An iterative method to compute the overlap Dirac operator at nonzero chemical potential

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Lattice 2007, Regensburg
Chiral symmetry on the lattice

- Chiral symmetry on the lattice – Ginsparg-Wilson relation:
  \[ \{D, \gamma_5\} = aD\gamma_5D \]

- Neuberger 1998: massless overlap Dirac-operator
  \[ D_{ov} = \mathbb{1} + \gamma_5 \text{sgn}(\gamma_5 D_w) \]

- \( D_{ov} \) satisfies GWR because \( \text{sgn}^2(A) = \mathbb{1} \)

- \( \gamma_5 D_w \) Hermitian: \( \gamma_5 D_{ov} = D_{ov}^\dagger \gamma_5 \) (\( \gamma_5 \)-Hermiticity)

- \( D_{ov} \) has exact zero modes with definite chirality reflecting the topological charge of the gauge configuration
Overlap operator at $\mu \neq 0$

- Replace $D_w$ by $D_w(\mu)$ in overlap definition

$$D_{ov}(\mu) = \mathbb{1} + \gamma_5 \text{sgn}(\gamma_5 D_w(\mu))$$


- Wilson Dirac-operator with quark chemical potential:

$$\left(D_w\right)_{yx}(\mu) = \delta_{yx} - \kappa \sum_{i=1}^{3} \left[ (1+\gamma_i)U_i(x)\delta_{y,x+i} + (1-\gamma_i)U_i^\dagger(x)\delta_{y,x-i} \right]$$

$$- \kappa \left[ e^{\mu} (1+\gamma_4)U_4(x)\delta_{y,x+4} + e^{-\mu} (1-\gamma_4)U_4^\dagger(x)\delta_{y,x-4} \right]$$

Hasenfratz-Karsch 1983, Kogut et al. 1983

- $D_{ov}(\mu)$ requires definition of sign of a non-Hermitian matrix
Function of a matrix

- function of a matrix defined by:

\[ f(A) = \frac{1}{2\pi i} \oint_{\Gamma} dz f(z)(z\mathbb{1} - A)^{-1} \]

where contour \( \Gamma \) encloses eigenvalues of \( A \)

- spectral form using Cauchy’s theorem:

  if \( A \) diagonalizable: \( A = U \text{ diag}\{\lambda_i\} U^{-1} \)

  \[ f(A) = U \text{ diag}\{f(\lambda_i)\} U^{-1} \]

  with \( \lambda_1, \ldots, \lambda_N \): complex eigenvalues

  \( U \in \text{Gl}(N, \mathbb{C}) \): eigenvector matrix

- if \( A \) not diagonalizable:

  extended spectral form derived from Jordan canonical form
Sign function of non-Hermitian matrix

- sign function of a (diagonalizable) non-Hermitian matrix

\[ \text{sgn}(A) = U \text{diag}\{\text{sgn}(\lambda_i)\} U^{-1} \]

J.D. Roberts, Int. J. Control 32 (1980) 677

- eigenvalues \( \lambda_i \) complex
- requires sign of complex number, \( z \in \mathbb{C} \):

\[ \text{sgn}(z) = \frac{z}{\sqrt{z^2}} = \text{sgn}(\text{Re } z) \]

- ensures \( \text{sgn}^2(z) = 1 \)
- gives correct result for \( z \in \mathbb{R} \)

- definition ensures \( \text{sgn}^2(A) = 1 \)
Properties $D_{ov}(\mu)$ of at $\mu \neq 0$

- satisfies Ginsparg-Wilson relation $\rightarrow$ lattice chiral symmetry
- naturally violates $\gamma_5$-Hermiticity
  - spectrum no longer on circle
  - no complex conjugate eigenvalue pairs $(\lambda, \lambda^*)$
- eigenvalue pairs $(\lambda, \frac{\lambda}{\lambda - 1})$, with eigenfunctions $(\psi, \gamma_5 \psi)$
- Anomaly relation and zero modes:
  \[ -\frac{1}{2} \text{tr}(\gamma_5 D_{ov}) = \text{index}(D_{ov}) = \frac{1}{2} \left( n_w^- - n_w^+ \right) \]

  with $n_w^\pm$: # of eigenvalues of $\gamma_5 D_w(\mu)$ with $\text{Re} \lambda \geq 0$
  $\rightarrow$ index of $D_{ov}$ determined by eigenvalues of $\gamma_5 D_w(\mu)$
- $D_{ov}(\mu)$ has exact zero modes with definite chirality: $\gamma_5 \psi = \pm \psi$
- Note:
  - equivalent overlap definition for $\mu = 0$: $D_{ov}(0) = 1 + \frac{D_w(0)}{\sqrt{D_w^\dagger(0)D_w(0)}}$
  - this is not a correct definition at $\mu \neq 0$ as it violates the GWR
Implementation and spectrum $4^4$ lattice

Implementation for small volume using spectral definition:
- full diagonalization of $\gamma_5 D_w(\mu)$ – LAPACK, Goto BLAS for QCDOC
- exact computation of complete sign matrix and overlap matrix $D_{ov}(\mu)$

→ Observation: overlap operator at $\mu \neq 0$ has exact zero modes
Validation of $D_{ov}(\mu)$

- Quenched lattice simulation on $4^4$ lattice ($\beta = 5.1$): microscopic density agrees with predictions of non-Hermitian chiral RMT for $\nu = 0$ and $\nu = 1$ (JB, Wettig - PRL97, 012003 (2006))

- Free fermion energy density has correct continuum limit (Gattringer, Liptak - arXiv:0704.0092 – see talk on Friday)

- Definition of $D_{ov}(\mu)$ consistent with Domain Wall fermions at $\mu \neq 0$ when $L_5 \to \infty$, $a_5 \to 0$
Domain Wall Fermions at $\mu \neq 0$

$$S_{\text{DW}F} = - \sum_{i=1}^{L_s} \left( \bar{\psi}_i A \psi_i - \bar{\psi}_i P_R \psi_{i+1} - \bar{\psi}_i P_L \psi_{i-1} \right)$$

where:

$$A = a_5 D_w(m_w, \mu) + 1$$

with boundary conditions:

$$P_R \psi_{L_s+1} = 0 \quad , \quad P_L \psi_0 = 0$$

i.e. a right handed chiral fermion on the $s = 1$ boundary, a left handed chiral fermion on the $s = L_s$ boundary when $L_s \to \infty$.

Integrating out the fermion fields (à la Edwards, Heller, Boriçi, Neuberger):

$$S_{\text{DW}F} = - \bar{\chi} \left( 1 + \gamma_5 \frac{1 - T^{L_s}}{1 + T^{L_s}} \right) \chi$$
Compute:

\[ \Sigma(\mu) = \frac{1 - T^{Ls}(\mu)}{1 + T^{Ls}(\mu)} \]

with transfer matrix:

\[ T(\mu) = \frac{1 - a_5 H_t(\mu)}{1 + a_5 H_t(\mu)} \]

and

\[ H_t(\mu) = \gamma_5 D_w(\mu)[2 + a_5 D_w(\mu)]^{-1} \]

Spectral decomposition: matrix function defined by function of eigenvalues

\[ \sigma = \frac{1 - \tau^{Ls}}{1 + \tau^{Ls}} \quad \text{with} \quad \tau = \frac{1 - \eta}{1 + \eta} \]

where \( \tau, \eta \in \mathbb{C} \) eigenvalues of \( T \) and \( a_5 H_t(\mu) \).
For $L_s \to \infty$:

$$
\sigma \to \begin{cases} 
1 & \text{if } |\tau| < 1 \\
-1 & \text{if } |\tau| > 1
\end{cases}
$$

Thus:

$$
\lim_{L_s \to \infty} \sigma = \text{sgn}(1 - |\tau|^2) = \text{sgn} \left( 1 - \frac{|1 - \eta|^2}{|1 + \eta|^2} \right) = \text{sgn}(\text{Re}(\eta))
$$

Corresponds to definition of sign of complex number, thus:

$$
\lim_{L_s \to \infty} D_{\text{DWF}}(\mu) = 1 + \gamma_5 \text{sgn}(H_t(\mu))
$$

For $a_5 \to 0$ recover overlap operator at $\mu \neq 0$:

$$
\lim_{a_5 \to 0} \lim_{L_s \to \infty} D_{\text{DWF}}(\mu) = 1 + \gamma_5 \text{sgn}(\gamma_5 D_w(\mu))
$$
Iterative method for sign function

- exact computation of $\text{sgn}(A)$ only possible for small volumes
  - memory requirements (store full matrix)
  - computation time (compute full diagonalization)

- develop iterative method to compute $f(A)b$ for non-Hermitian $A$

- exact result:
  If: polynomial $P_k(z)$ interpolates $f(z)$ at all eigenvalues of $A$
  Then: $P_k(A)b = f(A)b$ for any vector $b$

- approximation method for $y = f(A)b$:
  construct low degree polynomial approximation for $f$ on $\lambda(A)$ wrt $b$
  - depends on spectrum of $A$
  - depends on decomposition of $b$ in eigenvectors of $A$
Arnoldi method for non-Hermitian matrices

- **Krylov subspace**: $K_k(A, b) = \text{span}(b, Ab, A^2b, \ldots, A^{k-1}b)$.
  - contains all vectors resulting from action of arbitrary polynomial of degree $\leq k - 1$ on vector $b$
  - one of these vectors minimizes $\|P_{k-1}(A)b - f(A)b\|$ over all polynomials of degree $\leq k - 1 \rightarrow$ namely, the projection of $f(A)b$ on the Krylov subspace

- **Arnoldi method** uses the recursive scheme

$$AV_k = V_k H_k + \beta_k v_{k+1} e_k^T$$

with

$$V_k^+AV_k = H_k$$

This builds an orthonormal basis $V_k = (v_1, \ldots, v_k)$ in $K_k(A, b)$, where:

- $v_1 = b/|b|$  
- $H_k$ is a $k \times k$ Hessenberg matrix (upper triangular + one subdiagonal)
- eigenvalues of $H_k$ are Ritz values of $A$ w.r.t. $K_k(A, b)$
- $\beta_k$: normalization of $v_{k+1}$, $e_k$ is the $k$-th basis vector in $\mathbb{C}^k$. 

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Iterative method for overlap operator at $\mu \neq 0$
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projection of \( f(A)b \) on \( K_k(A, b) \):

\[
y \approx y_{\text{proj}} = V_k V_k^\dagger f(A) V_k V_k^\dagger b
\]

approximation to \( y_{\text{proj}} \) using \( V_k^\dagger f(A) V_k \approx f(H_k) \) (Ritz approximation)

\[
y_{\text{proj}} \approx \tilde{y} = \beta V_k f(H_k) e_1
\]

- \( \beta = |b| \)
- \( \tilde{y} \in K_k(A, b) \)
- problem reduced to computation of \( f(H_k) \) (\( \dim H_k \ll \dim A \))

\( f(H_k) \) computed exactly with spectral decomposition or suitable approximation method.

For sign function use Roberts’ matrix-iterative method:

\[
S^{n+1} = \frac{1}{2} \left[ S^n + (S^n)^{-1} \right] \quad , \quad \text{with} \quad S^0 = A
\]
Sign function and deflation – Hermitian case

- **Problem**: need large Krylov space if $A$ has small eigenvalues
- **Reason**: in region of $\mathbb{C}$ where $f$ changes rapidly → hard to approximate $f$ by low-degree polynomial
- **Solution**: improve efficiency by using exact value of $f$ for small eigenvalues of $A$
- **Hermitian case**: deflation simple because any # eigenvectors form subspace orthonormal to remaining eigenvectors:

$$f(A)b = UF(\Lambda)U^\dagger b = \sum_{i=1}^{m} f(\lambda_i)(u_i^\dagger \cdot b)u_i + f(A)b_{\perp}$$

- $u_i$ eigenvector corresp. to $\lambda_i$, and $b_{\perp} = b - \sum_{i=1}^{m}(u_i^\dagger \cdot b)u_i$
- Compute eigenvalues and eigenvectors needed for deflation once $\forall b$
- Approximation for $f(A)b_{\perp}$ in space $\perp \text{span}(u_1, \ldots, u_m)$
- Simple decomposition does not work in the non-Hermitian case since eigenvectors of $A$ are not orthonormal → subspaces mix
Non-Hermitian case I: Schur deflation

- construct approximate solution in subspace: 
  \[ \Omega_m + K_k(A, b) \]
- \( \Omega_m \) spanned by eigenvectors belonging to \( m \) critical eigenvalues of \( A \)
- Krylov subspace \( K_k(A, b) \)
- construct partial Schur decomposition for \( m \) critical eigenvalues of \( A \):
  \[ AS_m = S_m T_m \]
  - \( T_m \) is \( m \times m \) upper-triangular with eigenvalues of \( A \) on diagonal
  - orthonormal Schur vectors \( S_m = (s_1, \ldots, s_m) \) span space \( \Omega_m \)
  - \( \Omega_m \) is invariant under \( A \)
- apply modified Arnoldi method:
  \[
  \begin{align*}
  A \begin{pmatrix} S_m & V_k \end{pmatrix} &= \begin{pmatrix} S_m & V_k \end{pmatrix} \begin{pmatrix} T_m & S_m^\dagger AV_k \\ 0 & H_k \end{pmatrix} + \beta_k v_{k+1} e_k^T \\
  Q = \begin{pmatrix} S_m & V_k \end{pmatrix} &\text{ is orthonormal basis of } \Omega_m + K_k(A, b) \\
  v_1 = b_\perp / |b_\perp|, \text{ where } b_\perp = (1 - S_m S_m^\dagger) b &\text{ is projection of } b \text{ onto } \Omega_\perp. \\
  \text{non-Hermiticity } \rightarrow K_k(A, b) &\text{ mixes with } \Omega_m \text{ under operation of } A
  \end{align*}
  \]

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Iterative method for overlap operator at \( \mu \neq 0 \)

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Hessenberg matrix

\[ H = \begin{pmatrix} T_m & S_m AV_k \\ 0 & H_k \end{pmatrix} \]

satisfies

\[ H = Q^\dagger AQ \]

function approximation

\[ y \approx y_{\text{proj}} = QQ^\dagger f(A)QQ^\dagger b \approx Qf(H)Q^\dagger b \]

where

\[ f(H) = \begin{pmatrix} f(T_m) & Y \\ 0 & f(H_k) \end{pmatrix} \]

compute \( f(T_m), f(H_k) \) using suitable method

\( Y \) is solution of the Sylvester equation

\[ T_m Y - Y H_k = f(T_m)X - X f(H_k) \]

with \( X = S_m^\dagger AV_k \), which follows from the identity \( f(H)H = Hf(H) \).

Finally,

\[ f(A)b \approx (S_m \ V_k) \begin{pmatrix} f(T_m) & Y \\ 0 & f(H_k) \end{pmatrix} \begin{pmatrix} S_m^\dagger \\ V_k^\dagger \end{pmatrix} b \]
Non-Hermitian case II: Left-Right deflation

- use left and right eigenvectors belonging to \(m\) critical eigenvectors

\[
AR_m = R_m \Lambda_m
\]

\[
L_m^\dagger A = \Lambda_m L_m^\dagger
\]

- \(\Lambda_m\) is the diagonal eigenvalue matrix for the \(m\) critical eigenvalues
- \(R_m = (r_1, \ldots, r_m)\) is the matrix of right eigenvectors
- \(L_m = (\ell_1, \ldots, \ell_m)\) is the matrix containing the left eigenvectors
- \(L_m^\dagger R_m = I_m\), and \(R_m L_m^\dagger\) is oblique projector on the subspace \(\Omega_m\)

- decompose \(b\) as

\[
b = b_\parallel + b_\Theta
\]

where \(b_\parallel = R_m L_m^\dagger b\) is oblique projection of \(b\) on \(\Omega_m\) and \(b_\Theta = b - b_\parallel\)

\[
f(A)b = f(A)R_m L_m^\dagger b + f(A)b_\Theta
\]
1st term: exact contribution
\[ f(A)R_mL_m^\dagger b = R_m f(\Lambda_m)L_m^\dagger b \]

2nd term: Arnoldi method in the Krylov subspace \( K_k(A, b_\Theta) \)
\[ AV_k = V_kH_k + \beta_k v_{k+1} e_k^T \]

where \( v_1 = b_\Theta / |b_\Theta| \).

\( x_\Theta \): no components along the \( m \) critical eigendirections \( r_i \)
- successive operations of \( A \) yield no contributions along \( r_i \)
- hence \( K_k(A, b_\Theta) \) does not mix with \( \Omega_m \).

Finally,
\[ f(A)b \approx R_m f(\Lambda_m)L_m^\dagger b + \beta V_k f(H_k)e_1 \]

- compute \( f(H_k) \) with suitable method.
  E.g., for sign-function use Robert’s method.
- algorithm only needs first column of \( f(H_k) \)
- algorithm needs both left and right critical eigenvectors
method tested for $4^4$ and $6^4$ lattices

initialization phase: determine right (and left) eigenvectors of $\gamma_5 D_w(\mu)$ corresponding to eigenvalues with smallest magnitude using ARPACK

trade-off between the number of deflated eigenvalues and the size of the Krylov subspace

deflation is essential to reach satisfying efficiency

deflation efficiency grows with increasing lattice volume
Deflation and convergence for $D_{ov}(\mu)b$

$4^4$ lattice (dim=3072)

$6^4$ lattice (dim=15552)

CPU-time – $m = 32$ – LR-deflation

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<tr>
<th>$k$</th>
<th>Arnoldi</th>
<th>$\text{sgn}(H_k)$</th>
<th>total</th>
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<td>0.45</td>
<td>0.20</td>
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<td>400</td>
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<td>1.02</td>
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<tr>
<td>1000</td>
<td>10.84</td>
<td>12.33</td>
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CPU-time – $m = 128$ – LR-deflation

<table>
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<th>$\text{sgn}(H_k)$</th>
<th>total</th>
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<td>1000</td>
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## Summary

- connection between DWF and overlap operator at $\mu \neq 0$
- iterative method to compute $D_{ov}(\mu)b$

## In Progress

- further developments to iterative method (two-sided Lancos, etc)
- nested iteration methods for inversion of $D_{ov}(\mu)$
- unquenching by reweighting for small $\mu$ and comparison with unquenched chiral RMT
- compare individual peaks of spectral densities with latest RMT predictions → project with Gernot Akemann and Leonid Shifrin (see talk Leonid Shifrin on Friday)
- study phase of fermion determinant and compare with RMT (related to sign problem)