Going chiral: overlap versus Wilson twisted mass fermions

Karl Jansen



- 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



- \rightarrow discretization errors
- → chiral symmetry
- \rightarrow computational cost

Discretization Errors \leftrightarrow violation of chiral symmetry

Wilson-Dirac operator

$$D_{\mathrm{W}} = m_{q} + \frac{1}{2}\gamma_{\mu} \left[\nabla_{\mu} + \nabla_{\mu}^{*}\right] - ar_{\frac{1}{2}}\nabla_{\mu}^{*}\nabla_{\mu}$$
$$\nabla_{\mu}\psi(x) = \frac{1}{a} \left[U(x,\mu)\psi(x+a\hat{\mu}) - \psi(x)\right] , \ U = e^{iag_{0}A_{\mu}(x)}$$
$$\nabla_{\mu}^{*}\psi(x) = \frac{1}{a} \left[\psi(x) - U(x-a\hat{\mu},\mu)\psi(x-a\hat{\mu})\right]$$





- \rightarrow two definitions of quark mass
- → large discretization effect linear in the lattice spacing

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 $a \rightarrow 0$ combined fit of Wilson and Clover data 4 lattice spacings at fixed m_{π}^2

chiral extrapolation $m \rightarrow 0$

• linear: $\langle x \rangle_{\overline{\mathrm{MS}}} = 0.263(14)$

• non-linear:
$$\langle x \rangle_{\overline{\mathrm{MS}}} = 0.221^{+10+21}_{-9-13}$$

 \Rightarrow no data in interesting region of pion mass





in addition to natural slowing down as $m_\pi \to 0$ • very small eigenvalues

- slow down algorithms
- spoil signal

 \rightarrow problem appears for Wilson fermions

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

(staggered fermions: size of systematic error)

solution: Ginsparg-Wilson relation

$$\gamma_5 D + D\gamma_5 = 2aD\gamma_5 D$$

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

 D^{-1} anti-commutes with γ_5 at all non-zero distances

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

one solution of GW relation: overlap operator D_{ov} (Neuberger) (alternatives: domain wall fermions and perfect actions)

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

with $A = 1 + s - D_w(m_q = 0)$; s a tunable parameter, 0 < s < 1

Adding a mass term (naive definition)

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

 \rightarrow exact (lattice) chiral symmetry at $m_q=0$

- \rightarrow infrared safe: quark mass m_q \Leftarrow can reach very small quark masses
- \rightarrow O(a)-improved
- computationally very demanding,

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

Nevertheless: exist problems for overlap fermions: ϵ -regime of chiral perturbation theory, complicated operator mixings

Wilson (Frezzotti, Rossi) twisted mass QCD (Frezzotti, Grassi, Sint, Weisz)

equivalent Wilson-Dirac operator

$$D_{\rm W} = m_q e^{i\omega\gamma_5\tau^3} + \frac{\gamma_\mu}{2} \left[\nabla_\mu + \nabla^*_\mu \right] - a_{\overline{2}}^r \nabla^*_\mu \nabla_\mu + M_{\rm cr} \equiv m_q e^{i\omega\gamma_5\tau^3} + D_{\rm crit} + D_{\rm r}$$

 $\omega=0{\rightarrow}$ usual Wilson-Dirac operator

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

under parity, $R_5 = e^{i\omega\gamma_5 au^3}$

- $D_{\rm crit}$ invariant
- $m_q e^{i\omega\gamma_5\tau^3} \to -m_q e^{i\omega\gamma_5\tau^3}$
- $D_{\rm r} \rightarrow -D_{\rm r}$

 $\Rightarrow D_{\mathrm{W}}$ 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

$$\langle \mathcal{O} \rangle |_{(m_q,r)} = \left[\xi(r) + a m_q \eta(r) \right] \langle \mathcal{O} \rangle |_{m_q}^{\text{cont}} + a \chi(r) \left\langle \mathcal{O}' \right\rangle |_{m_q}^{\text{cont}}$$
$$\langle \mathcal{O} \rangle |_{(-m_q,-r)} = \left[\xi(-r) - a m_q \eta(-r) \right] \left\langle \mathcal{O} \right\rangle |_{m_q}^{\text{cont}} + a \chi(-r) \left\langle \mathcal{O}' \right\rangle |_{-m_q}^{\text{cont}}$$

in addition

$$\begin{aligned} \langle \mathcal{O} \rangle \big|_{m_q}^{\text{cont}} &= (-1)^P \left\langle \mathcal{O} \right\rangle \big|_{-m_q}^{\text{cont}} \\ \Rightarrow \quad \xi(r) &= +\xi(-r) \ , \ am_q \eta(r) = -am_q \eta(-r) \ , \ a\chi(r) = -a\chi(-r) \\ \Rightarrow \quad \frac{1}{2} \left[\left\langle \mathcal{O} \right\rangle \big|_{m_q,r} + \left\langle \mathcal{O} \right\rangle \big|_{-m_q,-r} \right] &= \xi(r) \left\langle \mathcal{O} \right\rangle \big|_{m_q}^{\text{cont}} + O(a^2) \end{aligned}$$

 \Rightarrow at $m_q = m_0 - M_{cr} = 0$ the Wilson average is O(a) improved

Wilson twisted mass QCD

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

 \Rightarrow choose $\omega=\pm\pi/2$ and bare quark mass the critical quark mass

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

Examples:

- hadron masses
- matrix elements
- form factors
- decay constants

Hopping paramter representation

$$\begin{split} \chi &\to \frac{\sqrt{2\kappa}}{a^{3/2}} \chi, \quad \bar{\chi} \to \frac{\sqrt{2\kappa}}{a^{3/2}} \bar{\chi}, \quad \kappa = \frac{1}{2am_0 + 8r} \\ S[\chi, \bar{\chi}, U] &= \sum_x \left\{ \overline{\chi}(x) \left(1 + 2ia\mu\kappa\gamma_5\tau_3 \right) \chi(x) \right. \\ &- \kappa \overline{\chi}(x) \sum_{\mu=1}^4 \left(U(x, \mu)(r + \gamma_\mu) \chi(x + a\hat{\mu}) \right. \\ &+ U^{\dagger}(x - a\hat{\mu}, \mu)(r - \gamma_\mu) \chi(x - a\hat{\mu}) \right) \right\} \end{split}$$

 \rightarrow maximal twist: $\kappa \rightarrow \kappa_{\rm crit}$

Frezzotti, Rossi: κ_{crit} to be known to O(a) we take κ_{crit} from pion mass intercept Aoki, Bär criticism \rightarrow talk by S. Aoki \rightarrow 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)

$$A_{\mu}^{\prime \alpha} = \cos(\omega)A_{\mu}^{\alpha} + \epsilon^{3\alpha\beta}\sin(\omega)V_{\mu}^{\beta}(\alpha = 1, 2)$$
$$= A_{\mu}^{3}(\alpha = 3)$$

$$V_{\mu}^{\prime \alpha} = \cos(\omega)V_{\mu}^{\alpha} + \epsilon^{3\alpha\beta}\sin(\omega)A_{\mu}^{\beta}(\alpha = 1, 2)$$
$$= V_{\mu}^{3}(\alpha = 3)$$

Scaling test at heavy mass

K.J., A. Shindler, C. Urbach, I. Wetzorke



open circles: twisted mass open squares: standard Wilson filled symbols: O(a) improved Wilson

Pion decay constant

definition of $F_{\rm PS}$: $\langle 0|A_0^1|PS\rangle = m_{\rm PS}F_{\rm PS}$

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

 $\partial_{\mu} \langle 0 | V_{\mu}^2 | \mathrm{PS} \rangle = F_{\mathrm{PS}} m_{\mathrm{PS}}^2 \; .$

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

$$F_{\rm PS}m_{\rm PS}^2 = \partial_\mu \langle 0|V_\mu^2|{\rm PS}\rangle = 2\mu_q \langle 0|P^1|PS\rangle$$

For asymptotic Euclidean times, the pseudoscalar correlation function f_P^1 assumes the form

$$f_P^1(t) = \frac{|\langle 0|P^1|PS\rangle|^2}{2m_{PS}} \cdot \left(e^{-m_{PS}t} + e^{-m_{PS}(T-t)}\right) , a \ll t \ll T .$$

fitting the pseudo scalar correlation function for large time separation, obtain the pseudoscalar mass and $|\langle 0|P^1|\text{PS}\rangle|^2/m_{\text{PS}}$

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

W. Bietenholz, T. Chiarappa, M. Hasenbusch, K.J., K. Nagai, M. Papinutto,

L. Scorzato, S. Shcheredin, A. Shindler, C. Urbach, U. Wenger, I. Wetzorke

here: only one $\beta = 5.85$



 \Rightarrow twisted mass simulations can reach quarks masses as small as overlap substantially smaller than O(a)-improved Wilson fermions





 \Rightarrow competition of Wilson term and twisted mass term

$$m_q \Lambda_{\rm QCD}^{-1} \gg a^2 \Lambda_{\rm QCD}^2$$

 \Rightarrow check continuum limit

PCAC quark masses

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



 \Rightarrow perfectly linear behaviour (?)

Renormalization constants





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

Cost comparison

T. Chiarappa, K.J., K. Nagai, M. Papinutto, L. Scorzato, A. Shindler, C. Urbach, U. Wenger, I. Wetzorke

- 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





Timings as function of quark mass





Cost comparison

| V, m_{π} | Overlap | ТМ | rel. factor |
|--------------------------|----------|---------|-------------|
| $12^4,720 Mev$ | 48.8(6) | 2.6(1) | 18.8 |
| $12^4,390 \mathrm{Mev}$ | 142(2) | 4.0(1) | 35.4 |
| $16^4,720 \mathrm{Mev}$ | 225(2) | 9.0(2) | 25.0 |
| $16^4, 390 \mathrm{Mev}$ | 653(6) | 17.5(6) | 37.3 |
| $16^4, 250 { m Mev}$ | 1949(22) | 22.1(8) | 88.6 |

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
- \rightarrow O(a)-improved
- \rightarrow safe against exceptionally small eigenvalues \Rightarrow allow for simulations at small quark masses
 - pion mass as small as 230 MeV
 - twisted mass: unexpected behaviour of, e.g., f_{π} at very small quark mass
 - \Rightarrow conceptual versus practical advantages