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A Method to Calculate Conserved Currents and Fermionic Force for the Lanczos Approximation to the Overlap Dirac Operator

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Introduction

The Overlap operator is defined as

$$D_{ov} := \frac{1}{a}\left(\mathbb{1} + \gamma_5 \text{sign}[\gamma_5 D_W]\right)$$

with the Wilson Dirac operator D_W and the lattice spacing a. It satisfies the Ginsparg-Wilson equation, preserves chiral symmetry in the limit $a \to 0$ and can be defined for finite chemical potential μ [1]. The matrix sign function makes the Overlap operator numerically very expensive and for realistic lattice sizes one usually has to rely on approximation methods.
In many situations we need to compute derivatives of the lattice Dirac operator, for example to compute the fermionic force in HMC simulations or to study conserved currents. To take derivatives of the Overlap operator we need to know how to differentiate the approximation of the sign function, which is often highly non-trivial. We present a method to compute derivatives of the Overlap operator.

The Lanczos Algorithm

An efficient method to approximate the matrix sign function is the nested, two-sided Lanczos algorithm[2]:

- Compute approximation to $\vec{y} = f(\mathbf{A})\vec{x}, \quad \mathbf{A} \in \mathbb{C}^{n\times n}$
- Krylov subspace method: $\mathcal{K}_k(\mathbf{A}, \vec{x}) := \text{span}(\vec{x}, \mathbf{A}\vec{x}, \ldots, \mathbf{A}^{k-1}\vec{x})$
- Works for finite μ, where $\gamma_5 D_W$ is non-hermitian
- Approximate $f(\mathbf{A})$ by a polynomial of degree $k-1$
- Information about $\vec{x}$ taken into account
- Scales like $\mathcal{O}(nk) + \mathcal{O}(k^3)$
- In General: Very good approximation already for $k \ll n$

The Problem

To evaluate the Overlap operator we use the Lanczos algorithm. Therefore we need to know:

How can we compute the derivative of the Lanczos algorithm?

Straight forward algorithmic differentiation turned out to be numerically unstable even for small matrix sizes.

References

[1] J. Bloch and T. Wettig. *Phys. Rev. Lett.*, 97:012003, 2006.

[2] J. Bloch and S. Heybrock. *Comput. Phys. Commun.*, 182:878–889, 2011.

[3] R. Mathias. *SIAM. J. Matrix Anal. & Appl.*, 17:610–620, 1996.

The Solution

Theorem (R. Mathias)[3]

Let $\mathbf{A}(t) \in \mathbb{C}^{n\times n}$ be differentiable at $t = 0$ and assume that the spectrum of $\mathbf{A}(t)$ is contained in an open subset $\mathcal{D} \subset \mathbb{C}$ for all t in some neighbourhood of 0. Let f be $2n-1$ times continuously differentiable on $\mathcal{D}$. We then have:

$$f\left(\begin{bmatrix} \mathbf{A}(0) & \dot{\mathbf{A}}(0) \\ 0 & \mathbf{A}(0) \end{bmatrix}\right) \equiv \begin{bmatrix} f(\mathbf{A}(0)) & \frac{d}{dt}\Big|_{t=0} f(\mathbf{A}(t)) \\ 0 & f(\mathbf{A}(0)) \end{bmatrix}$$

We can simultaneously compute the matrix sign function and its derivative!

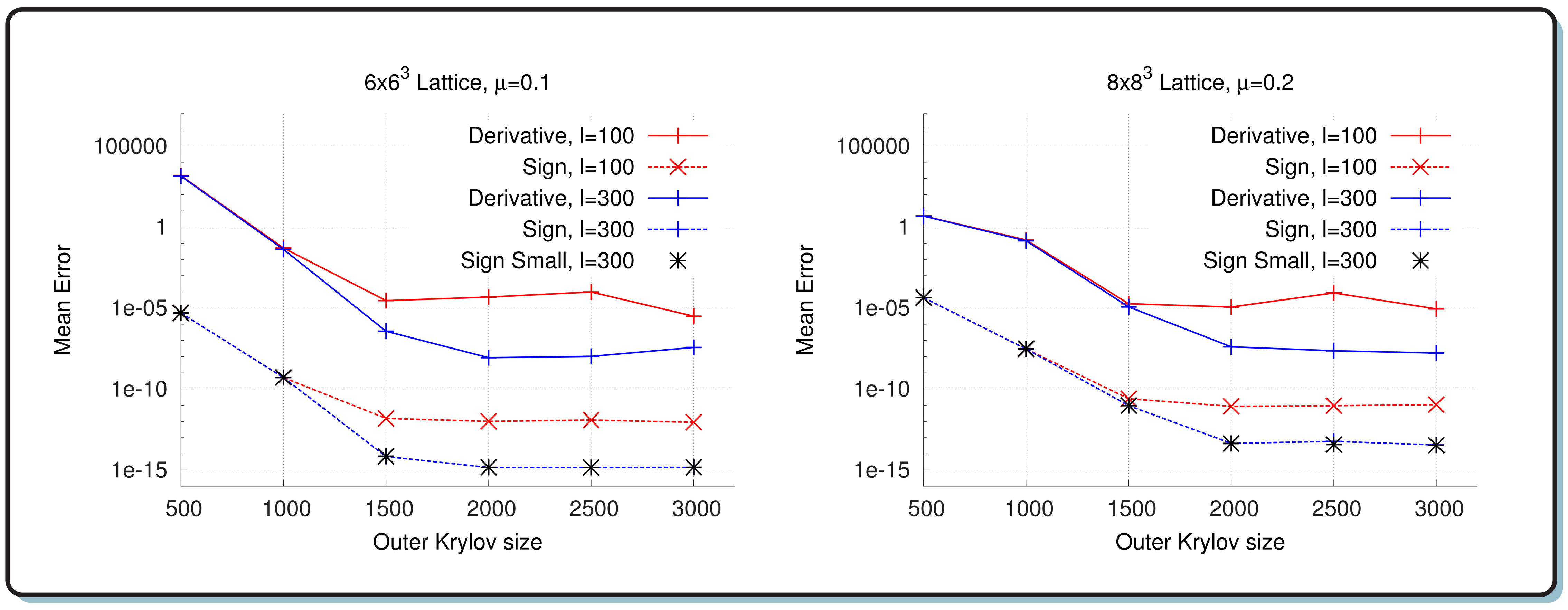
$$\text{sign}\left(\begin{bmatrix} \mathbf{A} & \dot{\mathbf{A}} \\ 0 & \mathbf{A} \end{bmatrix}\right)\begin{pmatrix} 0 \\ \vec{x} \end{pmatrix} = \begin{pmatrix} \frac{d}{dt}\text{sign}(\mathbf{A})\vec{x} \\ \text{sign}(\mathbf{A})\vec{x} \end{pmatrix}$$

Convergence of the Method

The convergence of the Lanczos algorithm depends on the spectrum of the matrix. Therefore it is important to study the properties of $\bar{\mathbf{A}} := \begin{bmatrix} \mathbf{A} & \dot{\mathbf{A}} \\ 0 & \mathbf{A} \end{bmatrix}$.

- $\det \bar{\mathbf{A}} = (\det \mathbf{A})^2$
- λ eigenvalue of $\mathbf{A} \Leftrightarrow \lambda$ eigenvalue of $\bar{\mathbf{A}}$
- $\vec{x}$ eigenvector of $\mathbf{A} \Leftrightarrow \begin{pmatrix} \vec{x} \\ 0 \end{pmatrix}$ eigenvetor of $\bar{\mathbf{A}}$
- Convergence depends only on $\mathbf{A}$

Numerical Results



- SU(3) configurations with improved action
- Compute derivatives with respect to background gauge field $\theta_\mu(x)$
- Matrix size 31104 ($6\text{x}6^3$) and 98304 ($8\text{x}8^3$)
- Finite chemical potential, $\gamma_5 D_W$ is not hermitian
- Nested Lanczos algorithm: Inner Krylov size l fixed, error ploted as function of the outer Krylov subspace size
- Results for simultaneous computation of the sign function and the derivative from the matrix $$\begin{bmatrix} \gamma_5 D_W & \frac{\partial}{\partial\theta_\mu(x)}(\gamma_5 D_W) \\ 0 & \gamma_5 D_W \end{bmatrix}$$
- Results for $\text{sign}(\gamma_5 D_W)$ ("Sign Small") lie on top of the results for the bigger block matrix.
- The Krylov subspace size needed to achieve a given precision does not nearly grow as fast as the matrix size when we go to larger lattices.

Summary and Outlook

- **Summary**
  - We present a method to compute derivatives of the Overlap operator
  - Tests on small lattices
  - First results are very promising
- **Outlook**
  - Generalisation to higher derivatives
  - Implement deflation
  - Calculation of conserved currents