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

$$\{\gamma_5, D\} = 2D\gamma_5 D$$

Overlap fermions

$$D_{\mathrm{ov}}(m) = 1 + \frac{m}{2\rho} + \left(1 - \frac{m}{2\rho}\right)\gamma_5 \operatorname{sgn} H_W$$

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.

$$\begin{aligned} \delta\psi &= \hat{\gamma}_5 \tau \psi \\ \delta\bar{\psi} &= \bar{\psi}\gamma_5 \tau \end{aligned}$$

with $\hat{\gamma}_5 = \operatorname{sgn} H_W$

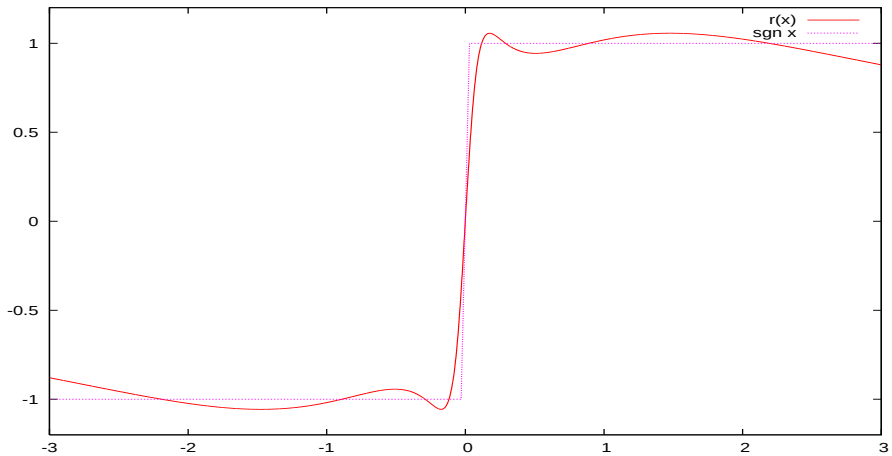
Numerics

$$D_{\mathrm{ov}} = 1 + \gamma_5 \operatorname{sgn} H_W$$

Approximate $\operatorname{sgn} x$ by rational function:

$$\operatorname{sgn}(x) \approx r(x) = x \sum_i \frac{\rho_i}{x^2 + \sigma_i}$$

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



Coefficients ρ_i, σ_i known analytically (Zolotarev)
Compute $\operatorname{sgn} H_W \psi$ 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:

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

with known coefficient b

Action:

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

with

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

Numerical value of $c(g)$:

$$c(g=1) \approx 30$$

Dynamical overlap fermions

Action:

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

Partition function:

$$\begin{aligned} Z &= \int DUD\bar{\Psi}D\Psi e^{-S(U,\Psi,\bar{\Psi})} \\ &= \int DU e^{-c\,\mathrm{tr}\,D_{\mathrm{ov}}(U)} (\det D_{\mathrm{ov}}(m,U))^{n_f} \\ &= \int DU \det O(U) \end{aligned}$$

with

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

Introducing pseudofermions:

$$\det O(U) = \int D\phi D\phi^* e^{-(\phi, O(U)^{-1}\phi)}$$

Hybrid Monte Carlo

Hamiltonian: $H(U, \phi, \pi) = S(U, \phi) + \frac{1}{2}(\pi, \pi)$
Start with gauge field U

- Heatbath initialization:

$$\begin{aligned} P(\pi) &\sim e^{-\frac{1}{2}(\pi,\pi)} \\ P(\eta) \sim e^{-(\eta,\eta)} &, \quad \phi := O^{1/2}\eta \end{aligned}$$

- Molecular dynamics evolution:
  Integrate Hamiltonian equations numerically, obtain U', π'
  Can use low-precision approximation here

$$\begin{aligned} \dot{U} &= \pi \\ \dot{\pi} &= -\frac{\partial}{\partial U} S \\ &= -\left(O^{-1}\phi, \frac{\partial O}{\partial U} O^{-1}\phi \right) \end{aligned}$$

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

$$\begin{aligned} O(U) &= f(M(U)) \\ M(U) &= D_{\mathrm{ov}}(U)^{\dagger} D_{\mathrm{ov}}(U) \\ f(x) &= e^{-\frac{1}{2}cx}\left((1-m^2)x + 4m^2\right)^{n_f} \end{aligned}$$

Rational HMC

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

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

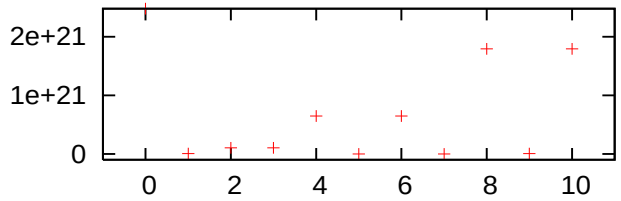
$$f(x)^{1/2} \approx r_s(x) = \sum_i \frac{\alpha'_i}{\beta'_i + x}$$

Coefficients $\alpha_i, \beta_i, \alpha'_i, \beta'_i$: Remez algorithm
Compute $r(M)\psi$ using multi-shift conjugate gradient
Coefficients β_i not always real
$\rightarrow$ can use 3-term CG

RHMC

Problem: condition number of O huge

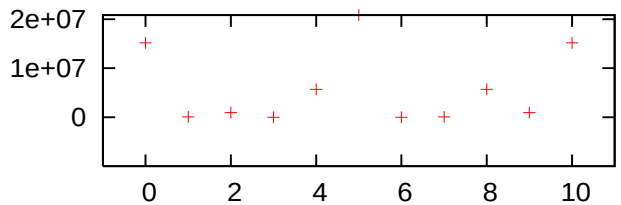
Coefficients $|\alpha_i|$:
$(c = 25, d = 11)$



$f(0) = O(1) \rightarrow$ enormous loss of precision
Possible solution (Clark, Kennedy):

$$\begin{aligned} \det O &= \left(\det(O^{\frac{1}{n}})\right)^n \\ &= \int d\Phi_1 \ldots \int d\Phi_n e^{\sum_i (\phi_i, O^{-\frac{1}{n}} \phi_i)} \end{aligned}$$

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



RHMC

Pseudofermion heatbath:

$$\phi_i = \sum_j \frac{\alpha'_j}{M + \beta'_j} \eta_i$$

Molecular dynamics:

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

Hamiltonian:

$$H = \sum_{i,j} \left(\phi_i, \frac{\alpha_j}{M + \beta_j} \phi_i \right) + \tfrac{1}{2}(\pi, \pi)$$

Overlap Derivative

"Inner" derivative: Need to compute

$$\left(\chi', \frac{\partial}{\partial U} D_{\mathrm{ov}} \chi\right)$$
$$= \left(\chi', \gamma_5 \frac{\partial}{\partial U} \operatorname{sgn} H_W \chi\right)$$

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

$$\operatorname{sgn} x \approx r(x) = x \sum_i \frac{\rho_i}{x^2 + \sigma_i}$$

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

Eigenvalue zero crossings

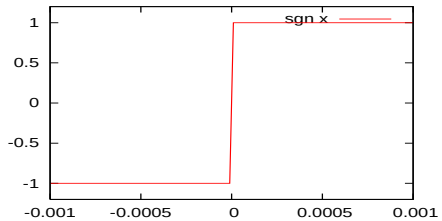
$D_{\mathrm{ov}}(U)$ discontinuous w.r.t. U
Different possibilities to treat discontinuity:

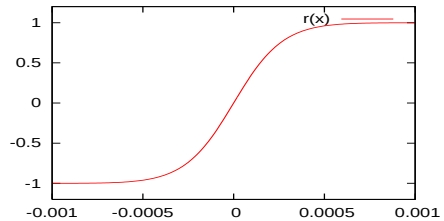
- Ignore it
  Correct algorithm, but no acceptance $\rightarrow$ inefficient
- Reflection/refraction step (Fodor et al.): Treat derivative exactly
- Use smooth approximation of sign function

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:

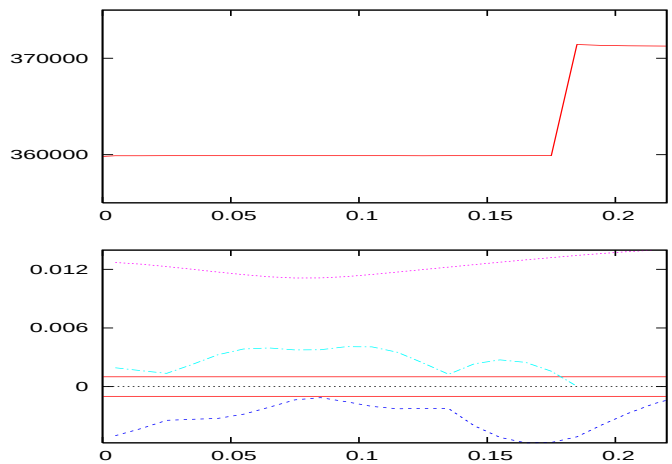


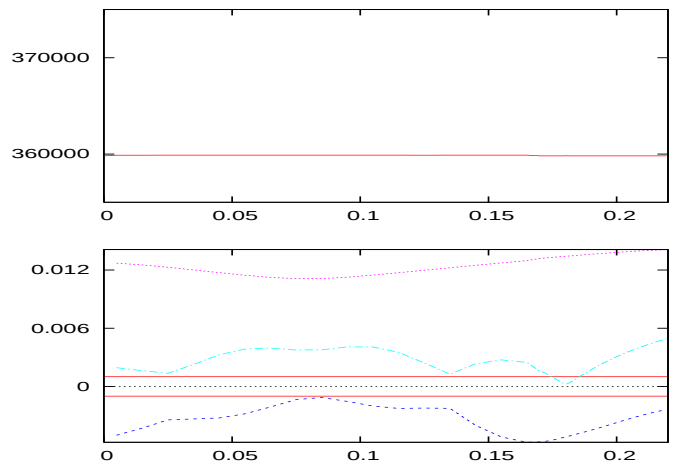


Heatbath/Metropolis

Molecular dynamics

Does not give satisfactory acceptance unless τ small enough:





$\tau = 0.01$

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

Test results

Simulation parameters:

$$
\begin{aligned}
V &= 8^4 \\
\rho &= 1.8 \\
am &= 0.5 \\
\tau_{\mathrm{MD}} &= 0.01 \\
c &\in \{25, 35, 45\} \\
a &= ?
\end{aligned}
$$

Energy conservation violation

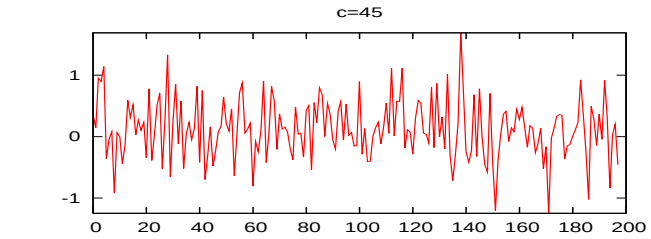
$$\delta H = H(U', \pi') - H(U, \pi)$$

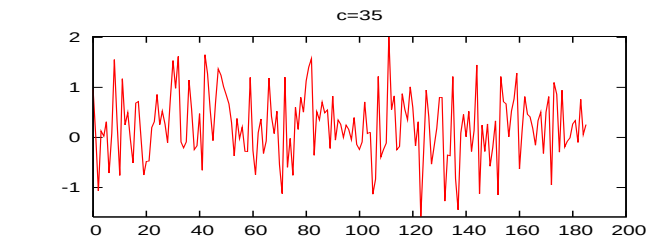
$c = 35, 45$:

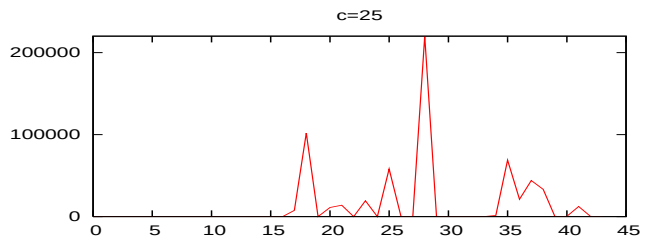
- δH acceptable for $\tau = 0.01$
- $\delta H \sim \tau^2$

$c = 25$:

- δH huge ($O(10^5)$) whenever eigenvalue crosses zero
- $\delta H \approx 1$ would require very small τ







Spectral density

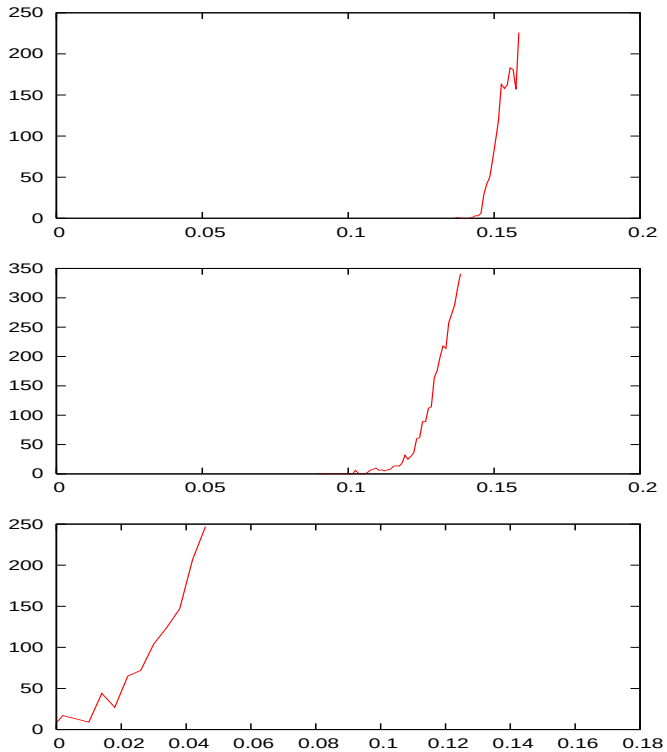
$\rho(H_W)$ spectral density of H_W

$c = 35, 45$:

- Gap around zero

$c = 25$:

- $\rho(0) > 0$



Summary

- Simulation of overlap gauge action possible with RHMC...
- ... but expensive
- Need to find c corresponding to $a \approx 0.1$fm
- Need better algorithm to treat zero crossings