New approach to the Dirac spectral density in lattice gauge theory applications

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We report tests and results from a new approach to the spectral density and the mode number distribution of the Dirac operator in lattice gauge theories. The algorithm generates the spectral density of the lattice Dirac operator as a continuous function over all scales of the complete eigenvalue spectrum. This is distinct from an earlier method where the integrated spectral density (mode number) was calculated efficiently for some preselected fixed range of the integration. The new algorithm allows global studies like the chiral condensate from the Dirac spectrum at any scale including the cutoff-dependent IR and UV range of the spectrum. Physics applications include the scale-dependent mass anomalous dimension, spectral representation of composite fermion operators, and the crossover transition from the \( \epsilon \)-regime of Random Matrix Theory to the \( p \)-regime in chiral perturbation theory. We present thorough tests of the algorithm in the 2-flavor sextet SU(3) gauge theory that we continue to pursue for its potential as a minimal realization of the composite Higgs scenario.

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1. Introduction and brief history

We introduce a new approach to the Dirac spectral density and mode number distribution in lattice gauge theories. The algorithm effectively generates the spectral density of the lattice Dirac operator as a continuous function over the entire range of the eigenvalue spectrum in large lattice volumes. This is distinct from an earlier method [1] where the integrated spectral density (mode number) was calculated efficiently for some preselected fixed range of the integration and averaged over gauge configurations. Motivated by [1] we set the goal to calculate efficiently the spectral density over the entire Dirac spectrum which can be integrated over any range to generate the mode number distribution on arbitrary scales in a single application to the gauge configuration before the average is taken over the gauge ensemble. Just like the method introduced in [1] for gauge theory applications, our method is also rooted in known applications of the Chebyshev expansion from approximation theory when combined with stochastic evaluation of operator traces in large vector spaces.

We have been developing and testing the reported lattice gauge theory algorithm over the last few years with results appearing in our earlier publications including [2, 3]. Our implementation of the algorithm itself was only presented for the first time in [4] with similar material to the one presented at this conference. We hope to motivate new work by our successful and thorough tests of this new lattice gauge theory application, implemented with staggered lattice fermions in our case. As an example, for extension to other type of lattice fermions, interesting new results were presented at this conference on the chiral condensate of the Dirac operator with domain wall lattice fermions using the same approach [5].

Based on the poster we presented at this conference, we demonstrate the effectiveness of the new algorithm. The plots in this short report are updated from the poster for better illustration of the algorithm and for pedagogical purposes. Section 2 is a brief summary of the method. In Section 3 we present some tests and implementations as applied to the spectral density of the chiral condensate and the mode number distribution. Section 4 is a brief illustration of physics applications where we present our first tests of the GMOR relation and the scale dependent mass anomalous dimension of the chiral condensate in the 2-flavor sextet SU(3) gauge theory that we continue to pursue for its viability as a minimal realization of the composite Higgs scenario. The method we present projects interesting new applications for future studies.

2. Resolution of spectral lines from a stochastic Chebyshev expansion

In [1] the projector operator was used for the determination of the mode number of the Dirac spectrum. A rational approximation to the projector operator was estimated by a Chebyshev polynomial expansion. Here we will approximate the δ-function of the Dirac operator, with its Chebyshev-Jackson polynomial approximation which will determine the moments of the spectral density to a preset high order. Similar methods have been found and referenced for the curious reader in [5] from recent history of approximation theory. Adding to the historical perspective, we note some very early work applying Chebyshev approximation to moments of spectral densities for Hamiltonian spectra [6], curiously with co-authors from the same institutional affiliation as one of us, but from an earlier era. Our method can be viewed as a similar approximation but has
broader scope and general applicability to a large class of Hamiltonian problems with stochastic implementation from the modern computer era.

We will describe the new algorithm for the spectrum of the staggered Dirac operator in a finite lattice volume, but the generalization to the spectrum of a large class of other operators under some general spectral conditions is straightforward. For a finite lattice four-volume $V$, with periodic or antiperiodic boundary conditions for fermions, the euclidean Dirac operator $D$ on any given gauge field configuration has purely imaginary eigenvalues $i\lambda_1, i\lambda_2, \ldots$, with the associated average spectral density $\rho(\lambda, m)$,

$$\rho(\lambda, m) = \frac{1}{N_{\text{eig}}} \sum_{i=1}^{N_{\text{eig}}} \langle \delta(\lambda - \lambda_i) \rangle.$$  \hspace{1cm} (2.1)

In Eq. (2.1) the sum over $N_{\text{eig}}$ individual $\lambda_i$ eigenvalues is averaged over gauge configurations which depend on the bare fermion mass $m$. The spectral density is a renormalizable quantity in gauge theories and the entire function in $\lambda$ can be computed at fixed $m$ on the lattice using the Chebyshev-Jackson expansion we will introduce. It is convenient to consider the mode number $\nu(M, m)$ of the positive definite hermitian operator $D^\dagger D + m^2$ in the integrated form of the spectral density as given by Eq. (2.2),

$$\nu(M, m) = V \int_{-\Lambda}^{\Lambda} d\lambda \rho(\lambda, m), \quad \Lambda = \sqrt{M^2 - m^2}.$$  \hspace{1cm} (2.2)

The important role of the mode number distribution in the analysis of the chiral condensate was emphasized in [1] with a demonstration of its renormalization group invariance $\nu_R(M_R, m_R) = \nu(M, m)$. After rescaling the spectrum of the Dirac operator $D$ and its equivalent $D^\dagger D$ quadratic form, the spectral density $\rho(t)$ depends on scaled eigenvalues $\tilde{\lambda}_i$ with

$$\rho(t) = \frac{1}{N_{\text{eig}}} \sum_{i=1}^{N_{\text{eig}}} \langle \delta(t - \tilde{\lambda}_i) \rangle_{\text{gauge ensemble}}$$  \hspace{1cm} (2.3)

where the variable $t$ is restricted to the [-1,1] interval with rescaled eigenvalues $\tilde{\lambda}_i$ in the [-1,1] interval. The implicit dependence on the bare fermion mass $m$ often will not be shown for convenience. The density function $\rho(t)$ can be expanded into a series of $T_k(t)$ Chebyshev polynomials of the first kind,

$$\rho(t) = \frac{1}{\sqrt{1-t^2}} \sum_{k=0}^{\infty} c_k T_k(t),$$  \hspace{1cm} (2.4)

with Chebyshev expansion coefficients

$$c_k = \begin{cases} \frac{2}{\pi} \int_{-1}^{1} T_k(t) \rho(t) dt & k = 0 \\ \frac{1}{\pi} \int_{-1}^{1} T_k(t) \rho(t) dt & k \neq 0. \end{cases}$$  \hspace{1cm} (2.5)

In practical implementations $D$ will be replaced by the positive definite $D^\dagger D$ operator and the Chebyshev coefficients can be expressed in terms of $D^\dagger D$ eigenvalues,

$$c_k = \begin{cases} \frac{2}{N_{\text{eig}}} \sum_{i=1}^{N_{\text{eig}}} T_k(\tilde{\lambda}_i^2) & k = 0 \\ \frac{1}{N_{\text{eig}}} \sum_{i=1}^{N_{\text{eig}}} T_k(\tilde{\lambda}_i^2) & k \neq 0. \end{cases}$$  \hspace{1cm} (2.6)
Based on Eq. (2.6), the evaluation of the operator traces $\text{Tr}(T_k(D^j D))$ is needed to calculate the spectral density function. We use the well-known stochastic evaluation with $\mathcal{Z}(2)$ noise vectors $\xi$,

$$\text{Tr}(T_k(D^j D)) \approx \frac{1}{N_{\text{noise}}} \sum_{n=1}^{N_{\text{noise}}} \xi_n^T \cdot T_k(D^j D) \cdot \xi_n.$$  

(2.7)

Recursion relations for Chebyshev polynomials of the operators,

$$T_{k+1}(D^j D)) \cdot \xi = 2D^j D \cdot T_k(D^j D) \cdot \xi - T_{k-1}(D^j D) \cdot \xi,$$

$$\xi^{(n)} = T_n(D^j D)) \cdot \xi^{(0)} \Leftrightarrow \xi^{(i+1)} = 2D^j D \cdot \xi^{(i)} - \xi^{(i-1)},$$  

(2.8)

are used in averages over noise vectors $\xi$ in repeated recursions. The series has to be truncated at some finite order which will provide the Dirac $\delta$-function and the Heaviside step function $\Theta$ at finite resolution. Figure 1 shows the spectral resolution of $\delta(\lambda)$ for a spectral line at $\lambda = 0.005$ and $\Theta(t)$ at step $t = 1$ for two different orders of the Chebyshev expansion. On the left panel, the resolution of the spectral function for a sharp $\delta$-function spectral line at $\lambda = 0.005$ is color coded. The width of the finite resolution is scaling with $1/N$ in the order $N$ of the Chebyshev expansion. In red color the resolution of the spectral density at truncation $N = 8000$ from the Chebyshev coefficients of Eq. (2.5) is shown for the sharp $\delta$-function spectral line. The truncation, as the insert of the left panel shows, introduces well-known Gibbs oscillations in the truncated spectral function at finite resolution. The Gibbs oscillations can be damped by the modified Chebyshev-Jackson expansion for the same spectral line at lower resolution consistent with $1/N$ scaling. Color coding on the right panel shows the resolution of the Heaviside step function comparing the Gibbs oscillation and its Jackson damping at the same Chebyshev order.

Figure 1: The left panel shows the sharp $\delta$-function spectral line in finite resolution with $1/N$ scaling and Gibbs oscillations (red insert) damped with Jackson coefficients in the main part of the left panel (red). The right panel shows the finite resolution of the Heaviside step function.
3. Spectral density and Mode number

To illustrate the efficiency of the method, Figure 2 shows results from the calculation of the spectral density and the related mode number distribution on all scales using the Chebyshev-Jackson expansion of Eq. (2.9). The calculation targets here an important BSM gauge theory with a fermion doublet in the two-index symmetric (sextet) representation of the SU(3) BSM color gauge group as reviewed in talks at this conference [8]. The upper left panel of the figure shows the spectral density of the staggered $D^3D$ Dirac operator using ten independent gauge configurations on the lattice volume with size $64^3 \times 96$ at bare gauge coupling set by $\beta = 3.25$ in the lattice action [8] and the fermion mass set at $m = 0.001$. Chebyshev polynomials up to order 8000 were used in the expansion with 20 noise vectors defined in Eq. (2.7). The size of the Jackknife errors in the spectral density is not visible on the scale of the upper left panel of the plot. The upper right panel shows the mode number counting the eigenmodes from the integral of the spectral density. It converges to the correct total count which is half of what is shown in the upper left panel from the implementation.

Figure 2: Tests with a fermion doublet in the two-index symmetric (sextet) representation of the SU(3) BSM color gauge group in the composite figure are discussed in the text. The black data points in the lower left panel come from direct diagonalization which is an important part of the testing procedure. The magenta line of the panel shows the result with $N=8000$ Chebyshev order in perfect match to the direct diagonalization data.
of $D^\dagger D$ on the staggered lattice counting only one of two degenerate eigenvalues of each pair in the spectrum. The lower left panel magnifies the far infrared (IR) scale of the spectral density illustrating the convergence of the Chebyshev-Jackson expansion as the polynomial order is increased. This panel also illustrates that the convergence rate is the slowest in the IR region and reached at polynomial order $N = 8000$ with the magenta line which is practically identical to the lowest blue line at $N = 7000$ even in the lowest eigenvalue range. Bands in the magnified IR part of the plot show the visible Jackknife errors of the spectral density. All tests were made with 20 noise vectors. Data points from the direct diagonalization of $D^\dagger D$ are in excellent agreement with the expansion even in the low IR region. The lower right panel shows the test when the number of noise vectors is varied at fixed expansion order which is kept lower. The results show no bias as a function of the noise vector number and with twenty (or fewer) noise vectors the variance is dominated by the fluctuations over the gauge ensemble. The increased size of the error band simply comes from the larger magnification.

4. Physics applications: GMOR and mass anomalous dimension

Excellent agreement between low eigenvalues from direct diagonalization of $D^\dagger D$ and the full spectral density function from the Chebyshev-Jackson expansion, as shown in Figure 2, provides checks on the GMOR relation for the chiral condensate as discussed in [2, 3]. Chiral perturbation theory of the effective chiral condensate $\Sigma_{\text{eff}}$, aided by the Chebyshev-Jackson expansion was used in our tests of the GMOR relation for added evidence of chiral symmetry breaking in the sextet BSM theory of the composite Higgs. The effective chiral condensate $\Sigma_{\text{eff}}$ was analyzed based on Eq. (4.1) as derived in [9],

$$\frac{\Sigma_{\text{eff}}}{\Sigma} = 1 + \frac{\Sigma}{32\pi^3N_F F^4} \left[ 2N_F^2 |\Lambda| \arctan \frac{|\Lambda|}{m} - 4\pi|\Lambda| - N_F^2 m \log \frac{\Lambda^2 + m^2}{\mu^2} - 4m \log \frac{|\Lambda|}{\mu} \right].$$

Figure 3: Results for the mass anomalous dimension $\gamma(M)$, as defined in the text, are shown for the model with a fermion doublet in the two-index symmetric (sextet) representation of the SU(3) BSM color gauge group. There are results at five different lattice spacings, one of them at exactly zero fermion mass. With the renormalization constants $Z_p$ and $Z_m$ determined in separate calculations, the continuum scale dependent mass anomalous dimension and its role in fermion mass generation is left for a future publication in preparation.
Additional probing of chiral symmetry breaking includes the study of the mass anomalous dimension $\gamma(M)$ as shown in Figure 3. The anomalous dimension of the chiral condensate can be determined from access to the mass anomalous dimension $\gamma(M)$ in the eigenmode function \[ \nu_R(M_R, m_R) = \nu(M, m) \approx \text{const} \cdot M^{4/\gamma(M)} \] (4.2)

The results are reported in Figure 3 with details left for a future publication in preparation.

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