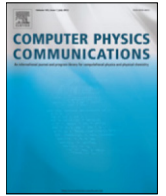




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# A numerical method to compute derivatives of functions of large complex matrices and its application to the overlap Dirac operator at finite chemical potential

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## ABSTRACT

We present a method for the numerical calculation of derivatives of functions of general complex matrices. The method can be used in combination with any algorithm that evaluates or approximates the desired matrix function, in particular with implicit Krylov–Ritz-type approximations. An important use case for the method is the evaluation of the overlap Dirac operator in lattice Quantum Chromodynamics (QCD) at finite chemical potential, which requires the application of the sign function of a non-Hermitian matrix to some source vector. While the sign function of non-Hermitian matrices in practice cannot be efficiently approximated with source-independent polynomials or rational functions, sufficiently good approximating polynomials can still be constructed for each particular source vector. Our method allows for an efficient calculation of the derivatives of such implicit approximations with respect to the gauge field or other external parameters, which is necessary for the calculation of conserved lattice currents or the fermionic force in Hybrid Monte-Carlo or Langevin simulations. We also give an explicit deflation prescription for the case when one knows several eigenvalues and eigenvectors of the matrix being the argument of the differentiated function. We test the method for the two-sided Lanczos approximation of the finite-density overlap Dirac operator on realistic  $SU(3)$  gauge field configurations on lattices with sizes as large as  $14 \times 14^3$  and  $6 \times 18^3$ .

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## 1. Introduction

Over the last decade matrix valued functions of matrices have become an essential tool in a variety of sub-fields of science and engineering [1]. An important application for matrix functions in the field of lattice QCD is the so-called overlap Dirac operator, which is a discretisation of the Dirac operator that respects the properly defined lattice chiral symmetry (Ginsparg–Wilson relations) and is free of doublers. Therefore the overlap Dirac operator is well suited for the non-perturbative study of strongly interacting chiral fermions. At finite chemical potential  $\mu$  the overlap Dirac operator is defined as [2]

$$D_{ov} := \frac{1}{a} (\mathbb{1} + \gamma_5 \operatorname{sgn}[H(\mu)]), \quad (1)$$

where  $H(\mu) := \gamma_5 D_w(\mu)$ ,  $D_w(\mu)$  is the Wilson–Dirac operator at chemical potential  $\mu$ ,  $\operatorname{sgn}$  is the matrix sign function and  $a$  stands for the lattice spacing. An explicit form of  $D_w(\mu)$  is given in Appendix A.

At finite chemical potential  $H$  is a non-Hermitian matrix with complex eigenvalues. Since the size of the linear space on which  $H$  is defined is typically very large ( $n \sim 10^4 \dots 10^7$ ), it is not feasible to evaluate the matrix sign function exactly. While at  $\mu = 0$  one can efficiently approximate the sign function of the Hermitian operator  $H$  by polynomials or rational functions [3–6], at nonzero  $\mu$  the operator  $H$  becomes non-Hermitian and such approximations typically become inefficient. However, having in mind that in practice the sign function  $\operatorname{sgn}[H(\mu)]$  is applied to some source vector, one can still construct an efficient polynomial approximation for each particular source vector by using Krylov subspace methods, such as Krylov–Ritz-type approximations. One of the practical Krylov–Ritz-type

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