Chiral symmetry breaking, instantons and the ultimate quenched calculation.

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We calculate the spectral density of the Dirac operator over an ensemble of configurations composed of overlapping instantons and anti-instantons. We find evidence that the spectral density diverges in the limit $\lambda \to 0$. This indicates the breaking of chiral symmetry and also provides evidence that quenched QCD may be pathological in nature.

1. Introduction

The reader is referred to [1,2] for background to this field. Preliminary results for this work have been given elsewhere [3].

The QCD Lagrangian for $N_f$ quarks in the chiral limit possesses a large family $SU_L(N_f) \otimes SU_R(N_f) \otimes U_A(1)$ of global symmetries. Phenomenologically we find that the non $U(1)$ part of this symmetry is dynamically broken to the diagonal subgroup, $SU_L(N_f) \otimes SU_R(N_f) \to SU_D(N_f)$. This chiral symmetry breaking ($\chi$SB) overcomes the degeneracy between parity partners (particles with opposite parities but otherwise identical quantum numbers) and gives rise to $N_f^2 - 1$ Goldstone bosons (a role played by the 3 pions for $N_f = 2$). The order parameter for $\chi$SB is given by:

$$\langle \bar{\psi} \psi \rangle = \lim_{m \to 0} i \int_0^\infty \frac{2m \overline{\rho} (\lambda, m)}{\lambda^2 + m^2}$$

where $\overline{\rho} (\lambda, m) = \lim_{V \to \infty} V^{-1} \rho (\lambda)_m$. We note that the spectral density $\overline{\rho} (\lambda, m)$ of the Dirac operator explicitly depends upon the mass $m$ via the fermion determinant. Conventionally the above integral is calculated in the appropriate limits to give

$$\langle \bar{\psi} \psi \rangle = \pi \overline{\rho} (0)$$

This however can break down if the spectral density is not smooth in $m$. To illustrate, $\overline{\rho} = \lambda^{-\alpha}, \alpha \in (0, 1)$ implies $\langle \bar{\psi} \psi \rangle = i \pi m^{-\alpha}$, hence the order parameter diverges in the chiral limit. If however $\overline{\rho} = (m/\lambda)^\alpha$ then we have a perfectly good order parameter in spite of the spectral density diverging in the limit of small eigenvalues. Our first conclusion is therefore that one should use (1) to calculate the chiral condensate at various masses and then extrapolate to the chiral limit. One can however rely on the Banks-Casher relationship (2) for quenched calculations, for here there is no fermion determinant to consider.

2. Calculation of spectral density

We construct an explicit matrix representation of the Dirac operator $i \mathcal{D}[A]$ for a given gauge field $A$ consisting of $n_-$ instantons (I) and $n_+$ anti-instantons ($\overline{I}$) (each object in isolation has gauge field $\overline{A}^\pm$). The matrix is of course defined by $(i \mathcal{D}[A])[j] = D_{kj} (k)$ in terms of some basis $\{|j\rangle\}$. If the basis is orthonormal then $D_{kj} = \langle k | i \mathcal{D}[j] \rangle$. The basis we choose to use is the basis of “would be zero-modes” $\{|\psi^+_0 \rangle, \ldots, |\psi^+_n \rangle, |\psi^-_0 \rangle, \ldots, |\psi^-_n \rangle\}$ where $(i \mathcal{D}[\overline{A}^\pm])[\psi^\pm_k] = 0$. We know that:

$$\langle \psi^+_k | i \mathcal{D}[\psi^+_k] \rangle = 0$$
$$\langle \psi^-_k | i \mathcal{D}[\psi^-_k] \rangle = 0$$
$$\langle \psi^+_k | i \mathcal{D}[\psi^-_j] \rangle = V_{kj} = V(x^+_k, \rho^+_j, x^-_j, \rho^-_j)$$
The first two follow from $\gamma_5|\psi^+_i\rangle = \pm|\psi^-_i\rangle$ and $\{\gamma_5, i\partial\} = 0$. The function $V$ (which is known approximately for a single $I$-$\Gamma$ pair) in the third equation depends upon the center and size of the two instantons. In general it should also depend upon their relative colour orientation but we choose to ignore this, this should be irrelevant as long as there are no non-trivial correlation effects in colour space. In terms of this basis we can construct the $(n_+ + n_-) \times (n_+ + n_-)$ matrix $D \equiv \langle \psi|i\partial|\psi\rangle$ which has block zeroes on the diagonal and $V, V^\dagger$ respectively off block diagonal.

There are two main objections to the matrix $D$ being a matrix representation of the Dirac operator. The first is that the “basis” we have chosen does not span the Hilbert space of wavefunctions. This is not too important for our considerations as wish to study the spectral density at small eigenvalues, these are the eigenvalues which have split from zero due to instanton interactions. The second more fundamental objection is that the “basis” we have chosen is not orthonormal.

$$
\langle \psi^+_i|\psi^+_j\rangle = U(x^+_i, \rho^+_i, x^+_j, \rho^+_j) \\
\langle \psi^-_i|\psi^-_j\rangle = U(x^-_i, \rho^-_i, x^-_j, \rho^-_j) \\
\langle \psi^+_i|\psi^-_j\rangle = 0
$$

hence the matrix $D$ is simply not a representation. We ignore the colour orientation of $U$ for the reason given in the consideration of $V$. The third equation equals zero again due to the $\gamma_5$ structure. We can however construct a new orthonormal basis $\{|\tilde{\psi}^+_i\rangle, |\tilde{\psi}^-_i\rangle\}$ using the standard Gram-Schmidt procedure.

$$
|\psi^+_i\rangle = R_{ij}|\tilde{\psi}^+_i\rangle \quad 1 \leq j \leq i \leq n_+ \\
|\psi^-_i\rangle = S_{ij}|\tilde{\psi}^-_i\rangle \quad 1 \leq j \leq i \leq n_-
$$

We are finally in a position to construct a matrix representation of the Dirac operator:

$$
i\partial \approx \tilde{D} \equiv \langle \tilde{\psi}|i\partial|\tilde{\psi}\rangle
$$

where

$$
\tilde{D}_{ij} = \begin{pmatrix}
0 & \tilde{V} = (R^{-1})^\dagger VS^{-1} \\
\tilde{V}^\dagger & 0
\end{pmatrix}
$$

This matrix representation shares many of the properties of the Dirac operator (as it must).

Firstly the matrix is endowed with a rich structure, the elements are not random. This must be so as vectors in a Hilbert space obey triangle inequalities (a fact which is crucial is attempting to orthogonalize the basis). Secondly, non-zero eigenvalues occur in pairs $\pm \lambda$ hence the matrix satisfies the $\gamma_5$ symmetry. Thirdly the Atiyah-Singer theorem is obeyed, a gauge field configuration with net winding number $Q = |n_- - n_+|$ does indeed have (at least) $Q$ exact zero eigenvalues. Fourthly our representation captures the essence of the mechanism by which eigenvalues are split away from zero. To see this simply consider the case of an $I$-$\Gamma$ pair and notice that if we choose the function $V$ appropriately then we will get the correct eigenvalue splitting. All these properties give us hope that the matrix representation indeed shares the essential qualities of the actual QCD Dirac operator for determining the spectrum at small eigenvalues.

The only other thing to decide is which functions to use for $U$ and $V$? Though these functions are known classically, there is little reason to believe that the classical forms dominate in the QCD vacuum. Pragmatically we use a variety of zero mode wavefunctions in calculating $U$ and $V$ (hard spheres, Gaussian and classical zero mode) and look for qualitative features of the resultant spectral densities which are independent of the functions used. In this talk we simplify and use the same functional form for both $U$ and $V$, we discuss the general case (amongst other things) in a subsequent publication [5], but it suffices to say that the conclusions are unaffected.

3. Results

Figure (1) shows the spectral density per unit volume for $N_f = 0$ (quenched) for two different volumes. The instanton gas is fairly dense, more dense than in the instanton liquid model [2] but less so than found in some recent investigations of the vacuum [4]. We have used the classical zero mode wavefunctions for the overlap integrals. The most noticeable thing about the resultant spectral density is the divergence at small eigenvalues. This divergence is independent of the functions used, see [5] for a more in
depth discussion. We can even use this method to generate a spectral density from real lattice data (where instanton positions and sizes are extracted as a study of the vacuum). This is shown in figure (2).

If we increase the density of instantons then we naively expect greater interactions, leading to eigenvalues splitting away further from zero. This should decrease the spectral density at small eigenvalues. This is indeed seen, as is the converse. The fact that we still see a divergence from the lattice data which is a dense gas shows the divergence to be a generic feature. Intriguingly we also see a difference if we position the objects at random, the spectral density increases at small eigenvalues. This shows that there may be non-trivial screening between instantons in the vacuum. When we include the effect of the fermion determinant and simulate unquenched QCD then we still find a divergence. This however results in a perfectly acceptable quark condensate and \( \langle Q^2 \rangle(m) \) distribution in the chiral limit. Our work however indicates that quenched QCD may be pathological in nature, it may have a divergent quark condensate. If this is so, then why has such a feature not been seen directly from the lattice? We believe that the spectral density is protected by lattice artefacts, there are no small eigenvalues on the lattice (unless by accident), hence the spectral density cannot diverge as required. However such a feature should be apparent in the “ultimate quenched calculation”.

REFERENCES