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Application of Gauss - Lanczos Algorithm to Determine Low Modes Density of Dirac Operator

Rudina Osmanaj [a1], **Dafina Xhako**[*b2], **Niko Hyka** [c3]

[1]Department of Physics, Faculty of Natural Sciences, University of Tirana, Bvd: "Zog I", Tirana, Albania

[2]Department of Physics Engineering, Faculty of Mathematical Engineering and Physical Engineering,
Polytechnic University of Tirana, Tirana, Albania

[3]Department of Diagnostics, Faculty of Medical Technical Sciences, Medical University of Tirana, Tirana, Albania

[a]rudina.zeqirllari@fshn.edu.al; *[b]dafinaxhako@yahoo.com; [c]nikohyka@gmail.com

ABSTRACT

There are numerous applications in physics, especially in Lattice QCD, where is required to bound entries and the trace of the inverse and the determinant of a large sparse matrix. This paper review one of the most popular methods which are used in lattice QCD to compute the determinant of the lattice Dirac operator: Gaussian integral representation. A modified algorithm can be used for other purposes too, for example for the determination of the density of eigenvalues of the Dirac operator near the origin. This because in Lattice QCD, low-lying Dirac modes are a suitable tool to understand chiral symmetry since they encode the nature of quark propagation as well as the condensate itself in the chiral regime. The formation of a non-zero chiral condensate is an effect of the accumulation of the low modes of the Dirac operator near zero. We review the development in Krylov subspace evaluation of matrix functions and we develop a practical numerical algorithm to achieve a reliable determination of the density of eigenvalues of the Dirac operator near the origin using the Gauss-Lanczos quadrature. We utilize the optimal properties of Krylov subspaces in approximating the distribution of the eigenvalues of the Dirac operator. In this work we have used the Boriçi - Creutz operator to test our method, as an example of using this algorithm in Lattice QCD.

Keywords: algorithm; Boriçi - Creutz operator; eigenvalues; Dirac operator; Gauss-Lanczos quadrature; lattice QCD; numerical simulation.

1. INTRODUCTION

Lattice QCD is a well - established non - perturbative approach to solving the quantum chromodynamics (QCD) theory of quarks and gluons. It is a lattice gauge theory formulated on a grid or lattice of points in space and time. When the size of the lattice is taken infinitely large and its sites infinitesimally close to each other, the continuum QCD is recovered [20]. But the simulation of light fermions on a lattice is always a challenging task. There are several prescriptions to circumvent or minimize the doubling problem

without spoiling the chiral symmetry on the lattice. By the no-go theorem [16], the minimum number of species one can have on a lattice with chiral symmetry is two what is known as a "minimally doubled" fermion.

There are several formulations of minimally doubled fermions, but we will be focused on Boriçi - Creutz (BC) fermions [4], [6]. These fermions share the desirable features of strict locality with traditional discretization, while preserving exact chiral symmetry for a degenerate doublet of quark fields, but breaks the hypercubic symmetry [3]. In order to correct this broken symmetry, can be add non-covariant counter terms through quantum corrections. The renormalization properties of the BC fermions at one loop in the perturbation theory have been investigated in reference [5], [21] and the free Dirac operator for Boriçi - Creutz fermions in momentum space is written as:

$$D_{BC}(\mathrm{p}) = \sum_{\mu}\left[i\gamma_{\mu}\sin(\mathrm{p}_{\mu}) + i\left(\Gamma - \gamma_{\mu}\right)\cos(\mathrm{p}_{\mu})\right] + i\left(c_3 - 2\right)\Gamma, \tag{1}$$

where c_3 is one of the counter terms added in the action by the authors of ref [5], [21], the most relevant term that contributes in the corrected action. The aim of the original study is to restore the broken symmetry by studying the chiral condensate, but in this paper, we will focus on the algorithm we have used in order to perform a part of the study, the Gauss - Lanczos quadrature. [1]

2. THE EFFECTIVE CONDENSATE

The Banks - Casher relation [2] links the spectral density ρ (λ, m) of the Dirac operator to the condensate as:

$$\lim_{\lambda\to 0}\lim_{m\to 0}\lim_{V\to\infty}\rho(\lambda,m) = \frac{\Sigma}{\pi}, \tag{2}$$

where

$$\Sigma = -\lim_{m\to 0}\lim_{V\to\infty}\left\langle\overline{\psi}\psi\right\rangle. \tag{3}$$

Let remember that in a space - time box of volume V with periodic or anti-periodic boundary conditions, the Euclidian massless Dirac operator D in presence of a given gauge field has purely imaginary eigenvalues $i\lambda_1$, $i\lambda_2$...., which may be ordered so that those with the lower magnitude come first. The associated average spectral density is given by:

$$\rho(\lambda,m) = \frac{1}{V}\sum_{k=1}^{\infty}\left\langle\delta\left(\lambda-\lambda_k\right)\right\rangle, \tag{4}$$

where the bracket <…> denotes the QCD (Quantum Chromo Dynamics) expectation value and m the current - quark mass.

The Banks - Casher relation can be read in both directions: a non-zero spectral density implies that the symmetry is broken by a non - vanishing Σ and vice - versa. As we mentioned above, spectral density and low - lying Dirac modes are very important for understanding spontaneous chiral symmetry breaking. Furthermore, the chiral condensate is a useful order parameter to distinguish the phases at T = 0, for minimally doubled

fermions [4], [7], [12], [20], [23-27]. In the continuum theory and for small masses, the mode number can be calculated analytically in chiral perturbation theory. In infinite volume, chiral perturbation theory yields an expansion of the spectral density ρ (λ, m) essentially in powers of λ and m. The leading term is given by the Bank - Casher formula which relates the mode number to the "effective chiral condensate" defined through:

$$\Sigma_{eff} = \frac{\pi}{2}\frac{\nu(\Lambda)}{\Lambda V}, \tag{5}$$

where

$$\Lambda = \sqrt{M^2 - m^2}. \tag{6}$$

So, instead of using spectral density, the average number $\nu(\Lambda)$ of eigenmodes of the massive Hermitian operator $D^{+}D + m^2$ with eigenvalues $\alpha \le M^2$, where M^2 is a chosen cutoff value, seems to be a more convenient quantity to deal with. Since:

$$\nu(\Lambda) = V\int_{-\Lambda}^{\Lambda} \rho(\lambda, m)\, d\lambda, \tag{7}$$

the mode number carries the same information as the spectral density [8], [10], [18], [23-27]. In the presence of a given gauge field, the number of eigen-modes of with eigenvalues can be determined by calculating the eigenvalues and their multiplicities numerically.

Spectral density and low–lying Dirac modes calculation is very important in order to understand the dynamics of spontaneous chiral symmetry breaking. There are several articles and studies on the spectral density of the Dirac operator, such as in references [6], [9], [10]. In these papers the Dirac modes number is calculated by approximating the operator for low-lying modes applying the spectral projector method. While in our work we propose a spectral method for the determination of the spectral density of Dirac operator near the origin using Gauss – Lanczos quadrature and we can show the dynamical spontaneous chiral symmetry breaking using chiral lattice fermions (Boriçi – Creutz fermions).

3. GAUSS - LANCZOS ALGORITHM

In this section, we show an alternative way to count efficiently the mode number and estimate the effective condensate. We utilise the optimal properties of Krylov subspaces in approximating the distribution of the eigenvalues of the Dirac operator. These properties allow us to use the Gauss - Lanczos quadrature in order to estimate the number of modes of the Dirac operator. What we propose is to use Lanczos algorithm in order to produce the tridiagonal and symmetric Lanczos matrix T_n. Its eigenvalues, or the so-called Ritz values, tend to approximate the eigenvalues of the original matrix $A_n = D_n^{\dagger}D$. The eigenvalues and eigenvectors of a symmetric and tridiagonal matrix can be computed by the QR method [1], [11]. In fact, Ritz values are the nodes of the Gauss - Lanczos quadrature with the corresponding weights being the first elements of the Ritz vectors squared. Bai, Fahey and Golub [1] observed that a vector-matrix-vector of the form $\psi^{\dagger} f(A)\psi$ can be expressed as an integral of the function $f(.)$ over a modified spectral measure. An *n*-point Gaussian quadrature approximation to this integral is then given by

$$\psi^{\dagger} f(A)\psi \approx \sum_{i=1}^{n} \omega_i f(\theta_i), \tag{8}$$

where the abscissas, θ_i, of this quadrature rule are given by the Ritz values. These are generated by the Lanczos algorithm applied with seed vector ψ, while the weights ω_i are the squares of the first components of the corresponding eigenvectors of T_n.

So, using Gauss - Lanczos quadrature we calculate the distribution of the eigenvalue's modes, and then we find the low-lying Dirac modes as:

$$\frac{\nu(\Lambda)}{V} = \sum_{i=1}^{k(\Lambda)} \omega(\theta_i), \tag{9}$$

since our function $f(\theta_i)$ is the Heaviside function:

$$f(\theta_i) = \begin{cases} 1 & i \le k(\Lambda) \\ 0 & i > k(\Lambda) \end{cases}. \tag{10}$$

Let $A \in C^{N \times N}$ be a Hermitian matrix and $b \in C^N$ a starting vector. Then the following algorithm computes the Gauss - Lanczos quadrature.

Gauss – Lanczos algorithm

Calculate α_i *dhe* β_i *using Lanczos algorithm for Ax=b*

Define $(T_n)_{i,i} = \alpha_i$, $(T_n)_{i+1,i} = (T_n)_{i,i+1} = \beta_i$, $(T_n)_{i,j} = 0$

Calculate the eigenvalue and eigenvectors of the matrix Tn, where i=1…. n

Sort the eigenvalues and eigenvectors in the increasing order of eigenvalues

Define k as the maximal index s, the maximum index which correspond to the cut-off eigenvalue

Define θ_i *as the positive square root of the original eigenvalue*

Define z_i *as the first elements of the eigenvectors* v_i, *i = 1…n*

Define $\omega_i = z_i^2$

Calculate the mode number $\vartheta_k = \sum_i^k \omega_i$

Let remember that the Lanczos algorithm (C. Lanczos, 1952) is as below: Let be D the Dirac matrix. In many cases in order to find the eigenvalues of a huge matrix, is sufficient to find the eigenvalues of the respective tridiagonal matrix, which eigenvalues are very close to those of the original matrix. Using Lanzcos algorithm, we define the element of the tridiagonal matrix.

Lanczos algorithm

% *Let be* $A = D^* D$ *and* $b = z_2$

% $\beta_0 = 0, \rho_1 = \|b\|_2^{-1}, q_0 = 0, q_1 = \rho_1 b$

for *i =1 .... n* ***do***

$\nu = A q_i$

$\alpha_i = q_i^{\dagger} \nu$

$\nu := \nu - q_i \alpha_i - q_{i-1} \beta_{i-1}$

$\beta_i = \|\nu\|_2$

$$\rho_{i+1} = \frac{\nu}{\beta_i}$$

$$\rho_{i+1} = -\frac{(\rho_i \alpha_i + \rho_{i-1}\beta_{i-1})}{\beta_i}$$

if $\left|\frac{\rho_1}{\rho_{i+1}}\right| < tol$ ***then***

$n = i$

stop

end if

end for

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4. RESULTS

In order to test our method, we have used BC fermions in the quenched approximation for $\beta = 6$ in a 24^4 lattice. For this kind of lattice fermions, the flavor number is $n_f = 2$ and the counter term we have chosen is $c_3 = 0.4$. Using Gauss - Lanczos quadrature we have calculated the mode number for minimally doubled fermions BC, and therefore the effective chiral condensate, in a background of 1000 gauge configurations, generated using the SU(3) theory. The simulations are made using the Hybrid Monte Carlo (HMC) algorithm and for the calculations we have used Lanczos algorithm [13], implemented in FermiQCD, a collection of C++ classes, functions and parallel algorithms for lattice QCD, based on Matrix Distributed Processing [22]. As a condition in order to stop the Lanzcos algorithm we have set that the residue is smaller than the tolerance *tol* = 10^{-3}, because the number of modes of the Dirac operator for 1000 configuration, considering the errors too, doesn't change for different values of the tolerance. This can be seen in the Figure 1, where is presented the number of modes for different tolerances for the minimally doubled fermions Boriçi – Creutz. The results are averaged over 1000 configurations. As expected by the chiral perturbation theory, the low modes of the operator condense and reach a "plateau", as can be seen in the Figure 2.

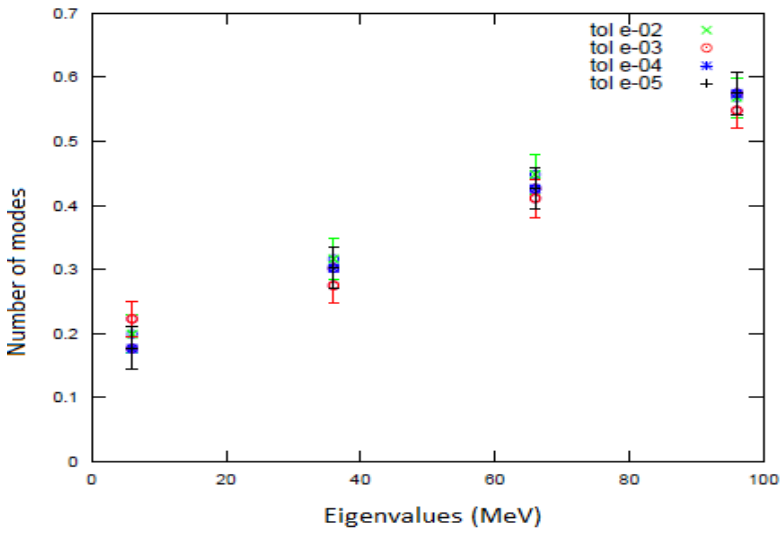

Figure 1. In this figure is presented the number of modes for certain eigenvalues for different tolerances for the minimally doubled fermions Boriçi – Creutz.

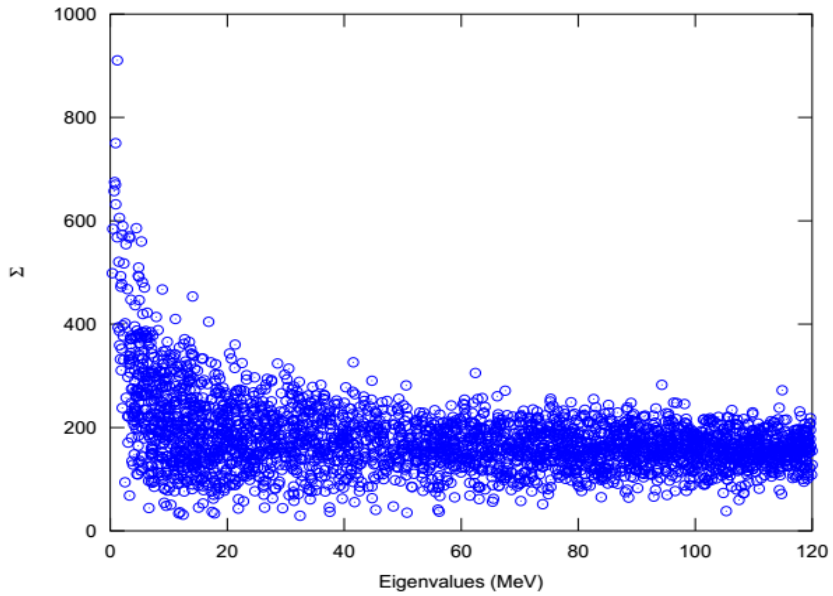

Figure 2. In this figure can be seen clearly the condensation of low modes of the Dirac Operator and the formation of a non-zero effective chiral condensate.

5. CONCLUSIONS

Although In this paper we presented one of the uses of Gauss - Lanczos quadrature in Lattice QCD: the evaluation of the low - lying Dirac modes. The methodology we propose, utilize the optimal properties of Krylov subspaces in approximating the distribution of the eigenvalues of the Dirac operator, not in calculating every eigenvalue of the operator. This is distinct from an earlier method where the integrated spectral density (mode number) was calculated efficiently for some preselected fixed range of integration. This algorithm can be used in Lattice QCD for different scopes, for exploring the phase structure of QCD for example, as was the main aim of our original study. Using this algorithm and the Boriçi - Creutz action with zero quark mass in the quenched approximation we take results that give an "expected" qualitative "behavior" of low-lying modes as predicted by the chiral theory.

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