Lattice QCD with two light Wilson twisted mass quarks

A status report

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with the
European Twisted Mass Collaboration (ETMC)

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Motivation

Quantumchromodynamics (QCD) – the theory of strong interactions

$$\mathcal{L}_{QCD} = \bar{\psi}(i\not{D} - m_q)\psi - \frac{1}{4}G_{\mu\nu}G^{\mu\nu}$$

- a simple and beautiful field theory,
- parameters are the quark masses m_q and the dimensionless gauge coupling,
- in the chiral limit a scale is generated through *dimensional transmutation*,
- all dimensionful quantities can be expressed in units of *one characteristic scale*, e.g. the proton mass,

Motivation

- exhibits a variety of non-perturbative phenomena like
  - colour confinement,
  - spontaneous breaking of chiral symmetry,
  - its restoration at high temperature or density.
- A qualitative and quantitative understanding of these phenomena provides
  - confirmation of the theoretical framework,
  - necessary input for SM phenomenology,
  - valuable contributions to the discovery of new physics beyond the SM.

$\Rightarrow$ Lattice QCD is a (the) non-perturbative method for such ab-initio calculations

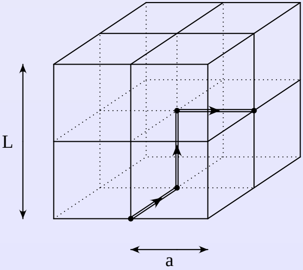
QCD on the Lattice I

Quantumchromodynamics is formally described by the Lagrange density:

$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}(i\not{D} - m_q)\psi - \frac{1}{4}G_{\mu\nu}G^{\mu\nu}$$

Lattice regularization: discretize Euclidean space-time

- hypercubic $L^3 \times T$-lattice with lattice spacing a
- derivatives $\Rightarrow$ finite differences
- integrals $\Rightarrow$ sums
- gauge potentials A_μ in $G_{\mu\nu}$ $\Rightarrow$ link matrices U_μ ('•⟶•')



Wilson Formulation

Wilson Dirac Operator

$$D_{\mathrm{W}}[U] + m_0 = \frac{1}{2} \sum_{\mu} \left[\gamma_\mu (\nabla_\mu + \nabla^*_\mu) \qquad\qquad \right] + m_0$$

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- with the covariant difference operators:

$$\nabla_\mu\psi(x) = \frac{1}{a}\left[U(x,\mu)\psi(x + a\hat{\mu}) - \psi(x)\right]$$
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- but:
  - chiral symmetry is explicitly broken, $\{D_\mathrm{W}, \gamma_5\} \neq 0$,
  - therefore m_0 renormalises additively (and multiplicatively)

$$m_q = m_0 - m_\mathrm{crit}\ ,$$

  - leading lattice artifacts are $\mathcal{O}(a)$,

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$$m_q = m_0 - m_{\mathrm{crit}} \ ,$$

  - leading lattice artifacts are $\mathcal{O}(a)$,
  - unphysically small eigenvalues of $D_{\mathrm{W}}[U] + m_0$.

QCD on the Lattice II

- Partition function $\mathcal{Z}_{\text{QCD}} = \int \left(\mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi\right) \mathrm{e}^{-S_{\text{QCD}}[U;\bar{\psi},\psi]}$
- Mathematically well defined in Euclidean space-time on a finite volume.
- Non-perturbative, gauge invariant regularisation:
  $\Rightarrow$ non-perturbative (low energy) physics
- Continuum limit $\Rightarrow a \to 0$:
  - Poincaré symmetries are restored automatically,
  - Universality guarantees irrelevance of discretisation details.
- The expectation value of an operator $\mathcal{O}$ is defined non-perturbatively by the functional integral

$$\langle \mathcal{O} \rangle \equiv \frac{1}{\mathcal{Z}_{\text{QCD}}} \int \left(\mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi\right) \mathrm{e}^{-S_{\text{QCD}}[U;\bar{\psi},\psi]} \mathcal{O}[\bar{\psi},\psi;U],$$

QCD on the Lattice III

- The finite number of finite integrals can be evaluated on a computer.
- Integrate out the fermion fields to obtain the fermion determinant $\int \mathcal{D}\psi\mathcal{D}\bar{\psi}e^{-\bar{\psi}D\psi} \propto \det(D)$:

$$\mathcal{Z} = \int (\mathcal{D}U) \det D(U) e^{-S_G[U]}$$

- Any operator $\mathcal{O}$ can be expressed in terms of the bosonic fields

$$\mathcal{O}'(U) = \mathcal{O}\left(\frac{\delta}{\delta\psi}, \frac{\delta}{\delta\bar{\psi}}; U\right) e^{-\bar{\psi}D\psi}\Big|_{\psi=\bar{\psi}=0}$$

e.g. the fermion propagator is $\langle\psi(x)\bar{\psi}(y)\rangle = D^{-1}(x,y)$.

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$\Rightarrow$ subtle interplay of limits

- We need

$$\begin{aligned} a &< 0.1\,\text{fm}, \\ L &> 2\,\text{fm}, \\ m_{\text{PS}} &< 300\,\text{MeV}. \end{aligned}$$

Why is it so expensive?

- We need to compute

$$\mathcal{Z}_{\mathrm{QCD}} \propto \int \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, e^{-\bar{\psi}(D+m_q)\psi} \propto \det(D+m_q).$$

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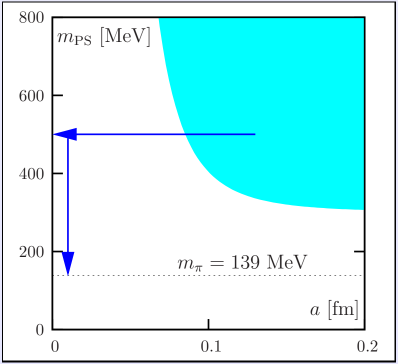
but calculating

$$\varphi = (D+m_q)^{-1}\phi$$

becomes very expensive for small quark mass and large lattice extent L/a.

Continuum and chiral extrapolation

- Cost of a simulation $\propto L^5 (m_{\mathrm{PS}})^{-6} a^{-7}$: [Ukawa '01]



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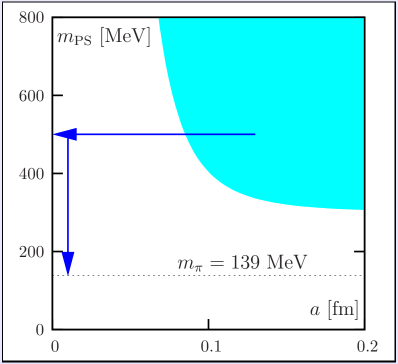

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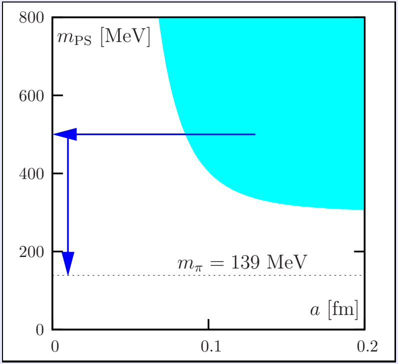

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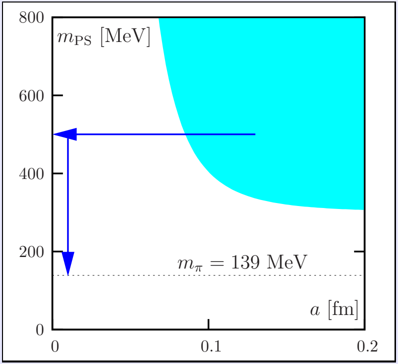

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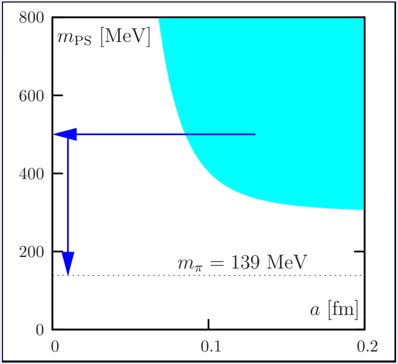

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. . . and better algorithms!

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- Molecular dynamics evolution of P and U by numerical integration of the corresponding equations of motion:
  - large forces cause small step size.
- Metropolis accept/reject step to correct for discretisation errors of the numerical integration.

Preconditioning

- The pseudo-fermion part ($Q = \gamma_5 D$, $N_f = 2$):

$$\det(Q^2) = \int \mathcal{D}\phi\, \mathcal{D}\phi^\dagger\, e^{-\phi^\dagger \frac{1}{Q^2} \phi} = \int \mathcal{D}\phi\, \mathcal{D}\phi^\dagger\, e^{-S_{\rm pf}}$$

can be preconditioned by

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  - n-th root trick [Clark & Kennedy '04]

Mass preconditioning (Hasenbusch Trick)

Mass preconditioning uses the following splitting:

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- Original idea: Choose σ such that the condition numbers of $Q^2+\sigma^2$ and $Q^2/(Q^2+\sigma^2)$ are equal [Hasenbusch & Jansen '02; ALPHA '03]:

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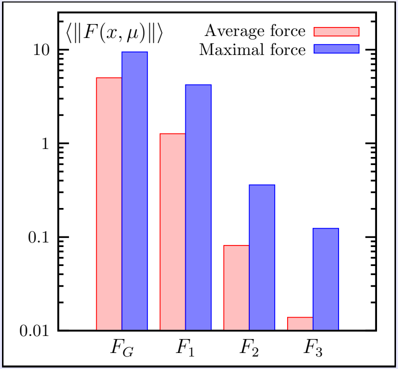
- Caveat: Q^2 must still be inverted.

Multiple time scales

Use mass preconditioning with multiple time scales [Urbach, Jansen, Shindler, U.W. '04]:

$$S_{\text{eff}} = S_G + S_1 + S_2 + \ldots + S_n$$



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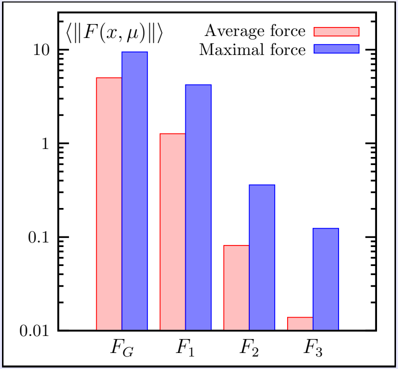

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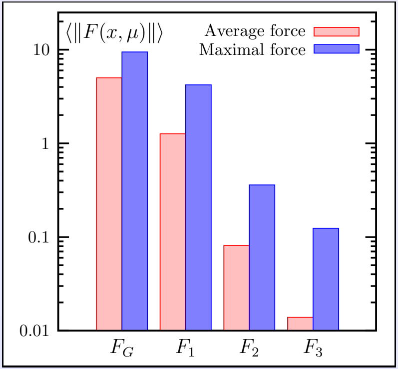

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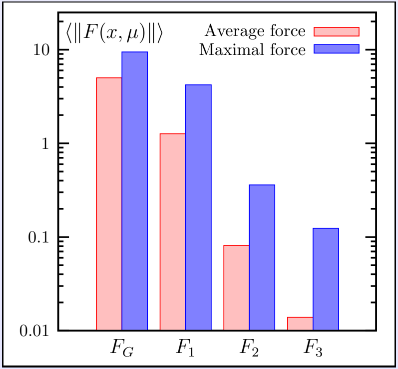
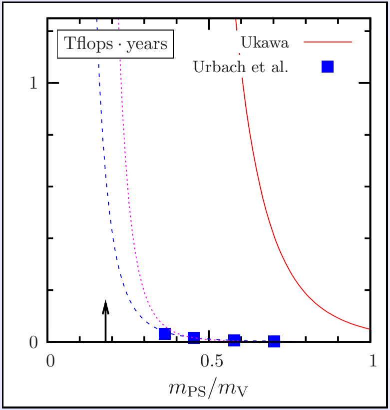


- Use different timescales $\Delta\tau_i$ for different parts in the action S_i [Sexton & Weingarten '92]
- $\|\Delta\tau_i F_i\| \approx \text{const}$
- most expensive A_i on largest timescale.

Cost Reduction

Cost for 1000 independent configurations, $a = 0.08$ fm



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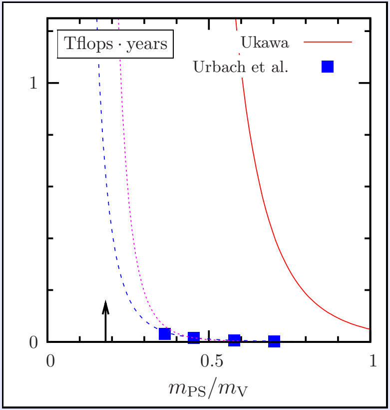

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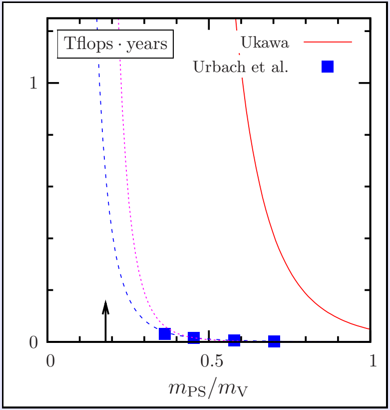

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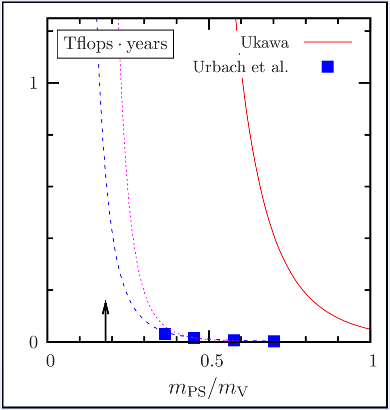

- much faster than standard HMC
- scales better in $m_{\mathrm{PS}}/m_{\mathrm{V}}$
- similar developments by other groups

  [QCDSF ’03; Lüscher ’04; Peardon et al.’05; Clark & Kennedy ’05]

Twisted Mass Fermions I

- Consider the continuum 2-flavour fermionic action

  [Frezzotti, Grassi, Sint, Weisz, '99]

$$S_F = \int d^4x \; \bar{\psi} \; [D + m_q + i\mu\gamma_5\tau_3] \; \psi$$

with

- twisted mass parameter μ,
- τ_3 third Pauli matrix acting in flavour space.

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  with

  - twisted mass parameter μ,
  - τ_3 third Pauli matrix acting in flavour space.

- Its form is invariant under a change of variables with twist angle ω:

$$\psi \rightarrow e^{i\omega\gamma_5\tau_3/2}\psi, \qquad \bar{\psi} \rightarrow \bar{\psi}e^{i\omega\gamma_5\tau_3/2}.$$

Twisted Mass Fermions II

- Remarks:
  - functional measure is invariant,
  - transformation corresponds to a chiral rotation from 'twisted' to 'physical' basis,

    $\Rightarrow \omega = 0$: standard action, $\omega = \pm\frac{\pi}{2}$: maximal twist,
  - mass terms transform as

$$m_q \to m_q \cos\omega + \mu \sin\omega, \quad \mu \to -m_q \sin\omega + \mu \cos\omega,$$

  - twisted axial and vector currents are connected to the physical ones by

$$\begin{aligned} A_\mu^a &\to A_\mu^a \cos\omega + \varepsilon^{3ab} V_\mu^b \sin\omega \quad \text{for } a = 1,2; \quad A_\mu^3 \to A_\mu^3, \\ V_\mu^a &\to V_\mu^a \cos\omega + \varepsilon^{3ab} A_\mu^b \sin\omega \quad \text{for } a = 1,2; \quad V_\mu^3 \to V_\mu^3. \end{aligned}$$

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Wilson Twisted Mass Dirac operator [Frezzotti, Grassi, Sint, Weisz, '99]

$$D_{\rm tm} = \frac{1}{2}\sum_\mu \left[\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - a\nabla^*_\mu\nabla_\mu\right] + m_0 + i\mu\gamma_5\tau_3$$

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...and most importantly:

- this difference can be tuned to obtain $\mathcal{O}(a)$ improvement.

$\mathcal{O}(a)$ Improvement

- If $\omega = \pi/2$ (maximal twist) then ...
  - observables are $\mathcal{O}(a)$ improved [Frezzotti & Rossi '03]:

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  - simplified pattern of operator mixing under renormalisation,
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- but...
  - parity and flavour symmetry are explicitly broken, the latter leading to $m_{\mathrm{PS}}^{\pm} - m_{\mathrm{PS}}^{0}$ splitting.

Idea of the Proof

$$\langle O(x)\rangle^{\mathrm{lat}} = \langle O(x)\rangle^{\mathrm{c}} - a\int dy\,\langle O(x)\mathcal{L}_1(y)\rangle^{\mathrm{c}} + a\sum_k \langle O_k(x)\rangle^{\mathrm{c}} + \mathcal{O}(a^2)$$

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- O must be even under $\tilde{\mathcal{P}}$, $\mathcal{L}_1$ is odd: term cancels in the expansion.

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- Choose an operator O not invariant under $\tilde{\mathcal{P}}$,

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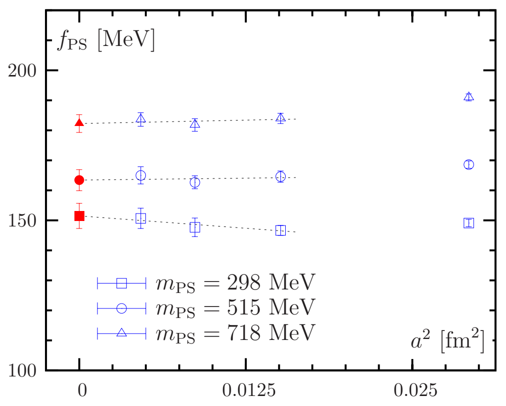
- Example:

$$m_{\mathrm{PCAC}} \equiv \frac{\langle \partial_\mu A^a_\mu(x) P^a(y) \rangle}{2\langle P^a(x) P^a(y) \rangle}\Big|_{m_{\mathrm{PS}}=m_{\mathrm{ref}}} = 0$$

with A^a_μ and P^a the axial vector current and the pseudo-scalar density, respectively.

Test in Quenched Approximation of QCD



[Jansen et al., ’05]

Outline

European Twisted Mass Collaboration

Members from many institutions all over Europe:

B. Blossier, Ph. Boucaud, P. Dimopoulos,
F. Farchioni, R. Frezzotti, V. Gimenez,
G. Herdoiza, K. Jansen, V. Lubicz,
G. Martinelli, C. McNeile, C. Michael,
I. Montvay, D. Palao, M. Papinutto,
O. Pène, J. Pickavance, G.C. Rossi,
L. Scorzato, A. Shindler, S. Simula,
C. Urbach, A. Vladikas, U. Wenger

Set-up

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- gauge action: treelevel Symanzik improved [Weisz '83].

$\beta = 3.90$, $a \approx 0.09$ fm

$a\mu$	$L^3 \times T$	$m_{\rm PS}$ [MeV]	$N_{\rm traj}$
0.0040	$24^3 \times 48$	280	5000
0.0064	$24^3 \times 48$	350	5000
0.0085	$24^3 \times 48$	390	5000
0.0100	$24^3 \times 48$	430	5000
0.0150	$24^3 \times 48$	510	5000
0.0040	$24^3 \times 32$	280	5000
0.0040	$20^3 \times 48$	-	17
0.0040	$32^3 \times 64$	280	5000

$\beta = 4.05$, $a \approx 0.07$ fm (preliminary)

$a\mu$	$L^3 \times T$	m_{PS} [MeV]	N_{traj}
0.003	$32^3 \times 64$	270	5000
0.006	$32^3 \times 64$	370	5000
0.008	$32^3 \times 64$	-	3000
0.012	$32^3 \times 64$	520	3000

$\beta = 3.80$, $a \approx 0.12$ fm (preliminary)

$a\mu$	$L^3 \times T$	m_{PS} [MeV]	N_{traj}
0.006	$20^3 \times 48$	-	
0.009	$20^3 \times 48$	-	
0.012	$20^3 \times 48$	-	
0.015	$20^3 \times 48$	-	

$\Rightarrow$ Tuning is ongoing...

Machines

- Many massively parallel machines throughout Europe:
  - IBM p960 Regatta and BlueGene/L at FZ-Jülich,
  - apeNEXT at DESY Zeuthen and Rome,
  - MareNostrum in Valencia,
  - QCDOC in Edinburgh,
  - Altix system at LRZ Munich (pending),
  - local PC-clusters and -farms, etc.

Machines

Tuning to Maximal Twist

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  - choose an operator odd under parity (in the physical basis) and vanishing in the continuum,
  - at finite a tune its v.e.v. to zero by adjusting am_0.

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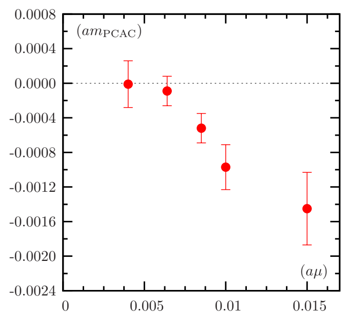
- It was not obvious at the beginning that this tuning is feasible!

Tuning to Maximal Twist

Tuning to full twist is possible with reasonable computer resources!



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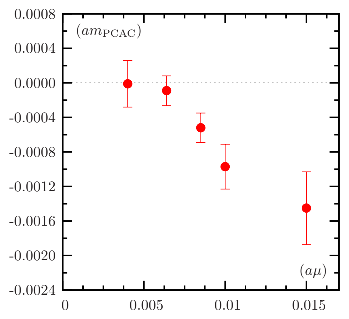

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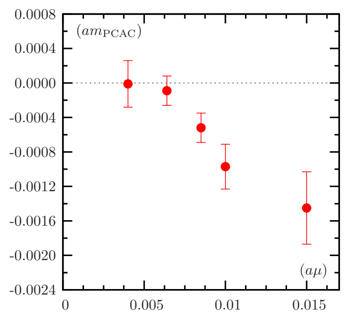

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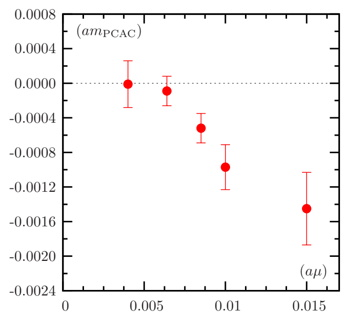

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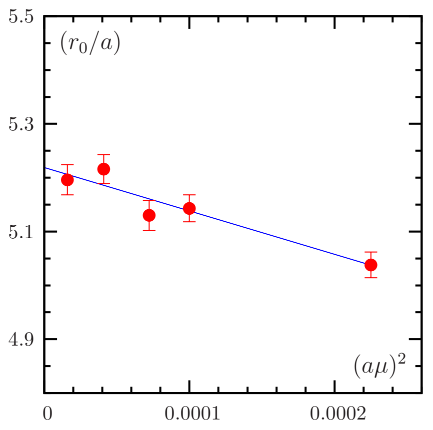
- $r_0 \approx 0.5\mathrm{fm}$ is only known approximately.

Sommer Parameter



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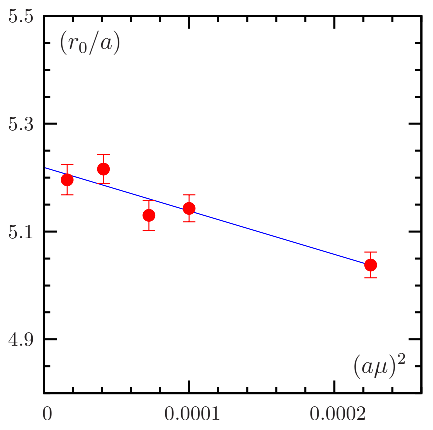

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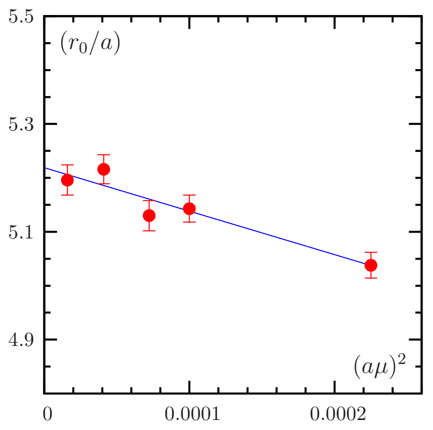

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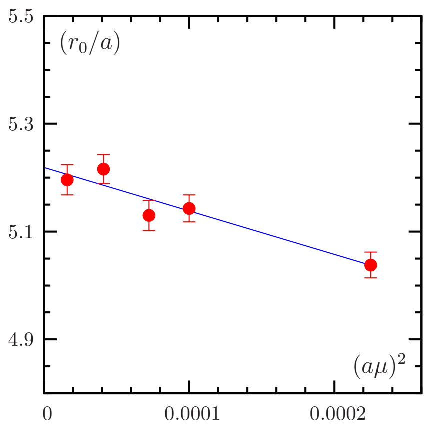

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$\Rightarrow$ $r_0/a = 5.22(2)$ at the physical point.

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  due to an exact lattice Ward identity [Frezzotti, Grassi, Sint, Weisz '01].
- No renormalisation factor needed!
  - since $Z_\mu = 1/Z_P$
  - similar to overlap fermions (exact chiral symmetry)
  - unlike pure Wilson

Description with Chiral Perturbation Theory

- Describe mass and L dependence with $N_f = 2$ χPT at NLO

[Gasser, Leutwyler '87; Colangelo, Dürr, Haefeli '05]

$$m_{\mathrm{PS}}^2 = 2B_0\mu \left[1 + \frac{1}{2}\xi\, \tilde{g}_1(\lambda)\right]^2 [1 + \xi \log(2B_0\mu/\Lambda_3^2)]$$

$$f_{\mathrm{PS}} = F_0 \; [1 - \xi\, \tilde{g}_1(\lambda)] \; [1 - 2\xi \log(2B_0\mu/\Lambda_4^2)]$$

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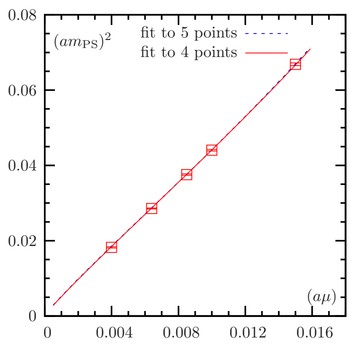
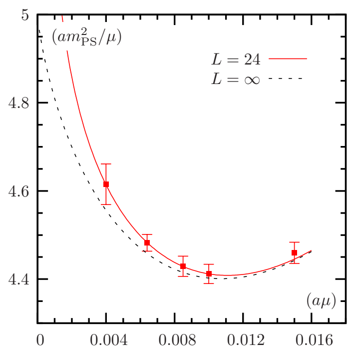
- Fit simultaneously to our data:
  fit parameters B_0, F_0, $\log\Lambda_3^2$, $\log\Lambda_4^2$

Pion Sector: m_{PS} at $\beta = 3.9$





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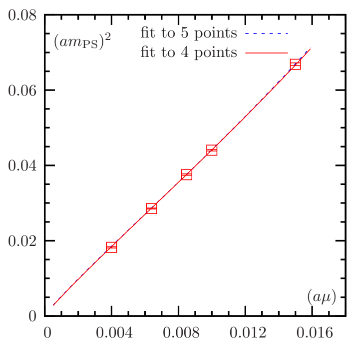

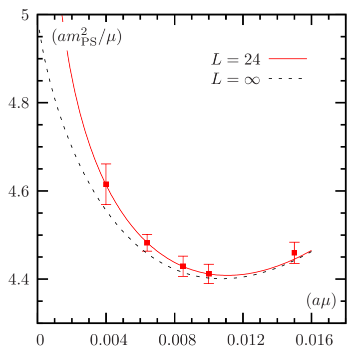

- excellent description by chiral perturbation theory,
- sensitivity to Λ_3 exposed.

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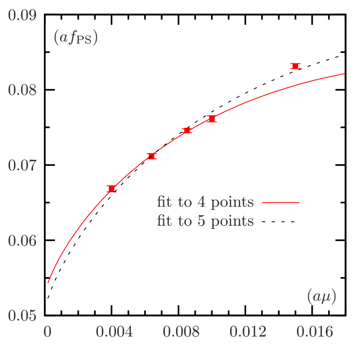

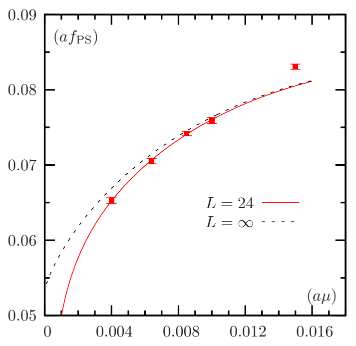

$$2aB_0 = 4.99(6), \quad aF = 0.0534(6)$$
$$a^2\,\bar{l}_3^2 \equiv \log(a^2\Lambda_3^2) = -1.93(10),$$
$$a^2\,\bar{l}_4^2 \equiv \log(a^2\Lambda_4^2) = -1.06(4)$$

Low Energy Constants

- determination of $\bar{l}_{3,4} \equiv \log(\Lambda_{3,4}/m_\pi)$:

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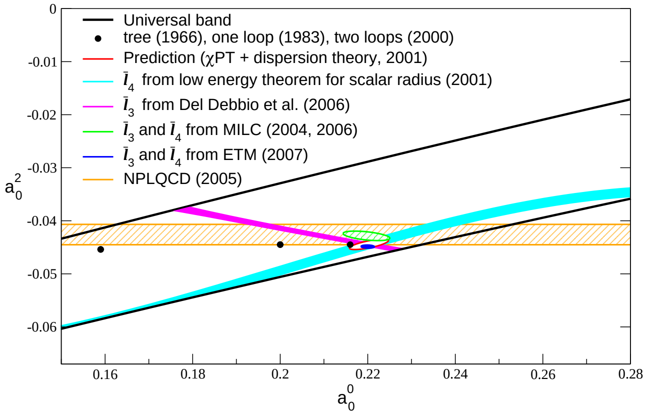
- determine the lattice spacing with $f_\pi = 130.7\ \mathrm{MeV}$

$$a = 0.087(1)\ \mathrm{fm} \quad \Rightarrow \quad r_0 = 0.454(7)\ \mathrm{fm}$$

$\pi\pi$ Scattering: S-wave scattering length a_0^0 and a_0^2

$$a_0^0 = 0.220 \pm 0.002, \quad a_0^2 = -0.0449 \pm 0.0003$$



[Leutwyler priv., cf. hep-ph/0612112]

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- we are assuming that finite size effects are correctly described by χPT to that order

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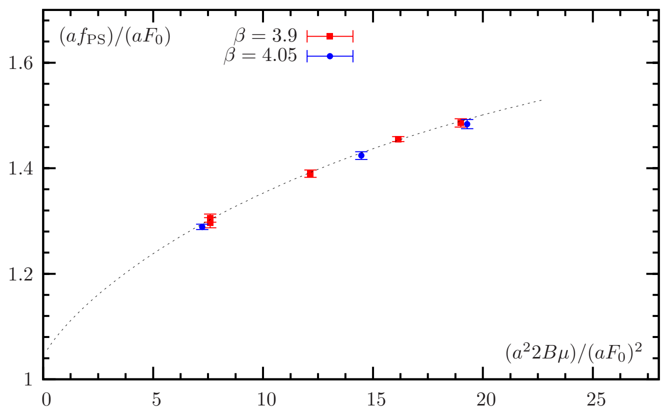
Preliminary Check for Lattice Artifacts

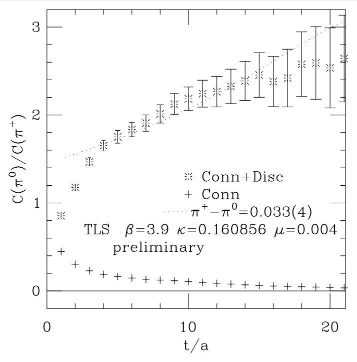
Combined fit of two lattice spacings:



Lattice artefacts seem to be very small!

Pion Mass Splitting

At finite lattice spacing flavour symmetry is broken at $\mathcal{O}(a^2)$:



- Isospin is broken at $a > 0$,
- strongest for $m_{\rm PS}^+ - m_{\rm PS}^0$,
- breaking vanishes as $m_{\rm PS}^+ - m_{\rm PS}^0 = c_2 a^2$,
- $\Delta \equiv (m_{\rm PS}^+ - m_{\rm PS}^0)/m_{\rm PS}^+ \sim 25\%$

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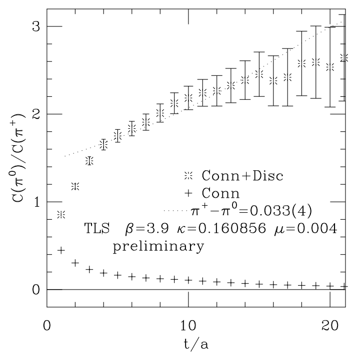

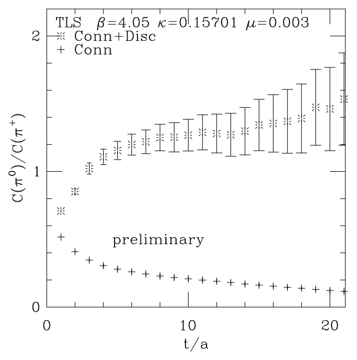

- at $\beta = 3.90$: splitting 25% of charged m_{PS}
- at $\beta = 4.05$: splitting 10% of charged m_{PS}

Pion Mass Splitting

- Neutral pion lighter than charged:
  - this is consistent with prediction from χPT,
  - problems for FS correction formula?
- Pion splitting decreases with a^2 as expected,
- disconnected contribution in π^0 is large and reduces the difference.
- Compared to quenched the effect is strongly reduced.

Quark Masses (PRELIMINARY)

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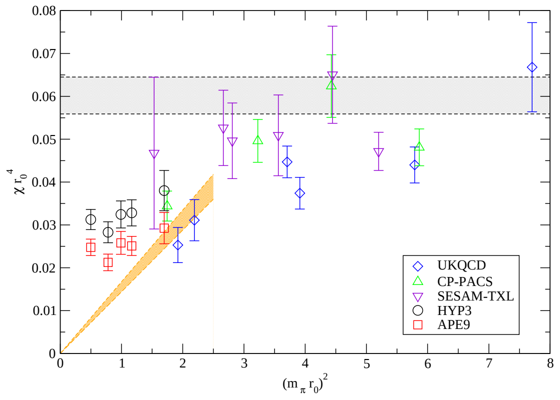
- as a first attempt: used renormalisation constants of bilinear quark operators from RI-MOM

Topological susceptibility (PRELIMINARY)



The cake is prepared...

Calculations under way or planned

- Other mesons: $\rho, a_0, b_1, \ldots,$
- Pion form factors: $F_{\mathrm{S,V}}$,
- Baryons: $N, P, \Delta^+, \Delta^{++}, \ldots$
- charm sector: $f_{\mathrm{D}},\ m_{\mathrm{D_S}}/m_{\mathrm{D}}$,
- string breaking, ρ-decay,
- topological susceptibility,
- Adler function: $g-2, \alpha_s$,

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  - tuning possible

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- We have a sound set-up:
  - $O(a)$ improvement with maximally twisted mass fermions,
  - highly tuned algorithms available,
- First physics results with light quarks on fine lattices:
  - m_{PS} as light as 280 MeV,
  - lattice spacings $\lesssim$ 0.1 fm,
  - volumes larger 2 fm,
  - stable simulations,
  - lattice artifacts seem to be small.

Outlook

- Simulate larger volumes and check for finite size effects,
- continuum extrapolation,
- mixed action approach:
  Neuberger fermions in the valence sector $\rightarrow$ e.g. B_{K},
- long term objective: $2+1+1$ flavours of quarks.