Simulating a gauge action from the Overlap Operator with RHMC

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Work with

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Outline

Introduction

Overlap gauge action

RHMC

Test results
Lattice chiral symmetry

Continuum:

\[ \{D, \gamma_5\} = 0 \]

Not possible on lattice without doublers (Nielsen-Ninomiya theorem)
But: exact chiral symmetry with overlap fermions (Neuberger),
Domain wall fermions (Kaplan),...
Ginsparg-Wilson relation

\[ \{\gamma_5, D\} = 2D\gamma_5D \]
Overlap fermions

\[ D_{ov}(m) = 1 + \frac{m}{2\rho} + \left(1 - \frac{m}{2\rho}\right) \gamma_5 \text{sgn} \: H_W \]

with Hermitian Wilson-Dirac operator

\[ H_W = \gamma_5 D_W(-\rho), \: \rho \in (0, 2) \]

Exact chiral \( SU(n) \times SU(n) \times U(1) \) symmetry for \( n \) massless flavours, e.g.

\[ \delta \psi = \hat{\gamma}_5 \tau \psi \]
\[ \delta \bar{\psi} = \bar{\psi} \gamma_5 \tau \]

with \( \hat{\gamma}_5 = \text{sgn} \: H_W \)
$D_{ov} = 1 + \gamma_5 \text{sgn } H_W$

Approximate sgn $x$ by rational function:

\[ \text{sgn}(x) \approx r(x) = x \sum_i \frac{\rho_i}{x^2 + \sigma_i} \]

such that $|\text{sgn}(x) - r(x)| < \epsilon$
for $x \in \text{spec } H_W$

Coefficients $\rho_i, \sigma_i$ known analytically (Zolotarev)

Compute sgn $H_W \psi$ using multi-mass solver
Cost for applying $D_{ov}$ determined by cond $H_W$
Can be improved by

- Projecting out few small eigenvalue/eigenvector pairs
- Using an improved gauge action (Iwasaki, Lüscher-Weisz, DBW2, ...)
- Link smearing (Stout, HYP, ...)

Our approach: Construct gauge action from $D_{ov}$ itself
Gauge action from $D_{ov}$

Classical continuum limit:

$$\text{tr}_{CS} \left( D_{ov}(x, x) - D_{ov}^{\text{free}}(x, x) \right) = b \text{tr} F_{\mu\nu}(x) F_{\mu\nu}(x)$$

with known coefficient $b$

Action:

$$S(U, \psi, \bar{\psi}) = c \text{tr} D_{ov}$$

with

$$c = \frac{1}{2bg^2}$$

Numerical value of $c(g)$:

$$c(g = 1) \approx 30$$
Dynamical overlap fermions

Action:

\[ S(U, \psi, \bar{\psi}) = c \text{tr} D_{ov}(U) + \sum_{i=1}^{n_f} \bar{\psi}_i D_{ov}(U, m) \psi_i \]

Partition function:

\[ Z = \int DUD\bar{\Psi} D\Psi e^{-S(U, \psi, \bar{\psi})} \]
\[ = \int DU e^{-c \text{tr} D_{ov}(U)} (\text{det} D_{ov}(m, U))^{n_f} \]
\[ = \int DU \text{det} O(U) \]

with

\[ O(U) = e^{-cD_{ov}(U)} D_{ov}(m, U)^{n_f} \]

Introducing pseudofermions:

\[ \text{det} O(U) = \int D\phi D\phi^* e^{-(\phi, O(U)^{-1}\phi)} \]
Hybrid Monte Carlo

Hamiltonian: \( H(U, \phi, \pi) = S(U, \phi) + \frac{1}{2}(\pi, \pi) \)

Start with gauge field \( U \)

- **Heatbath initialization:**

  \[
  P(\pi) \sim e^{-\frac{1}{2}(\pi, \pi)} \\
  P(\eta) \sim e^{-(\eta, \eta)}, \quad \phi := O^{1/2} \eta
  \]

- **Molecular dynamics evolution:**
  Integrate Hamiltonian equations numerically, obtain \( U', \pi' \)
  Can use low-precision approximation here

\[
\begin{align*}
\dot{U} &= \pi \\
\dot{\pi} &= -\frac{\partial}{\partial U} S \\
&= - \left( O^{-1} \phi, \frac{\partial O}{\partial U} O^{-1} \phi \right)
\end{align*}
\]
HMC

- Metropolis step:
  Compute $\delta H = H(U', \pi') - H(U, \pi)$
  Accept $U'$ with probability

$$p = \max \left( 1, e^{-\delta H} \right)$$

Need to compute:

- $O(U)^{1/2} \psi$ (in heatbath)
- $O(U)^{-1} \psi$ (in molecular dynamics, Metropolis step)

where

$$O(U) = f(M(U))$$
$$M(U) = D_{ov}(U) \dagger D_{ov}(U)$$
$$f(x) = e^{-\frac{1}{2}cx} \left( (1 - m^2)x + 4m^2 \right)^{nf}$$
Rational HMC

RHMC algorithm (Clark, Kennedy): Approximate \( f(x)^{-1}, f(x)^{1/2} \) by rational functions:

\[
f(x)^{-1} \approx r_i(x) = \sum_i \frac{\alpha_i}{\beta_i + x}
\]

\[
f(x)^{1/2} \approx r_s(x) = \sum_i \frac{\alpha'_i}{\beta'_i + x}
\]

Coefficients \( \alpha_i, \beta_i, \alpha'_i, \beta'_i \): Remez algorithm

Compute \( r(M)\psi \) using multi-shift conjugate gradient

Coefficients \( \beta_i \) not always real

\( \rightarrow \) can use 3-term CG
Problem: condition number of $O$ huge

Coefficients $|\alpha_i|$: 
$(c = 25, d = 11)$

$f(0) = O(1) \rightarrow$ enormous loss of precision

Possible solution (Clark, Kennedy):

$$\det O = \left(\det(O_1^n)\right)^n = \int d\Phi_1 \ldots \int d\Phi_n e^{\sum_i (\phi_i, O^{-1}_n \phi_i)}$$

Coefficients $|\alpha_j|$: 
$(c = 25, d = 11, n = 6)$
RHMC

Pseudofermion heatbath:

\[ \phi_i = \sum_j \frac{\alpha_j'}{M + \beta_j'} \eta_i \]

Molecular dynamics:

\[ \frac{\partial S}{\partial U} = -\sum_{i,j} \alpha_j \left( (M + \beta^*)^{-1} \phi_j, \frac{\partial M}{\partial U} (M + \beta)^{-1} \phi_j \right) \]

Hamiltonian:

\[ H = \sum_{i,j} \left( \phi_i, \frac{\alpha_j}{M + \beta_j} \phi_i \right) + \frac{1}{2} (\pi, \pi) \]
Overlap Derivative

“Inner” derivative: Need to compute

\[
\left( \chi', \frac{\partial}{\partial U} D_{ov} \chi \right) = \left( \chi', \gamma_5 \frac{\partial}{\partial U} \text{sgn} H_W \chi \right)
\]

Derivative of rational approximation (Fodor et al, Cundy):

\[
\text{sgn} x \approx r(x) = x \sum_i \frac{\rho_i}{x^2 + \sigma_i}
\]

\[
\frac{\partial r(H_W)}{\partial U} = \sum_i \rho_i (H_W^2 + \sigma_i)^{-1} \left[ \sigma_i \frac{\partial H_W}{\partial U} - H_W \left( \frac{\partial H_W}{\partial U} \right) H_W \right] (H_W^2 + \sigma_i)^{-1}
\]
Eigenvalue zero crossings

\( D_{ov}(U) \) discontinuous w.r.t. U

Different possibilities to treat discontinuity:

- Ignore it
  Correct algorithm, but no acceptance \( \rightarrow \) inefficient

- Reflection/refraction step (Fodor et al.): Treat derivative exactly

- Use smooth approximation of sign function

If gauge action suppresses rough gauge fields, there should be no crossings anyway \( \rightarrow \) topological charge remains fixed

Ergodicity?
Eigenvalue zero crossings

Our choice: Approximate sign function smoothly during molecular dynamics:

Heatbath/Metropolis
Does not give satisfactory acceptance unless $\tau$ small enough:

$$\tau = 0.01$$

$\tau = 0.001$ for $t > 0.17$
Test results

Simulation parameters:

\[ V = 8^4 \]
\[ \rho = 1.8 \]
\[ am = 0.5 \]
\[ \tau_{MD} = 0.01 \]
\[ c \in \{25, 35, 45\} \]
\[ a = ? \]
Energy conservation violation

\[ \delta H = H(U', \pi') - H(U, \pi) \]

\( c = 35, 45: \)
- \( \delta H \) acceptable for \( \tau = 0.01 \)
- \( \delta H \sim \tau^2 \)

\( c = 25: \)
- \( \delta H \) huge (\( O(10^5) \)) whenever eigenvalue crosses zero
- \( \delta H \approx 1 \) would require very small \( \tau \)
Spectral density

$\rho(H_W)$ spectral density of $H_W$

c $= 35, 45$:
  - Gap around zero

c $= 25$:
  - $\rho(0) > 0$
Simulation of overlap gauge action possible with RHMC... but expensive

Need to find \( c \) corresponding to \( a \approx 0.1 \text{fm} \)

Need better algorithm to treat zero crossings