Lattice QCD Simulations with 2+1 Flavors and Open Boundaries

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Perspectives and Challenges in Lattice Gauge Theory
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Outline

Outline

- Motivation, Introduction
- Simulation Details, Algorithmic Setup
- Tuning Strategy
- Scale Setting
- Autocorrelations
- Reweighting
- Measurements
- Outlook and Summary

for more details $\rightarrow$ hep-lat 1411.3982

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

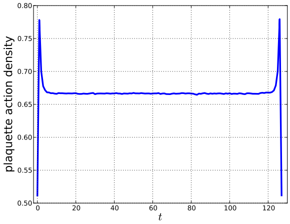
- lattice simulations get stuck in topological sectors
- problems begin at $a \approx 0.05\ \mathrm{fm}$

$\Rightarrow$ 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

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

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

Action

Open Boundaries

- open boundary conditions imposed in temporal direction
- coefficients of the boundary improvement terms are set to their tree level values

Gauge Action

- Lüscher–Weisz action

  $\to$ tree level coefficients $c_0 = 5/3$ and $c_1 = -1/12$
- $\beta = 6/g_0^2$ with the bare gauge coupling g_0

$$S_g[U] = \frac{\beta}{6}\left(c_0 \sum_p \mathrm{tr}\{1 - U(p)\} + c_1 \sum_r \mathrm{tr}\{1 - U(r)\}\right)$$

plaquettes p and the rectangles r

Action

Fermion Action

- non-perturbatively improved Wilson Clover action
- c_{sw} from [Bulava2013]
- 2+1 flavor:
  - degenerate up and down quark masses
  - strange-quark mass $m_{0,\mathrm{s}}$ is tuned as a function of light quark mass

$$D_{\mathrm{W}}(m_0) = \frac{1}{2}\sum_{\mu=0}^{3}\{\gamma_\mu(\nabla^*_\mu + \nabla_\mu) - a\nabla^*_\mu\nabla_\mu\} + ac_{sw}\sum_{\mu,\nu=0}^{3}\frac{i}{4}\sigma_{\mu\nu}\widehat{F}_{\mu\nu} + m_0$$

$$S_{\mathrm{f}}[U,\overline{\psi},\psi] = a^4\sum_{f=1}^{3}\sum_{x}\overline{\psi}_f(x)\,D_{\mathrm{W}}(m_{0,f})\,\psi_f(x), \qquad m_{0,f} = \frac{1}{2a}\left(\frac{1}{\kappa_{\mathrm{f}}} - 8\right)$$

Choice of Parameters

Scale setting and quark masses

- set the scale through Wilson flow t_0
- quark masses are set using m_π and m_K
- we use $m_\pi = 134.8(3)$ MeV and $m_K = 494.2(4)$ MeV
  $\rightarrow$ isospin limit from FLAG report
- $\sqrt{8t_0} = 0.4144(59)(37)$ fm from BMW collaboration
  (n_f =2+1 flavors at physical point, continuum extrapolated)

$$\phi_2 = 8t_0 m_\pi^2 \quad \rightarrow \quad \phi_2^{\text{phys}} = 0.0801(27)$$

$$\phi_4 = 8t_0(m_K^2 + \frac{1}{2}m_\pi^2) \quad \rightarrow \quad \phi_4^{\text{phys}} = 1.117(38)$$

Choice of Parameters

Note

- $\phi_2 \propto (m_\mathrm{u} + m_\mathrm{d})$ and $\phi_4 \propto (m_\mathrm{u} + m_\mathrm{d} + m_\mathrm{s})$ in leading order ChPT
- no renormalization constants or chiral extrapolation needed
- large cutoff effects in the various definitions of t_0/a^2 at our largest lattice spacings
- t_0 is not an experimentally accessible observable and only known from other lattice simulations.

Scale Setting

Scale setting with t_0

- Wilson flow equation: $\partial_t V_t(x,\mu) = -g_0^2 \{\partial_{x,\mu} S_W(V_t)\} V_t(x,\mu)$ with $V_t(x,\mu)\big|_{t=0} = U(x,\mu)$
- Wilson flow $\langle E(t) \rangle$ of Yang-Mills action density with flow time t
- Definition: $t_0^2 \langle E(t_0) \rangle = 0.3$

One goal of these simulations: $\rightarrow$ independent crosscheck of t_0 value

Estimate of lattice spacing

β	3.4	3.55	3.7
$a \approx$	0.086fm	0.064fm	0.05fm

Ensemble Overview

id	β	N_s	N_t	κ_u	κ_s	m_π[MeV]	m_K[MeV]	$m_\pi L$
B105	3.40	32	64	0.136970	0.13634079	280	460	3.9
H101	3.40	32	96	0.13675962	0.13675962	420	420	5.8
H102	3.40	32	96	0.136865	0.136549339	350	440	4.9
H105	3.40	32	96	0.136970	0.13634079	280	460	3.9
C101	3.40	48	96	0.137030	0.136222041	220	470	4.7
D100	3.40	64	128	0.137090	0.136103607	130	480	3.7
H200	3.55	32	96	0.137000	0.137000	420	420	4.4
N200	3.55	48	128	0.137140	0.13672086	280	460	4.4
D200	3.55	64	128	0.137200	0.136601748	200	480	4.2
N300	3.70	48	128	0.137000	0.137000	420	420	5.1
N301	3.70	48	128	0.137005	0.137005	410	410	4.9
J303	3.70	64	192	0.137123	0.1367546608	260	470	4.1

Chiral Trajectory

Fixed $\mathrm{Tr}M = \sum_f m_f$

$$a\sum_{f=1}^{3}(m_{0,\mathrm{f}} - m_{\mathrm{cr}}) = \mathrm{const} \quad \Leftrightarrow \quad a\sum_{f=1}^{3} m_{0,\mathrm{f}} = \mathrm{const} \quad \Leftrightarrow \quad \sum_{f=1}^{3}\frac{1}{\kappa_\mathrm{f}} = \mathrm{const}\,.$$

Note for $\mathcal{O}(a)$-improvement of coupling constant

$$\tilde{g}_0^2 = g_0^2\left\{1 + \frac{b_\mathrm{g}}{3}a\sum_f(m_{0,\mathrm{f}} - m_{\mathrm{cr}})\right\}$$

- b_g is small at one loop in perturbation: $b_\mathrm{g} = 0.012\,N_f\,g_0^2$

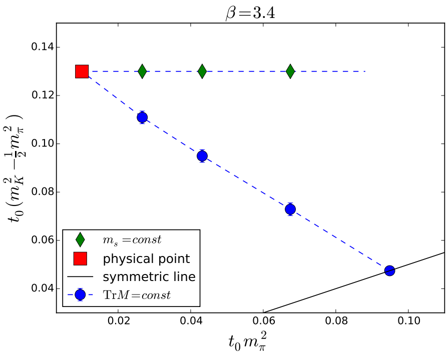
  $\rightarrow$ but non-perturbative result is not known
- $\tilde{g}_0$ is constant at fixed $\mathrm{Tr}M$ $\rightarrow$ constant lattice spacing for each β

  $\rightarrow$ also sum of improved PCAC quark masses is constant up to $\mathcal{O}(a)(am_{ud})$ effects

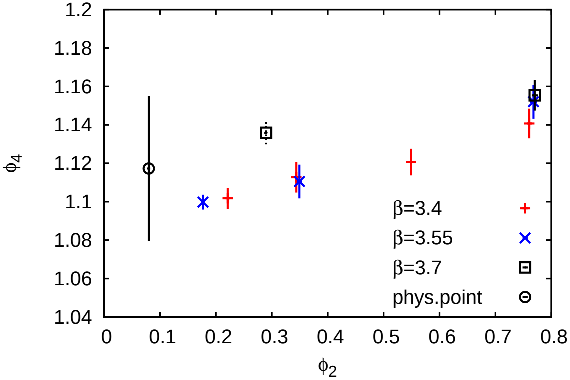
Tuning Strategy

Tuning Strategy

- At fixed β match lattices with different lattice spacings at flavor symmetric point (i.e. $m_{ud} = m_s \to m_\pi = m_K \approx 420\ \mathrm{MeV}$)
- We have determining the slope of ϕ_4 as a function of ϕ_2 at $\beta = 3.4$ from a set of preliminary runs: $\phi_4\big|_{m_{ud}=m_s} = 1.15$



Tuning Strategy



Note

- good accuracy is achieved
- no significant cutoff effects ($\beta = 3.7$ is still under production and its error therefore not yet trustworthy)
- moderate quark mass effect, around 5% between the chiral limit and the symmetric point (as expected from ChPT)

openQCD and Reweighting

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.

$\Rightarrow \langle O \rangle = \frac{\langle WO \rangle}{\langle W \rangle}$ with Observable O and reweighting factor W

Software

openQCD software package (available versions 1.0, 1.2, 1.4)

Supercomputers

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

Twisted-Mass Reweighting

Motivation

- Wilson Dirac operator is not protected against eigenvalues below the quark mass

$\rightarrow$ not a problem at a sufficiently large volume and quark mass

$\rightarrow$ small eigenvalues can lead to instabilities during the simulation

Introducing a twisted-mass term

$$\det Q^2 = \det{}^2 Q_{\rm oo} \det \hat{Q}^2 \rightarrow \det{}^2 Q_{\rm oo} \det \frac{\hat{Q}^2 + \mu_0^2}{\hat{Q}^2 + 2\mu_0^2} \det\left(\hat{Q}^2 + \mu_0^2\right)$$

- even-odd preconditioning: $\hat{Q} = Q_{\rm ee} - Q_{\rm eo} Q_{\rm oo}^{-1} Q_{\rm oe}$
- reweighting factor $W_0 = \det \frac{(\hat{Q}^2 + 2\mu_0^2)\,\hat{Q}^2}{(\hat{Q}^2 + \mu_0^2)^2} \rightarrow \langle O \rangle = \frac{\langle W_0 O \rangle}{\langle W_0 \rangle}$

Further Algorithmic Improvements

Hasenbusch mass factorization with a twisted mass

$$\det\left(\hat{Q}^2+\mu_0^2\right)=\det\left(\hat{Q}^2+\mu_{N_{\rm mf}}^2\right)\times\prod_{i=1}^{N_{\rm mf}}\det\frac{\hat{Q}^2+\mu_{i-1}^2}{\hat{Q}^2+\mu_i^2}$$

tower of increasing values of $\mu_0<\mu_1<\cdots<\mu_{N_{\rm mf}}$

Light fermion action

$$S_{\rm ud,eff}[U,\phi_0,\ldots,\phi_{N_{\rm mf}+1}]=\left(\phi_0,\frac{\hat{Q}^2+2\mu_0^2}{\hat{Q}^2+\mu_0^2}\phi_0\right)+\sum_{i=1}^{N_{\rm mf}}\left(\phi_i,\frac{\hat{Q}^2+\mu_i^2}{\hat{Q}^2+\mu_{i-1}^2}\phi_i\right)$$
$$+\left\{\left(\phi_{N_{\rm mf}+1},\frac{1}{\hat{Q}^2+\mu_{N_{\rm mf}}^2}\phi_{N_{\rm mf}+1}\right)-2\log\det Q_{\rm oo}\right\}$$

Strange quark simulation details

RHMC Algorithm: square root is approximated by a rational function

$$\det Q = \det Q_{\rm oo} \det \sqrt{\hat{Q}^2} = \det Q_{\rm oo} \det\big(A^{-1} \prod_{i=1}^{N_{\rm p}} \frac{\hat{Q}^2 + \bar{\mu}_i^2}{\hat{Q}^2 + \bar{\nu}_i^2}\big) \times W_1$$

- Zolotarev's approximation of inverse square root in interval $[r_a, r_b]$ with $N_{\rm p}$ poles
- reweighting factor W_1 to account for errors in the rational approximation

Strange quark action

$$S_{\rm s,eff}[U, \phi_0, \ldots, \phi_{N'_{\rm p}}] = \sum_{i=0}^{N'_{\rm p}-1} \big(\phi_i, \frac{\hat{Q}^2 + \bar{\nu}^2_{N_{\rm p}-i}}{\hat{Q}^2 + \bar{\mu}^2_{N_{\rm p}-i}} \phi_i\big) + \big(\phi_{N'_{\rm p}}, \prod_{j=1}^{N_{\rm p}-N'_{\rm p}} \frac{\hat{Q}^2 + \bar{\nu}_j^2}{\hat{Q}^2 + \bar{\mu}_j^2} \phi_{N'_{\rm p}}\big) - \log\det Q_{\rm oo}$$

- multi-shift conjugate gradient algorithm for the last factor with the large shifts
- deflated solver for the terms involving the smaller $\bar{\mu}_i$

Hybrid Monte Carlo

More details

- trajectory length $\tau = 2$ in all simulations
- acceptance rate ~ 0.95
- three-level integration scheme with OMF2/OMF4

Locally deflated solver [Lüscher2007, Frommer2013]

- local deflation subspace: deflation block size 4^4 (mostly)
- number of deflation modes per block: $20 - 32$

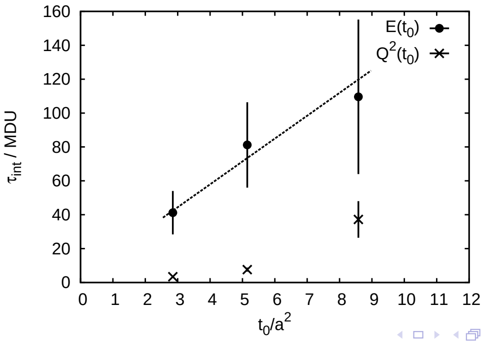
RQCD

Autocorrelations

Integrated autocorrelation time

$$\tau_{int}(A) = \frac{1}{2} + \sum_{t=1}^{\infty} \rho_A(t) \equiv \frac{1}{2} + \sum_{t=1}^{\infty} \frac{\Gamma_A(t)}{\Gamma_A(0)}$$

$\Gamma_A(t) = \langle A_t \, A_0 \rangle - \langle A \rangle^2$ with Monte Carlo time t



Scaling of the Integrated Autocorrelation Time

Topological charge $Q^2(t_0)$ and action density $E(t_0)$ at flow time t_0

- expectation: Langevin scaling $\tau_{int} \propto a^{-2}$
- very good scaling for action density E
- topological charge shows significant scaling violations

  $\rightarrow$ at larger a topological charge decorrelates significantly faster than predicted by the scaling hypothesis (very similar to the pure gauge case)

  $\rightarrow$ cutoff effects eventually large for topological charge scaling (similar to pure gauge: $\tau_{int} \propto a^{-2}(c + da^2)$?)

Costs

- we find $\tau_{exp} \approx 14(3)\, t_0/a^2$
- desired statistics: $\mathcal{O}(50) \times \tau_{exp}$

  $\rightarrow \beta = 3.4 \rightarrow 2000\,\mathrm{MDU}$

  $\rightarrow \beta = 3.55 \rightarrow 3600\,\mathrm{MDU}$

  $\rightarrow \beta = 3.7 \rightarrow 6000\,\mathrm{MDU}$

Twisted-Mass Reweighting Factor

Choice of μ

$$\langle A \rangle = \frac{\langle AW \rangle_W}{\langle W \rangle_W}\,, \quad W = W_0 W_1$$

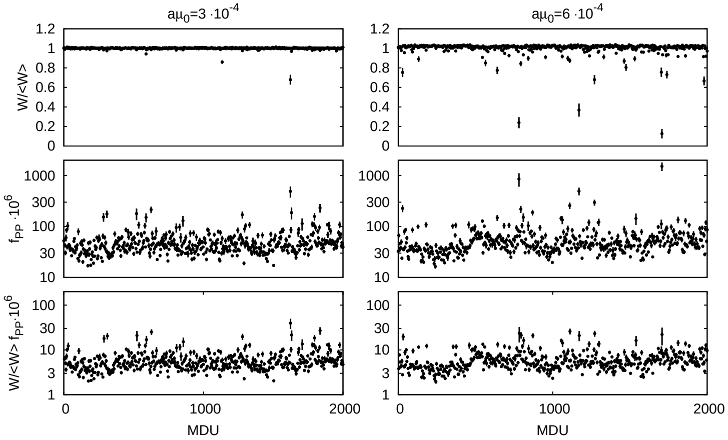
- value of μ has to be tuned to balance fluctuations (depends on observable!)

$\rightarrow$ small μ to control fluctuations (small error) $\Leftrightarrow$ large μ to increase HMC stability

Correlations of reweighting factor and observable has to be considered

- gluonic observables
  - $\rightarrow$ only small correlations
  - $\rightarrow$ effective reduction in statistics is small $\rightarrow \langle \mathrm{var}(W) \rangle \ll \langle W \rangle^2$
- fermionic observables
  - $\rightarrow$ correlations can be large
  - $\rightarrow$ cancellations between reweighting factor and observable

Reweighting and the PS Correlation Function



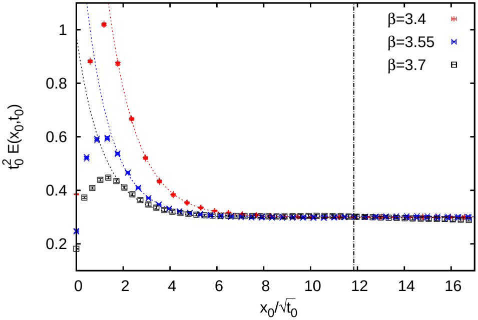
→ time history of W (top), $f_{\rm PP}(x_0)$ (center), $Wf_{\rm PP}(x_0)$ (bottom) at $x_0 = (T + a)/2$ with different $a\mu_0 = 0.0003, 0.0006$ at $m_\pi = 220 MeV$

Reweighting Factors

Remarks

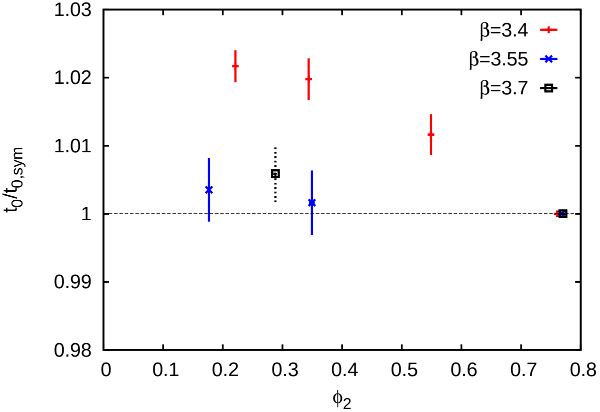
- computation of reweighting factors using stochastic estimators
  $\rightarrow$ computationally cheap
- 12-36 estimators for twisted mass reweighting factor W_0
- 1 estimator for strange reweighting factor W_1 is enough
- splitting of twisted mass reweighting factor beneficial when larger fluctuations occur

Boundary Effects



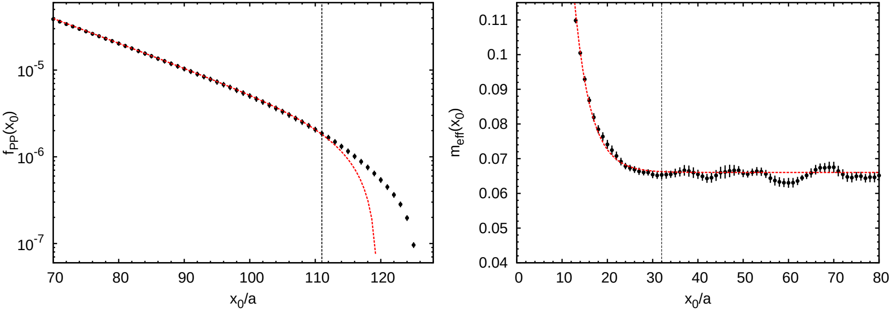
- time translational invariance lost
- large cutoff effects close to the boundary
- Dirac operator is only tree-level improved at the boundary
- no sizable dependence on the quark mass
- fit form $E(x_0, t) = E(t) + c_0 \cosh\{-m(x_0 - \frac{T}{2})\}$

Quark Mass Dependence of t_0



- $t_{0,\mathrm{sym}}$ is the value at $m_{\mathrm{ud}} = m_{\mathrm{s}}$
- one expects constant behavior to leading order ChPT

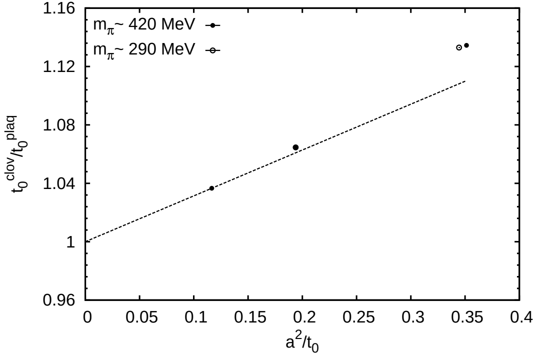
Pseudoscalar Masses



$$f_{\rm PP}(x_0, y_0) = -\frac{a^6}{L^3} \sum_{\vec{x},\vec{y}} \langle P^{rs}(x) P^{sr}(y) \rangle \,, \quad P^{rs} = \bar{\psi}^r \gamma_5 \psi^s$$

- 'wiggles' $\Leftrightarrow$ broken translational invariance in temporal direction
- $U(1)$ stochastic source fields at $y_0 = a$ and $y_0 = T - a$
- fit form: $f_{\rm PP}(x_0) = A \sinh\left(m_{\rm PS}(\tilde{T} - x_0)\right)$

Cutoff Effects in t_0



$t_0^{clov} \Leftrightarrow t_0^{plaq}$: t_0 from two different discretizations of $F_{\mu\nu}$ (plaquette and clover)

- $t_0^{clov}/t_0^{plaq} = 1$ in the continuum limit
- dashed line $\leftarrow$ assume perfect scaling for $\beta = 3.7$

  $\rightarrow$ scaling violations are small at $\beta = 3.55$ and sizeable at $\beta = 3.4$

Outlook

Generation of CLS gauge configurations

- currently ongoing:

  $\rightarrow$ ensembles with m_s fixed at $\beta = 3.4, 3.55$

  $\rightarrow$ ensembles with different volumes for $\mathrm{Tr}M$ fixed at $\beta = 3.4$

- planned:

  $\rightarrow$ more statistics for D100 ensemble (physical point at $\beta = 3.4$)

  $\rightarrow$ additional lattice spacing for fixed $\mathrm{Tr}M$

Measurements

- currently starting:
  - for both trajectories with m_s fixed and $\mathrm{Tr}M$ fixed at $\beta = 3.4$

  $\rightarrow$ Hadron massess (including charm), PCAC masses, decay constants, meson and baryon distribution amplitudes,...

- same measurements will start soon afterwards at $\beta = 3.5$ (also 3-point functions)

Summary

Lattice Simulations with Open Boundaries

- 2+1f simulations with non-perturbatively improved Wilson Clover action
- open boundaries $\rightarrow$ avoid topological freezing as $a \rightarrow 0$
- boundary effects are under control
- tuning strategy works fine, high accuracy can be achieved
- autocorrelations scale as expected
- twisted mass reweighting works nicely but needs some tuning
- large set of ensemble already generated and more are in production
- long term effort within CLS

Baryon Spectrum: Setup

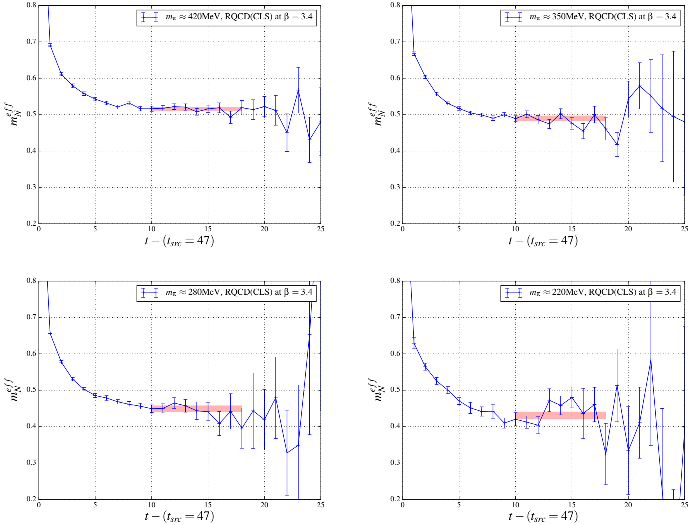
Setup

- 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

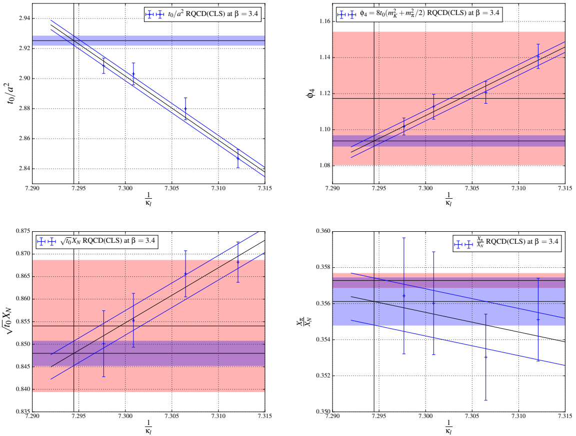
Baryon Spectrum: Effective Mass (Nucleon)

preliminary



Baryon Spectrum: Chiral Extrapolation

preliminary



SU(3) Chiral Perturbation Theory

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

e.g. [Bernard et al. 1993]

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

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

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

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

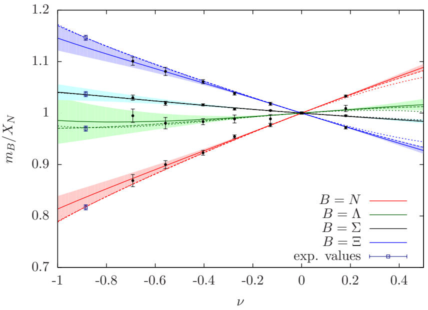
Average nucleon mass

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

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

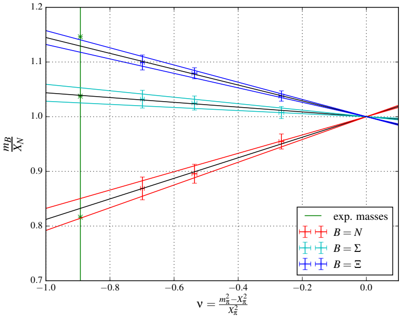
Baryon Spectrum: Fan Plot

preliminary



[Bruns, Greil, Schaefer 2013]

based on QCDSF data



preliminary RQCD(CLS) data

⇒ consistency with other studies (QCDSF, RQCD)