Improved Chiral Lattice Fermion Actions

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Summary

- Introduction:
  - Lattice Fermions and Chiral symmetry
  - Domain Wall Fermions
  - Overlap
  - “Perfect” Fermions
- The Ginsparg-Wilson relation
- Implementations
- Improvements on the implementation
  - Gauge actions
  - Mobius fermions
  - Continued Fraction
- What is the best thing to do?
- Conclusions and future
Kaplan’s Fermions

Continuum 5D fermions:

\[ 
\bar{\psi}(x, s) + \gamma_5 \partial_5 \psi(x, s) + m(s) \psi(x, s) = 0 
\]

The zero mode:

\[ 
\psi_0 = \phi^\pm(s) u_\pm \quad \gamma_5 u_\pm = \pm u_\pm \quad [\pm \partial_5 + m(s)] \phi^\pm(s) = 0 
\]

and

\[ 
\phi^+(s) = e^{-m |s|} 
\]

is the only normalizable state
Domain Wall Fermions for QCD

Formulate the 5D Wilson fermions with mass $M \neq 0$ in $s \in [1, L_s]$

For $-2 < M < 0$, light chiral modes are bound on the walls. Only one Dirac fermion without doublers remains.

Fermion mass is introduced by explicitly coupling $m_f$ of the walls. [Shamir, Furman & Shamir]
Ward Identity

\[ q(x) = P_L \psi(x, 0) + P_R \psi(x, L_s - 1) \]
\[ \overline{q}(x) = \overline{\psi}(x, L_s - 1) P_L + \overline{\psi}(x, 0) P_R \]
\[ q_{mp}(x) = P_L \psi(x, \frac{L_s}{2} + 1) + P_R \psi(x, \frac{L_s}{2}) \]
\[ \overline{q}_{mp}(x) = \overline{\psi}(x, \frac{L_s}{2}) P_L + \overline{\psi}(x, \frac{L_s}{2} + 1) P_R \]
\[ P_{R/L} = \frac{1}{2} (1 \pm \gamma_5) \]

\[ \Delta_\mu \langle A^a_\mu(x) \mathcal{O} \rangle = 2 m_f \langle J^a_5(x) \mathcal{O} \rangle + 2 \langle J^a_{5q}(x) \mathcal{O} \rangle + i \langle \delta^a_x \mathcal{O} \rangle \]

\[ J^a_5(x) = \overline{q}(x) \tau^a \gamma_5 q(x) \]
\[ J^a_{5q}(x) = \overline{q}_{mp}(x) \tau^a \gamma_5 q_{mp}(x) \]
\[ A^a_\mu(x) = \sum_{s=0}^{L_s-1} \text{sign} \left( s - \frac{L_s - 1}{2} \right) j^a_\mu(x, s) \]

\[ \lim_{L_s \to \infty} \langle J^a_{5q}(x) \mathcal{O} \rangle = 0 \] : Exact chiral symmetry at finite lattice spacing
Overlap Fermions
Narayanan - Neuberger

- Develop Kaplan’s idea
  \[ e^{-S(U)} = \langle 0_- | 0_+ \rangle \]

- Derive the 4D effective action

- The overlap formula
  \[ D_{ov}^0 = \frac{1}{2} + \frac{1}{2} \gamma_5 \varepsilon [\gamma_5 D(M_5)] \]
  \[ D_{0ov}^0 = \frac{1}{2} + \frac{1}{2} \gamma_5 \varepsilon [\gamma_5 D(M_5)] \]
  \[ M_5 < 0 \]

\[ D_{xy}^{Wilson}(M_5) = (4 + M_5) \delta_{x,y} - \frac{1}{2} [(1 - \gamma_\mu) U_\mu(x) \delta_{x+\mu,y} + (1 + \gamma_\mu) U_\mu^\dagger(y) \delta_{x,y+\mu}] \]
Ginsparg-Wilson Relation

Renormalization group transformation:

\[ e^{-S'[\Phi]} = \int D\phi \, e^{-S[\phi]-T[\Phi;\phi]}, \]

The fixed point operator satisfies (massless case):

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

Luscher symmetry:

\[ \delta \psi = \gamma_5 (1 - 2D) \psi \quad \delta \bar{\psi} = \bar{\psi} \gamma_5 \]

- The overlap satisfies the GW relation
- What about the DWF?
Is the GW relation enough?

• Take the overlap formula with $M_5 > 0$

$$D^0_{ov} = \frac{1}{2} + \frac{1}{2}\gamma_5 \varepsilon[\gamma_5 D(M_5)]$$

• It satisfies the GW relation

$$\gamma_5 D + D \gamma_5 = \gamma_5 + \frac{1}{2}\varepsilon[\gamma_5 D(M_5)] + \frac{1}{2}\gamma_5 \varepsilon[\gamma_5 D(M_5)] \gamma_5 = 2 D \gamma_5 D$$

• It does not have chiral modes!
DWF and the GW relation

- DWF are at heart the same as the overlap
- It’s easy to show that
  \[ D_{ov}(m) = \frac{1 + m}{2} + \frac{1 - m}{2} \gamma_5 \mathcal{E}_{Ls}[\gamma_5 D(M_5)] \]
  \[ D(M_5) = \frac{a_5 D^W(M_5)}{2 + a_5 D^W(M_5)} \]
- The physical quark propagator is
  \[ \frac{1}{D_{eff}} \equiv \langle \bar{q}q \rangle = \frac{1}{1 - m} \left( \frac{1}{D_{ov}} - 1 \right) \]
- This is just a particular approximation of the sign function
  \[ \mathcal{E}_{Ls}(x) = \frac{\prod_s^{Ls}(1 + x) - \prod_s^{Ls}(1 - x)}{\prod_s^{Ls}(1 + x) + \prod_s^{Ls}(1 - x)} \]
- The GW relation
  \[ 2\gamma_5 \Delta_L \equiv \frac{1}{2} \left[ 1 - \mathcal{E}_{Ls}^2 \right] = \gamma_5 D_{ov}^0 + D_{ov}^0 \gamma_5 - 2D_{ov}^0 \gamma_5 D_{ov}^0 \]
- The violation is positive for \( L_S \) even
The DWF approximation

\[ \varepsilon_{L_s}(x) = \frac{\prod_{s}^{L_s}(1 + x) - \prod_{s}^{L_s}(1 - x)}{\prod_{s}^{L_s}(1 + x) + \prod_{s}^{L_s}(1 - x)} \]

- No flexibility in the approximation
- Only \( L_s \) can be changed and hope for the best....
Changing the gauge action

- DBW2 gauge action works for quenched (2GeV cutoff)
- Dynamical with 1.7GeV cutoff only a factor of 2 better
Why do we still work with DWF?

- For the overlap it seems there are a lot of tricks one can play (Zolotarev, continued fractions, double pass, Nested iteration prec. etc.)

- The physical picture is compelling for DWF (Axial current)

- The 5D action is local. New algorithms can exploit this feature.

- Dynamical: Easy force computation. (other 5D methods have this feature too)

- Computing the inverse is easier than computing the matrix and then inverting!

- A little flexibility would not hurt!
The Mobius Fermions

\[
D_{dwf}^{(5)} = \begin{bmatrix}
D_+ & -D_+ P_- P_+ 0 0 & \cdots & 0 \\
-D_- P_+ P_- P_+ & D_+ D_- D_+ 0 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
m D_- P_- & m D_- P_+ 0 \cdots & \cdots & -P_+ D_- P_+ \\
\end{bmatrix}
\]

\[
D_+ = 1 + b_5 D_w \\
D_- = 1 - c_5 D_w \\
P_+ = \frac{1 + \gamma_5}{2} \\
P_- = \frac{1 - \gamma_5}{2}
\]
The Mobius overlap

With a little high school algebra we get

\[ \mathcal{P}^{-1} \frac{1}{D_{wf}(m)} D_{wf}(m) \mathcal{P} = \begin{bmatrix}
(1 - m)T^{-L_s/2+1} & 0 & \cdots & 0 \\
\frac{1}{1 - T^{-L_s/2+1}T_{L_s}} & 1 & 0 & \cdots & 0 \\
(1 - m)T^{-L_s/2+2} & 0 & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots \\
(1 - m)T^{-L_s/2} & 0 & \cdots & 1 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
(1 - m)T^{-L_s} & 0 & \cdots & 0 & 1 & \cdots & \ddots \\
\end{bmatrix} \]

\[ \mathcal{P} = \begin{bmatrix}
P_+ & P_+ & \cdots & 0 \\
0 & P_+ & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & P_+ \\
P_+ & 0 & \cdots & P_- \\
\end{bmatrix} \quad L = \begin{bmatrix}
1 & 0 & 0 & \cdots & 0 \\
-T^{-L_s+1}M_+ & 1 & 0 & 0 & \cdots \\
-T^{-L_s+2}M_+ & 0 & 1 & \cdots & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots \\
-T^{-1}M_+ & 0 & \cdots & 0 & 1 \\
\end{bmatrix} \quad M_- = P_- - mP_+ \quad M_+ = P_+ - mP_- \quad T^{-1} = \frac{1 + H_T}{1 - H_T} \quad H_T = \gamma_5D \]

\[ D_{ov}(m) = \frac{1 + m}{2} + \frac{1 - m}{2} \gamma_5 \mathcal{E}_{L_s} [\gamma_5D(M_5)] \]

\[ \varepsilon_{L_s} = \frac{T^{-L_s} - 1}{T^{-L_s} + 1} = \frac{(1 + H_T)^{L_s} - (1 - H_T)^{L_s}}{(1 + H_T)^{L_s} + (1 - H_T)^{L_s}} \]

\[ D = \frac{(b_5 + c_5)}{2 + (b_5 - c_5)} \frac{D_w}{D_w} = \alpha \frac{D_w}{2 + a_5D_w} \]

- Overlap: \( \alpha=2, a_5=0 \) (Borici)
- DWF: \( \alpha=1, a_5=1 \) (Shamir)
What do we gain?

- Keep $a_5$ fixed
- Tune the scale $\alpha$
- Shift the eigenvalues to better fit the approximation window
Ward Identity

\[ q(x) = P_- \psi(x, 0) + P_+ \psi(x, L_s - 1) \]
\[ \bar{q}(x) = \bar{\psi}(x, L_s - 1)D_- P_- + \bar{\psi}(x, 0)D_- P_+ \]
\[ q_{mp}(x) = P_- \psi(x, \frac{L_s}{2} + 1) + P_+ \psi(x, \frac{L_s}{2}) \]
\[ \bar{q}_{mp}(x) = \bar{\psi}(x, \frac{L_s}{2})D_- P_- + \bar{\psi}(x, \frac{L_s}{2} + 1)D_- P_+ \]

\[ \Delta \mu \langle A_{\mu}^a(x) \mathcal{O} \rangle = 2 m_f \langle J_5^a(x) \mathcal{O} \rangle + 2 \langle J_{5q}^a(x) \mathcal{O} \rangle + i \langle \delta_x^a \mathcal{O} \rangle \]

\[ J_5^a(x) = \bar{q}(x) \tau^a \gamma_5 q(x) \]
\[ J_{5q}^a(x) = \bar{q}_{mp}(x) \tau^a \gamma_5 q_{mp}(x) \]

- The axial current is now more complicated
Chiral symmetry breaking

\[ \Delta \mu \langle A^a_\mu(x)\mathcal{O}\rangle = 2 m_f \langle J^a_5(x)\mathcal{O}\rangle + 2\langle J^a_{5q}(x)\mathcal{O}\rangle + i\langle \delta^a_x\mathcal{O}\rangle \]

- The size of \( \langle J^a_{5q}(x)\mathcal{O}\rangle \) measures chiral symmetry breaking
- Let's use for the operator \( \mathcal{O} = J^a_5(0) \)
- Assume at long distances \( J^a_{5q} \sim J^a_5 \)
- The proportionality constant is the residual mass

\[ M_{\text{res}} = \frac{\sum_{x,y}\langle J^a_{5q}(y,t)J^a_5(x,0)\rangle}{\sum_{x,y}\langle J^a_5(y,t)J^a_5(x,0)\rangle} \bigg|_{t \geq t_{\text{min}}} \]
Residual Mass vs time
Residual mass and the GW

\[2\gamma_5 \Delta L \equiv \frac{1}{2} \gamma_5 \left[1 - \varepsilon_{Ls}^2\right] = \gamma_5 D_{ov}^0 + D_{ov}^0 \gamma_5 - 2D_{ov}^0 \gamma_5 D_{ov}^0\]

- The violation of the GW relation is related to the residual mass

\[M_{\text{res}} = \frac{\sum_{x,y} \langle J^a_5(y) J^a_5(x) \rangle}{\sum_{x,y} \langle J^a_5(y) J^a_5(x) \rangle} = \frac{\text{Tr} \Delta L \frac{1}{D_{ov}^\dagger D_{ov}}}{\text{Tr} G_\pi}\]
**Even-odd preconditioning**

\[
Q_{DWF} = \begin{pmatrix}
Q_{ee} & Q_{eo} \\
Q_{oe} & Q_{oo}
\end{pmatrix} = \begin{pmatrix}
Q_{ee} & 0 \\
0 & Q_{oo}
\end{pmatrix} \times \begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix} \times \begin{pmatrix}
1 & 0 \\
0 & 1 - Q_{oo}^{-1} Q_{oe} Q_{ee} Q_{eo}^{-1}
\end{pmatrix} \times \begin{pmatrix}
1 & Q_{ee}^{-1} Q_{eo} \\
0 & 1
\end{pmatrix}
\]

- The mobius extra terms do not allow 5d even-odd preconditioning

For the 4d preconditioning the even-even and odd-odd are non-trivial they do not depend on the gauge fields and can be inverted with few extra flops
Residual Mass: Quenched

- Quenched 2GeV cutoff
- Almost 40% speedup
- Change the scale as we change $L_s$
- Speed up approaches a factor of infinity!
What’s best for Dynamical

with R. Brower, R. Edwards, B. Joo, T. Kennedy, H. Neff and U. Wenger

• Define a metric for efficiency

• Ask: What is the cost for given residual mass

• Tested Mobius and Continued Fraction 5D algorithms

• Use RBC dynamical light mass configurations
  (25cnfs $M_\pi \sim 500\text{MeV}$)

• Open question: How small chiral symmetry can we tolerate?

• We do not have to have exact chiral symmetry to do QCD
Residual Mass: dynamical
Dependence on $L_s$

\[ \Delta m_{\pi} \]

$m_q = 0.0138$

LHPC data on MILC lattices
Checks if \( m_\pi^2 = C(m_q + m_{\text{res}}) \)

\[ m_q = 0.0138 \]

LHPC data on MILC lattices
Mobius and Zolotarev

• An other approximation to the sign function

\[ \varepsilon_{L_s}(x) = \frac{\prod_s^{L_s}(1 + \alpha_s x) - \prod_s^{L_s}(1 - \alpha_s x)}{\prod_s^{L_s}(1 + \alpha_s x) + \prod_s^{L_s}(1 - \alpha_s x)} \]

• The error in the approximation

\[ \frac{1}{4}[1 - \varepsilon_{L_s}^2(x)] = \frac{\prod_s^{L_s}(1 + \alpha_s x) \prod_s^{L_s}(1 - \alpha_s x)}{[\prod_s^{L_s}(1 + \alpha_s x) + \prod_s^{L_s}(1 - \alpha_s x)]^2} \]

• The error is zero for \( x = \pm 1/\alpha_s \)

• Zolotarev: Find \( \alpha_s \) so that the approximation is optimal in a given interval
- Single zeros produce negative error.
- The residual mass is not positive!
- Possibility of exceptional configurations for $m>0$
- The problem can be fixed: Use double zeros
No free lunch theorem

• The Zolotarev Mobius operator is badly conditioned

• The cost of the calculation explodes if any of the $\alpha_s > 5$

• Zolotarev is impractical for Mobius

• We need to find a preconditioner that solves the problem

• We do have some ideas we are exploring....
Improved HMC for DWF

Two objectives:

- Achieve good accuracy of chiral symmetry
  - Increasing $L_s$ also causes acceptance problems
  - HMC scales with $V_{5d}^{4/5}$

- Avoid **critical slowing** down as we approach the chiral limit
  - This seems most important
Current algorithms

What has been done?

- Fleming - Vranas and RBC (old)

\[ \text{det} D_{ov}^{\dagger} D_{ov} = \int d\phi_0 \cdots d\phi_{L_s-1} d\phi_0^{pv} \cdots d\phi_{L_s-1}^{pv} \exp \left( -\phi^{\dagger} P^{\dagger} \frac{1}{D_{dwf}} D_{dwf}^{\dagger} P \phi + \phi^{pv\dagger} P^{\dagger} D_{pv}^{\dagger} D_{pv} P \phi^{pv} \right) \]

- Dawson and RBC (new)

\[ \text{det} D_{ov}^{\dagger} D_{ov} = \int d\phi_0 \cdots d\phi_{L_s-1} \exp \left( -\phi^{\dagger} P^{\dagger} D_{pv}^{\dagger} \frac{1}{D_{dwf}} D_{dwf}^{\dagger} D_{pv} P \phi \right) \]
New HMC algorithms

Try to accelerate the approach to the chiral limit

\[
det[M^\dagger M] = det[M_p^\dagger M_p] \times det \left[ M^\dagger \frac{1}{M_p^\dagger} \frac{1}{M_p} M \right] = \int D\phi D\psi e^{-\phi^\dagger \frac{1}{M_p^\dagger} \frac{1}{M_p} \phi - \psi^\dagger M_p \frac{1}{M^\dagger} \frac{1}{M} M_p \psi}
\]

- Luscher SAP algorithm
- Hasenbusch algorithm
- Hopefully new DWF preconditioners can be found...
Conclusions

- Dynamical chiral fermions with good chiral symmetry require enormous resources

- We need every possible algorithmic trick we can get

**H. Nueberger:** My main message in this paper is that in the context of dynamical fermion simulations there are many alternatives and tricks that have not been yet explored, and it might be a waste to exclusively focus on the most literal numerical implementations of the recent theoretical advances on the topic of chiral symmetry on the lattice.

- We are working on improving HMC and preconditioners for the DWF operators

- Future looks promising!