The physical point: results and challenges - ETM collaboration

Lattice QCD at the physical pion mass: results, challenges and modern techniques
2017 DESY - Zeuthen

Jacob F. Finkenrath

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Approaching the physical point

- finite volume effects
  - $\rightarrow$ set $L \cdot m_\pi \geq 3$ better ≥ 4
    this implies large lattices for small pion masses
- small lattice artefact's $\longrightarrow$ *in ETMC ensembles ?*
  - $\rightarrow$ use $\mathcal{O}(a)$ improvement
  - $\rightarrow$ use fine lattice spacings
- stable algorithms $\longrightarrow$ *in ETMC software ?*
  - $\rightarrow$ control of the smallest eigenvalue
  - $\rightarrow$ efficient solvers
- large statistics $\mathcal{O}(100)$ to $\mathcal{O}(1000)$
  - $\rightarrow$ control of numerical costs
  - $\rightarrow$ control of autocorrelation times $\longrightarrow$ *in ETMC ensembles ?*
  - $\rightarrow$ control of statistical errors $\longrightarrow$ *in ETMC ensembles ?*
- physical quark masses
  - $\rightarrow$ use efficient tunning conditions $\longrightarrow$ *in ETMC simulation effort?*

Overview- ETMC - Ensembles

$n_f = 2+1+1,$
$c_{sw} = 0$
$a \sim 0.089,\ 0.082,\ 0.062$
$\min(m_\pi) = 210$ MeV

$n_f = 2,\ c_{sw} \neq 0$
$a \sim 0.094$ fm
$\min(m_\pi) = 130$ MeV

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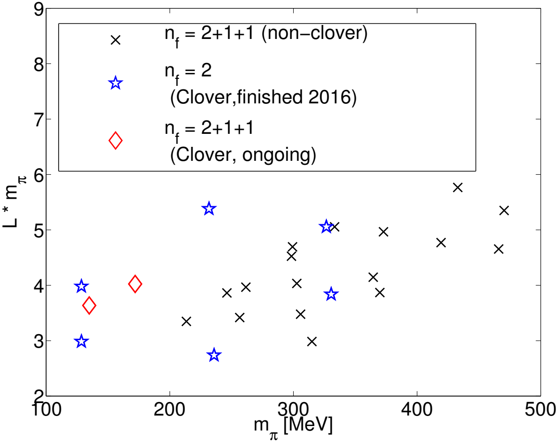

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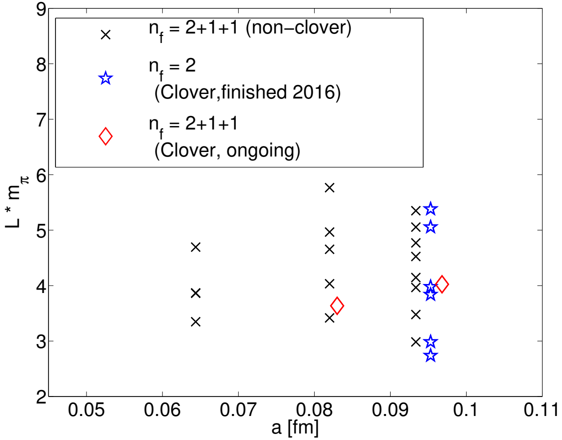


ETMC - light sector

$n_f = 2$ mass degenerated twisted mass operator:

$$D = D_W(\kappa, c_{sw}) \otimes 1 + i\mu\gamma_5 \otimes \tau_3 = \begin{bmatrix} D_W + i\gamma_5\mu & 0 \\ 0 & D_W - i\gamma_5\mu \end{bmatrix}$$

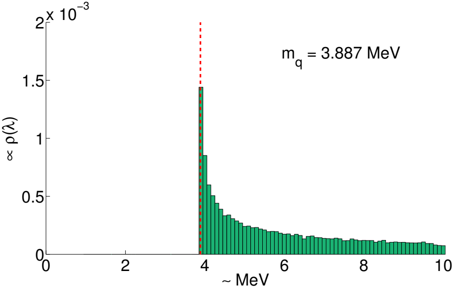
where $1, \tau_3$ is acting in flavor space

- γ_5-hermiticity:
  $\rightarrow$ Determinant is positive and real
- for the squared operator follows:
  $D^\dagger D = D_W^\dagger D_W + \mu^2$
  smallest eigenvalue is protected by μ
- $\mathcal{O}(a)$-improvement
  $m_{PCAC}(\kappa) \longrightarrow 0$
  $\kappa \longrightarrow \kappa_{crit}$

needs to be tuned

[Frezzotti, Rossi 2003]

Eigenvalue density of
$H_{eo} = \gamma_5(D_{ee} - D_{eo}D_{oo}^{-1}D_{eo})$



The heavy mass – sector

Heavy sector: $n_f = 1{+}1$ mass non-degenerated twisted mass operator:

$$D_h = D_W \otimes 1 + i\overline{\mu}\gamma_5 \otimes \tau_3 - \overline{\epsilon} \otimes \tau_1 = \begin{bmatrix} D_W + i\gamma_5\overline{\mu} & -\overline{\epsilon} \\ -\overline{\epsilon} & D_W - i\gamma_5\overline{\mu} \end{bmatrix}$$

where $1, \tau_3, \tau_1$ is acting in flavor space

- Volume increases by factor 2
  - smallest eigenvalues around strange quark mass
- $\gamma_5 \otimes \tau_1$ - hermiticity ensures real and positive determinant
  $\det D_h = \det\sqrt{D_h^\dagger D_h}$
  for HMC hermitian operator necessary (square root)
  using rational approximation of the square root

Algorithm - Setup of HMC

Software: *tmLQCD* with *DDalphaAMG*

https://github.com/etmc/tmLQCD
https://github.com/sbacchio/DDalphaAMG

- Integrator: nested OMF-scheme order 2

  [Omelyan,Mryglod,Folk 2003]

- Solver: Multi-Grid for twisted mass fermions
  mixed-precision CG

  [see next slides]

- Force for light sector:
  Hasenbusch mass preconditioning
  $\rightarrow$ to suppress IR-noise
  with factorization $\rho \sim 0.001;\ 0.01;\ 0.1$

  [Hasenbusch 2001]

- force for $1+1$ sector:
  rational approximation

cost at the physical point ?

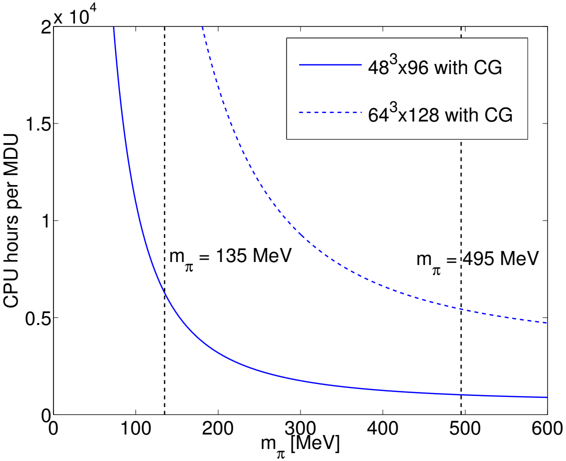
Solver - Using DD-alphaAMG for light quark sector

Work with Simone Bacchio, Karsten Karl, Matthias Rottmann, Andreas Frommer

- CG critical slowing down for $m_\pi \to 135$ MeV
  $L \cdot m_\pi \gtrsim 3$ becomes expensive

Conjugate gradient solver: $cost \propto 1/m_\pi^2$

Data generated on
$V = 96 \times 48^3$
$a = 0.094$ fm
$m_\pi = 130$ MeV



[432 Haswell Xeon Processors E5-2697 on SuperMUC]

Solver - Using DD-alphaAMG for light quark sector

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- CG critical slowing down for $m_\pi \to 135$ MeV
  $L \cdot m_\pi \gtrsim 3$ becomes expensive

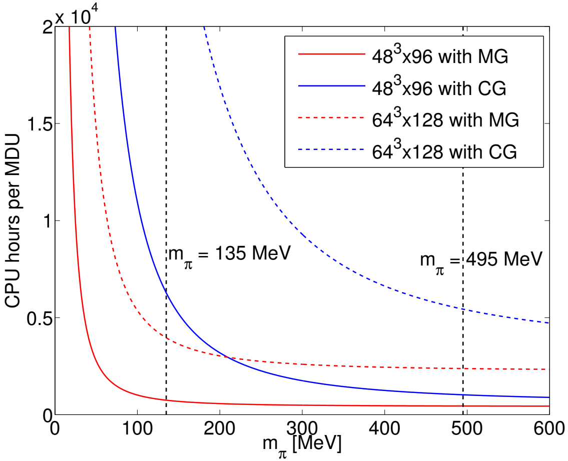
Adapting DDalphaAMG solver to tm operator

- using a trick on the coarse lattice by $\mu_c \sim 5\mu$

Results:

- speed up of CG by a factor 100
- speed up of the HMC by a factor ~ 8

See also Simones Poster, Karsten Karls talk, [Frommer et al. 2016]



[432 Haswell Xeon Processors E5-2697 on SuperMUC]

DD-alpha AMG

Using DDalphaAMG solver for light quark sector: Speed up the HMC by a factor ~ 8
$\Rightarrow$ Strange quark becomes expensive (more than a factor 2)

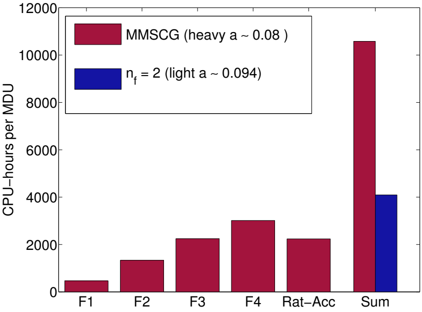
Adapting DDalphaAMG solver for heavy quark sector

- extending projectors to flavor space
- use same coarse subspace as for the light sector

Results:

- speed up of a factor 5 (F4)
- speed up of the HMC by a factor 2

[Simone Bacchio]



[Data from 4096 SuperMUC Haswell Xeon Processors E5-2697]

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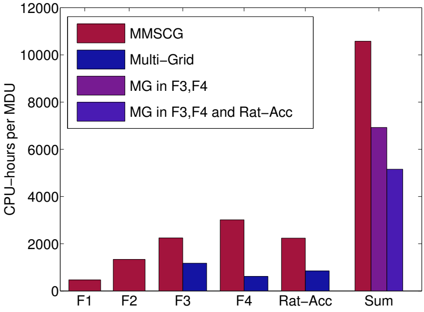

[Data from 4096 SuperMUC Haswell Xeon Processors E5-2697]

Algorithmic part - Summary

for $n_f = 2 + 1 + 1$

lattice size of $V = 128 \times 64^3$ at the physical point

$\longrightarrow$ around 2.5 hours on 4096 CPUs

to reach larger lattices more code and algorithmic development to simulate even finer lattice spacings $a \lesssim 0.75$ fm

Approaching the physical point

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    this implies large lattices for small pion masses
- small lattice artefact's
  - → use $\mathcal{O}(a)$ improvement
  - → use fine lattice spacings
- stable algorithms
  - → control of the smallest eigenvalue
  - → efficient solvers

large statistics $\mathcal{O}(100)$ to $\mathcal{O}(1000)$

- → control of numerical costs
- → control of autocorrelation times
- → control of statistical errors

- physical quark masses
  - → use efficient tunning conditions

Isospin - Symmetry

twisted mass discretization breaks Isospin symmetry

$\Rightarrow$ Pion triplet is splitted up:
neutral pion mass is lighter than the charged

in chiral perturbation theory

$$(m^2_{\pi^0} - m^2_{\pi^\pm}) = -c_0 \cdot a^2$$

$\rightarrow$ vanished for $a \rightarrow 0$

for $c_0 > 0$:
neutral pion mass can be zero for non-zero light quark masses

$\rightarrow$ phase transition close to small neutral pion masses

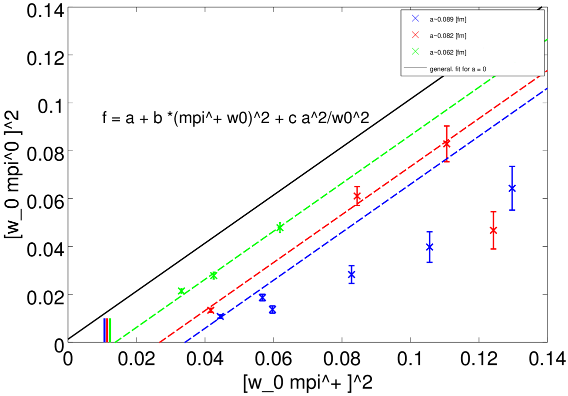
- physical quark masses can not be reached if the isospin splitting is too large
- autocorrelation times increases
  $\rightarrow$ tunning of κ_{crit} becomes a non-trivial task for $\mu \rightarrow \mu_{phys}$
  $\longrightarrow$ lets look to our ensembles

Isospin breaking in $n_f = 2+1+1$ (non-clover)

using the fit-function:
$w_0 m_{\pi^0}^2 = \alpha + \beta [m_{\pi^\pm} w_0]^2 + \gamma a^2 / w_0^2$

- $\alpha = 0.001(1)$
- $\beta = 1.003(26)$
- $\gamma = -0.102(2)$

large isospin breaking in the pion system



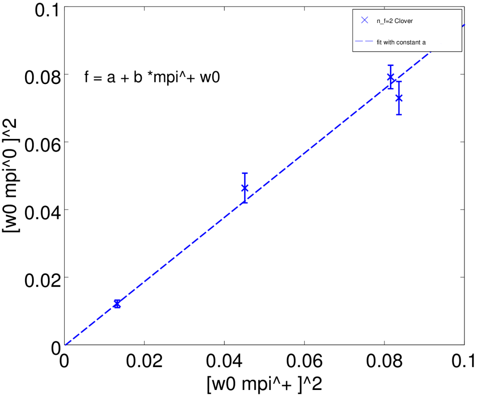
Isospin breaking in $n_f = 2$ (clover)

For $n_f = 2$ with clover term the error is larger than the splitting

using the fit-function:
$m_{\pi^0} = \alpha + \beta m_{\pi^\pm} w_0$

- $\alpha = 0.0003(14)$
- $\beta = 0.94(4)$
- ($\gamma = --$
  one lattice spacing)

pion mass difference is for lattice spacing of $a \sim 0.0936$ neglect-able



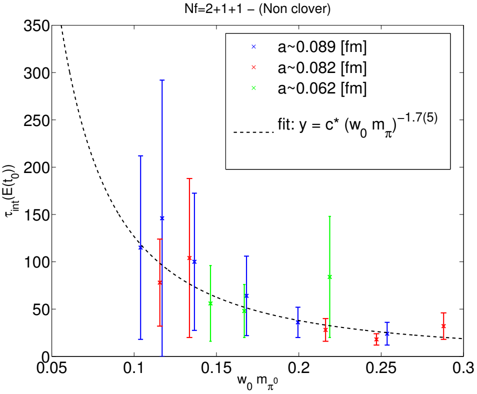
Autocorrelation in $n_f = 2+1+1$ (non-clover)

- here we use m_{π^0} instead of $m_{\pi^\pm}$
- no a-dependence for $a \in [0.06;\ 0.09]$

using the fit-function:
$\tau_{int} = c \cdot (w_0 m_{\pi^0})^{\alpha}$

- $\alpha = -1.7(5)$

$\rightarrow$ τ_{int} scales with $m_{\pi^0}^{-2}$



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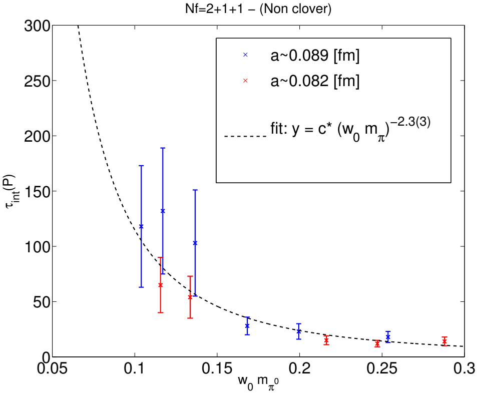
- $\alpha = -2.3(3)$

$\rightarrow \tau_{int}$ scales with $m_{\pi^0}^{-2}$



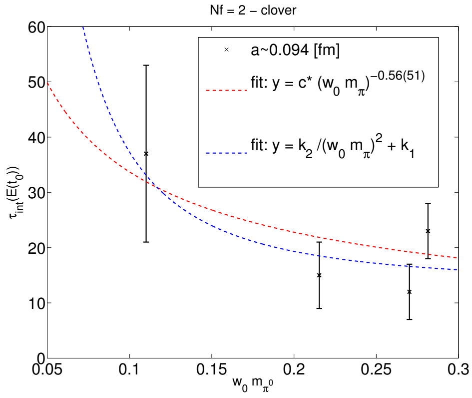
Autocorrelation in $n_f = 2$ (clover)

- using m_{π^0} although (here $n_f = 2$) is similar to $m_{\pi^\pm}$)
- only one lattice spacing $a = 0.094$ fm

using the fit-function:
$\tau_{int} = c \cdot (w_0 m_{\pi^0})^\alpha$

- $\alpha = -0.56(51)$

when assuming τ_{int} scales with $m_{\pi^0}^{-2}$ looks OK



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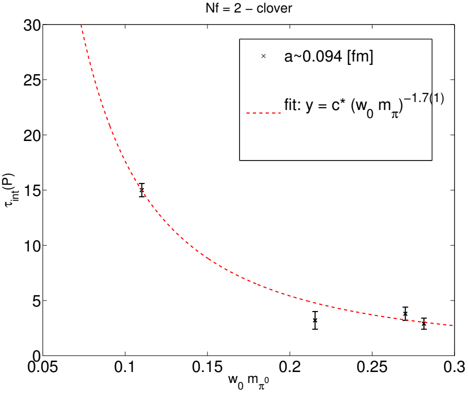


Error analysis on $n_f = 2$ clover ensembles with $a = 0.094$ fm

Error Scaling at the physical point:

We will use the standard deviation with the integrated autocorrelation time:

$$\sigma = \sqrt{2}\sigma_{standart} \cdot \sqrt{\tau_{int}}$$

we know that

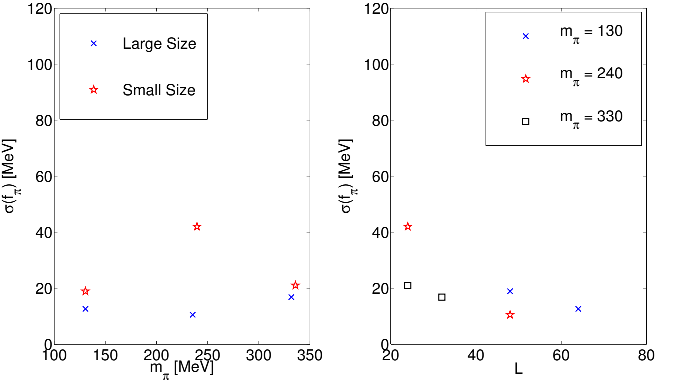
$$\tau_{int} \propto \frac{1}{m_\pi^2}$$

$\longrightarrow$ standard deviation will have a pion mass dependence

here we will use the $n_f = 2$ ensembles
to understand the error
(preliminary, no-error for the standard deviation)

Error Scaling in $n_f = 2$ - Pion decay constant

$\alpha = -1.8$
$\beta = -1.1$



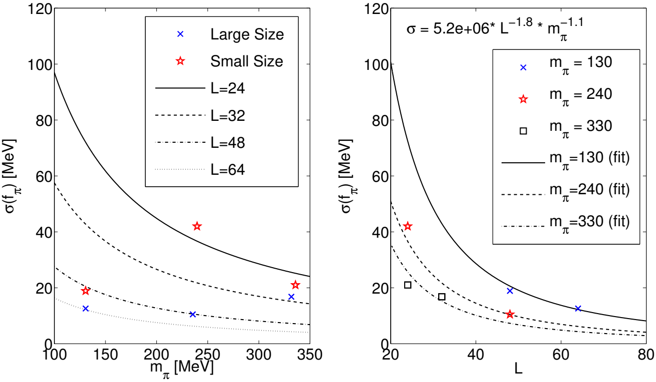
Error Scaling in $n_f = 2$ - Pion decay constant

using the fit-function:

$$\sigma_f(L, m_\pi) = kL^\alpha m_\pi^\beta$$

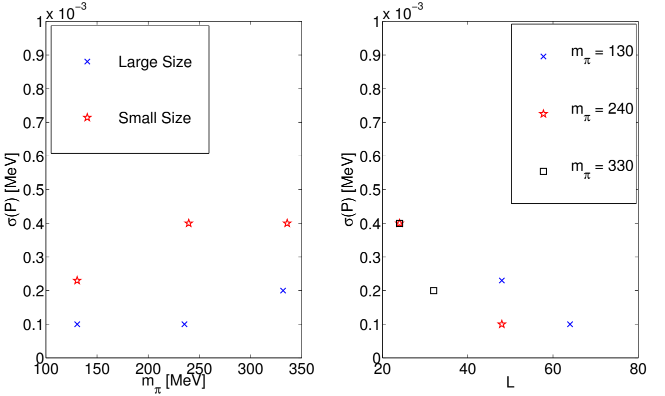
expected L dependence $\propto 1/\sqrt{L^3}$
(time-slice sources)

$\alpha = -1.8$
$\beta = -1.1$



Error Scaling in $n_f = 2$ - Plaquette

$\alpha = -2.1$
$\beta = -0.96$



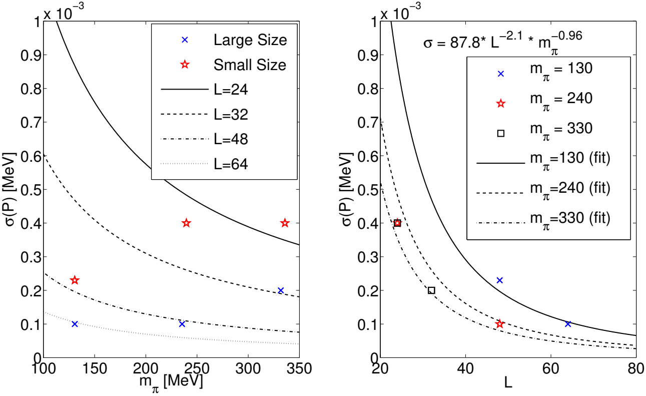
Error Scaling in $n_f = 2$ - Plaquette

using the fit-function:

$$\sigma_P(L, m_\pi) = k L^\alpha m_\pi^\beta$$

expected L dependence $\propto 1/\sqrt{(T \cdot L^3)} = 1/(\sqrt{2}L^2)$
(Volume average)

$\alpha = -2.1$
$\beta = -0.96$



ETMC effort in $n_f = 2+1+1$ - tunning

Tunning of κ_{crit}

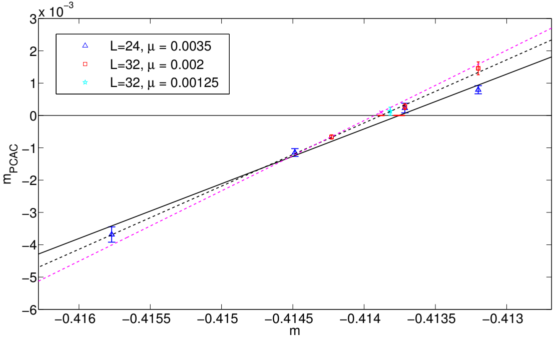
$$m_{PCAC}(\kappa) \to 0$$

$m_{PCAC} = a(\mu) + b(\mu)\kappa$ becomes a fine tuning problem

$$cost(L, m_\pi) \propto \frac{1}{m_\pi^{2[3]}} L^{5[6]}$$

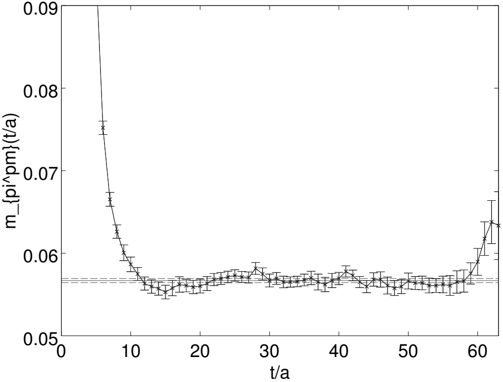
if for each μ need new three κ-values

it becomes expensive at $L \geq 48$



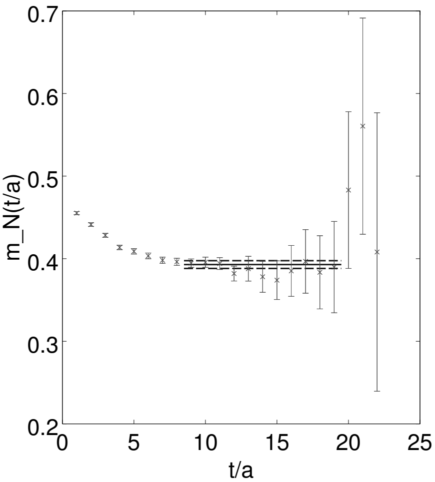
ETMC effort in $n_f = 2 + 1 + 1$ - effective pion–mass at the physical point

effective mass plateau of the pion on $n_f = 2 + 1 + 1$ clover, $V = 128 \times 64^3$



ETMC effort in $n_f = 2 + 1 + 1$ - effective nucleon–mass at the physical point

effective mass plateau of the nucleon on $n_f = 2 + 1 + 1$ clover, $V = 128 \times 64^3$, 64 configs a 8 point sources



Approaching the physical point - Conclusion

- finite volume effects
  - → set $L \cdot m_\pi \geq 3$ better ≥ 4
    this implies large lattices for small pion masses ⟶ *on-going simulations OK*
- small lattice artefact's ⟶ *twisted mass is order a-improved*
  - → use $\mathcal{O}(a)$ improvement
  - → use fine lattice spacings
- stable algorithms, ⟶ *tmLQCD with DDalphaAMG*
  - → control of the smallest eigenvalue ⟶ *smallest EV bounded by μ*
  - → efficient solvers ⟶ *MG solver works for efficient for small pion mass*
- large statistics $\mathcal{O}(100)$ to $\mathcal{O}(1000)$
  - → control of numerical costs ⟶ *feasible for $V = 128 \times 64^3$*
  - → control of autocorrelation times ⟶ *scales with $1/m_{\pi^0}^2$*
  - → control of statistical errors ⟶ *works for large lattices (at least in $f_\pi, P \ldots$)*
- physical quark masses
  - → use efficient tunning conditions ⟶ *can become complicated for large lattices and small pion masses*

Thanks

to the audience

to all members of the ETM collaboration
especially which are involved in the Simulation effort

special thanks to Urs Wenger and Carsten Urbach for providing data used here