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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Quantum chromodynamics (QCD) – the theory of strong interactions

\[ \mathcal{L}_{\text{QCD}} = \bar{\psi}(i\slashed{D} - m_{q})\psi - \frac{1}{4} G_{\mu \nu} G^{\mu \nu} \]

- 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,
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.

⇒ Lattice QCD is a (the) non-perturbative method for such ab-initio calculations
Quantum chromodynamics is formally described by the Lagrange density:

$$\mathcal{L}_{\text{QCD}} = \bar{\psi} (i D - m_q) \psi - \frac{1}{4} G_{\mu \nu} G^{\mu \nu}$$

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 $A_\mu$ in $G_{\mu \nu} \Rightarrow$ link matrices $U_\mu$ ('\[\text{•} \rightarrow \text{•}\]')
### Wilson Dirac Operator

\[
D_W[U] + m_0 = \frac{1}{2} \sum_\mu \left[ \gamma_\mu (\nabla_\mu + \nabla_\mu^*) \right] + m_0
\]
Wilson Formulation

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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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suffers from a fermion doubling problem.
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  - solves the fermion doubling problem,
- but:
  - chiral symmetry is explicitly broken, \(\{D_W, \gamma_5\} \neq 0\),
  - therefore \(m_0\) renormalises additively (and multiplicatively)
  \[ m_q = m_0 - m_{\text{crit}} \]
- leading lattice artifacts are \(O(a)\),
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    \[ m_q = m_0 - m_{\text{crit}} \],
  - leading lattice artifacts are \(\mathcal{O}(a)\),
  - unphysically small eigenvalues of \(D_W[U] + m_0\).
Partition function \( Z_{\text{QCD}} = \int (\mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi) \ e^{-S_{\text{QCD}}[U; \bar{\psi}, \psi]} \)

- 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

\[
\langle \mathcal{O} \rangle \equiv \frac{1}{Z_{\text{QCD}}} \int (\mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi) \ e^{-S_{\text{QCD}}[U; \bar{\psi}, \psi]} \mathcal{O}[\bar{\psi}, \psi; U],
\]
The finite number of finite integrals can be evaluated on a computer.

Integrate out the fermion fields to obtain the fermion determinant $\int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-\bar{\psi}D\psi} \propto \text{det}(D)$:

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

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

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

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

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$\Rightarrow$ subtle interplay of limits

We need

$$a \ < \ 0.1 \text{ fm},$$

$$L \ > \ 2 \text{ fm},$$

$$m_{PS} \ < \ 300 \text{ MeV}.$$
Why is it so expensive?

- We need to compute

\[ Z_{\text{QCD}} \propto \int \mathcal{D}\bar{\psi} \mathcal{D}\psi \ e^{-\bar{\psi}(D+m_q)\psi} \propto \det(D + m_q). \]
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but calculating

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

becomes very expensive for small quark mass and large lattice extent \( L/a \).
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  ⇒ Use bigger computers ... ... and better algorithms!
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Molecular dynamics evolution of $P$ and $U$ by numerical integration of the corresponding equations of motion:
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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.
The pseudo-fermion part \( Q = \gamma_5 D, \ N_f = 2 \):

\[
\det(Q^2) = \int \mathcal{D}\phi \mathcal{D}\phi^\dagger \ e^{-\phi^\dagger \frac{1}{\alpha^2} \phi} = \int \mathcal{D}\phi \mathcal{D}\phi^\dagger \ e^{-S_{pf}}
\]

can be preconditioned by

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\det(Q^2) = \det(A_1) \cdot \det(A_2) \cdot \ldots \cdot \det(A_n)
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- mass preconditioning (Hasenbusch trick) \[\text{[Hasenbusch '01]}\]
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- \(n\)-th root trick [Clark & Kennedy '04]
Mass pre-conditioning uses the following splitting:

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\det(Q^2) = \det\left(\frac{Q^2}{Q^2 + \sigma^2}\right) \cdot \det(Q^2 + \sigma^2)
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Original idea: Choose \( \sigma \) 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.
Use mass preconditioning with multiple time scales \cite{Urbach, Jansen, Shindler, U.W. '04}:

\[ S_{\text{eff}} = S_G + S_1 + S_2 + \ldots + S_n \]
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- Use different timescales $\Delta \tau_i$ for different parts in the action $S_i$

\[ \langle \| F(x, \mu) \| \rangle \]

\begin{center}
\begin{tabular}{c c c c}
$F_G$ & $F_1$ & $F_2$ & $F_3$
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- most expensive \( A_i \) on largest timescale.
Cost for 1000 independent configurations, $a = 0.08 \text{ fm}$

![Graph showing the cost in Tflops · years for different values of $m_{PS}/m_V$. The graph compares the results of Urbach et al. and Ukawa.](image-url)
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- much faster than standard HMC
- scales better in $m_{PS}/m_V$
- similar developments by other groups

[QCDSF '03; Lüscher '04; Peardon et al.'05; Clark & Kennedy '05]
Consider the continuum 2-flavour fermionic action

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

with
- twisted mass parameter \( \mu \),
- \( \tau_3 \) third Pauli matrix acting in flavour space.
Consider the continuum 2-flavour fermionic action

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with

- twisted mass parameter \( \mu \),
- \( \tau_3 \) third Pauli matrix acting in flavour space.

Its form is invariant under a change of variables with twist angle \( \omega \):

\[ \psi \rightarrow e^{i\omega \gamma_5 \tau_3 / 2} \psi, \quad \bar{\psi} \rightarrow \bar{\psi} e^{i\omega \gamma_5 \tau_3 / 2}. \]
Twisted Mass Fermions II

Remarks:

- functional measure is invariant,
- transformation corresponds to a chiral rotation from 'twisted' to 'physical' basis,
  \[ \Rightarrow \omega = 0 : \text{standard action}, \quad \omega = \pm \frac{\pi}{2} : \text{maximal twist}, \]
- mass terms transform as
  \[ m_q \rightarrow m_q \cos \omega + \mu \sin \omega, \quad \mu \rightarrow -m_q \sin \omega + \mu \cos \omega, \]
- twisted axial and vector currents are connected to the physical ones by
  \[ A^a_\mu \rightarrow A^a_\mu \cos \omega + \varepsilon^{3ab} V^b_\mu \sin \omega \quad \text{for} \quad a = 1, 2; \quad A^3_\mu \rightarrow A^3_\mu, \]
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Wilson Twisted Mass Dirac operator \cite{Frezzotti, Grassi, Sint, Weisz, '99}

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- \( D_{tm} \) is protected against unphysically small eigenvalues,
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**Wilson Twisted Mass Dirac operator**  \[D_{tm} = \frac{1}{2} \sum_{\mu} \left[ \gamma_\mu (\nabla_\mu + \nabla^*_\mu) - a \nabla^*_\mu \nabla_\mu \right] + m_0 + i \mu \gamma_5 \tau_3\]

- \(D_{tm}\) is protected against unphysically small eigenvalues,
- has a strictly positive measure,
- differs from Wilson formulation only by lattice artifacts
  because Wilson term \(a \nabla^*_\mu \nabla_\mu\) is not invariant under change of variables,

...and most importantly:
- this difference can be tuned to obtain \(O(a)\) improvement.
\( \mathcal{O}(a) \) Improvement

- If \( \omega = \pi/2 \) (maximal twist) then ...
  - observables are \( \mathcal{O}(a) \) improved [Frezzotti & Rossi '03]:
  - shown to work in practice for various observables in the quenched approximation [Jansen et al. '04-'05; Abdel-Rehim et al. '04-'05],
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- simplified pattern of operator mixing under renormalisation,
- only one parameter $\omega$ must be tuned,

but...
- parity and flavour symmetry are explicitly broken, the latter leading to $m^\pm_{PS} - m^0_{PS}$ splitting.
Idea of the Proof

\[
\langle O(x) \rangle^{\text{lat}} = \langle O(x) \rangle^c - a \int dy \langle O(x) L_1(y) \rangle^c + a \sum_k \langle O_k(x) \rangle^c + O(a^2)
\]

[Rossi, Frezzotti, Martinelli, Papinutto '05]
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- **example:** cont. symmetry modified Parity

\[\tilde{\mathcal{P}} : \begin{cases} 
\psi(\bar{x}, t) & \rightarrow \gamma_0 \exp(i \omega \gamma_5 \tau_3) \psi(-\bar{x}, t) \\
\bar{\psi}(\bar{x}, t) & \rightarrow \bar{\psi}(-\bar{x}, t) \exp(i \omega \gamma_5 \tau_3) \gamma_0
\end{cases} \]
\[ \langle O(x) \rangle_{\text{lat}} = \langle O(x) \rangle^c - a \int dy \langle O(x) L_1(y) \rangle^c + a \sum_k \langle O_k(x) \rangle^c + \mathcal{O}(a^2) \]

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- \( O \) must be even under \( \tilde{\mathcal{P}} \), \( L_1 \) is odd: term cancels in the expansion.
Choose an operator $O$ not invariant under $\tilde{P}$,
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tune $m_0$ such that $O$ has vanishing expt. value at each lattice spacing and fixed physical situation,
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Example:

$$m_{PCAC} \equiv \left. \frac{\langle \partial_\mu A^a_\mu(x) P^a(y) \rangle}{2 \langle P^a(x) P^a(y) \rangle} \right\vert_{m_{PS}=m_{ref}} = 0$$

with $A^a_\mu$ and $P^a$ the axial vector current and the pseudo-scalar density, respectively.
Lattice Formulation of QCD
HMC Algorithm
Wilson Twisted Mass Fermions

Test in Quenched Approximation of QCD

\[ f_{PS} \text{ [MeV]} \]

\[ a^2 \text{ [fm}^2] \]

- \( m_{PS} = 298 \text{ MeV} \)
- \( m_{PS} = 515 \text{ MeV} \)
- \( m_{PS} = 718 \text{ MeV} \)

[Jansen et al., '05]
Members from many institutions all over Europe:

Set-up

\( N_f = 2 \) flavours of degenerate quarks, maximally twisted,
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- lattice volumes of spatial extension larger than 2 fm,
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- gauge action: treelevel Symanzik improved \cite{Weisz '83}. 
<table>
<thead>
<tr>
<th>$a\mu$</th>
<th>$L^3 \times T$</th>
<th>$m_{PS}$ [MeV]</th>
<th>$N_{\text{traj}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0040</td>
<td>$24^3 \times 48$</td>
<td>280</td>
<td>5000</td>
</tr>
<tr>
<td>0.0064</td>
<td>$24^3 \times 48$</td>
<td>350</td>
<td>5000</td>
</tr>
<tr>
<td>0.0085</td>
<td>$24^3 \times 48$</td>
<td>390</td>
<td>5000</td>
</tr>
<tr>
<td>0.0100</td>
<td>$24^3 \times 48$</td>
<td>430</td>
<td>5000</td>
</tr>
<tr>
<td>0.0150</td>
<td>$24^3 \times 48$</td>
<td>510</td>
<td>5000</td>
</tr>
<tr>
<td>0.0040</td>
<td>$24^3 \times 32$</td>
<td>280</td>
<td>5000</td>
</tr>
<tr>
<td>0.0040</td>
<td>$20^3 \times 48$</td>
<td>-</td>
<td>17</td>
</tr>
<tr>
<td>0.0040</td>
<td>$32^3 \times 64$</td>
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<td>5000</td>
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</tbody>
</table>
\[ \beta = 4.05, \ a \approx 0.07 \text{ fm (preliminary)} \]

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<tr>
<td>0.003</td>
<td>$32^3 \times 64$</td>
<td>270</td>
<td>5000</td>
</tr>
<tr>
<td>0.006</td>
<td>$32^3 \times 64$</td>
<td>370</td>
<td>5000</td>
</tr>
<tr>
<td>0.008</td>
<td>$32^3 \times 64$</td>
<td>-</td>
<td>3000</td>
</tr>
<tr>
<td>0.012</td>
<td>$32^3 \times 64$</td>
<td>520</td>
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<td>0.006</td>
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<tr>
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<td>-</td>
<td>-</td>
</tr>
<tr>
<td>0.015</td>
<td>( 20^3 \times 48 )</td>
<td>-</td>
<td>-</td>
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\( \Rightarrow \) Tuning is ongoing...
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
Many different choices are possible:

- 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 $a m_0$. 
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We tune

$$m_{PCAC} = \frac{\sum_x \langle \partial_0 A_0^a(x) P^a(0) \rangle}{2 \sum_x \langle \partial_0 P^a(x) P^a(0) \rangle} = 0, \quad a = 1, 2$$

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Involves at each value of $a$ several (expensive) tuning simulations.

It was not obvious at the beginning that this tuning is feasible!
Tuning to full twist is possible with reasonable computer resources!

- needs to be done on the target lattice volume,
Tuning to Maximal Twist

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- we see deviations for the other $\mu$-values (as expected),
- $\mu$-dependence is a $O(a)$ cut-off effect modifying the $O(a^2)$ artefacts in physical obervables.
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$r_0 \approx 0.5\text{fm}$ is only known approximately.
Sommer Parameter

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\[ (r_0/a) \]

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$\Rightarrow$ $r_0/a = 5.22(2)$ at the physical point.
Pion Sector: \( m_{PS} \) and \( f_{PS} \)

- \( m_{PS} \) from exponential decay of appropriate correlation functions
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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
Describe mass and $L$ dependence with $N_f = 2$ $\chi$PT at NLO

\[ m_{PS}^2 = 2B_0\mu \left[ 1 + \frac{1}{2} \xi \tilde{g}_1(\lambda) \right]^2 \left[ 1 + \xi \log\left(\frac{2B_0\mu}{\Lambda^2_3}\right) \right] \]

\[ f_{PS} = F_0 \left[ 1 - \xi \tilde{g}_1(\lambda) \right] \left[ 1 - 2\xi \log\left(\frac{2B_0\mu}{\Lambda^2_4}\right) \right] \]

with $\xi = \frac{2B_0\mu}{(2\pi F_0)^2}$, $\lambda = \sqrt{2B_0\mu L^2}$ and $\tilde{g}_1(\lambda)$ is a known function.
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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 $\beta = 3.9$

- **excellent description by chiral perturbation theory**,
Pion Sector: $m_{PS}$ at $\beta = 3.9$

- excellent description by chiral perturbation theory,
- sensitivity to $\Lambda_3$ exposed.
Pion Sector: \( f_{PS} \) at \( \beta = 3.9 \)

\[
2aB_0 = 4.99(6), \quad aF = 0.0534(6)
\]

\[
a^2 \overline{t}_3^2 \equiv \log(a^2 \Lambda_3^2) = -1.93(10),
\]

\[
a^2 \overline{t}_4^2 \equiv \log(a^2 \Lambda_4^2) = -1.06(4)
\]
determination of $\bar{l}_{3,4} \equiv \log(\Lambda_{3,4}/m_\pi)$:

$$\bar{l}_3 = 3.65 \pm 0.12, \quad \bar{l}_4 = 4.52 \pm 0.06$$

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

$$a = 0.087(1) \text{ fm} \quad \Rightarrow \quad r_0 = 0.454(7) \text{ fm}$$
\( a_0^0 = 0.220 \pm 0.002, \quad a_0^2 = -0.0449 \pm 0.0003 \)
Note: all errors are statistical only!

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All this needs to be checked!
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- we are assuming that lattice artifacts are negligible
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- we are assuming that finite size effects are correctly described by $\chi$PT to that order

All this needs to be checked!
Preliminary Check for Lattice Artifacts

Combined fit of two lattice spacings:

\[
\frac{(a f_{PS})}{(a F_0)} \quad \beta = 3.9
\]

\[
\frac{(a f_{PS})}{(a F_0)} \quad \beta = 4.05
\]

Lattice artefacts seem to be very small!
At finite lattice spacing flavour symmetry is broken at $\mathcal{O}(a^2)$:

- Isospin is broken at $a > 0$,
- strongest for $m_{PS}^+ - m_{PS}^0$,
- breaking vanishes as $m_{PS}^+ - m_{PS}^0 = c_2 a^2$,
- $\Delta \equiv (m_{PS}^+ - m_{PS}^0)/m_{PS}^+ \sim 25\%$
At finite lattice spacing flavour symmetry is broken at $\mathcal{O}(a^2)$:

- at $\beta = 3.90$: splitting 25% of charged $m_{PS}$
- at $\beta = 4.05$: splitting 10% of charged $m_{PS}$
Neutral pion lighter than charged:
- this is consistent with prediction from $\chi$PT,
- problems for FS correction formula?

Pion splitting decreases with $a^2$ as expected,

disconnected contribution in $\pi^0$ is large
and reduces the difference.

Compared to quenched the effect is strongly reduced.
Prime example for lattice calculations.
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Estimates of quark masses:

\[ m_{u,d}^{\overline{\text{MS}}, 2 \text{ GeV}} = 4.1(2) \text{ MeV} \]

\[ m_{s}^{\overline{\text{MS}}, 2 \text{ GeV}} = 115(2) \text{ MeV} \]

\[ m_{c}^{\overline{\text{MS}}, 2 \text{ GeV}} = 1.4(1) \text{ GeV} \]
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m_c(\overline{\text{MS}}, 2 \text{ GeV}) &= 1.4(1) \text{ GeV}
\end{align*}
\]

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

Pion Sector

Other Physics

Topological susceptibility

(PRELIMINARY)
The cake is prepared...
Calculations under way or planned

- Other mesons: $\rho, a_0, b_1, \ldots$
- Pion form factors: $F_{S,V}$
- Baryons: $N, P, \Delta^+, \Delta^{++}, \ldots$
- Charm sector: $f_D, m_{D_S}/m_D$
- String breaking, $\rho$-decay
- Topological susceptibility
- Adler function: $g - 2, \alpha_s$
And what about the strange ...?

With twisted mass $N_f = 2 + 1 + 1$ flavours are possible

[Frezzotti & Rossi '03]
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$O(a)$ improvement at maximal twist
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- algorithms are ready  [Montvay & Scholz ’05; Chiarappa, Frezzotti, Urbach ’05]
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We have a sound set-up:

- $O(a)$ improvement with maximally twisted mass fermions,
- highly tuned algorithms available,
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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.
Simulate larger volumes and check for finite size effects,
continuum extrapolation,
mixed action approach:
Neuberger fermions in the valence sector → e.g. $B_K$,
long term objective: $2 + 1 + 1$ flavours of quarks.