Going chiral: overlap versus Wilson twisted mass fermions

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- Why new lattice actions
- Scaling with Wilson twisted mass fermions
  extended scaling test → A. Shindler
- Comparison of overlap and Wilson twisted mass fermions
  - approach to the chiral limit
  - simulation cost
- Conclusions
There are dangerous lattice animals

→ discretization errors
→ chiral symmetry
→ computational cost
Discretization Errors $\leftrightarrow$ violation of chiral symmetry

Wilson-Dirac operator

$$D_W = m_q + \frac{1}{2} \gamma_\mu \left[ \nabla_\mu + \nabla^*_\mu \right] - ar\frac{1}{2} \nabla^*_\mu \nabla_\mu$$

$$\nabla_\mu \psi(x) = \frac{1}{a} \left[ U(x, \mu) \psi(x + a\hat{\mu}) - \psi(x) \right], \quad U = e^{ia g_0 A_\mu(x)}$$

$$\nabla^*_\mu \psi(x) = \frac{1}{a} \left[ \psi(x) - U(x - a\hat{\mu}, \mu) \psi(x - a\hat{\mu}) \right]$$
Chiral extrapolation

ZeRo collaboration (Guagnelli, K.J., Palombi, Petronzio, Shindler, Wetzorke) perform continuum extrapolation of a twist-2, non-singlet pion operator

- Linear continuum extrapolation $a \to 0$
- Combined fit of Wilson and Clover data
- 4 lattice spacings at fixed $m_\pi^2$
- Chiral extrapolation $m \to 0$
  - Linear: $\langle x \rangle_{\overline{MS}} = 0.263(14)$
  - Non-linear: $\langle x \rangle_{\overline{MS}} = 0.221^{+10+21}_{-9-13}$

$\Rightarrow$ no data in interesting region of pion mass
Why are we not able to reach realistic pion mass?

in addition to
natural slowing down as $m_\pi \to 0$

- very small eigenvalues
- slow down algorithms
- spoil signal

→ problem appears for Wilson fermions

→ similar (maybe worse) for O(a)-improved Wilson fermions

(staggered fermions: size of systematic error)
solution: **Ginsparg-Wilson relation**

\[
\gamma_5 D + D \gamma_5 = 2a D \gamma_5 \]

\[
\Rightarrow D^{-1} \gamma_5 + \gamma_5 D^{-1} = 2a \gamma_5
\]

\(D^{-1}\) anti-commutes with \(\gamma_5\) at all non-zero distances

\(\rightarrow\) only mild (i.e. local) violation of chiral symmetry

Ginsparg and Wilson arrived at this expression already in the early days of lattice gauge theories from a completely different path

\(\Leftarrow\) block spinning from the continuum

one solution of GW relation: overlap operator \(D_{ov}\) (Neuberger)

(alternatives: domain wall fermions and perfect actions)

\[
D_{ov} = \left[ 1 - A(A^\dagger A)^{-1/2} \right]
\]

with \(A = 1 + s - D_w(m_q = 0); s\) a tunable parameter, \(0 < s < 1\)
Adding a mass term (naive definition)

\[ D_{ov} = m_q + [1 - A(A^{\dagger}A)^{-1/2}] \]

→ exact (lattice) chiral symmetry at \( m_q = 0 \)

→ infrared safe: quark mass \( m_q \)
  \( \Leftarrow \) can reach very small quark masses

→ O(a)-improved

\( \Leftarrow \) computationally very demanding,

O(10-100) more expensive than standard Wilson fermions

Nevertheless: exist problems for overlap fermions: \( \epsilon \)-regime of chiral perturbation theory, complicated operator mixings
**Wilson** *(Frezzotti, Rossi)* twisted mass QCD *(Frezzotti, Grassi, Sint, Weisz)*

equivalent Wilson-Dirac operator

\[
D_W = m_q e^{i \omega \gamma_5 \tau^3} + \frac{\gamma_\mu}{2} \left[ \nabla_\mu + \nabla^*_\mu \right] - a_r^2 \nabla_\mu \nabla^*_\mu + M_{cr} \equiv m_q e^{i \omega \gamma_5 \tau^3} + D_{crit} + D_r
\]

\(\omega = 0\) → usual Wilson-Dirac operator

\(\omega = \pi/2 \rightarrow i \gamma_5 \tau_3 m_q\) : twisted mass term at zero quark mass

under parity, \(R_5 = e^{i \omega \gamma_5 \tau^3}\)

- \(D_{crit}\) invariant
- \(m_q e^{i \omega \gamma_5 \tau^3} \rightarrow -m_q e^{i \omega \gamma_5 \tau^3}\)
- \(D_r \rightarrow -D_r\)

\(\Rightarrow D_W\) invariant under \(R_5 \times (r \rightarrow -r) \times (m_q \rightarrow -m_q)\)
Wilson twisted mass QCD

it can be shown than

$$\langle \mathcal{O} \rangle |_{(m_q, r)} = (-1)^P \langle \mathcal{O} \rangle |_{(-m_q, -r)}$$

- action invariant under $R_5$
- change of integration measure compensated by the parity transformation of operator
Wilson twisted mass QCD

Symanzik expansion

\[
\langle O \rangle\big|_{(m_q, r)} = [\xi(r) + a m_q \eta(r)] \langle O \rangle_{mq}^{cont} + a \chi(r) \langle O' \rangle_{mq}^{cont}
\]

\[
\langle O \rangle\big|_{(-m_q, -r)} = [\xi(-r) - a m_q \eta(-r)] \langle O \rangle_{mq}^{cont} + a \chi(-r) \langle O' \rangle_{-m_q}^{cont}
\]

in addition

\[
\langle O \rangle_{mq}^{cont} = (-1)^P \langle O \rangle_{-m_q}^{cont}
\]

\[
\Rightarrow \quad \xi(r) = +\xi(-r) , \quad a m_q \eta(r) = -a m_q \eta(-r) \quad , \quad a \chi(r) = -a \chi(-r)
\]

\[
\Rightarrow \quad \frac{1}{2} \left[ \langle O \rangle_{m_q, r} + \langle O \rangle_{-m_q, -r} \right] = \xi(r) \langle O \rangle_{mq}^{cont} + O(a^2)
\]

\[
\Rightarrow \quad \text{at } m_q = m_0 - M_{cr} = 0 \quad \text{the Wilson average is } O(a) \text{ improved}
\]
Wilson twisted mass QCD

\[ \langle O \rangle|_{m_q, r, \omega = \pi/2} = \frac{1}{2} \left[ \langle O \rangle|_{m_q, r, \omega = \pi/2} + \langle O \rangle|_{m_q, -r, \omega = \pi/2} \right] \]

⇒ choose \( \omega = \pm \pi/2 \) and bare quark mass the critical quark mass

⇒ all quantities even in \( \omega = \pm \pi/2 \) are automatic \( O(a) \) improved

Examples:

• hadron masses

• matrix elements

• form factors

• decay constants
Hopping parameter representation

\[ \chi \rightarrow \sqrt{2}\kappa \frac{a^{3/2}}{\chi}, \quad \bar{\chi} \rightarrow \sqrt{2}\kappa \frac{a^{3/2}}{\bar{\chi}}, \quad \kappa = \frac{1}{2am_0+8r} \]

\[ S[\chi, \bar{\chi}, U] = \sum_x \left\{ \bar{\chi}(x) \left( 1 + 2ia\mu\kappa\gamma_5\tau_3 \right) \chi(x) \right. \]

\[ - \kappa \bar{\chi}(x) \sum_{\mu=1}^{4} \left( U(x, \mu)(r + \gamma_\mu)\chi(x + a\hat{\mu}) \right) \]

\[ + \left. U^\dagger(x - a\hat{\mu}, \mu)(r - \gamma_\mu)\chi(x - a\hat{\mu}) \right\} \]

→ maximal twist: \( \kappa \rightarrow \kappa_{\text{crit}} \)

Frezzotti, Rossi: \( \kappa_{\text{crit}} \) to be known to \( O(a) \)

we take \( \kappa_{\text{crit}} \) from pion mass intercept

Aoki, Bär criticism → talk by S. Aoki

→ talk by A. Shindler
Field rotations and bilinears

field rotations

\[ \psi(x) \equiv e^{i\frac{\omega}{2}\gamma_5\tau_3} \chi(x) = \left( \cos \frac{\omega}{2} + i\gamma_5\tau_3 \sin \frac{\omega}{2} \right) \chi(x) \]

\[ \overline{\psi}(x) \equiv \overline{\chi}(x) e^{i\frac{\omega}{2}\gamma_5\tau_3} = \overline{\chi}(x) \left( \cos \frac{\omega}{2} + i\gamma_5\tau_3 \sin \frac{\omega}{2} \right) \]

bilinears example: axial and vector currents

“physical basis” (unprimed quantities)

“twisted basis” (primed quantities)

\[ A'^{\alpha}_{\mu} = \cos(\omega) A^{\alpha}_{\mu} + \epsilon^{3\alpha\beta} \sin(\omega) V^{\beta}_{\mu}(\alpha = 1, 2) \]

= \[ A^{3}_{\mu}(\alpha = 3) \]

\[ V'^{\alpha}_{\mu} = \cos(\omega) V^{\alpha}_{\mu} + \epsilon^{3\alpha\beta} \sin(\omega) A^{\beta}_{\mu}(\alpha = 1, 2) \]

= \[ V^{3}_{\mu}(\alpha = 3) \]
Scaling test at heavy mass
K.J., A. Shindler, C. Urbach, I. Wetzorke

$D_{\text{crit}} (\kappa_{\text{crit}})$ determined with pure Wilson fermions correlation function

$$f_P^\alpha(t) = \sum_x \langle P^\alpha(x) P^\alpha(0) \rangle$$

$$r_0 m_\pi = 1.79 \approx 750 \text{MeV}$$

open circles: twisted mass
open squares: standard Wilson
filled symbols: $O(a)$ improved Wilson
**Pion decay constant**

definition of $F_{PS}$: $\langle 0|A^1_0|PS \rangle = m_{PS}F_{PS}$

twisted basis, at $\omega = \pi/2$, the axial current is related to the vector current

$$\partial_\mu \langle 0|V^2_\mu|PS \rangle = F_{PS}m^2_{PS}.$$

vector ward identity implies $Z_P = Z^{-1}_\mu$

$$F_{PS}m^2_{PS} = \partial_\mu \langle 0|V^2_\mu|PS \rangle = 2\mu_q \langle 0|P^1|PS \rangle$$

For asymptotic Euclidean times, the pseudoscalar correlation function $f^1_P$ assumes the form

$$f^1_P(t) = \frac{|\langle 0|P^1|PS \rangle|^2}{2m_{PS}} \cdot (e^{-m_{PS}t} + e^{-m_{PS}(T-t)}) \quad \text{for } a \ll t \ll T.$$

fitting the pseudo scalar correlation function for large time separation, obtain the pseudoscalar mass and

$$|\langle 0|P^1|PS \rangle|^2 / m_{PS}$$

from which we get $|\langle 0|P^1|PS \rangle|$.
Pion decay constant

scaling result and comparison to O(a) improved Wilson fermions

open symbols: twisted mass

filled symbols: O(a) improved Wilson
twisted mass against overlap fermions: pion mass


here: only one $\beta = 5.85$

⇒ twisted mass simulations can reach quarks masses as small as overlap substantially smaller than $O(a)$-improved Wilson fermions
twisted mass against overlap fermions: pseudoscalar decay constant

\[ F_{\pi} a \]

\[ (M_\pi a)^2 \]

\[ m_q \Lambda_{QCD}^{-1} \gg a^2 \Lambda_{QCD}^2 \]

⇒ competition of Wilson term and twisted mass term

⇒ check continuum limit
PCAC quark masses

\[ m_{\text{PCAC}}^{OV} = \frac{\sum_x \langle \partial_0 A_0^a(x) \, P^a(0) \rangle}{\sum_x \langle P^a(x) P^a(0) \rangle}, \quad m_{\text{PCAC}}^{tm} = \frac{\epsilon^{3ab} \sum_x \langle \partial_0 V_0^b(x) \, P^a(0) \rangle}{\sum_x \langle P^a(x) P^a(0) \rangle} \quad a = 1, 2 \]

\[ \Rightarrow \text{perfectly linear behaviour (¿)} \]
Renormalization constants

compute $m_{\text{PCAC}}/m_{\text{bare}}$

overlap data

twisted mass data
twisted mass against overlap fermions: $m_\rho$ and baryon masses

- for too small $(m_\pi a)$:
  - signal noisy
  - difficult to extract ground state
Cost comparison

- testing different solvers
  CG, MR, CGS, GMRES, SUMR

- testing pion masses $m_\pi = 720\text{MeV}$, $m_\pi = 390\text{MeV}$ and $m_\pi = 250\text{MeV}$
  also one larger mass

- lattices $12^4, 16^4$

- variety of algorithmic improvements
  - adaptive precision
  - chiral projection
  - eigenvalue deflation
  - multiple mass solver

- missing: preconditioning (running)

- tested also eigenvalue computation
Best algorithm for overlap fermions

12^4, m_{ov} = 0.10
12^4, m_{ov} = 0.03
16^4, m_{ov} = 0.10
16^4, m_{ov} = 0.03
Best algorithm for twisted mass fermions

\[
\begin{array}{c}
12^4, \mu = 0.0125 \\
12^4, \mu = 0.042 \\
16^4, \mu = 0.0125 \\
16^4, \mu = 0.042
\end{array}
\]
Timings as function of quark mass

Timings for the inversion of the overlap operator
$16^4$ lattice, $\beta=5.85$, $s=0.6$, 40 $Q^2$ eigenvectors projected, on JUMP

Inversion timings for TM
$16^4$ lattice, $\beta=5.85$
### Cost comparison

<table>
<thead>
<tr>
<th>$V, m_\pi$</th>
<th>Overlap</th>
<th>TM</th>
<th>rel. factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>$12^4, 720\text{MeV}$</td>
<td>48.8(6)</td>
<td>2.6(1)</td>
<td>18.8</td>
</tr>
<tr>
<td>$12^4, 390\text{MeV}$</td>
<td>142(2)</td>
<td>4.0(1)</td>
<td>35.4</td>
</tr>
<tr>
<td>$16^4, 720\text{MeV}$</td>
<td>225(2)</td>
<td>9.0(2)</td>
<td>25.0</td>
</tr>
<tr>
<td>$16^4, 390\text{MeV}$</td>
<td>653(6)</td>
<td>17.5(6)</td>
<td>37.3</td>
</tr>
<tr>
<td>$16^4, 250\text{MeV}$</td>
<td>1949(22)</td>
<td>22.1(8)</td>
<td>88.6</td>
</tr>
</tbody>
</table>

*Best absolute timings in seconds on one node of JUelich MultiProzessor (JUMP)*

IBM p690 Regatta in Juelich

find: Wilson twisted mass fermions are **20-80** cheaper than overlap fermions
Conclusion

★ overlap and Wilson twisted mass fermions

→ $O(a)$-improved

→ safe against exceptionally small eigenvalues
  ⇒ allow for simulations at small quark masses
  - pion mass as small as 230 MeV
  - twisted mass: unexpected behaviour of, e.g., $f_\pi$ at very small quark mass

⇒ conceptual versus practical advantages