Lattice QCD with 2+1 Flavors and Open Boundaries: First Results of the Baryon Spectrum

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Lattice 2014
The 32nd International Symposium on Lattice Field Theory
June 25th, 2014

Outline

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- Motivation, Introduction
- Simulation Details, Reweighting
- Scale Setting
- Baryon Spectrum
- Outlook and Summary

Motivation

Today's lattice QCD simulations

- more computing power and better algorithms $\rightarrow$ better precision of lattice QCD results
- more and more important $\rightarrow$ good control of systematics

$\Rightarrow$ obviously, very important: good control of continuum limit

Problem when lattice spacing $a \rightarrow 0$

$\Rightarrow$ freezing of topology

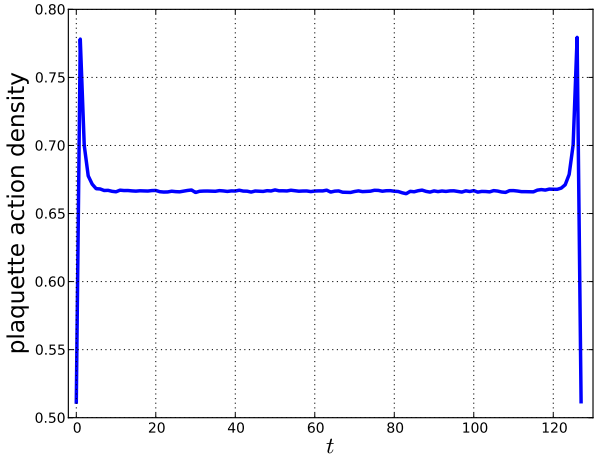
- lattice simulations get stuck in topological sectors
- problems begin at $a \approx 0.05\ \mathrm{fm}$

$\Rightarrow$ elegant solution: lattice simulations with open boundary conditions

[Lüscher and Schaefer 2011]

$\rightarrow$ topology can flow in and out through the boundary

Lattice QCD with Open Boundaries



Open Boundaries

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

Major CLS effort

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

See also talks by

- Piotr KORCYL, Monday, 16.30h
- Mattia BRUNO, Tuesday, 14.35h

Simulation Details

Lattice Action

- Non-perturbatively improved Wilson Clover action
- Tree-level improved Symmanzik gauge action
- Two degenerate light quarks and one strange quark
- Simulations at fixed $\sum_q \frac{1}{\kappa_q}$ (QCDSF strategy)

Note: $\mathrm{Tr}(aM) = 2am_{ud} + am_s = const. + \mathcal{O}(a)$

Lattice spacing (preliminary)

$\beta = 6/g^2 = 3.4 \quad \rightarrow \quad a \approx 0.086\ \mathrm{fm}$ ($\beta = 3.3, 3.55, 3.7$ not presented in this talk)

Meson masses (preliminary)

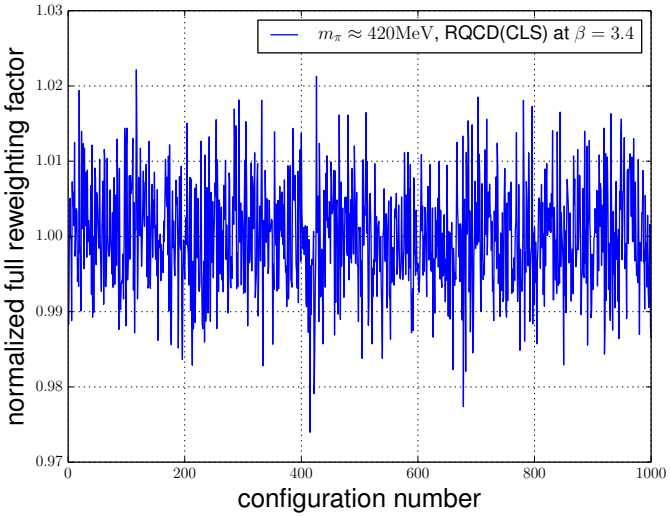
run id	H101	H102	H105	C101
m_π	420 MeV	355 MeV	280 MeV	230 MeV
m_K	420 MeV	440 MeV	465 MeV	475 MeV

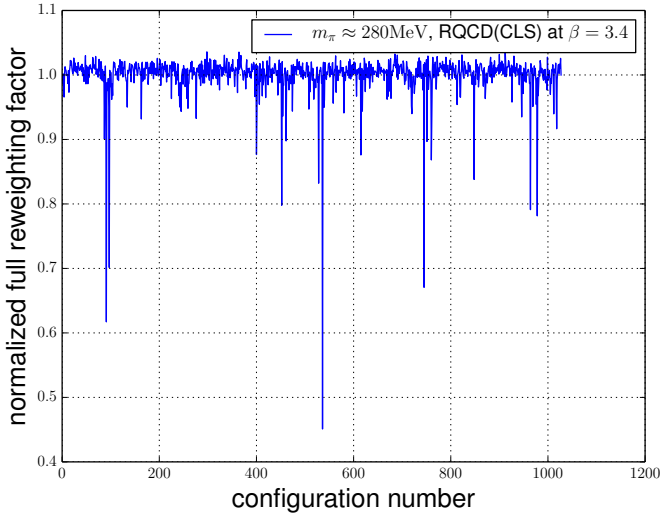
Geometry

$32^3 \times 96$ and $48^3 \times 96$ (smallest m_π) $\quad \Rightarrow \quad m\pi L > 4$ for all ensembles

openQCD and Reweighting

preliminary





Simulations and reweighting

- twisted mass reweighting
  $\rightarrow$ add a twisted mass term to light quark action in the simulations to stabilize HMC runs
- strange quark mass reweighting
  $\rightarrow$ accounts for errors in the rational approx.

$\Rightarrow \langle O \rangle = \frac{\langle RO \rangle}{\langle R \rangle}$ with Observable O and rwt. factor R

Software

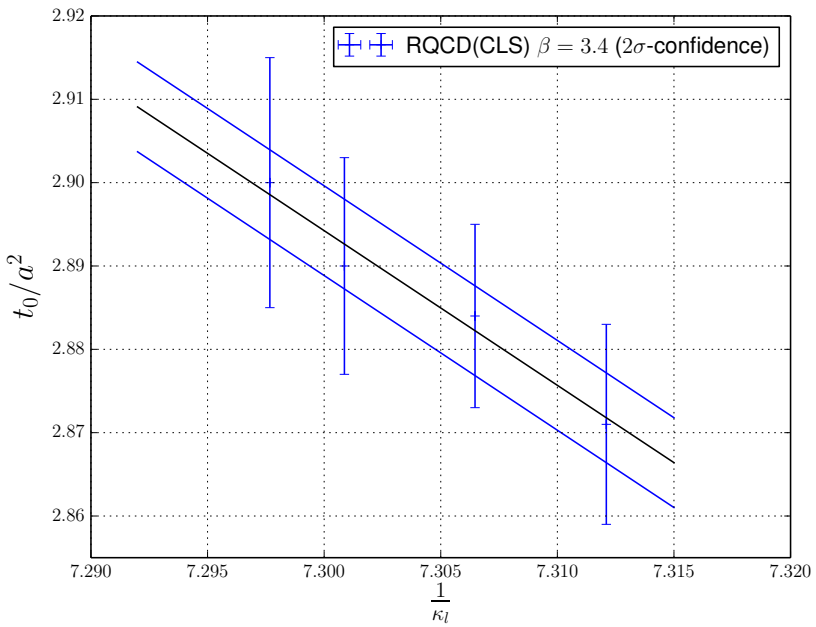
openQCD and CHROMA software package

Supercomputers

Simulations are mainly performed at LRZ@Munich, JSC@Juelich, FERMI@Bologna

Scale Setting

preliminary



Scale setting with t_0

- Wilson flow $\langle E(t) \rangle$ of Yang-Mills action density with flow time t
- $t_0^2 \langle E(t_0) \rangle = 0.3$
- compare to literature [Borsanyi *et. al.* 2012]

$$\sqrt{t_0^{BMW}} = 0.1465(21)(13)\ \mathrm{fm}$$

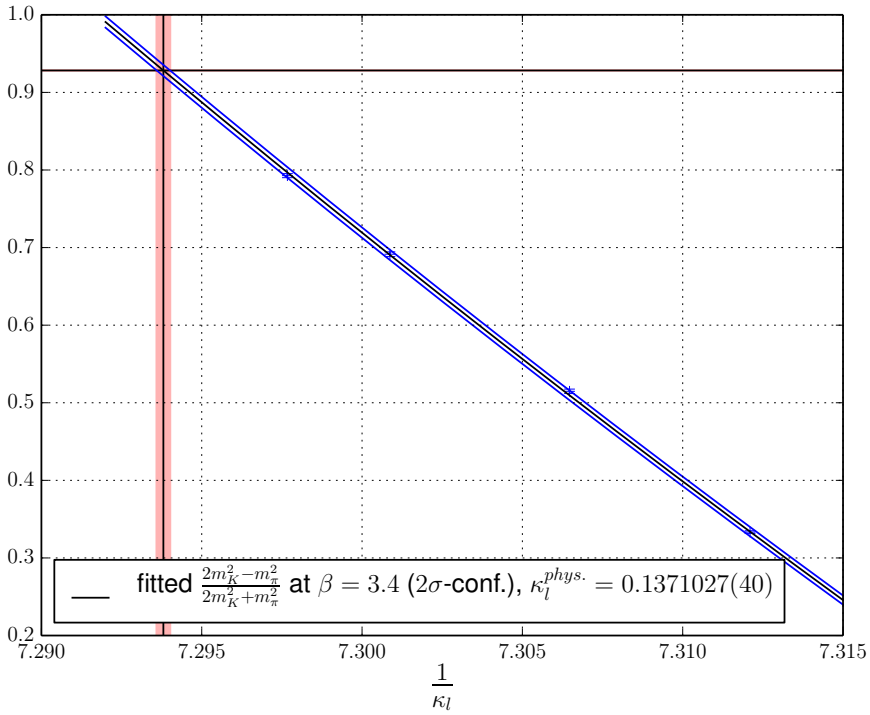
Wilson fermions, continuum extrapolated, at physical point

Goal: $\rightarrow$ independent crosscheck of t_0 value

Mesons: Chiral Extrapolations and Scale Setting

To fix $\left(\kappa_l, \sum_q \frac{1}{\kappa_q}, a\right)$ to the physical point requires 3 measurements, e.g. (m_π, m_K, t_0)

Note: $\sum_q \frac{1}{\kappa_q}$ is fixed in our simulation, but need to check for correct value
$\Rightarrow$ remain to fix κ_l and a



preliminary

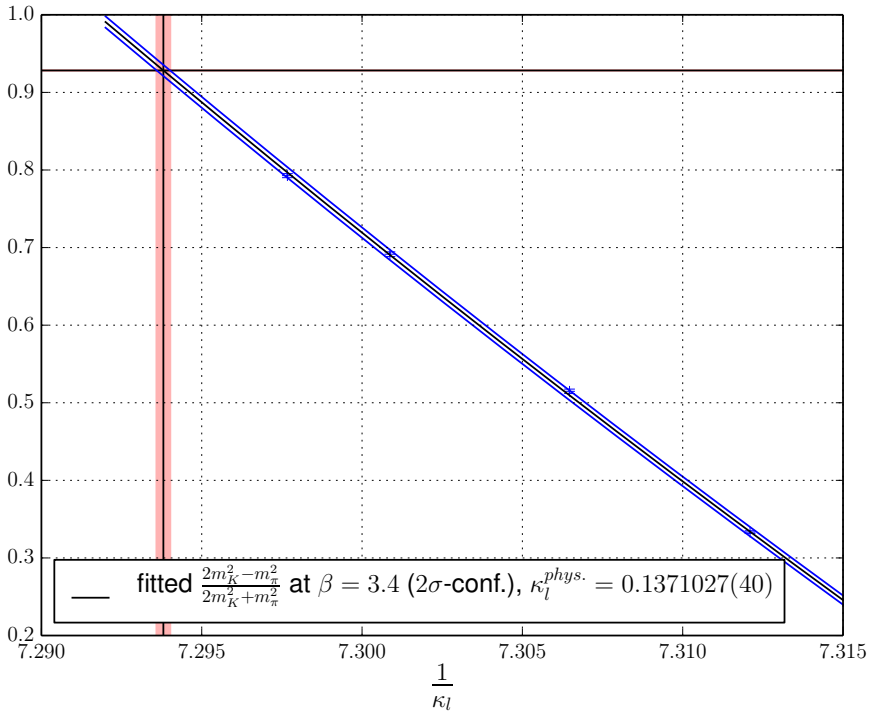
Note:

- $(am_\pi)^2, (am_K)^2 \underset{\sim}{\propto} \frac{1}{\kappa_l}$
- $2(am_K)^2 + (am_\pi)^2 \approx const$
- $\frac{2m_K^2-m_\pi^2}{2m_K^2+m_\pi^2}$ takes its physical value where $\frac{m_K}{m_\pi}$ has its physical value

Mesons: Chiral Extrapolations and Scale Setting

Physical Point

Define physical point where, e.g., $\frac{2m_K^2 - m_\pi^2}{2m_K^2 + m_\pi^2}$ takes its physical value [FLAG] and extract $\kappa_l^{phys.}$
$\Rightarrow$ remain to fix a (choose a specific scale setting)



preliminary

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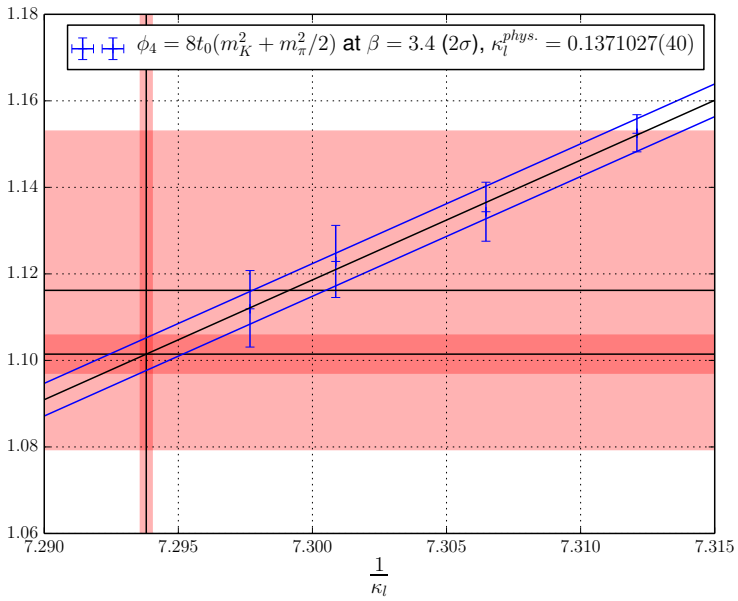
Mesons: Chiral Extrapolations and Scale Setting

Two scenarios

1. set scale with t_0^{BMW} $\Rightarrow$ consistency means we have chosen $\sum_q \frac{1}{\kappa_q}$ correctly
2. set scale with $2m_K^2 + m_\pi^2$ $\Rightarrow$ extract t_0, but need to check for correct $\sum_q \frac{1}{\kappa_q}$
   $\Rightarrow \sqrt{t_0} = 0.1455(3)$ fm
   $\Rightarrow$ consistent with BMW continuum extrapolated value $\left(\sqrt{t_0^{BMW}} = 0.1465(21)(13)\text{ fm}\right)$



Look at, e.g., $\phi_4 = 8t_0(m_K^2 + m_\pi^2/2)$

at physical point ($\kappa_l = \kappa_l^{phys.}$)
$\Rightarrow \phi_4 = 1.1015(6)$

Compare to

$$\phi_4 = 8t_0^{BMW}(m_{K,phys.}^2 + m_{\pi,phys.}^2/2) = 1.116(37)$$

preliminary

Mesons: Chiral Extrapolations and Scale Setting

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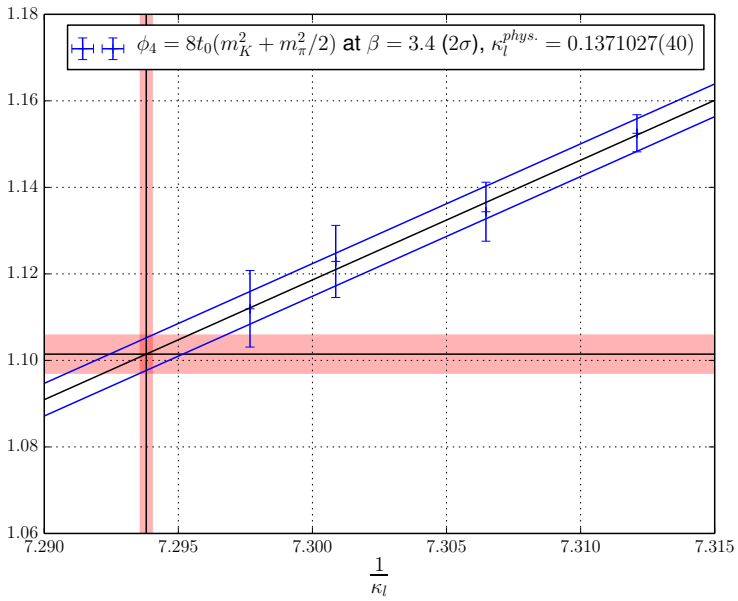

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preliminary

Baryon Spectrum: Setup

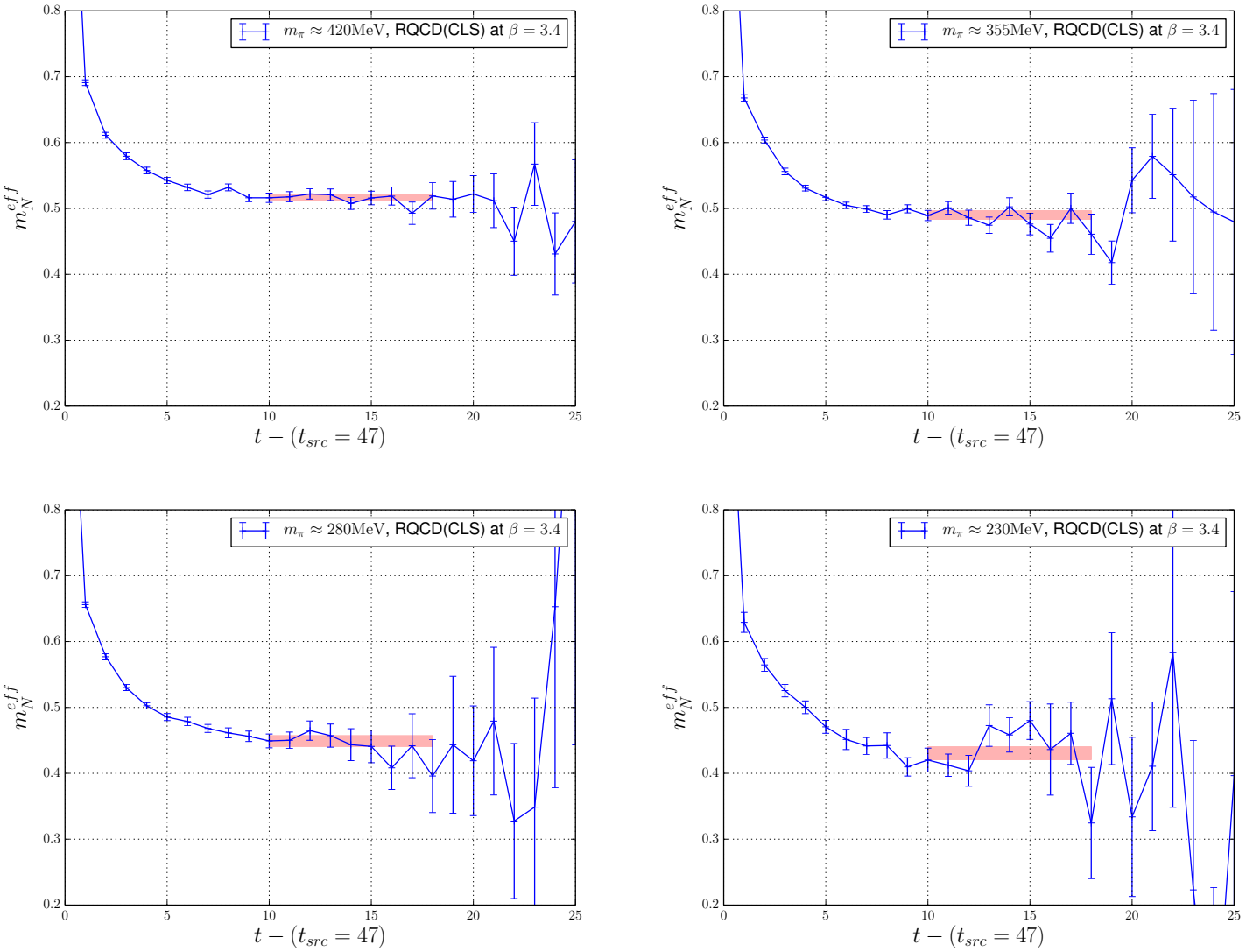
Setup

- relativistic interpolators: $I_N = \epsilon_{abc} u_a \left(u_b^T C \gamma_5 d_c \right), \ldots$
- fixed temporal source position at center $t_{src} = 47$, $(N_\tau = 96)$
- random spatial source position
- one source per configuration, configurations separated by 4 MDU
- smeared-smeared correlator
  $\rightarrow$ 100 steps of Wuppertal smearing on APE smeared gauge links (for both source and sink)
- fit range = $[10, 18]$

run id	H101	H102	H105	C101
stats.	2000	2000	2000	500

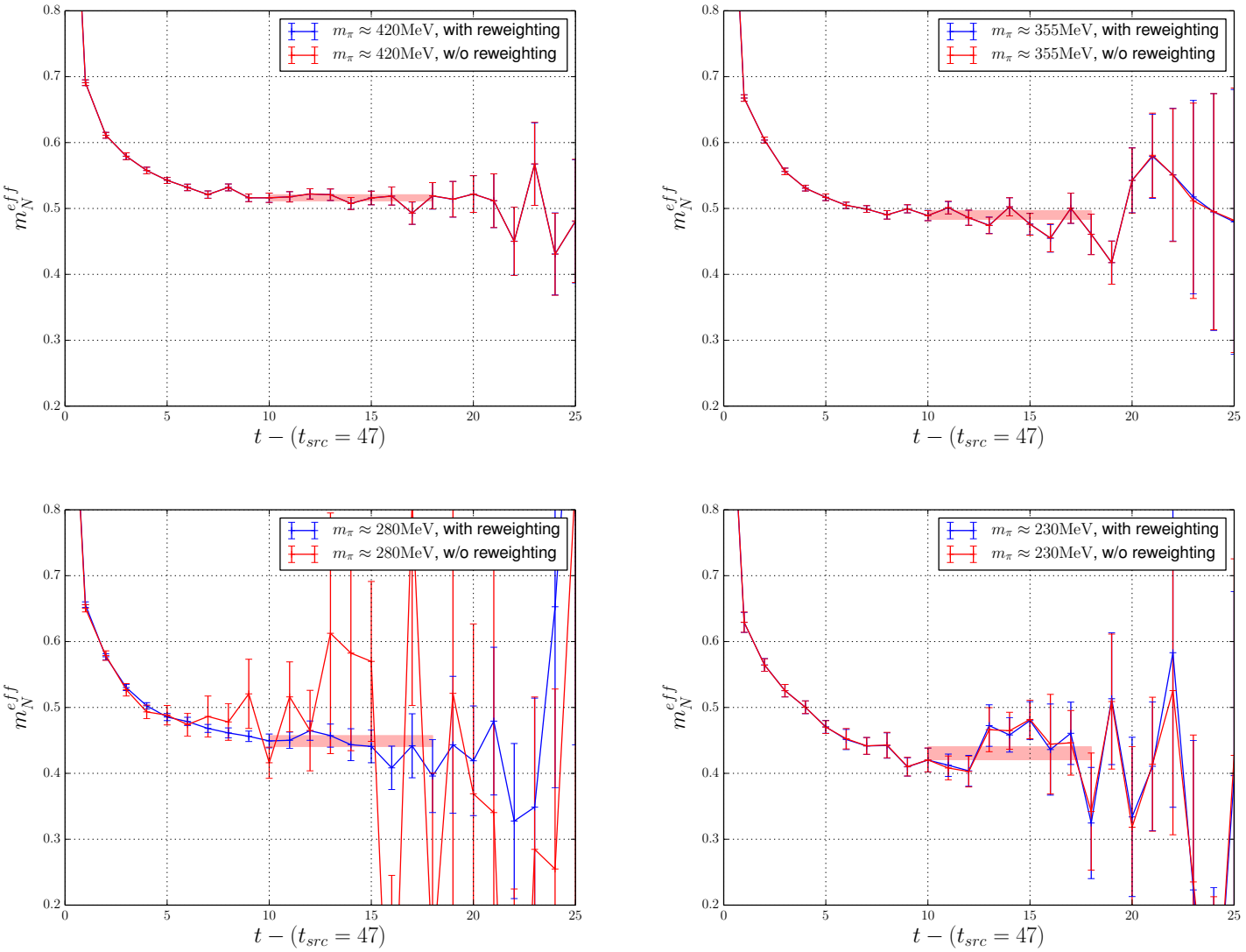
Baryon Spectrum: Effective Mass (Nucleon)

preliminary



Baryon Spectrum: Reweighting (Nucleon)

preliminary



SU(3) Chiral Perturbation Theory

Octet baryon masses to $\mathcal{O}(p^2)$ in BChPT

e.g. [Bernard et al. 1993]

$$m_N = m_0 - 4b_D\dot{M}_K^2 + 4b_F\left(\dot{M}_K^2 - \dot{M}_\pi^2\right) - 2b_0\left(2\dot{M}_K^2 + \dot{M}_\pi^2\right) + \cdots ,$$

$$m_\Lambda = m_0 + \frac{4}{3}b_D\left(-4\dot{M}_K^2 + \dot{M}_\pi^2\right) - 2b_0\left(2\dot{M}_K^2 + \dot{M}_\pi^2\right) + \cdots ,$$

$$m_\Sigma = m_0 - 4b_D\dot{M}_\pi^2 - 2b_0\left(2\dot{M}_K^2 + \dot{M}_\pi^2\right) + \cdots ,$$

$$m_\Xi = m_0 - 4b_D\dot{M}_K^2 - 4b_F\left(\dot{M}_K^2 - \dot{M}_\pi^2\right) - 2b_0\left(2\dot{M}_K^2 + \dot{M}_\pi^2\right) + \cdots .$$

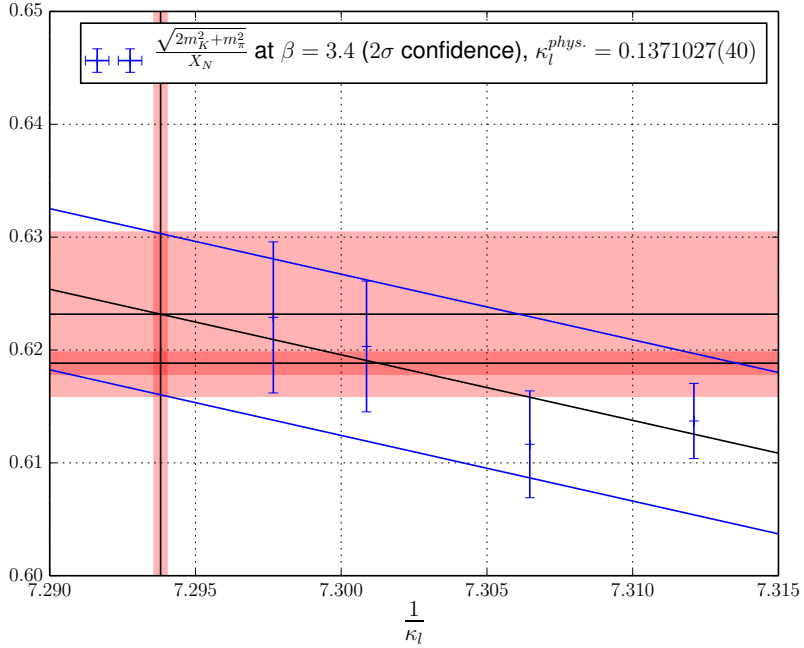
Average nucleon mass

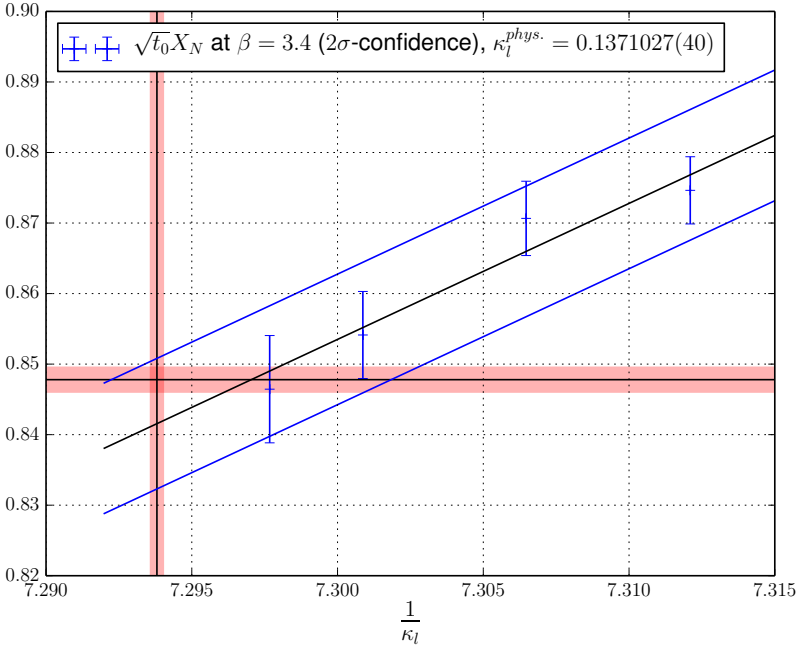
(remember: $2m_K^2 + m_\pi^2 \approx const.$)

$$X_N = \frac{1}{3}\left(m_N + m_\Sigma + m_\Xi\right) = m_0 - 2b_0\left(2\dot{M}_K^2 + \dot{M}_\pi^2\right) + \cdots$$

Baryon Spectrum: $X_N = \frac{1}{3}(m_N + m_\Sigma + m_\Xi)$

preliminary





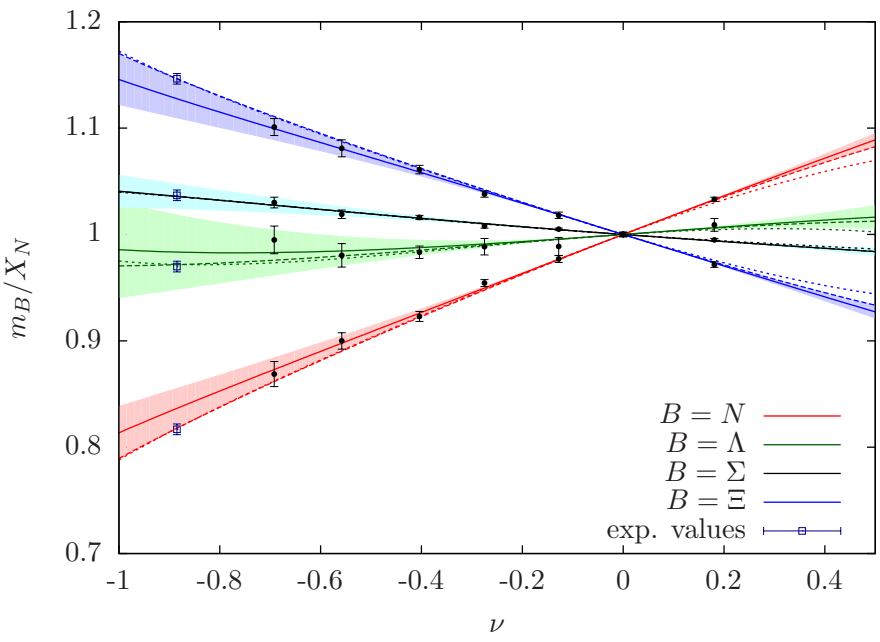
Compare to $\kappa_l^{phys.}$ and t_0 from our determination above

$\rightarrow$ find consistency for $\frac{\sqrt{2m_K^2+m_\pi^2}}{X_N}$, $\sqrt{t_0}X_N \Rightarrow$ we have chosen $\sum_q \frac{1}{\kappa_q}$ correctly

Note: more detailed study of systematics necessary (work in Progress)

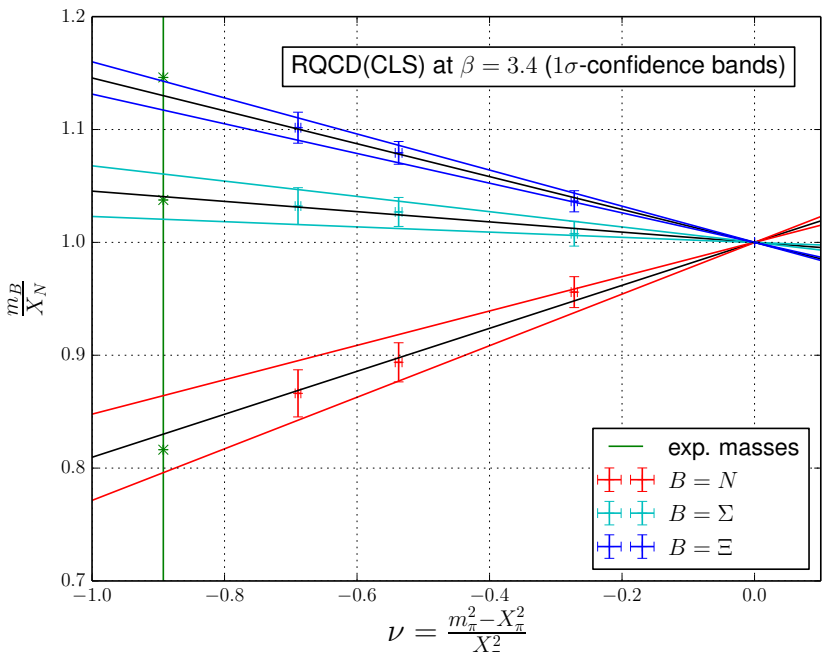
Baryon Spectrum: Fan Plot

preliminary



[Bruns, Greil, Schaefer 2013]

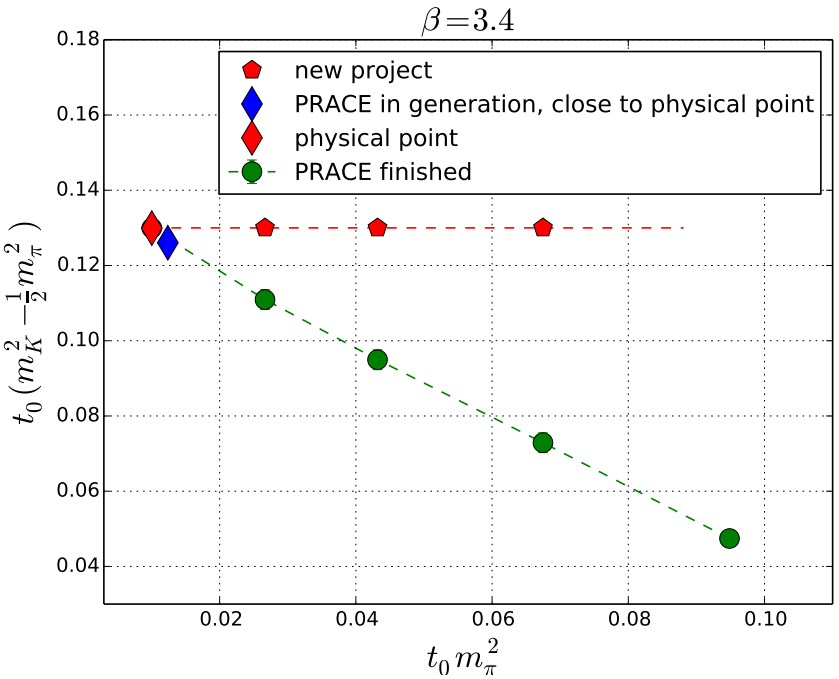
based on QCDSF data



preliminary RQCD(CLS) data

$\Rightarrow$ consistency with other studies (QCDSF, RQCD)

Outlook: Simulations at Fixed Strange Quark Mass



$m_s^{PCAC} = m_{s,phys.}^{PCAC} = const.$

- additional simulations at $\beta = 3.4$
- project has just started

$\Rightarrow$ obtain also $\mathrm{SU}(2)$ low energy constants

Summary

Lattice Simulations with Open Boundaries

- avoid topological freezing as $a \to 0$
- long term effort within CLS

Scale Setting

- example case presented for scale setting

$\to$ consistency found for t_0 with value from BMW + correct choice for $\sum_q \frac{1}{\kappa_q}$

Baryon Spectrum

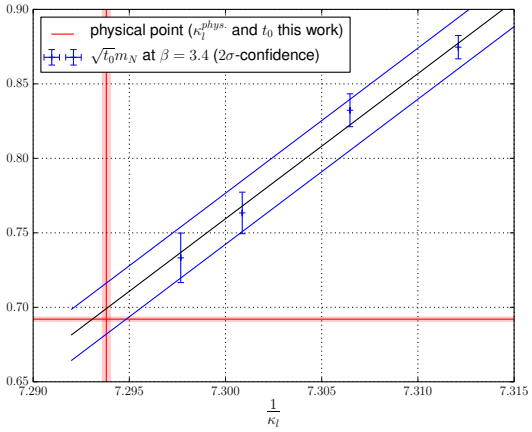
- 'fan plot' consistent with results from literature

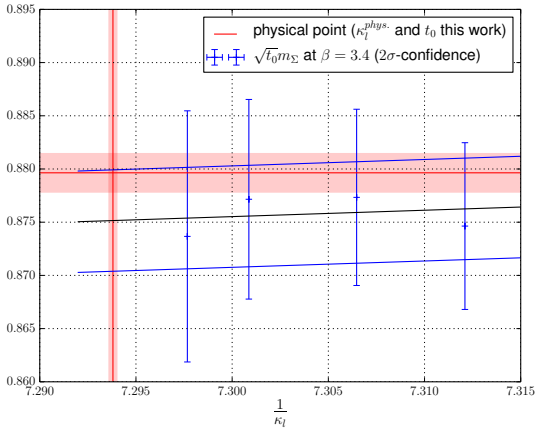
Outlook

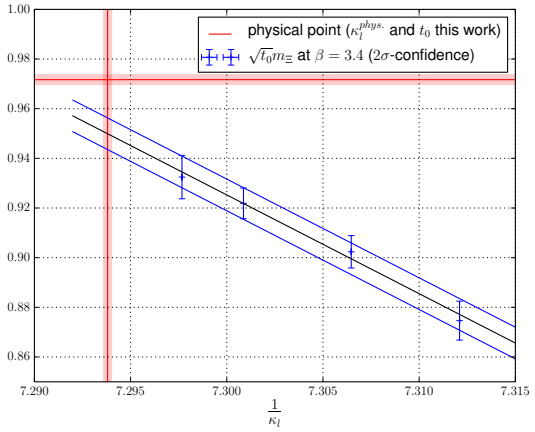
- more detailed study with increased stats., more observables, smaller m_π, lattice spacing
- additional simulations in preparation at fixed $m_s^{PCAC} = m_{s,phys.}^{PCAC}$

Baryon Spectrum: Chiral Extrapolation

preliminary







$\kappa_l^{phys.}$ and t_0 from our determination above

$\rightarrow$ consistency of t_0 at $\kappa_l^{phys.}$ for N and Σ

$\rightarrow$ $\approx$ 2% deviation for Ξ

- study of systematics in more detail (work in Progress)