On the extraction of spectral quantities with open boundary conditions

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32nd International Symposium on Lattice Field Theory - Columbia University, New York

June 24, 2014

Setup of the simulations

- Lüscher-Weisz gauge action
- 2+1 O(a)-improved Wilson fermions

  Hasenbusch factorization of fermion determinant

  strange quark simulated with RHMC

  for more details see P. Korcyl's talk

- Open boundary conditions in time [Lüscher,Schaefer,2011]

  cutoff effects close to the boundaries

  how the analysis changes in presence of open BC

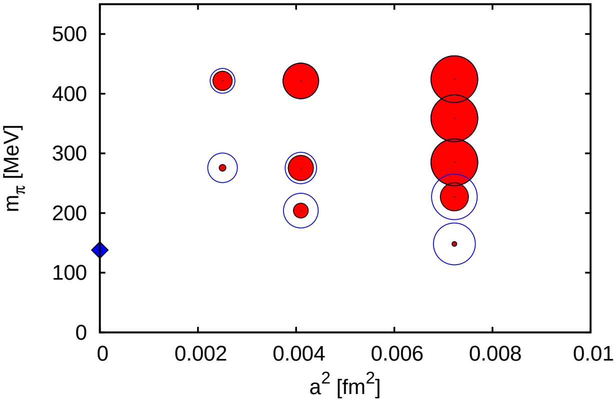
- Twisted-mass reweighting à la Lüscher-Palombi

  how the reweighting affects observables

High statistics

8000 MDU per ensemble

Ensemble Map



Focus on trajectories:

tr$M$ constant at $a \approx 0.085$ fm

continuum limit at symmetric point

Area: MDU$/\tau_{\rm exp}$; Blue circles: available statistics at the end of project

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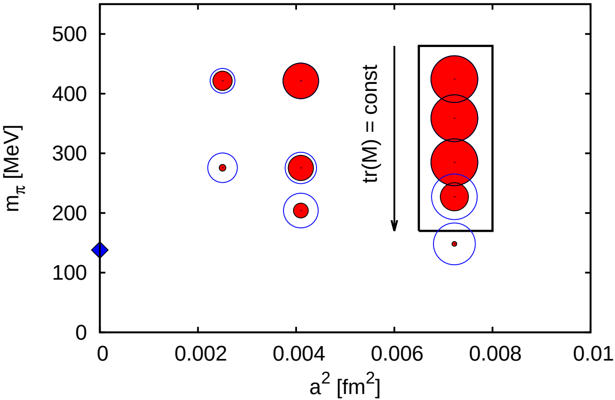

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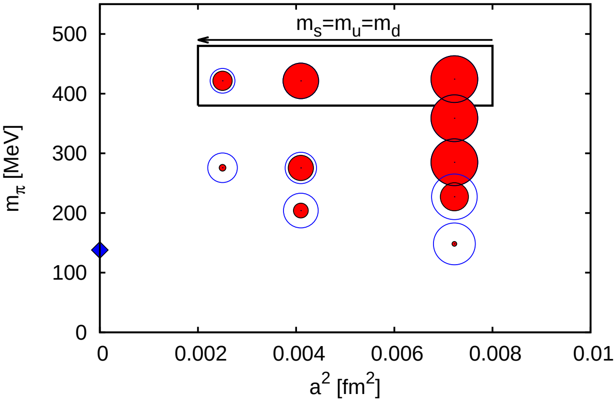

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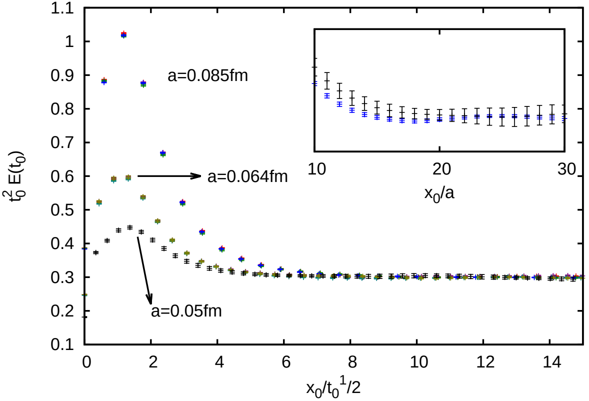
Energy density - Boundaries



Wilson flow: [Lüscher,'10]

Signature of the boundaries:

- no pion mass dependence
- large cutoff effects
- fluctuations in the center of lattice

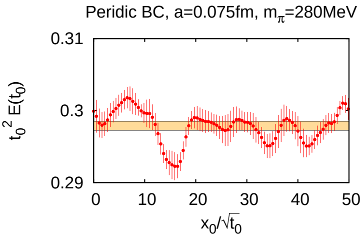
Boundary effects are dominantly $O(a)$ effects $\rightarrow$ plateau starts at fixed $x_0/a \approx [15:20]$

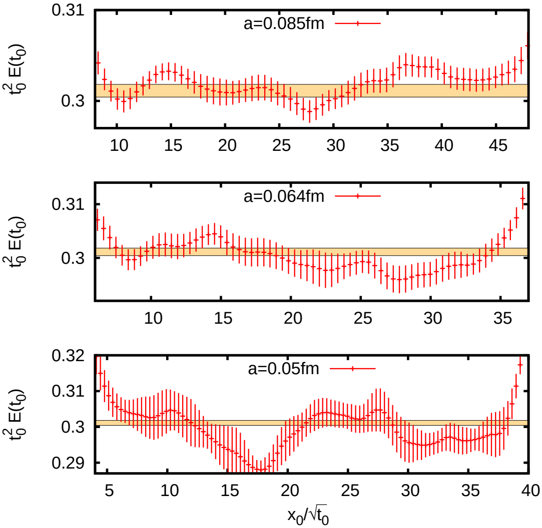
Energy density - Bulk

smoothing effect

slow-mode effect calls for proper error analysis ($\tau_{\rm exp}$) [Schaefer et al.,'11]

same fluctuations observed in periodic BC

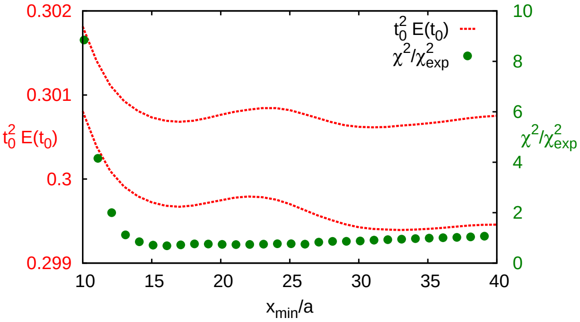




Where does the plateau start?

Study χ^2 as a function of the distance from boundary $x_{\min}$

$\chi^2_{\exp}$: expected χ^2 in presence of correlations [Bunk,'80s]



$t_0^2 E_{t_0}(x_{\min})$ from plateau $[x_{\min}$: fixed$]$

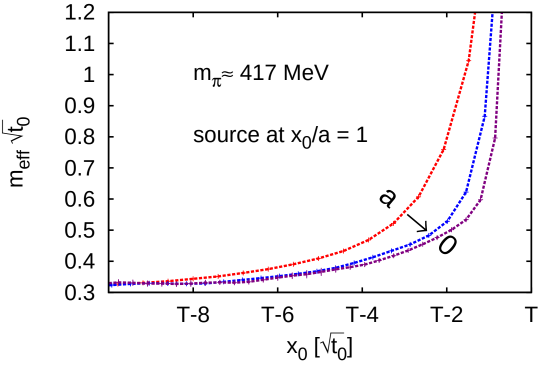
In the bulk

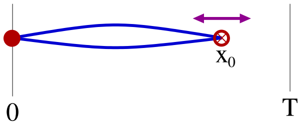
waves consequence of limited statistics only

Sufficient statistics for error computation

Mass - Boundaries

$$a^3 f_{\mathrm{P}}(x_0) = \frac{a^3}{L^3} \sum_{\mathbf{x}} \langle P(x_0, \mathbf{x}) P(0, \mathbf{x}) \rangle \,,\; a m_{\mathrm{eff}}(x_0 + \frac{a}{2}) = \log \frac{f_{\mathrm{P}}(x_0)}{f_{\mathrm{P}}(x_0 + a)}$$



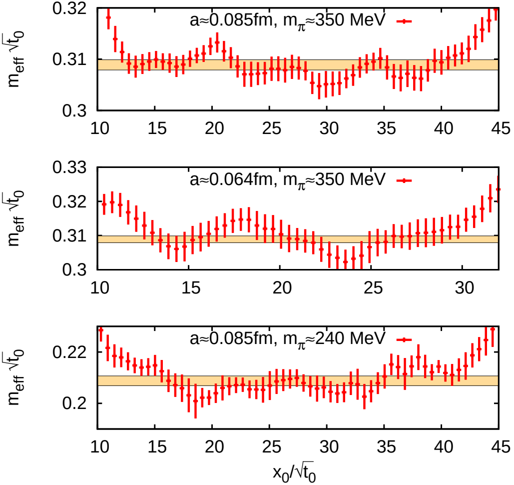


Large cutoff effects close to boundary

Small dependence on pion mass

Mass - Bulk

In the center of the lattice we find waves.



Fluctuations of 1-2 σ

Few per cent w.r.t. the scale of the observable

[Aoki et al.,'96]:

1. cov. matrix
2. finite statistical precision
3. fixed source position

$\Downarrow$

Waves in $m_{\rm eff}$ of 1-2 σ

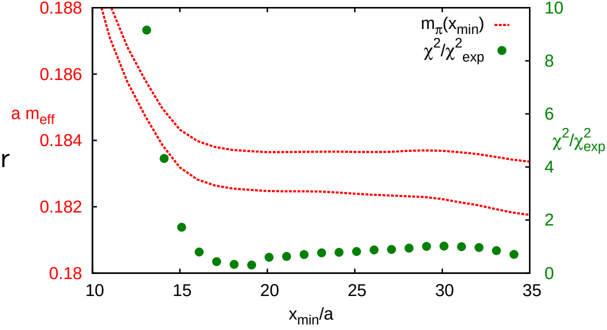
Waves in the bulk

$$am_\pi(x_{\min}) \text{ from plateau } [x_{\min} : x_{\max}]\,, \quad x_{\max} = \text{fixed}\,.$$

Plateau starts when $\chi^2/\chi^2_{\rm exp} \lesssim 1$

0.25 fm safe distance for excited states

Waves are a pure statistical fact



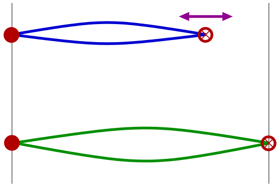
π decay constant

$$a^3 f_{\mathrm{A}}(x_0, y_0) = \frac{a^3}{L^6} \sum_{\mathbf{x},\mathbf{y}} \langle A_0(x_0, \mathbf{x}) P(y_0, \mathbf{y}) \rangle \, ,$$

From Transfer matrix difference to periodic BC $\rightarrow A(y_0)$:
$A(y_0)$ amplitude depends on distance from boundary

$$f_{\mathrm{A}}(x_0, y_0) = A(y_0) \hat{f}_\pi e^{-m_\pi(x_0 - y_0)} \, , \; f_{\mathrm{P}}(T - y_0, y_0) = A^2(y_0) e^{-m_\pi(T - 2y_0)}$$

[Guagnelli et al.,'99]: Transfer matrix applied to Schrödinger functional

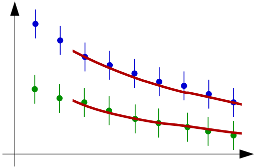


$$F_\pi^{\mathrm{bare}} \propto \frac{f_{\mathrm{A}}(x_0, y_0)}{\sqrt{f_{\mathrm{P}}(T - y_0, y_0)}} e^{m_\pi(x_0 - T/2)}$$

Cancellation of $A(y_0)$ via ratio

Plateau in x_0, if $0 \ll x_0 \ll T$

Strategies

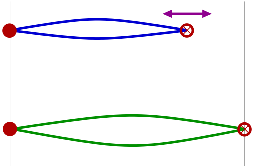


Global fit to f_A, f_P

$$f_\mathrm{A}(x_0, y_0) = A(y_0)\hat{f}_\pi e^{-m_\pi(x_0-y_0)}$$

$$f_\mathrm{P}(T-y_0, y_0) = A^2(y_0) e^{-m_\pi(T-2y_0)}$$

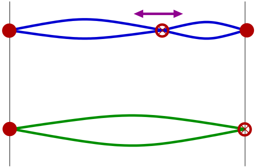
Note $\hat{f}_\pi \leftrightarrow F_\pi^{\mathrm{bare}}$ one-particle normalization



Cancellation of $e^{-m\cdots}$ factor using:

$$m_\mathrm{eff}(x_0),\ m_\mathrm{eff}^{\mathrm{average}},\ m_\mathrm{eff}^{\mathrm{fit}}$$

$$F_\pi^{\mathrm{bare}}(x_0, y_0) \propto \frac{f_\mathrm{A}(x_0, y_0)}{\sqrt{f_\mathrm{P}(T-y_0, y_0)}} e^{m_\mathrm{eff}(x_0 - T/2)}$$

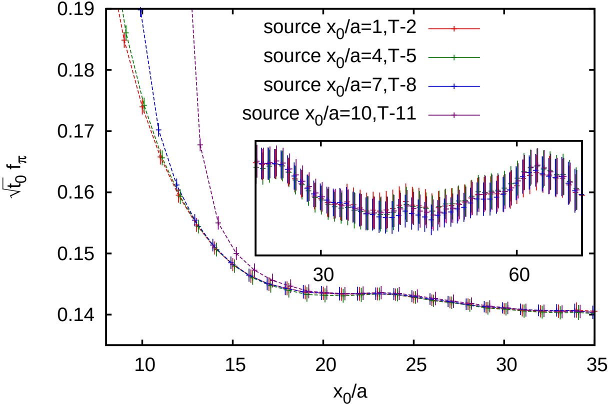


Cancellation of exp factor with $f_\mathrm{A}(x_0, T-y_0)$

Our proposal

$$F_\pi^{\mathrm{bare}}(x_0, y_0) \propto \sqrt{\frac{f_\mathrm{A}(x_0, y_0) f_\mathrm{A}(x_0, T-y_0)}{f_\mathrm{P}(T-y_0, y_0)}}\,.$$

Dependence on source position



Strong correlation between sources

Waves in the center of the lattice as for m_π, $E(t)$

Loss of translation invariance in time

No advantage in averaging correlators from displaced sources.

Different methods

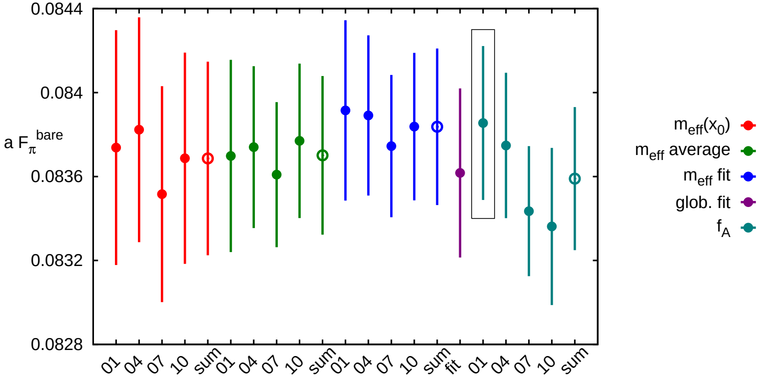
Test ensemble H101:

$m_\pi \approx 415$ MeV, $m_\pi L \approx 4.8$

$a \approx 0.085$ fm, stat$\approx 100\tau_{\text{exp}}$

Result

$$am_\pi = 0.18306(57)$$
$$aF_\pi^{\text{bare}} = 0.08385(37)$$
$O(0.5\%)$ precision



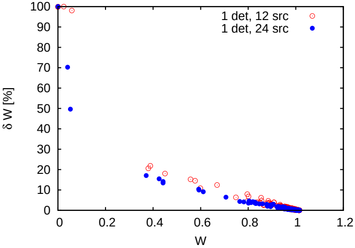
Reweighted Observables

Twisted-Mass (type II) reweighting is under investigation

$$S_f \propto -\log\det\frac{(Q^2+\mu^2)^2}{Q^2+2\mu^2}\,, \quad W = \det\frac{Q^2(Q^2+2\mu^2)}{(Q^2+\mu)^2}\,, \quad Q=\gamma_5 D$$

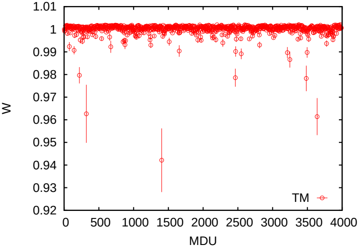
Weights computed from stochastic sources:

- is the number of sources, the method safe?



Fluctuations with gauge configurations

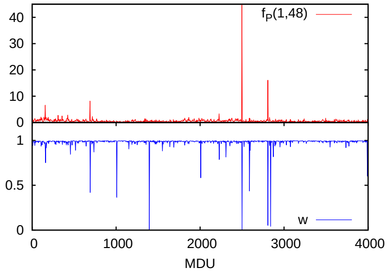
- how do these affect the observables?



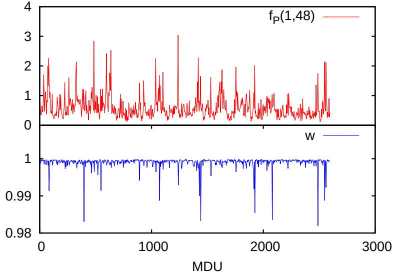
Back reaction -I

On a given configuration with small eigenvalues λ of D

observables like $f_\mathrm{P} \sim \lambda^{-2}\,, \quad \langle W \rangle_\mathrm{src} \sim \lambda^2$



$\mu \to \mu/2$



Prob. $\det \frac{(Q^2+\mu^2)^2}{Q^2+2\mu^2}$:

Regions of fields space with small λ now accessible with $\mu > 0$, good for ergodicity

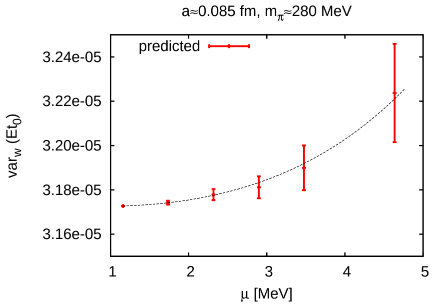
if μ is large $\to$ large fluctuations in observables

Back reaction - II

Predict error of observables in simulations with weight w

$$(\Delta O)^2 = \frac{\mathrm{var}_w(O)}{N}\,, \quad \langle O\rangle = \frac{\langle Ow\rangle_w}{\langle w\rangle_w}$$

It can be expressed as observable in underlying theory:



Error of gluonic observables (un-correlated) degrades slower

$$\leftarrow \mathrm{var}_w(O) = \langle w^{-1}\rangle\langle (O-\bar{O})^2 w\rangle$$

Fermionic observables more problematic, still under investigation

Conclusions

Open boundary conditions:

- loss of translation invariance in time is not a problem
- decay constants can be computed with desired precision (at $a \sim 0.085$ fm)
- we introduced a new strategy to compute F_π

Reweighting factors:

- better sampling of region of small EV of the Dirac operator
- affect observables $\rightarrow$ careful tuning of μ
- have to be computed properly

Thanks for your attention!