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

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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

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Lattice formulation of QCD On-shell chiral symmetry Approximations and representations

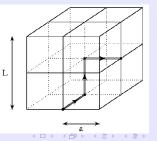
QCD on the Lattice I

Quantumchromodynamics is formally described by the Lagrange density:

$$\mathcal{L}_{ ext{QCD}} = ar{\psi}(i \not\!\!\!\! D - m_q) \psi - rac{1}{4} G_{\mu
u} G^{\mu
u}$$

Lattice regularization: discretize Euclidean space-time

- hypercubic *L*⁴-lattice with lattice spacing *a*
- derivatives \Rightarrow finite differences
- Integrals ⇒ sums
- gauge potentials A_μ in G_{μν} ⇒
 link matrices U_μ (' →→→ ')



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QCD on the Lattice II

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

$$Z = \int (\mathcal{D}U) \det D(U) \mathrm{e}^{-\mathcal{S}_{\mathsf{G}}[U]}$$

- 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
 ⇒ restoration of chiral symmetry requires fine tuning

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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

$$\psi \to \mathbf{e}^{i\alpha\gamma_5(1-aD)}\psi; \quad \overline{\psi} \to \overline{\psi}\mathbf{e}^{i\alpha(1-aD)\gamma_5}$$

and the Dirac operator must be invariant:

$$D
ightarrow e^{ilpha(1-aD)\gamma_5}De^{ilpha\gamma_5(1-aD)}=D$$

For an infinitesimal transformation this implies that

$$(1-aD)\gamma_5D+D\gamma_5(1-aD)=0$$

which is the Ginsparg-Wilson relation

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

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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

$$aD_{GW}=rac{1}{2}(1+\gamma_5\hat{\gamma}_5); \quad \hat{\gamma}_5^\dagger=\hat{\gamma}_5; \quad aD_{GW}^\dagger=\gamma_5aD_{GW}\gamma_5$$

This satisfies the GW relation if $\hat{\gamma}_5^2 = 1$

And it must have the correct continuum limit

$$D_{GW}
ightarrow \hat{\partial} \Rightarrow \hat{\gamma}_5 = \gamma_5 (2a\partial - 1) + O(a^2)$$

• Both conditions are satisfied if we define

$$\hat{\gamma}_5 = \gamma_5 \frac{D-M}{\sqrt{(D-M)^{\dagger}(D-M)}} = \operatorname{sgn}\left[\gamma_5(D-M)\right]$$

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Overlap Dirac operator II

• The resulting overlap Dirac operator:

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

- 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 $sgn(H) \simeq R_{n,m}(H) = \frac{P_n(H)}{Q_m(H)}$
 - Choice of representation:
 - \Rightarrow continued fraction, partial fraction, Cayley transform

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Zolotarev's Approximation I

• By means of Zolotarev's theorem we have:

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

$$\diamond \quad \mathbf{C}_{\mathbf{r}} = \frac{\operatorname{sn}^{2}(\frac{rK'}{n}, k'^{2})}{1 - \operatorname{sn}^{2}(\frac{rK'}{n}, k'^{2})}$$

♦ $\xi = sn(u, k)$ is the Jacobian elliptic function defined by the elliptic integral

$$u = \int_0^{\varepsilon} \frac{dt}{\sqrt{(1 - t^2)(1 - k^2 t^2)}}, \, 0 < k < 1.$$

Setting x = k ⋅ sn(u, k) we obtain the best uniform rational approximation on [-1, -k] ∪ [k, 1]:

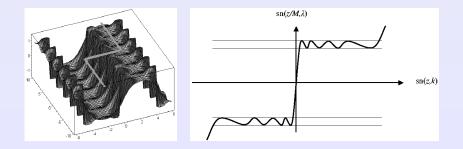
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Zolotarev's Approximation II

$$sgn(x) \simeq R_{n+1,n}(x) = (1-l)\frac{x}{kD}\prod_{r=1}^{\lfloor \frac{n}{2} \rfloor} \frac{x^2 + k^2 c_{2r}}{x^2 + k^2 c_{2r-1}}$$



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Partial Fraction Representation

 Partial fraction decomposition is obtained by matching poles and residues:

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

- 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 ⇒ extra dimension
 - five-dimensional representation of the sgn-function
 - nested Krylov space problem reduces to single 5d Krylov space solution

Schur complement Continued fractions Partial fractions Cayley transform

Schur Complement

- Consider the block matrix $\begin{pmatrix} A & B \\ C & D \end{pmatrix}$
 - It may be block diagonalised by a LDU decomposition (Gaussian elimination)

$$\left(\begin{array}{cc} 1 & 0 \\ CA^{-1} & 1 \end{array}\right) \cdot \left(\begin{array}{cc} A & 0 \\ 0 & D - CA^{-1}B \end{array}\right) \cdot \left(\begin{array}{cc} 1 & A^{-1}B \\ 0 & 1 \end{array}\right)$$

The bottom right block is the <u>Schur complement</u>
In particular we have

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A) \det(D - CA^{-1})$$

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Continued fractions I

Consider a five-dimensional matrix of the form

$$\left(\begin{array}{cccc} A_0 & 1 & 0 & 0 \\ 1 & A_1 & 1 & 0 \\ 0 & 1 & A_2 & 1 \\ 0 & 0 & 1 & A_3 \end{array}\right)$$

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

$$\left(\begin{array}{cccc} 1 & 0 & 0 & 0 \\ S_0^{-1} & 1 & 0 & 0 \\ 0 & S_1^{-1} & 1 & 0 \\ 0 & 0 & S_2^{-1} & 1 \end{array} \right) \left(\begin{array}{cccc} S_0 & 0 & 0 & 0 \\ 0 & S_1 & 0 & 0 \\ 0 & 0 & S_2 & 0 \\ 0 & 0 & 0 & S_3 \end{array} \right) \left(\begin{array}{cccc} 1 & S_0^{-1} & 0 & 0 \\ 0 & 1 & S_1^{-1} & 0 \\ 0 & 0 & 1 & S_2^{-1} \\ 0 & 0 & 0 & 1 \end{array} \right)$$

• The Schur complement of the matrix is the continued fraction $S_3 = A_1 - \frac{1}{S_2} = A_1 - \frac{1}{A_2 - \frac{1}{S_1}} = A_1 - \frac{1}{A_2 - \frac{1}{A_1 - \frac{1}{A_2}}}$

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Continued fractions II

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

$$sgn_{n-1,n}(H) = k_0H + \frac{c_1}{c_1k_1H + \frac{c_1c_2}{c_2k_2H + \cdot \cdot + \frac{c_{n-1}c_n}{c_nk_nH}}}$$

as the Schur complement of the five-dimensional matrix

$$\begin{pmatrix} \mathbf{k}_{0}\mathbf{H} & \mathbf{c}_{1} \\ \mathbf{c}_{1} & -\mathbf{c}_{1}^{2}\mathbf{k}_{1}\mathbf{H} & \mathbf{c}_{1}\mathbf{c}_{2} \\ \mathbf{c}_{1}\mathbf{c}_{2} & \mathbf{c}_{2}^{2}\mathbf{k}_{2}\mathbf{H} \\ & & \ddots & \\ & & & \ddots & \\ & & & \mathbf{c}_{n-1}\mathbf{c}_{n} \\ & & & \mathbf{c}_{n-1}\mathbf{c}_{n} \end{pmatrix}$$

 Class of operators related through equivalence transformations parametrised by c_i's

Schur complement Continued fractions Partial fractions Cayley transform

Partial fractions

Consider a five-dimensional matrix of the form:

$$\left(\begin{array}{ccccc} A_1 & 1 & 0 & 0 & 1 \\ 1 & -B_1 & 0 & 0 & 0 \\ 0 & 0 & A_2 & 1 & 1 \\ 0 & 0 & 1 & -B_2 & 0 \\ -1 & 0 & -1 & 0 & R \end{array}\right)$$

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:

$$sgn_{n-1,n}(H) = H \sum_{j=1}^{n} \frac{p_j}{H^2 + q_j}$$

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Schur complement Continued fractions Partial fractions Cayley transform

Cayley Transform

Consider a five-dimensional matrix of the form (transfer matrix form):

with its Schur complement $1 - A_0 A_1 A_2 A_3$

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

$$\operatorname{sgn}_{n-1,n}(H) = \frac{1 - \prod_{j=1}^{n} T_j(H)}{1 + \prod_{j=1}^{n} T_j(H)}$$

• This is the standard Domain Wall Fermion formulation

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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

 \Rightarrow the overlap Dirac operator

 ...each five-dimensional operator has different symmetry properties

 \Rightarrow different calculational behaviour

• ...there is no physical significance to the standard Domain Wall formulation

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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 π propagator
 - it can be calculated directly in four and five dimensions
- $m_{\rm res}$ is just the first moment of Δ_n
 - higher moments might be important for other physical quantities

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Setup

 We use 15 gauge field backgrounds from dynamical DWF dataset:

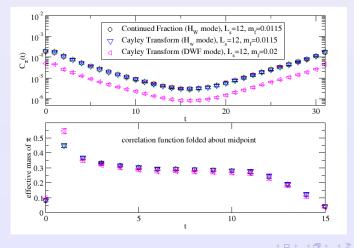
 $V = 16^3 \times 32$, $L_s = 8, 12, 16$, $N_f = 2$, $\mu = 0.02$

- Matched π mass for all representations
- All operators are eve-odd preconditioned

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Comparison of Representations

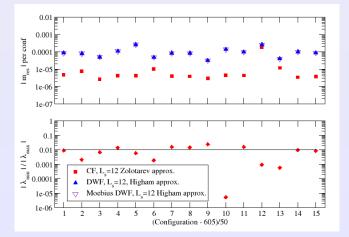


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m_{res} per configuration



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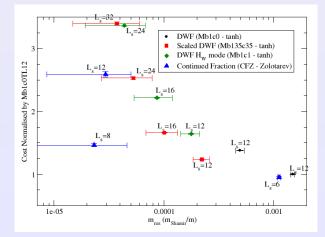
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Cost versus *m*_{res}



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Conclusions

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?

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