij}(T - x_0) = -\frac{a^3}{3L^3} \sum_{\mathbf{x}} \left\langle A_0^{ij}(x)\, \mathcal{O}'^{ji} \right\rangle$$

$$g_{\mathrm{P}}^{ij}(T - x_0) = -\frac{a^3}{3L^3} \sum_{\mathbf{x}} \left\langle P^{ij}(x)\, \mathcal{O}'^{ji} \right\rangle$$

$$\mathcal{O}'^{ji} = a^6 \sum_{\mathbf{u},\mathbf{v}} \bar{\zeta}'_j(\mathbf{u})\, \gamma_5\, \zeta'_i(\mathbf{v})$$

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Simulation details

- openQCD for the SF simulations

  (SF-specific choices $C = C' = 0$ and $\theta = 0$)

  [M Lüscher and S Schaefer, [arXiv:1206.2809 [hep-lat]], Comput. Phys. Commun. **184** (2013) 519]

  http://luscher.web.cern.ch/luscher/openQCD/

- $N_f = 3$ mass-degenerate flavors Wilson-clover fermions
  tree-level improved Lüscher–Weisz gauge action

- non-perturbative $c_{\mathrm{SW}}, c_{\mathrm{A}}$

  [J Bulava and S Schaefer, [arXiv:1304.7093 [hep-lat]], Nucl. Phys. B **874** (2013) 188]

  [J Bulava *et al.* [ALPHA], [arXiv:1604.05827 [hep-lat]], Phys. Rev. D **93** (2016) no.11, 114513]

- RHMC reweighting factors

  [A D Kennedy, I Horvath and S Sint, [hep-lat/9809092], Nucl. Phys. Proc. Suppl. **73** (1999) 834]
  . [M A Clark and A D Kennedy, [hep-lat/0608015], Phys. Rev. Lett. **98** (2007) 051601]
  [M Lüscher and F Palombi,[arXiv:0810.0946 [hep-lat]], PoS LATTICE **2008** (2008) 049]

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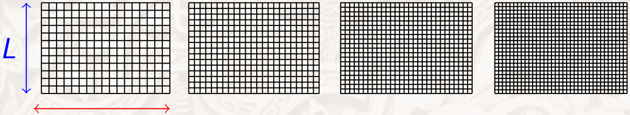
continuum limit

- $L \approx 1.2\,\mathrm{fm}\,,\ Lm_{11} \approx 0.0\,,\ Lm_{22} \approx 0.25,\ 0.5,\ 0.75,\ 1.0$
- $a \approx 0.09\,\mathrm{fm} \longrightarrow 0.045\,\mathrm{fm}$



$T = 3L/2 - a$

$L^3 \times T/a^4$	β	κ	# REP	# MDU	ID
$12^3 \times 17$	3.3	0.13652	10	10240	A1k1
		0.13660	10	13048	A1k2
$12^3 \times 19$	3.3	0.13652	10	10468	A2k1
$16^3 \times 23$	3.512	0.13700	2	20480	B1k1
		0.13703	1	8192	B1k2
		0.13710	3	24560	B1k3
$16^3 \times 23$	3.47	0.13700	1	8176	B2k1
$20^3 \times 29$	3.676	0.13680	1	7848	C1k1
		0.13700	4	15232	C1k2
		0.13719	4	15472	C1k3
$24^3 \times 35$	3.810	0.13712	7	15448	D1k1

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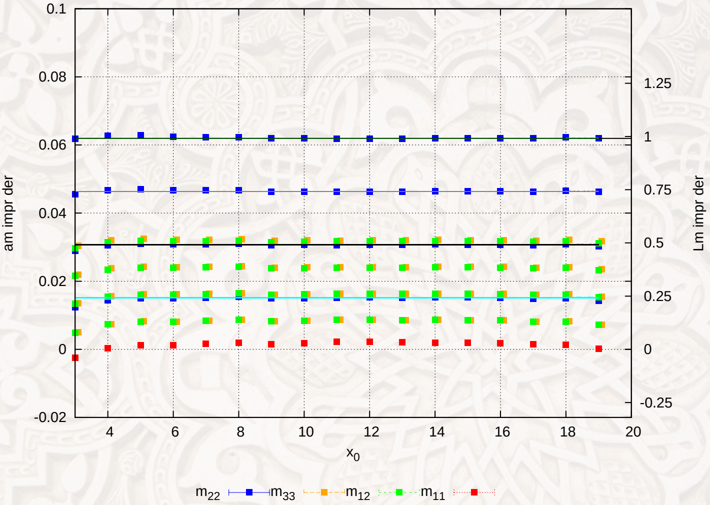
from: [J. Bulava *et al.* [ALPHA], [arXiv:1604.05827 [hep-lat]], Phys. Rev. D **93** (2016) no.11, 114513]

Masses (B1k3 ens)



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Consistency check

$$
\begin{cases}
\frac{1}{2}(m_{22}-m_{11}) & = Z\,\delta\,\left(1+aA^{(\mathrm{sea})}+2\,a\bar{m}\,b_{\mathrm{mPA}}\right)+\ldots \\
(m_{22}-m_{33}) & = Z\,\delta\,\left(1+aA^{(\mathrm{sea})}+(2\,a\bar{m}+a\delta)\,b_{\mathrm{mPA}}\right)+\ldots \\
(m_{33}-m_{11}) & = Z\,\delta\,\left(1+aA^{(\mathrm{sea})}+(2\,a\bar{m}-a\delta)\,b_{\mathrm{mPA}}\right)+\ldots \\
(m_{22}-m_{12}) & = Z\,\delta\,\left(1+aA^{(\mathrm{sea})}+2\,a\bar{m}\,b_{\mathrm{mPA}}+a\delta\,b_{\mathrm{PA}}\right)+\ldots \\
(m_{12}-m_{11}) & = Z\,\delta\,\left(1+aA^{(\mathrm{sea})}+2\,a\bar{m}\,b_{\mathrm{mPA}}-a\delta\,b_{\mathrm{PA}}\right)+\ldots
\end{cases}
$$

$$a\bar{m}=(am_{q,2}+am_{q,1})/2, \qquad a\delta=(am_{q,2}-am_{q,1})/2$$

$$Z=Z(g_0)=\frac{Z_{\mathrm{m}}(g_0,L)Z_{\mathrm{P}}(g_0,L)}{Z_{\mathrm{A}}(g_0)}, \qquad aA^{(\mathrm{sea})}=(x\,b_{\mathrm{PA}}+\bar{b}_{\mathrm{mPA}})\,a\,\mathrm{tr}\,\hat{m}^{(\mathrm{sea})}$$

$$b_{\mathrm{mPA}}=b_{\mathrm{m}}+b_{\mathrm{P}}-b_{\mathrm{A}}, \qquad b_{\mathrm{PA}}=b_{\mathrm{P}}-b_{\mathrm{A}}$$

$$\frac{1}{4}\,\frac{(m_{22}-m_{11})\,(m_{22}-m_{11})}{(m_{22}-m_{33})\,(m_{33}-m_{11})}=1+O(a^2)$$

$$\frac{1}{4}\,\frac{(m_{22}-m_{11})\,(m_{22}-m_{11})}{(m_{22}-m_{12})\,(m_{12}-m_{11})}=1+O(a^2)$$

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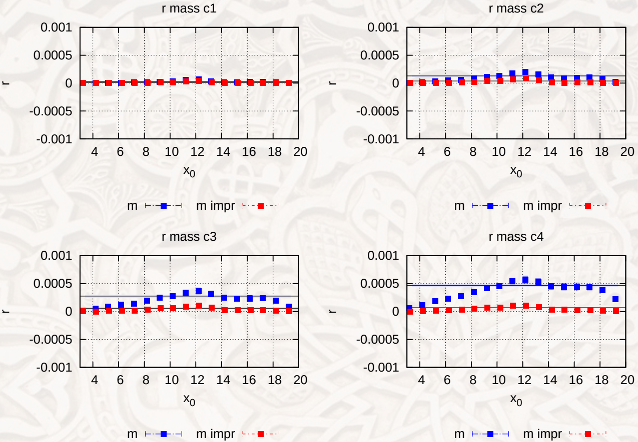
Consistency check (B1k3 ens)



$$r_1 = \frac{1}{4}\frac{(m_{22}-m_{11})(m_{22}-m_{11})}{(m_{22}-m_{33})(m_{33}-m_{11})} - 1 = O(a^2)$$

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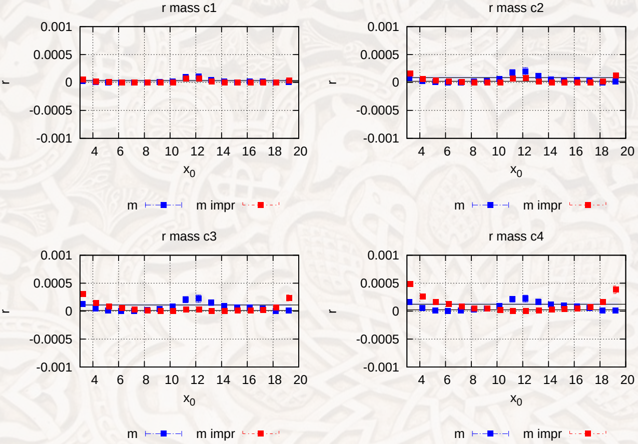
Consistency check (B1k3 ens)



$$r_2 = \frac{1}{4}\frac{(m_{22}-m_{11})(m_{22}-m_{11})}{(m_{22}-m_{12})(m_{12}-m_{11})} - 1 = O(a^2)$$

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Numerical definitions of $b_{\rm A} - b_{\rm P}$, $b_{\rm m}$, Z

$$R_{\rm AP} = \frac{2\,(2m_{12} - m_{11} - m_{22})}{(m_{11} - m_{22})\,(am_{q,1} - am_{q,2})} = b_{\rm A} - b_{\rm P} + O(am_{q,1} + am_{q,2})$$

$$R_{\rm m} = \frac{4\,(m_{12} - m_{33})}{(m_{11} - m_{22})\,(am_{q,1} - am_{q,2})} = b_{\rm m} + O(am_{q,1} + am_{q,2})$$

$$R_Z = \frac{m_{11} - m_{22}}{m_{q,1} - m_{q,2}} + (R_{\rm AP} - R_{\rm m})\,(am_{11} + am_{22}) = Z + O(a\,{\rm tr}\,\hat{m}^{\rm (sea)})$$

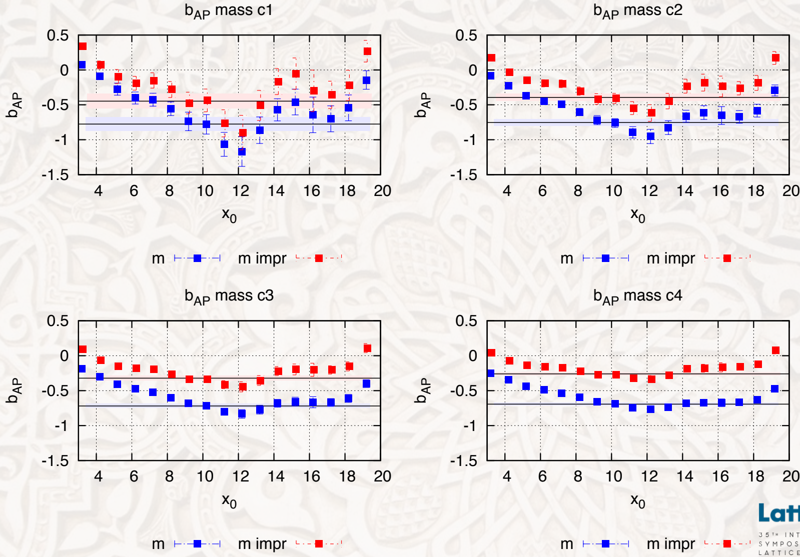
$$Z = Z(g_0) = \frac{Z_{\rm m}(g_0, L) Z_{\rm P}(g_0, L)}{Z_{\rm A}(g_0)}$$

$L \approx 1.2\,{\rm fm}$ $\qquad Lm_{11} \approx 0.0$

$Lm_{22} \approx 0.25,\ 0.5,\ 0.75,\ 1.0$

$m_{0,3} = \frac{1}{2}(m_{0,1} + m_{0,2})$

$(b_A - b_P)$ vs x_0 (B1k3 ens)



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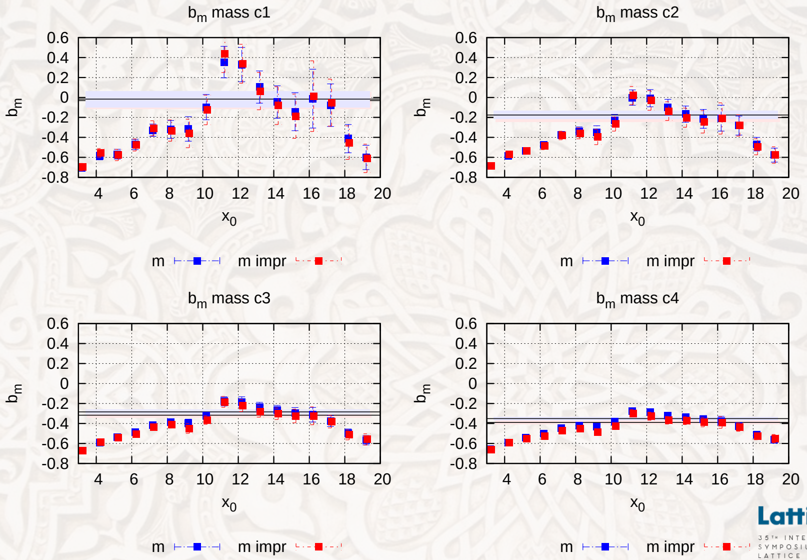
b_m vs x_0 (B1k3 ens)



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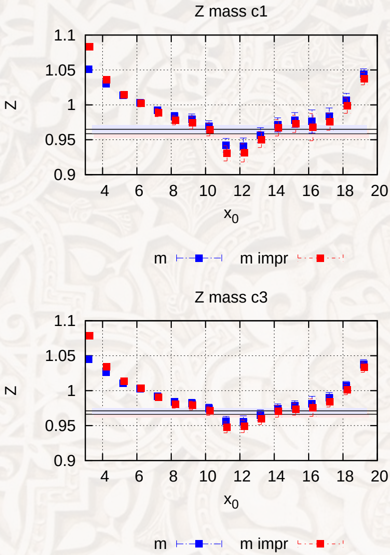
Z vs x_0 (B1k3 ens)



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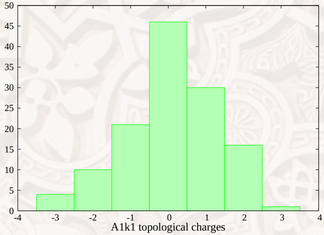
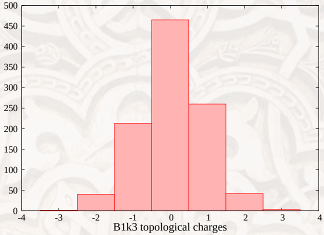
Topological sectors





- Project to trivial topological sector ($Q_{top}(t) = 0$)

$$Q_{top}(t) = -\frac{a^4}{32\pi^2} \sum_x \epsilon_{\mu\nu\alpha\beta}\, \mathrm{tr}\{G_{\mu\nu}(x,t)\, G_{\alpha\beta}(x,t)\}$$

$t =$ "flow time" of the gradient flow (covariant) diffusion

$$\begin{cases} \partial_t B_\mu(t,x) = D_\nu G_{\nu\mu}(t,x) \\ B_\mu(0,x) = A_\mu(x) \end{cases}$$

$$D_\mu = \partial_\mu + [B_\mu,\ \ ]$$

$$G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu]$$

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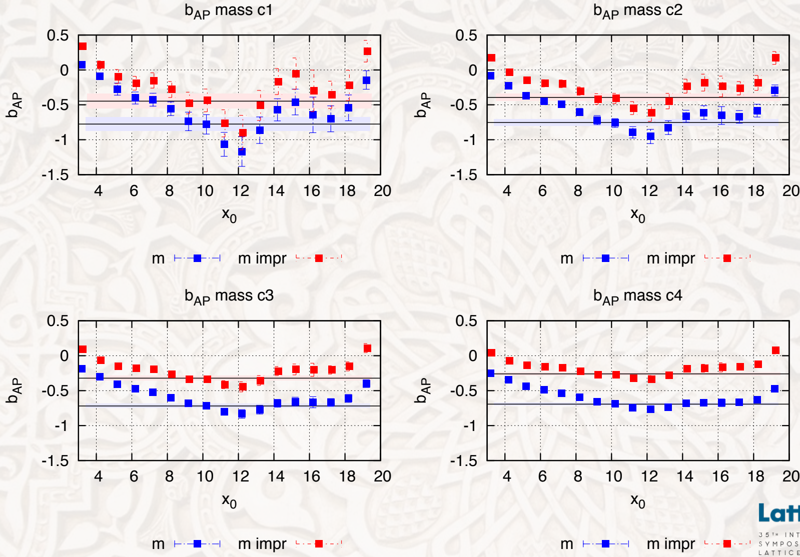
$(b_\mathrm{A} - b_\mathrm{P})$ vs x_0, $Q_{top}(t) = 0$ (B1k3 ens)



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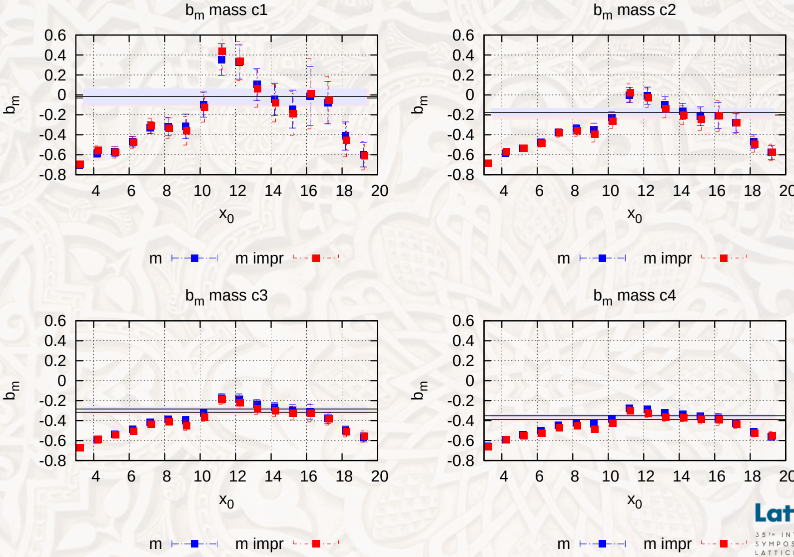
b_{m} vs x_0, $Q_{top}(t) = 0$ (B1k3 ens)



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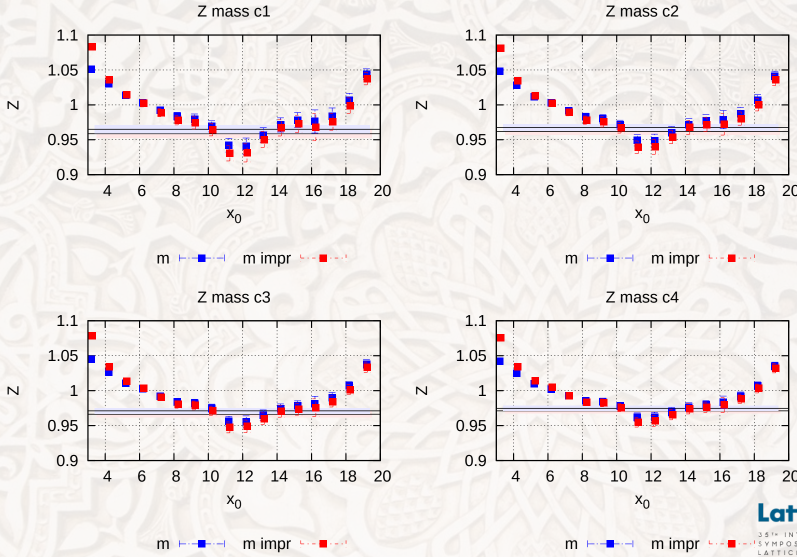
Z vs x_0, $Q_{top}(t) = 0$ (B1k3 ens)



Conclusion & Outlooks

- Results for b_{AP} sensitive to the choice of the lattice derivative (standard or improved)
- No significant dependence on the topological charge
- $\Longrightarrow$ Compute the correlators for the finer lattices
- $\Longrightarrow$ Reconstruct the Padè fits

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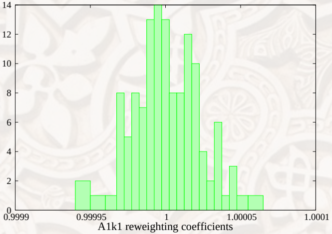
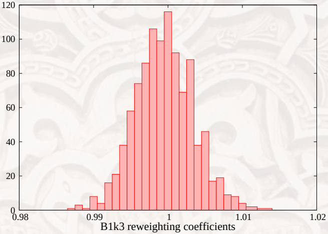
RHMC





- RHMC reweighting factors

[A D Kennedy, I Horvath and S Sint, [hep-lat/9809092], Nucl. Phys. Proc. Suppl. **73** (1999) 834]

[M A Clark and A D Kennedy, [hep-lat/0608015], Phys. Rev. Lett. **98** (2007) 051601]

[M Lüscher and F Palombi,[arXiv:0810.0946 [hep-lat]], PoS LATTICE **2008** (2008) 049]

$$\langle A \rangle = \frac{\langle AW \rangle_W}{\langle W \rangle_W}$$

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