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Deflation and polynomial preconditioning in the application of the overlap operator at nonzero chemical potential

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Solving linear systems is oftentimes the most demanding computation in lattice QCD simulations. The overlap discretization, which allows the implementation of chiral symmetry on the lattice, requires the solution of particularly demanding linear systems. When solving $D_{ov}x = b$ with an iterative method, with D_{ov} the overlap operator, every iteration requires applying the sign function of another operator over some vector, which at nonzero chemical potential takes the form $\text{sign}(Q_\mu)b$, where $Q_\mu = \Gamma_5 D_\mu$, with D_μ the Dirac operator at nonzero chemical potential μ and $Q_\mu^H \neq Q_\mu$.

The evaluation of the application of the sign function over a vector, with a non-Hermitian operator Q_μ , is in general very demanding in both time and memory. We describe here how to substantially reduce both the time and memory required by this sign function evaluation via polynomial preconditioning when using an Arnoldi approximation. For this, a polynomial $q(Q_\mu^2)$ approximating $(Q_\mu^2)^{-1/2}$ is pre-built, followed by the evaluation of the sign function by means of an Arnoldi process on $q^2(Q_\mu^2)Q_\mu^2$. We show the effectiveness of this method via numerical experiments on a realistic configuration.

Furthermore, we describe how deflation can be combined with this form of preconditioning for the same problem of evaluating the sign function in the overlap discretization. In particular, we use LR deflation, and via numerical experiments illustrate the benefits of combining deflation and polynomial preconditioning for the problem at hand.

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