Chiral Fermions on the Lattice:
A Flatlander’s Ascent into Five Dimensions

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with
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In the flatland
- Lattice formulation of QCD
- On-shell chiral symmetry
- Approximations and representations

Into five dimensions
- Schur complement
- Continued fractions
- Partial fractions
- Cayley transform

The view from above
- Panorama view
- Chiral symmetry breaking
- Numerical studies

Summary
- Conclusions
Quantumchromodynamics is formally described by the Lagrange density:

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

Lattice regularization: discretize Euclidean space-time

- hypercubic $L^4$-lattice with lattice spacing $a$
- derivatives $\Rightarrow$ finite differences
- integrals $\Rightarrow$ sums
- gauge potentials $A_\mu$ in $G_{\mu\nu}$ $\Rightarrow$ link matrices $U_\mu$ (‘"
  “\’
)
QCD on the Lattice II

- Partition function $Z = \int (DUD\bar{\psi}D\psi) \ e^{-S[U;\bar{\psi},\psi]}$
- Integrating out the fermions yields

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

- Mathematically well defined theory
- Non-perturbative, gauge invariant regularisation (low energy physics)
- Continuum limit $\Rightarrow a \rightarrow 0$
  - Poincaré symmetries are restored automatically
  - Naive discretisation of Dirac operator introduces doublers
    $\Rightarrow$ restoration of chiral symmetry requires fine tuning
On-shell chiral symmetry

- It is possible to have chiral symmetry on the lattice without doublers if we only insist that the symmetry holds on shell.
- Such a transformation should be of the form

\[ \psi \rightarrow e^{i\alpha \gamma_5 (1-aD)} \psi; \quad \overline{\psi} \rightarrow \overline{\psi} e^{i\alpha (1-aD)\gamma_5} \]

and the Dirac operator must be invariant:

\[ D \rightarrow e^{i\alpha (1-aD)\gamma_5} D e^{i\alpha \gamma_5 (1-aD)} = D \]

- For an infinitesimal transformation this implies that

\[ (1 - aD)\gamma_5 D + D\gamma_5 (1 - aD) = 0 \]

which is the Ginsparg-Wilson relation

\[ \gamma_5 D + D\gamma_5 = 2aD\gamma_5 D \]
Overlap Dirac operator I

- We can find a solution $D_{GW}$ of the Ginsparg-Wilson relation as follows:
  - Let the lattice Dirac operator be of the form
    \[
    aD_{GW} = \frac{1}{2} (1 + \gamma_5 \hat{\gamma}_5); \quad \hat{\gamma}_5 = \gamma_5; \quad aD_{GW}^\dagger = \gamma_5 aD_{GW} \gamma_5
    \]
    This satisfies the GW relation if $\hat{\gamma}_5^2 = 1$
  - And it must have the correct continuum limit
    \[
    D_{GW} \to \emptyset \Rightarrow \hat{\gamma}_5 = \gamma_5 (2a\emptyset - 1) + O(a^2)
    \]
  - Both conditions are satisfied if we define
    \[
    \hat{\gamma}_5 = \gamma_5 \frac{D - M}{\sqrt{(D - M)^\dagger (D - M)}} = \text{sgn} [\gamma_5 (D - M)]
    \]

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Overlap Dirac operator II

The resulting overlap Dirac operator:

\[ D(H) = \frac{1}{2}(1 + \gamma_5 \text{sgn}[H(-M)]) \]

- has exact zero modes with exact chirality \( \Rightarrow \) index theorem
- no additive mass renormalisation, no mixing

Three different variations:
- Choice of kernel, e.g. \( H = \gamma_5 D_W(-M) \)
- Choice of approximation:
  - polynomial approximations, e.g. Chebyshev
  - rational approximations \( \text{sgn}(H) \approx R_{n,m}(H) = \frac{P_n(H)}{Q_m(H)} \)
- Choice of representation:
  \( \Rightarrow \) continued fraction, partial fraction, Cayley transform
Zolotarev’s Approximation I

By means of Zolotarev’s theorem we have:

\[ \text{sn} \left( \frac{u}{M}, \lambda \right) = \frac{\text{sn}(u, k)}{M} \prod_{r=1}^{\left\lceil \frac{n}{2} \right\rceil} \frac{1 + \frac{\text{sn}^2(u, k)}{c_{2r}}}{1 + \frac{\text{sn}^2(u, k)}{c_{2r-1}}} \]

- \( c_r = \frac{\text{sn}^2(\frac{nK'}{k}, k'^2)}{1 - \text{sn}^2(\frac{nK'}{k}, k'^2)} \)
- \( \xi = \text{sn}(u, k) \) is the Jacobian elliptic function defined by the elliptic integral

\[ u = \int_0^\xi \frac{dt}{\sqrt{(1 - t^2)(1 - k^2 t^2)}}, \quad 0 < k < 1. \]

Setting \( x = k \cdot \text{sn}(u, k) \) we obtain the best uniform rational approximation on \([-1, -k] \cup [k, 1] \):
Zolotarev’s Approximation II

\[ \text{sgn}(x) \simeq R_{n+1,n}(x) = (1 - l) \frac{x^{\left\lfloor \frac{n}{2} \right\rfloor}}{kD} \prod_{r=1}^{\left\lfloor \frac{n}{2} \right\rfloor} \frac{x^2 + k^2 c_{2r}}{x^2 + k^2 c_{2r-1}} \]
Partial Fraction Representation

- Partial fraction decomposition is obtained by matching poles and residues:

\[ \text{sgn}(x) \simeq R_{2n+1,2n}(x) = x \left( c_0 + \sum_{k=1}^{n} \frac{c_k}{x^2 + q_k} \right) \]

- Use a multi-shift linear system solver
- Physics requires inverse of \( D(\mu) \) (propagators, HMC force)
  - Leads to a two level nested linear system solution
- How can this be avoided?
  - Introduce auxiliary fields \( \Rightarrow \) extra dimension
  - Five-dimensional representation of the \( \text{sgn} \)–function
  - Nested Krylov space problem reduces to single 5d Krylov space solution
Consider the block matrix \( \begin{pmatrix} A & B \\ C & D \end{pmatrix} \)

It may be block diagonalised by a LDU decomposition (Gaussian elimination)

\[
\begin{pmatrix} 1 & 0 \\ CA^{-1} & 1 \end{pmatrix} \cdot \begin{pmatrix} A & 0 \\ 0 & D - CA^{-1}B \end{pmatrix} \cdot \begin{pmatrix} 1 & A^{-1}B \\ 0 & 1 \end{pmatrix}
\]

The bottom right block is the **Schur complement**

In particular we have

\[
\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A) \det(D - CA^{-1}B)
\]
Continued fractions I

Consider a five-dimensional matrix of the form

\[
\begin{pmatrix}
A_0 & 1 & 0 & 0 \\
1 & A_1 & 1 & 0 \\
0 & 1 & A_2 & 1 \\
0 & 0 & 1 & A_3 \\
\end{pmatrix}
\]

and its LDU decomposition where \( S_0 = A_0; \quad S_n + \frac{1}{S_{n+1}} = A_n \)

\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
S_0^{-1} & 1 & 0 & 0 \\
0 & S_1^{-1} & 1 & 0 \\
0 & 0 & S_2^{-1} & 1 \\
\end{pmatrix}
\begin{pmatrix}
S_0 & 0 & 0 & 0 \\
0 & S_1 & 0 & 0 \\
0 & 0 & S_2 & 0 \\
0 & 0 & 0 & S_3 \\
\end{pmatrix}
\begin{pmatrix}
1 & S_0^{-1} & 0 & 0 \\
0 & 1 & S_1^{-1} & 0 \\
0 & 0 & 1 & S_2^{-1} \\
0 & 0 & 0 & 1 \\
\end{pmatrix}
\]

The Schur complement of the matrix is the continued fraction

\[
S_3 = A_1 - \frac{1}{S_2} = A_1 - \frac{1}{A_2 - \frac{1}{S_1}} = A_1 - \frac{1}{A_2 - \frac{1}{A_1 - \frac{1}{A_0}}}
\]
Continued fractions II

- We may use this representation to linearise our continued fraction approximation to the sign function:

\[
\text{sgn}_{n-1,n}(H) = k_0 H + \frac{c_1}{c_1 k_1 H + \frac{c_1 c_2}{c_2 k_2 H + \cdots + \frac{c_{n-1} c_n}{c_n k_n H}}} 
\]

as the Schur complement of the five-dimensional matrix

\[
\begin{pmatrix}
  k_0 H & c_1 & 0 & \cdots & 0 \\
  c_1 & -c_1^2 k_1 H & c_1 c_2 & \cdots & 0 \\
  0 & c_1 c_2 & -c_2^2 k_2 H & \cdots & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & 0 & \cdots & c_{n-1} c_n & -c_n^2 k_n H
\end{pmatrix}
\]

- Class of operators related through equivalence transformations parametrised by \( c_i \)’s
Partial fractions

Consider a five-dimensional matrix of the form:

\[
\begin{pmatrix}
A_1 & 1 & 0 & 0 & 1 \\
1 & -B_1 & 0 & 0 & 0 \\
0 & 0 & A_2 & 1 & 1 \\
0 & 0 & 1 & -B_2 & 0 \\
-1 & 0 & -1 & 0 & R
\end{pmatrix}
\]

where \( A_i = \frac{x}{p_i}, B_i = \frac{p_i x}{q_i} \)

Compute its LDU decomposition and find its Schur complement

\[
R + \frac{p_1 x}{x^2 + q_1} + \frac{p_2 x}{x^2 + q_2}
\]

So we can use this representation to linearise the partial fraction approximation to the sgn-function:

\[
\text{sgn}_{n-1,n}(H) = H \sum_{j=1}^{n} \frac{p_j}{H^2 + q_j}
\]
Consider a five-dimensional matrix of the form (transfer matrix form):

\[
\begin{pmatrix}
1 & -A_1 & 0 & 0 \\
0 & 1 & -A_2 & 0 \\
0 & 0 & 1 & -A_3 \\
-A_0 & 0 & 0 & 1
\end{pmatrix}
\]

with its Schur complement \( 1 - A_0A_1A_2A_3 \)

So we can use this representation to linearise the Cayley transform of the approximation to the sgn-function:

\[
\text{sgn}_{n-1,n}(H) = \frac{1 - \prod_{j=1}^{n} T_j(H)}{1 + \prod_{j=1}^{n} T_j(H)}
\]

This is the standard **Domain Wall Fermion** formulation
What do we see . . .

- each representation of the rational function leads to a different five-dimensional Dirac operator
- they all have the same four-dimensional, effective lattice fermion operator
  ⇒ the overlap Dirac operator
- each five-dimensional operator has different symmetry properties
  ⇒ different calculational behaviour
- there is no physical significance to the standard Domain Wall formulation
Chiral symmetry breaking

- Ginsparg-Wilson defect \( \gamma_5 D + D\gamma_5 - 2aD\gamma_5 D = \gamma_5 \Delta \)
  - using the approximate overlap operator
    \( aD = \frac{1}{2}(1 + \gamma_5 R_n(H)) \) it measures chiral symmetry breaking
    \( a\Delta_n = \frac{1}{2}(1 - R_n(H)^2) \)

- The residual quark mass is \( m_{res} = \frac{\langle G^\dagger \Delta_n G \rangle}{\langle G^\dagger G \rangle} \)
  - \( G \) is the \( \pi \) propagator
  - it can be calculated directly in four and five dimensions
  - \( m_{res} \) is just the first moment of \( \Delta_n \)
    - higher moments might be important for other physical quantities
Setup

- We use 15 gauge field backgrounds from dynamical DWF dataset:
  \[ V = 16^3 \times 32, \quad L_s = 8, 12, 16, \quad N_f = 2, \quad \mu = 0.02 \]
- Matched \( \pi \) mass for all representations
- All operators are eve-odd preconditioned
Comparison of Representations

![Graph showing comparison of representations with different symbols representing different modes and parameters.](image-url)
$m_{\text{res}}$ per configuration

![Graph showing $m_{\text{res}}$ per configuration.]
Cost versus $m_{\text{res}}$
Conclusions

- We have a thorough understanding of various five dimensional formulations of chiral fermions
- More freedom and possibilities in 5 dimensions
- Physically they are all the same
- From a computational point of view there are better alternatives than the commonly used Domain Wall Fermions
- Hybrid Monte Carlo simulations: 5 versus 4 dimensional dynamics?