CLS 2+1 flavor simulations

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on behalf of the CLS based collaboration

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Introduction

Problems

Lattice simulations close to the physical point are difficult because

- autocorrelations grow, $\tau_{\rm exp} \propto 1/a^2 +$ topology freezing
- accidental zero-modes of the Dirac operator are encountered
- the condition number of the Dirac operator grows as $m_{u,d} \to 0$

Proposed solutions

To circumvent the above issues a number of improvements has been proposed, namely

- open boundary conditions
- twisted mass infrared regulator
- deflated solver

$\Rightarrow$ in this talk we will present first impressions of large volume simulations with 2+1 flavors which implement the above improvements.

Introduction

CLS: Coordinated Lattice Simulations

Joint effort of:
CERN, DESY / NIC, Dublin, Berlin HU, Mainz, Madrid, Milan, Münster, Odense/CP3-Origins, Regensburg, Roma-La Sapienza, Roma-Tor Vergata, Valencia, Wuppertal

Simulations

2 PRACE projects ⇒ computer time granted at LRZ's SuperMuc in Munich (Germany) and CINECA's Fermi in Bologna (Italy)

3 national projects ⇒ Gauss-Center in Jülich (Germany), NIC in Jülich (Germany), CSCS in Lugano (Switzerland)

Bruno, Djukanovic, Engel, Francis, Herdoiza, Horch, Korcyl, Korzec, Schaefer, Scholz, Simeth, Soeldner

General setup: openQCD-1.2

Gauge action

tree-level Symanzik improved action ($c_0 = \frac{5}{3}$, $c_1 = -\frac{1}{12}$)

Fermion action

Wilson $\mathcal{O}(a)$-improved fermions with c_{SW} determined non-perturbatively

[Bulava, Schaefer '13]

Open boundary conditions means

$$F_{0k}(x)\big|_{x_0=0} = F_{0k}(x)\big|_{x_0=T} = 0, \qquad k = 1, 2, 3,$$

and

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

[Lüscher '10, Lüscher, Schaefer '11]

General setup: openQCD-1.2

Fermion action: 2+1

- twisted mass regulator $\det(D^\dagger D) \to \left(\frac{\det(D^\dagger D+\mu^2)^2}{\det(D^\dagger D+2\mu^2)} + \text{reweighting} \right)$
- RHMC with reweighting

[Lüscher, Palombi '08, Lüscher, Schaefer '13]

Light quarks: frequency splitting

$$\frac{\det(D^\dagger D+\mu^2)^2}{\det(D^\dagger D+2\mu^2)} = \det(D^\dagger D+\mu_n^2)\frac{\det(D^\dagger D+\mu_0^2)}{\det(D^\dagger D+2\mu_0^2)}\prod_{k=0}^{n-1}\frac{\det(D^\dagger D+\mu_k^2)}{\det(D^\dagger D+\mu_{k+1}^2)}$$

with typically $n \sim 5-6$. [Hasenbusch '01, Hasenbusch, Jansen '03]

Nested MD integrators

- 3 level hierarchy ($\sim$ 10 steps on the coarsest level)
- 2nd (level 2) and 4th (levels 0 and 1) order Omelyan integrators

Strategy: our way to the physical point

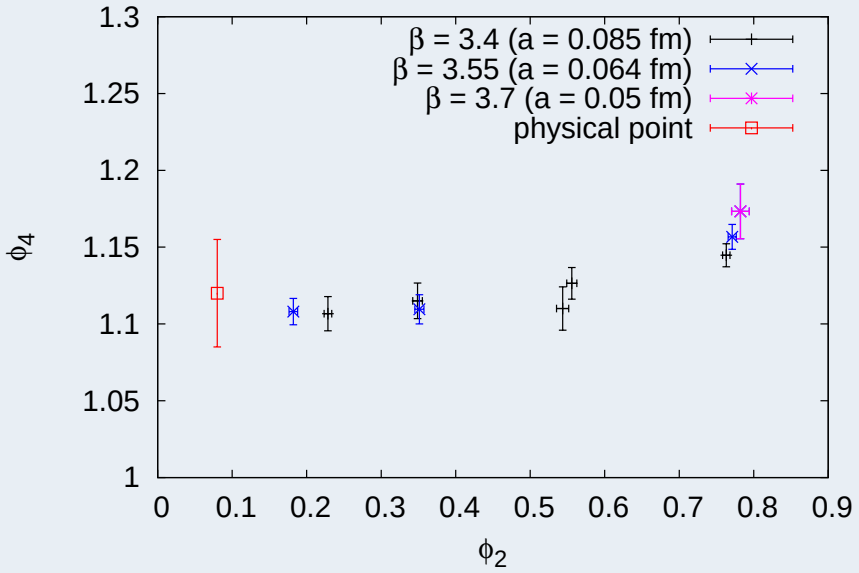
Matching

$$\phi_2(\beta, \kappa_u, \kappa_s) = 8t_0 m_\pi^2 \propto m_{ud} + \mathcal{O}(m_{ud}^2)$$

$$\phi_4(\beta, \kappa_u, \kappa_s) = 8t_0(m_K^2 + \frac{1}{2}m_\pi^2) \propto \mathrm{tr}M + \mathcal{O}(\mathrm{tr}M^2)$$

$$\sum_{i=u,d,s} \frac{1}{\kappa_i} = \mathrm{const} \Leftrightarrow \mathrm{tr}M_\mathrm{R} = \mathrm{const} + \mathcal{O}(a)$$

Line of constant $\mathrm{tr}M_R$



Physical point: m_π and m_K from PDG, $\sqrt{t_0} = 0.1465$ fm from S. Borsanyi *et al.* '12.

Strategy: our way to the physical point

Overview: lattice spacings and pion masses

		0.085 fm	0.064 fm	0.05 fm	a [fm]
m_K	m_π	3.4	3.55	3.7	β
415 MeV	415 MeV	$32^3 \times 96$	$32^3 \times 96$	$48^3 \times 128$	
440 MeV	350 MeV	$32^3 \times 96$			
470 MeV	280 MeV	$32^3 \times 96$	$48^3 \times 128$	$64^3 \times 192$	
480 MeV	220 MeV	$48^3 \times 96$	$64^3 \times 128$		
490 MeV	150 MeV	$64^3 \times 128$			

First impressions: open boundary conditions

Wilson flow observables

$$\dot{V}_t(x,\mu) = -g_0^2\left\{\partial_{x,\mu} S(V_t)\right\} V_t(x,\mu), \qquad V_t(x,\mu)\Big|_{t=0} = U(x,\mu)$$

[Lüscher '10]

History of the smoothed topological charge and its τ_{int}

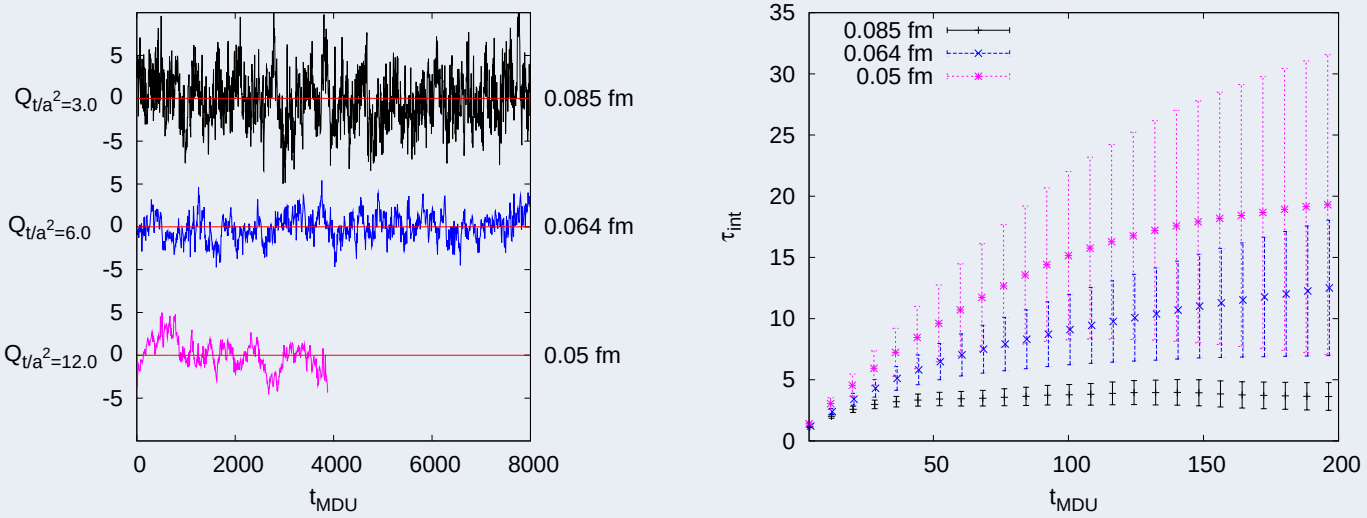
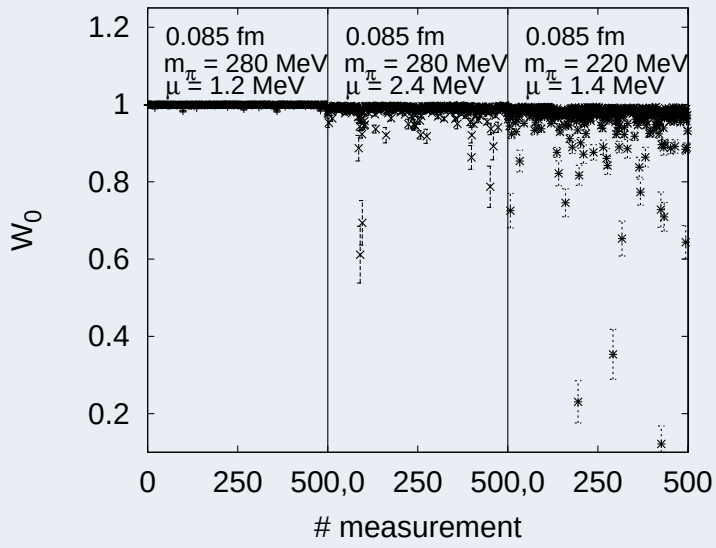


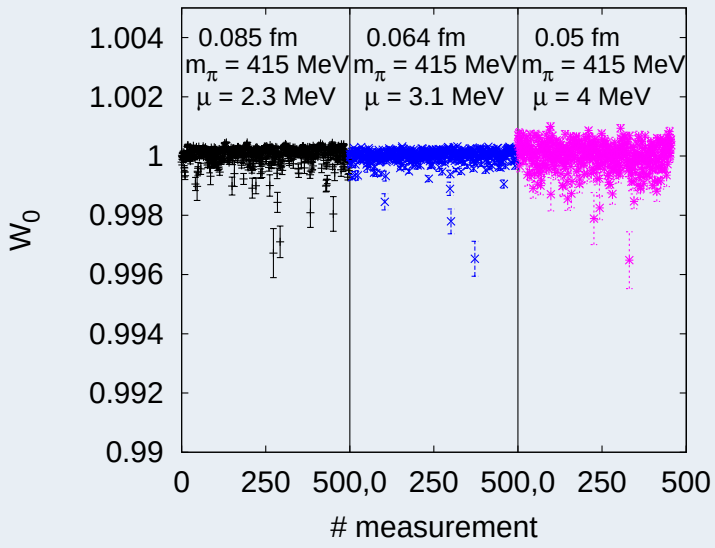
Figure: Topological charge at the symmetric point at flow times $t/a^2 = 3.0, 6.0, 12.0$.

First impressions: twisted mass reweighting

Infrared regulated Dirac operator

$$\det(D^\dagger D) \to \frac{\det(D^\dagger D + \mu^2)^2}{\det(D^\dagger D + 2\mu^2)} \qquad W_0 = \frac{\det(D^\dagger D)\det(D^\dagger D + 2\mu^2)}{\det(D^\dagger D + \mu^2)^2}$$





→ impact of reweighting on precision: see Mattia Bruno's talk Tue 14:35

First impressions: rational approximation reweighting

Rational approx. of $\left(\sqrt{D_s^\dagger D_s}\right)^{-1}$

$$\det D_s = W_1 \det R^{-1},$$

$$R = C \prod_{k=0}^{m-1} \frac{D_s^\dagger D_s + \omega_k^2}{D_s^\dagger D_s + \nu_k^2}.$$

Any inaccuracy of the rational approximation is dealt with by reweighting instead of an additional Metropolis step:

$$W_1 = \det(D_S R) \sim$$

$$\sim \exp\left\{-\phi\left(-\frac{1}{2}Z + \frac{3}{8}Z^2 - \dots\right)\phi\right\}$$

with $Z = D_s^\dagger D_s R^2 - 1$.

Reweighting factors

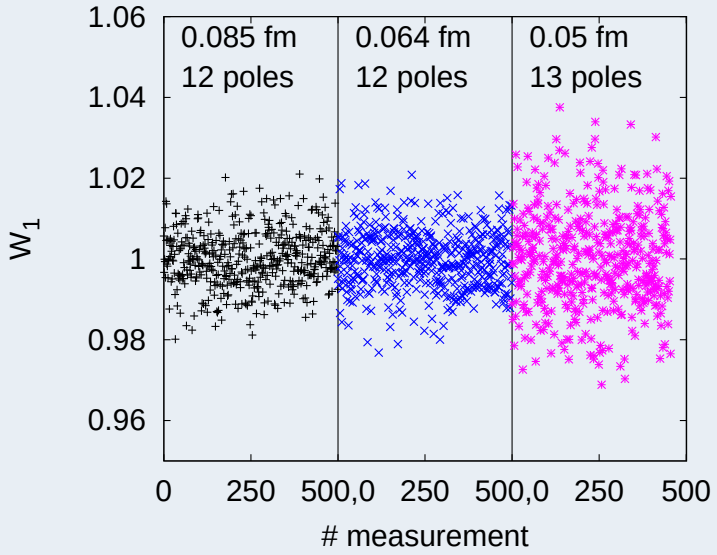


Figure: History of the rational approx. reweighting factor at the symmetric point.

$\Rightarrow$ works prefectly!

First measurements: Wilson flow observables

A renormalization-free observable is

$$\bar{E}(t, x_0) = \frac{1}{4} \sum_{\vec{x}} G^a_{\mu\nu}(t, x) G^a_{\mu\nu}(t, x)$$

and can be used to exhibit the growth of autocorrelations.

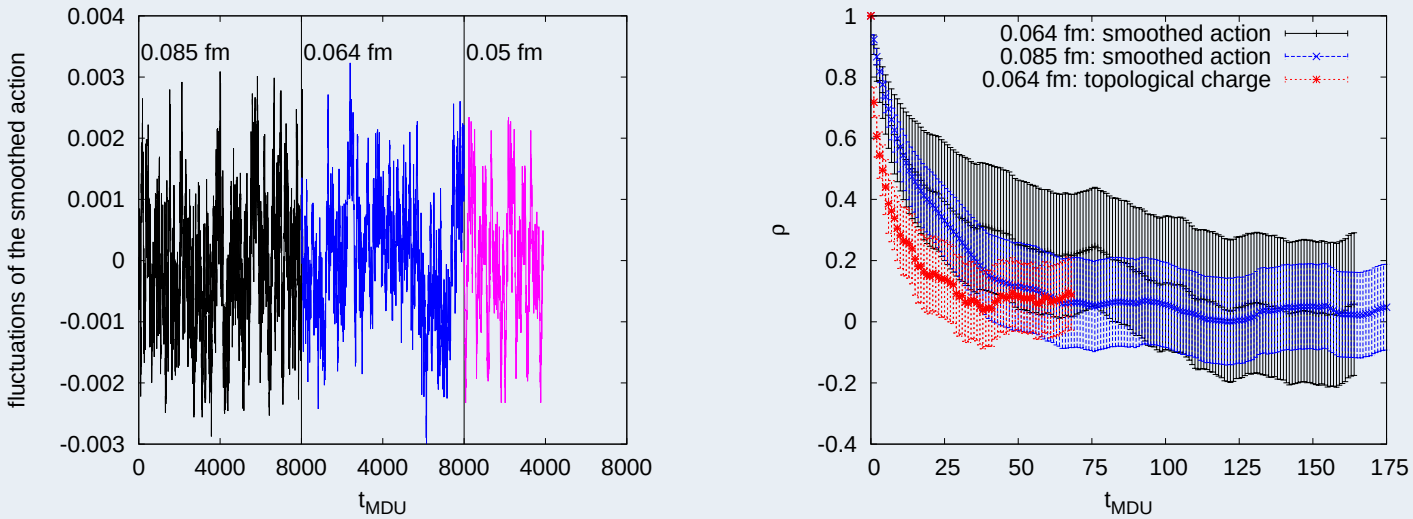


Figure: Smoothed YM action at the symmetric point at flow time $t/a^2 = 3.0, 6.0, 12.0$. Scaling of $\tau_{\rm int}$ consistent with $1/a^2$.

First measurements: t_0

t_0

$$\left\{ t^2 \langle \bar{E}(t, x_0 = T/2) \rangle \right\} \Big|_{t=t_0} = 0.3$$

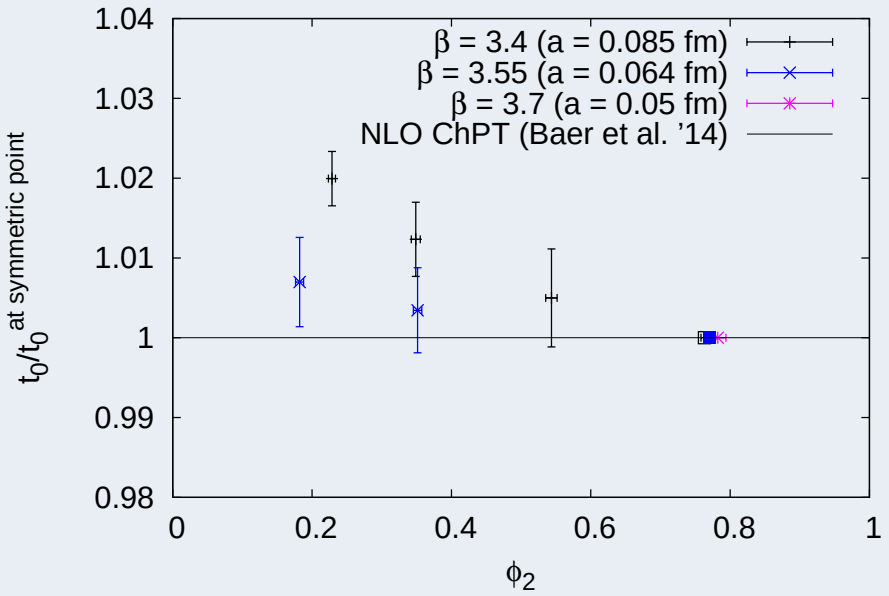


Figure: Dependence of t_0/t_0^{ref} on m_π at different lattice spacings.

First measurements: open boundary conditions

There's no free lunch

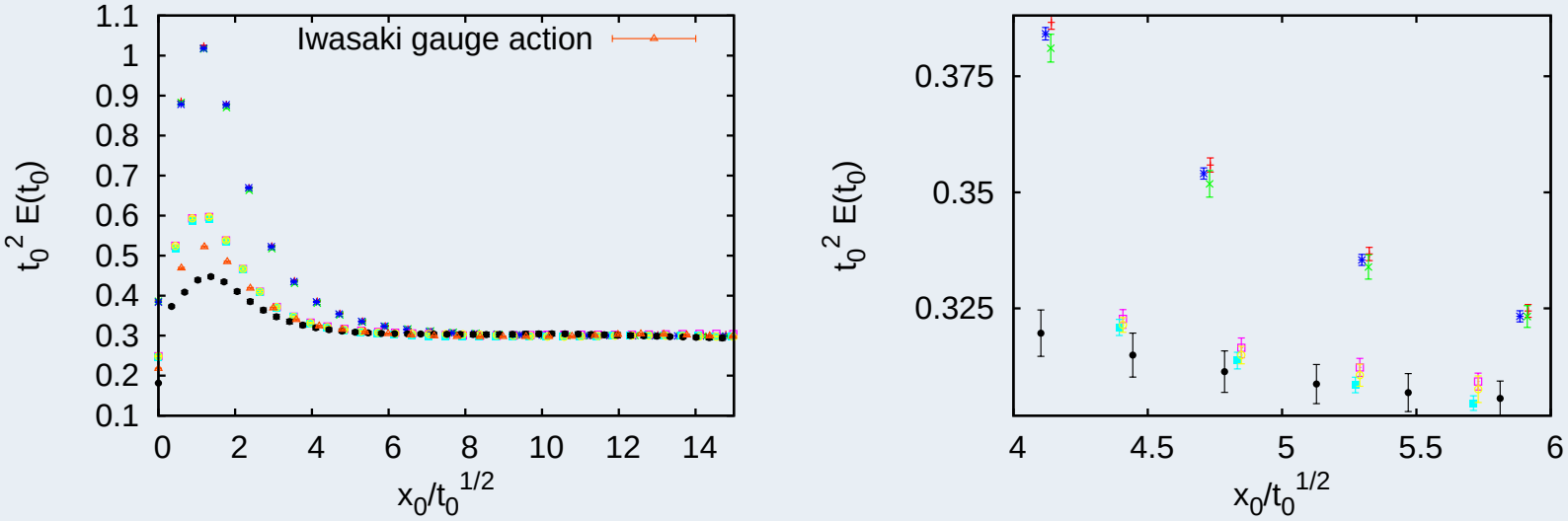


Figure: Cutoff effects at the boundaries.

First measurements: open boundary conditions

There's no free lunch

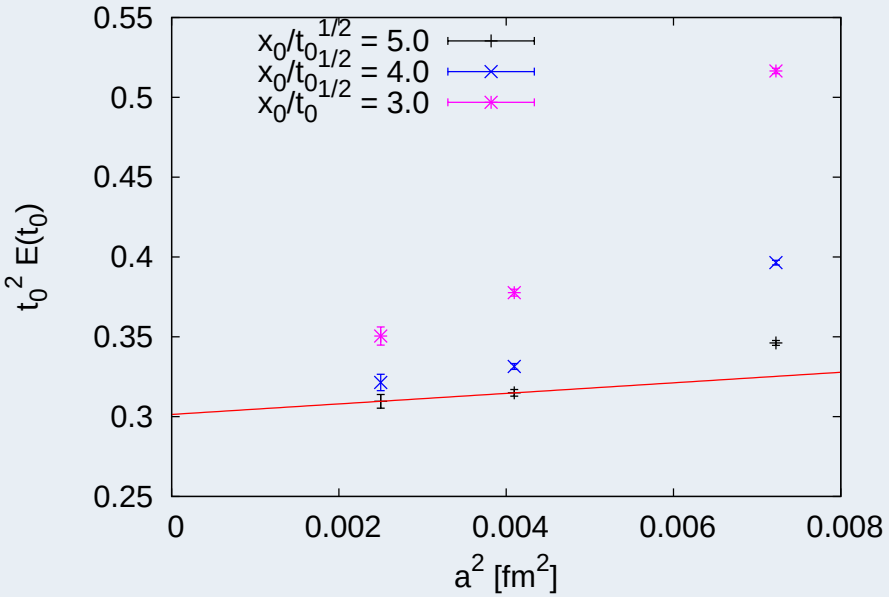
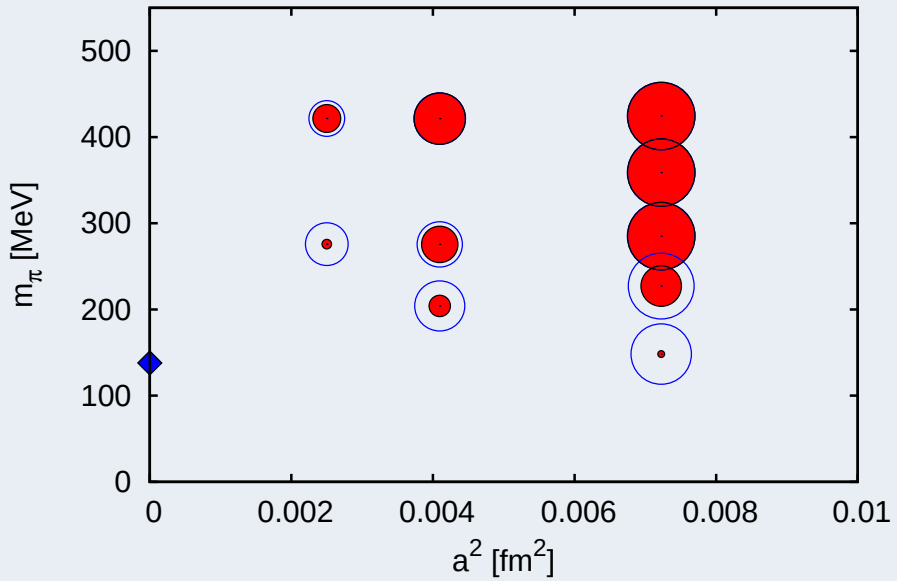


Figure: Cutoff effects at the boundaries.

Conclusions

Project under way!



- area of points: MDU/τ_{exp}
- area of circles: target MDU/τ_{exp}

Related talks

- impact of twisted mass reweighting on precision → Mattia Bruno's talk Tue 14:35
- baryon spectrum → Wolfgang Soeldner's talk Wed 9:20