Sign Function Notes

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We describe here some basic theoretical and notational aspects regarding the problem being solved with this code, namely the computation of the sign function as part of the overlap discretization in Lattice QCD, in the presence of a chemical potential.

1 The overlap operator

As described in [1], presented in Eq. (1) therein, the overlap operator takes the following form:

$$D_{ov}(\mu) = 1 + \Gamma_5 \text{sgn}(\Gamma_5 D_w(\mu)). \tag{1}$$

In Eq. 1, the parameter μ is the chemical potential. With $\mu \neq 0$, the operator $\Gamma_5 D_w(\mu)$ is rendered non-Hermitian, contrary to the usual situation of being Hermitian when $\mu = 0$. As mentioned in [1] and explained in [3], the "mass" parameter in the Wilson-Dirac operator i.e. m_w should be set carefully. **Note**: m_w does not correspond to either μ above or the traditional m_0 in the Wilson-Dirac operator, but it is rather a shift in m_0.

In Lattice QCD computations, one wants to typically apply the inverse of $D_{ov}(\mu)$ on some vector w. Solving this linear system will be done by some iterative method, which will imply applying $D_{ov}(\mu)$ in each iteration of said method. Hence, the expensive computation in solving $D_{ov}^{-1}(\mu)w$ is the frequent application of $\text{sgn}(\Gamma_5 D_w(\mu))v$, for some arbitrary vector v. We focus now, then, on obtaining $f(A)b$ with $f = \text{sgn}$ and $A = \Gamma_5 D_w(\mu)$.

2 The sign function in Lattice QCD

The interest here is on computing the sign function on $\Gamma_5 D_w(\mu)$, which can be explicitly written as [3]

$$\text{sgn}(B) = B\left(B^2\right)^{-1/2}, \quad B = \Gamma_5 D_w(\mu). \tag{2}$$

Again, special attention has to be put on the values μ and the mass parameter m_w. Also, it is important to note: $\text{sgn}^2(B) = I$.

3 Preconditioning the square root inverse

The new development, illustrated in part via the code presented here, is the use of polynomial preconditioning in the square root inverse. Let us write this down explicitly in Eq. 2 (we focus on right preconditioning here):

$$\mathrm{sgn}(B) = Bq(B)\left(B^2q^2(B)\right)^{-1/2}, \quad B = \Gamma_5 D_w(\mu), \tag{3}$$

where $q^2(B)$ should approximate well the inverse of B^2, which in turn implies that $q(B)$ should be a polynomial built to approximate well the inverse of $\Gamma_5 D_w(\mu)$. It is well known how to build efficient polynomials for preconditioning when solving a linear system of equations, see e.g. [2].

4 Krylov approximation to Eq. 3

To compute an approximation of the application of the sign function in Eq. 3 to some vector b, we run an Arnoldi on $B^2q^2(B)$, with the first Arnoldi vector being b normalized, leading to the relation

$$V_m^H B^2 q^2(B) V_m = H_m, \tag{4}$$

where it is important to note that H_m comes out of the Arnoldi on $B^2q^2(B)$. Then:

$$\mathrm{sgn}(B)b \approx \|b\|_2 B Z_m (H_m^{-1/2} e_1),\ Z_m = q(B)V_m,\ B = \Gamma_5 D_w(\mu). \tag{5}$$

This last one, Eq. 5, is the version that is implemented in this code.

5 Can we use mixed precision?

In principle, no. The Arnoldi has to be done in double precision, B has to be applied in double precision, and the polynomial has to be applied in double precision.

But, what about the **construction** of $q(D_w(\mu)$? This could be done in single precision, then the Lejas casted to double precision, and the subsequent application done in double precision. We will have a compilation flag that will allow us to choose either single or double precision for the construction of the polynomial.

6 Is Classical Gram-Schmidt good enough if we use high-degree polynomials?

Without polynomial preconditioning, due to the number of Arnoldi vectors being very large, we have to use Modified Gram-Schmidt. But, if the degree of the

polynomial preconditioner is large enough, the number of Arnoldi vectors might then be small enough such that Classical Gram-Schmidt is accurate enough. This could be explored later on via the compilation flag `-DORTH_CGS`.

7 TO-DOs / questions

- check with the lattice group for setting an appropriate value of μ for the 64×32^3 lattice that we will be using here
- check with the lattice group for setting an appropriate value of m_w for the 64×32^3 lattice that we will be using here
- is the usual polynomial construction, described e.g. in [2], appropriate for the "shifted" matrix $\Gamma_5 D_w(\mu)$?

8 References

References

[1] Jacques Bloch, Andreas Frommer, Bruno Lang, and Tilo Wettig. An iterative method to compute the sign function of a non-hermitian matrix and its application to the overlap dirac operator at nonzero chemical potential. *Computer Physics Communications*, 177(12):933–943, 2007.

[2] Jennifer A Loe and Ronald B Morgan. Toward efficient polynomial preconditioning for gmres. *Numerical Linear Algebra with Applications*, 29(4):e2427, 2022.

[3] Artur Strebel. *Advanced Applications For Algebraic Multigrid Methods In Lattice QCD*. PhD thesis, Dissertation, Wuppertal, Bergische Universität, 2020, 2020.