Simulation of an ensemble of $N_f = 2 + 1 + 1$ twisted mass clover-improved fermions at physical quark masses

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June 20, 2017

Approaching the physical point

* Lattice action: Twisted mass approach
  → Why simulation at the physical point are possible ?

* Tuning
  → How to tune physical quark masses ?

* Stable algorithm
  → Are the properties of the molecular dynamics under control ?

* Observables
  → Are we at the physical point ?

Results shown in this talk are part of the ongoing simulation effort of the European Twisted Mass Collaboration

ETMC - light sector

$n_f = 2$ mass degenerated twisted mass operator:

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

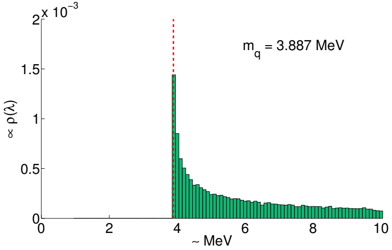
- $\mathcal{O}(a)$-improvement
  $m_{PCAC}(\kappa) \longrightarrow 0$
  $\kappa \longrightarrow \kappa_{crit}$
  needs to be tuned

  [Frezzotti, Rossi 2003]

- for the squared operator follows:
  $D^\dagger D = D_W^\dagger D_W + \mu^2$
  smallest eigenvalue is protected by μ

- Isospin breaking
  $(m_{\pi^0}^2 - m_{\pi^\pm}^2) \approx -c_0 \cdot a^2$

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



Simulating twisted mass fermions at the physical point

twisted mass discretization breaks Isospin symmetry

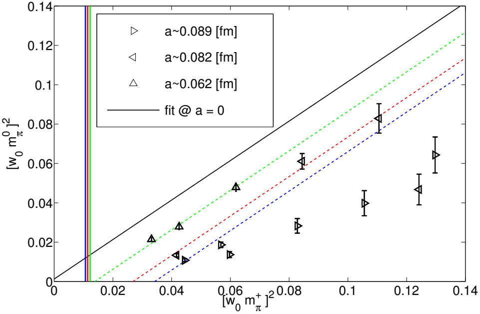
Finite twisted mass term ⇒ Isospin violation: pion triplet is splitted up (lattice χpt):

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

$n_f = 2+1+1$ ensembles
$c_{SW} = 0$
$\min(m_\pi) \sim 210\text{MeV}$

@ physical point
$\rightarrow m^0_\pi = 0$

Simulations not possible



@ physical point → simulations feasible
[Abdel-Rehim et. al. 2015]

Simulating twisted mass fermions at the physical point

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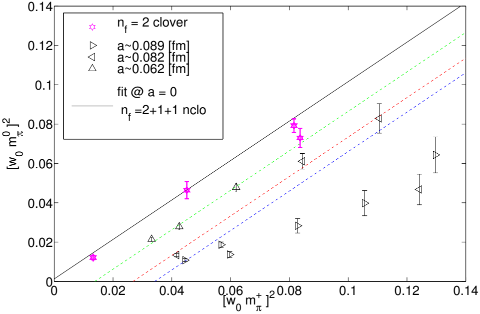
$$(m^2_{\pi^0} - m^2_{\pi^\pm}) = -c_0 \cdot a^2$$

$n_f = 2$ ensembles
$c_{SW} = 1.57551$
$\min(m_\pi) \sim 130\text{MeV}$

$|m^2_{\pi^0} - m^2_{\pi^\pm}| < [4\ \text{MeV}]^2$
(@ $m_\pi = 130$ MeV)



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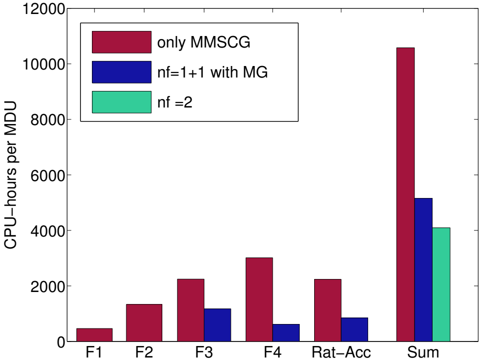
[Abdel-Rehim et. al. 2015]

DDalphaAMG in twisted mass

Speeding up: tmLQCD with DDalphaAMG

See talk by Simone Bacchio [Monday at Algorithms and Machines]

- using DDalphaAMG solver in the rational approximation
- gives a factor 2



$\longrightarrow$ 8 $\times$ speed up of the $n_f = 2$
$\longrightarrow$ 2 $\times$ speed up of the $n_f = 1 + 1$

Setup

Twisted mass with clover term

Target: lattice space $a = 0.08$ fm
$n_f = 2 + 1 + 1$ twisted mass fermions @ physical quark masses with $V = 128 \times 64^3$

sketch of the parameter tuning work (done):

tune: $\kappa \to \kappa_{crit}$
check: c_{sw} (estimate from 1-loop tadpole boosted PT), lattice spacing a, heavy quark sector

- start $L = 24$ with 4 κ's and $m_\pi \sim 310\mathrm{MeV}$
  $\to$ estimate κ_{crit}, check c_{sw} and lattice spacing a
- generate $L = 32$ at $\kappa_{crit}|_{L=24}$
  check heavy quark sector $\to$ re-tune
- re-run at $L = 32$ with 3 κ's and $m_\pi \sim 230\mathrm{MeV}$
  $\to$ estimate κ_{crit}
- start run $L = 64$ with $m_\pi \sim 135$ MeV

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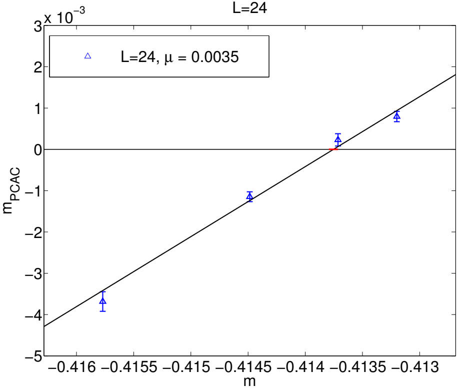
Light Quark Sector

Tuning of κ_{crit}:

$$\frac{Z_A m_{PCAC}(\kappa)}{\mu} \lesssim 0.1 \qquad \text{with} \quad Z_A \sim 0.8$$

such that $a\Lambda_{QCD}|Z_A m_{PCAC}/\mu| \lesssim a^2\Lambda_{QCD}^2$ [P. Boucaud et al. 2008]

- start with $L = 24$
- at $\kappa \in \{0.1394, 0.13942, 0.13945, 0.1394$
- and using: $m_{PCAC} = b + s(\mu)\kappa^{-1}$



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- after re-tune heavy quark masses
- re-tune on $L = 32$
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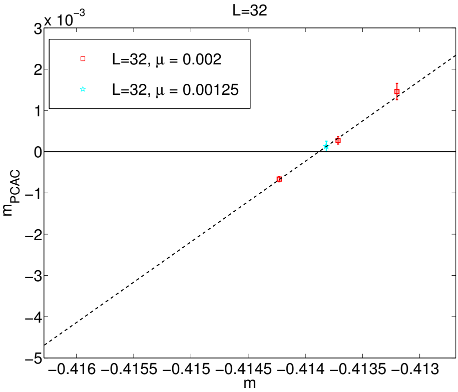

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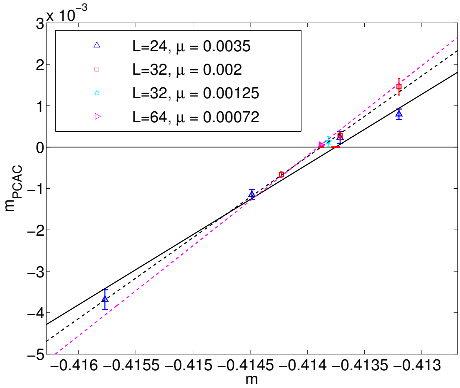


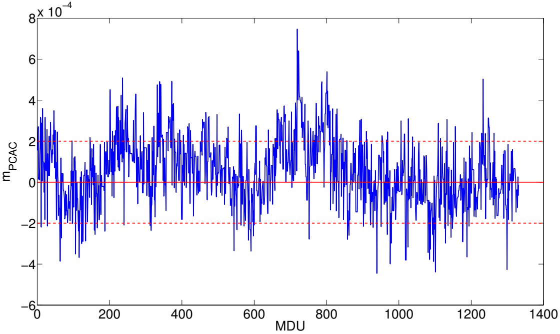
Summary:

- $s(\mu)$ increase moderate with μ
- possible to reach physical μ

Light Quark sector @ $L = 64$

PCAC mass at $\mu = 0.00072$ on $V = 128 \times 64^3$

PRELIMINARY



$\longrightarrow |m_{PCAC}| < 0.00005$

$\longrightarrow$ up to MDU 800: larger autocorrelation times

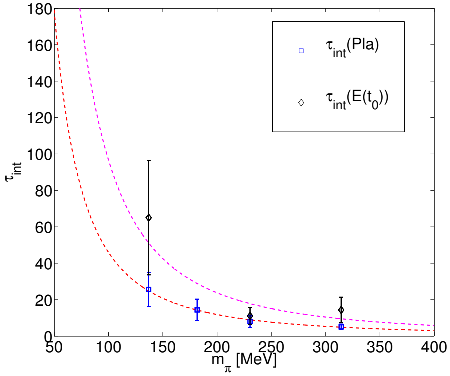
Autocorrelations

Reaching physical point is not trivial:
Autocorrelations increases with the pion mass

$$\tau_{int} = c_0 \cdot m_\pi^{c_1}$$

for plaquette:
$c_1 = -1.95(54)$

for $E(t_0)$:
$c_1 = -2.0(8)$



$\Rightarrow$ fine tuning problem: $cost \propto V^{5/4}/m_\pi^2$ and $m_{PCAC}/\mu \lesssim 0.1$

Heavy Quark Sector

Non Degenerated twisted mass operator:

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

two parameters: $\overline{\mu}, \overline{\epsilon} \rightarrow$ determinant real but charm sector difficult to access

$\Rightarrow$ valence sector: Osterwalder Seiler- fermions observables with strange and charm following [Frezzotti, Rossi 2004]

two parameters: μ_s , μ_c

tuning conditions:
$A_1 = \frac{\mu_c}{\mu_s} \equiv 11.8$

$B_2 = \frac{m_{D_s}}{f_{D_s}} \equiv 7.9$

Tunning of the ND-parameters:
matching via Kaons

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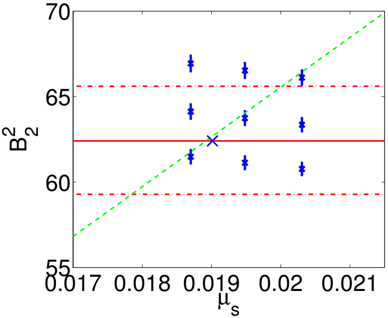


Stable algorithms

Max. forces of the $n_f = 2$ sector:
with Hasenbusch mass-preconditioning $F = \partial[1 + \rho_j \phi^\dagger Q^{-2}(\rho_{j-1})\phi]/\partial U$

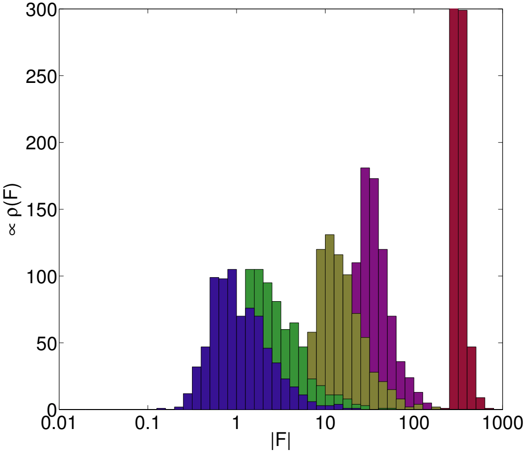
$\rho = 0.003$
(blue)

$\rho = 0.0012$
(green)

$\rho = 0.01$
(beige)

$\rho = 0.1$
(purple)

full operator
(red)



Stable algorithms

Max. forces of the $n_f = 1+1$ sector:
with rational approximation $F = \partial \left[\prod_{i=1}^{10} \phi^\dagger (Q^2+\mu_i)/(Q^2+\nu_i)\phi \right] / \partial U$

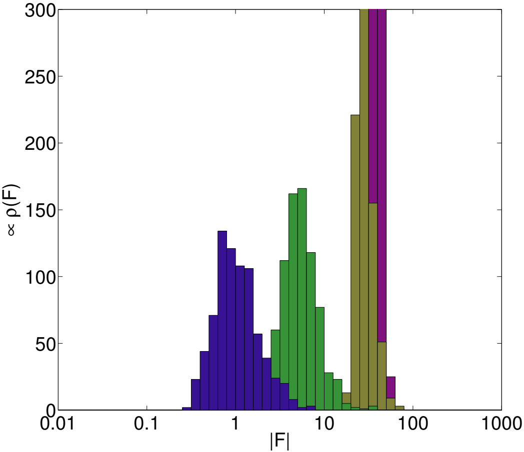
interval of
rat. approx:
$[0.000014 \;\; 1]$

$i = 9, 10$
(blue)

$i = 7, 8$
(green)

$i = 6, 5, 4$
(beige)

$i = 3, 2, 1$
(purple)



Stable algorithms

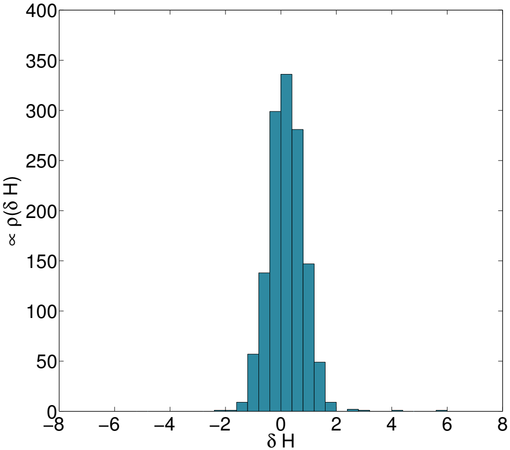
Discretization errors during integration:
$\delta H = H(U(\tau = 1)) - H(U(\tau = 0))$

order 2 OMF-scheme nested integration:

$[12, 24, 48, 96, 192]$

acceptance $= 77\%$

$\max(\delta H) = 5.67$

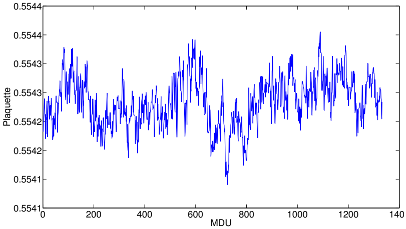


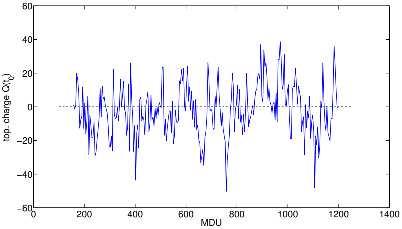
$\longrightarrow$ Hasenbusch mass preconditioning and finite twisted mass term are efficient against instabilities.

Stable algorithms

Plaquette and topological charge

PRELIMINARY





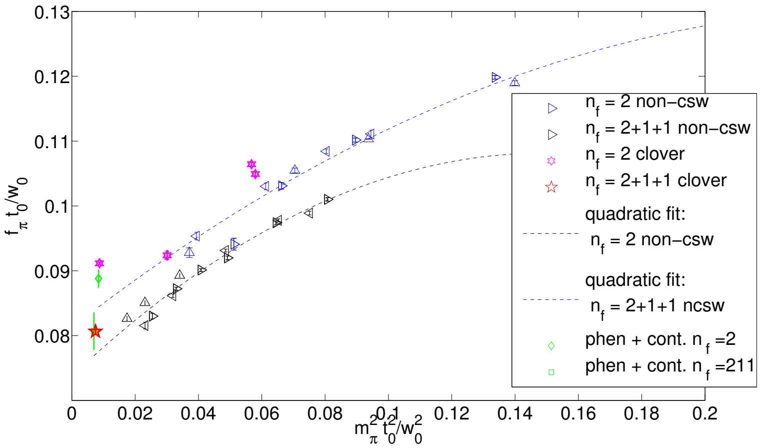
$\longrightarrow$ plaquette shows larger autocorrelation for $MDU < 800$ ($\tau_{int} = 31(13)$)

$\longrightarrow$ topological charge fluctuates ($\tau_{int} = 8(3)$)

Observables

Pion decay constant f_π

PRELIMINARY



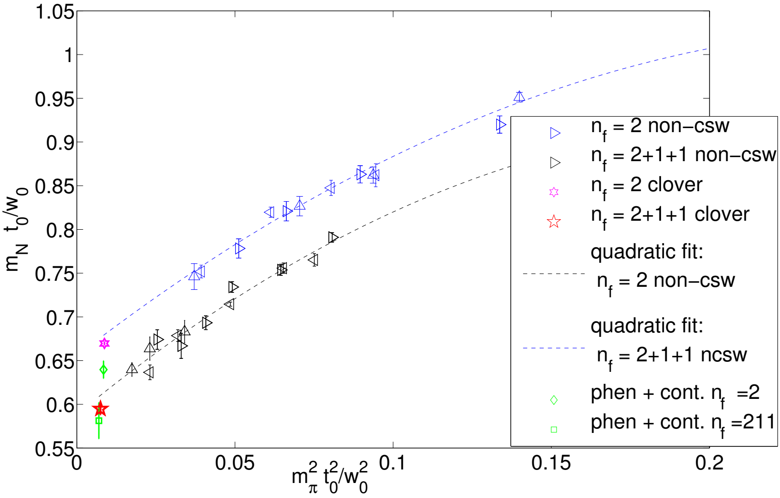
f_π agrees within statistical errors with the physical value

green points: t_0 and w_0 obtained by
$n_f = 2$ [Bruno, Lottini, Sommer 2013],$n_f = 2 + 1$ [BMW 2012]

Observables

Nucleon mass m_N

PRELIMINARY



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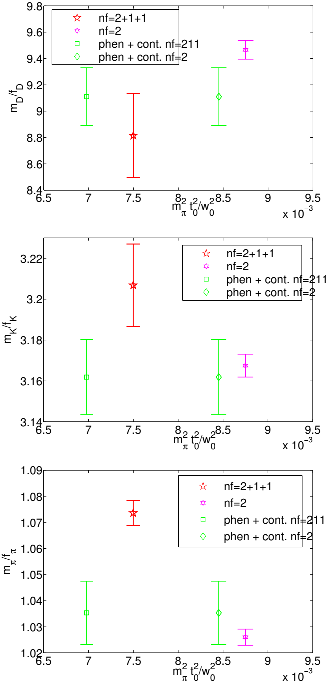
Observables

m_{PS}/f_{PS}
PRELIMINARY

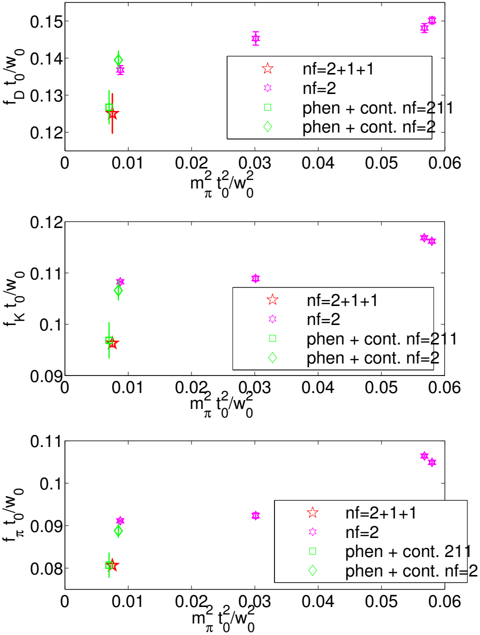
- Using to fix μ_s and μ_c tuning conditions:
  $A_1 = \mu_s/\mu_c$ and
  $B_2 = m_{D_s}/f_{D_s}$
- light quark mass:
  seems to a bit heavier
  $\rightarrow$ 140 MeV Pions more likely
- $n_f = 2$ corresponds to a lattice with 130 MeV pions



Observables

Pseudoscalar decay constants

PRELIMINARY



- f_{PS} agrees within statistical errors with the physical value

Conclusion

* Lattice action: Twisted mass approach
  - Why simulation at the physical point are possible ?

  $\rightarrow$ Clover term is efficient to reduce isospin splitting

  $\rightarrow$ Multigrid approach tames critical slowing down for $m_\pi \rightarrow m_{\pi,phys}$

* Tuning
  - How to tune physical quark masses ?

  $\rightarrow$ with tamed isospin violation possible, however still fine tuning problem $\propto V^{5/4} m_\pi^{-2}$

* Stable algorithm
  - Are the properties of the molecular dynamics under control ?

  $\rightarrow$ Hasenbusch mass preconditioning and finite twisted mass term are efficient against instabilities.

* Observables
  - Are we at the physical point ?

  $\rightarrow$ Wilson clover twisted mass fermions allow to reach this point at $a \sim 0.08$ fm

Thank you for your attention !