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Quenched Chiral Artifacts for Wilson-Dirac Fermions

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Abstract

We examine artifacts associated with the chiral symmetry breaking induced through the use of Wilson-Dirac fermions in lattice Monte Carlo computations. For light quark masses, the conventional quenched theory can not be defined using direct Monte Carlo methods due to the existence of nonintegrable poles in physical quantities. These poles are associated with the real eigenvalue spectrum of the Wilson-Dirac operator. We show how this singularity structure can be observed in the analysis of both QED in two dimensions and QCD in four dimensions.

1 Introduction

During the past twenty years, considerable progress has been achieved in studying the nonperturbative structure of gauge field theory through numerical computations of lattice field theory. The principal method of analysis has involved Monte Carlo computations of physical quantities such as meson correlation functions where fermions have been treated using the quenched approximation. The quenched approximation omits the contribution of the fermion determinant to the functional integral defining the transition amplitudes. This approximation is known to be quite sensitive to the particular formulation used to define fermions on the lattice. In this paper we will address certain problems associated with the study of light fermions using the Wilson-Dirac formulation [1] of lattice fermions.

In the continuum the usual Dirac operator defining the fermion action preserves a chiral symmetry structure in the presence of gauge interactions which is broken only by the addition of fermion mass terms or Yukawa interactions. In the Wilson-Dirac formulation of lattice fermions, this chiral structure is explicitly broken by the analogue of second derivative terms which are needed to remove the doubling degeneracy of the naive lattice action for Dirac fermions. This chiral symmetry breaking modifies the eigenvalue spectrum of the Wilson-Dirac operator from that expected for the continuum Dirac operator. In Euclidean space, the chiral structure of the usual Dirac operator implies a purely imaginary spectrum for its eigenvalues. However, the Wilson-Dirac operator will have a spectrum of complex eigenvalues which fill a region of the complex plane [2, 3]. In particular, there will be a spread in the values of the real part of these eigenvalues which means that the massless fermion limit cannot be uniquely specified and the chiral limit can only be defined through ensemble averages of physical quantities. Unfortunately, the relevant physi-

cal quantities, such as the pion correlator, are singular functions of the Wilson-Dirac eigenvalues in the standard quenched approximation and there is growing evidence [4] that ensemble averages may not exist for sufficiently small fermion masses. We will give explicit evidence that this is the case for Wilson fermion theories in two and four dimensions including QED2 and QCD4.

In previous work [4, 5] we have shown that the precisely real eigenvalues of the Wilson-Dirac operator play a special role in the quenched theory. These eigenvalues are the analogue of the zero modes of the continuum theory which are associated with the topological structure of the background gauge field. In the lattice formulation of the theory, these modes are responsible for the singular behavior of the quenched theory for light fermion masses. The singularities arise when the fermion mass is chosen to lie within the band of real eigenvalues which exists because of the chiral symmetry breaking property of the Wilson-Dirac operator. This is well known and is the principal reason for the "exceptional" configurations observed in Monte Carlo calculations of the quenched theory [6]. Indeed, we have previously made a careful analysis [4] of the correlation between the behavior of the real eigenvalue spectrum and the observation of exceptional configurations. However, the problem associated with these exceptional configurations goes beyond the annoying problem of an occasional large contribution of a single configuration and its implication for the statistical errors of the associated ensemble averages. We have previously pointed out that this problem cannot be solved simply by accumulating larger statistical samples as the exceptional configurations are expected to occur at a level where, even in large statistical samples, the statistical errors will not diminish even in the limit of infinite statistics.

The singularities associated with the real eigenvalues are related to both the chi-

ral symmetry breaking associated with the Wilson-Dirac operator and the quenched approximation which enhances singularities of the fermion propagators that are normally suppressed in the full unquenched theory. The fermion propagator can be written as a sum over the eigenvalues of the Wilson-Dirac operator, λ_i,

$$S_F(x, y, A(x)) = \sum_i v_i(x, A) w_i(y, A)/(\lambda_i + m_0) \tag{1}$$

where v (resp. w) are left (resp. right) eigenmodes in a particular background gauge field, $A(x)$.

In the continuum, the fermion mass parameter being nonzero implies that there are no singular terms in the sum when the gauge fields are smoothly varied. However, this is not the case on the lattice. As the background gauge field is varied, isolated real eigenvalues are restricted to remain on the real axis. The symmetries of the Wilson-Dirac operator [4, 7] imply that the complex eigenvalues occur in complex conjugate pairs and a single real eigenvalue cannot become two complex-conjugate eigenvalues via smooth variation of the gauge potentials. Because of this constraint, the contribution of the real eigenvalue modes to the functional integral over the gauge potential can be reduced to a one- dimensional integral corresponding to the position of the real eigenvalue. Hence, the quenched functional integral will contain nonintegrable singularities associated with the contribution of the real modes if the fermion mass is chosen to lie within the band associated with the spread of the real eigenvalues. For example, the nonsinglet meson propagator is obtained by squaring the quark propagator and, therefore, the real modes will generate a dipole contribution to the meson correlator. If the bare fermion mass is chosen to lie within the band of real eigenvalues, the Monte Carlo calculation will smoothly sample eigenvalues in the neighborhood of fermion mass corresponding to a one-dimensional integration parameter even though the original gauge integration corresponds to a

very high dimensional space of integration variables. Hence, the sum for the meson correlator effectively reduces to

$$\int \mathcal{D}A \frac{\mathrm{Res}(A)}{(\lambda_{\mathrm{pole}}(A) + m_o)^2} \to \int d\lambda \frac{\mathrm{Res}(\lambda)}{(\lambda + m_o)^2} \tag{2}$$

which is not directly defined. For this reason we argue that the naive quenched theory does not exist. The "exceptional" configurations observed in Monte Carlo calculations are not strictly speaking an exceptional feature but are, instead, a *generic* property of the quenched theory signaling the breakdown of the naive theory for light fermion masses. The Monte Carlo averages simply do not converge for sufficiently large statistical samples. Indeed, this singular behavior of the naive quenched theory led us to propose [5] a modification of the quenched theory, MQA, where these lattice fermion artifacts are explicitly removed in the evaluation of the quenched correlation functions by restoring the chiral structure of the continuum theory. Others have recently proposed that the entire band of light fermion masses might be associated with a massless phase of the theory [8]. Unfortunately, we shall argue below that this interpretation cannot be directly applied because the naive quenched hadronic correlation functions simply are not defined in this region for the reasons given above.

While we have given a general argument concerning the difficulties of defining the naive quenched theory, we will now show explicit evidence of this singular behavior in a number of calculations in QED2 and QCD4. In particular, we wish to show in this paper that nonintegrable singularities in the quenched functional integral have a characteristic and clearly detectable statistical signature in a Monte Carlo simulation. In Section 2, the singularity structure of quenched 2-dimensional QED is explored using a variety of detailed statistical signatures. Explicit numerical evidence is provided to show that the quenched functional integral of physical

correlators contains nonintegrable singularities and is therefore undefined. A convenient statistical diagnostic for revealing the existence and strength of nonintegrable singularities in a quenched path integral is introduced and applied. Section 3 illustrates certain universal aspects of the statistical behavior of the Monte Carlo simulation of divergent integrals using a simple one-dimensional test function with essentially identical behavior to meson correlators in quenched lattice gauge theory. The analysis of Section 2 for QED2 is repeated in Section 4 using data from a full 4 dimensional quenched QCD simulation at relatively strong coupling (β=5.7) - one infected with frequent "exceptional" configurations. In Section 5 we comment on the use of spectral characteristics of the hermitian Wilson-Dirac operator in studying new phases of quenched gauge theory with Wilson fermions, and emphasize the need for a regularized version of quenched theory in studying otherwise undefined correlator averages.

2 Quenched Singularity Structure of QED2

The two-dimensional version of massive quantum electrodynamics, the massive Schwinger model, has frequently been used as a testbed for studying the structure of fermions in lattice field theory [2]. It shares many features in common with four dimensional quantum chromodynamics, including aspects of chiral symmetry, a nontrivial topological structure, fermion doubling problems on the lattice, and the exceptional configuration artifacts of Wilson-Dirac fermions.

In a previous paper [4], we have emphasized the role that exactly real eigenvalues play in generating exceptional configurations. In QED2 with Wilson-Dirac fermions, the real eigenvalues occur in bands rather than at a particular critical

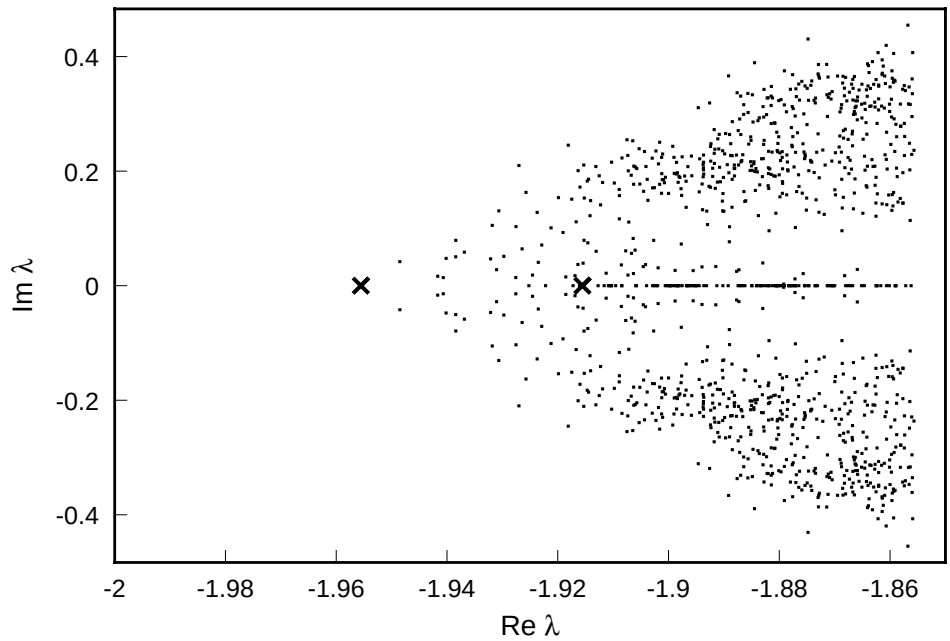

Figure 1: Wilson-Dirac spectrum near the left critical branch [QED2]. The eigenvalue positions corresponding to $m_q = 0.10$ and $m_q = 0.06$ are denoted by crosses.

value associated with the zero modes of the continuum theory. The bands tend to narrow for gauge configurations generated with larger values of β corresponding to the approach to the continuum theory.

We have carried out simulations of QED2 defined on a 10x10 lattice at β= 4.5. According to the analysis of Smit and Vink [2], the massless theory is associated with a bare fermion mass given by the approximate relation $m_0 = m_c \simeq$2.0-0.65/β = 1.9155. In Fig(1), we show the spectrum of accumulated eigenvalues of the Wilson-Dirac operator in a typical set of 500 consecutive (uncorrelated) configurations in a quenched simulation at β=4.5. Only eigenvalues with a real part less than the critical value of Smit and Vink are shown in this plot. Both real and complex

eigenvalues exist in this region. Because the real eigenvalues are less than the critical value, they will produce poles in the fermion propagators at positive values of the fermion mass, leading to a singular behavior of physical quantities constructed from these propagators in the quenched theory. We have marked the positions where real eigenvalues would produce poles for $m_q \equiv m_0 - m_c$=0.06 and 0.10, respectively. The smaller fermion mass, m_q=0.06, lies within the band of real eigenvalues, while the larger mass, m_q=0.10, lies outside this region and should not be associated with singular behavior.

In the quenched theory, various physical quantities, such as correlation functions, can be computed from products of the valence fermion propagator. The propagators in turn can be written as a spectral sum involving eigenfunctions of the Wilson-Dirac operator and associated eigenvalues as in Eq(1). The pseudoscalar ("pion") propagator is then given as a sum over the eigenvalues:

$$J_{55}(x,y) = \sum_{ij} \frac{\mathrm{Tr}\gamma_5 r_{ij}(x,y,A)\gamma_5 r_{ji}(y,x,A)}{(\lambda_i(A)+m_0)(\lambda_j(A)+m_0)} \tag{3}$$

where $m_0 = m_q + m_c$. The eigenvalue dependence of the denominators exhibits the potential for double pole singular behavior in an integral over A (for heavy-light mesons, one would encounter a single pole, for light-light-light baryons in QCD4, a *triple* pole in the quenched functional integral).

As an example of this divergence, we computed the pseudoscalar propagator at Euclidean time t=2 for m_q=0.06 and 0.10. In Fig(2) the cumulative averages and associated statistical errors are plotted for a sample of 1000 quenched gauge configurations separated by 10 Metropolis sweeps. The propagator averages for the lighter mass clearly reflect the presence of singularities in the functional integral. After *apparent* convergence with the first 100 configurations, the contributions of a number of exceptional configurations become dominant and no reliable average

value can be extracted from the simulation. For this mass value, we are within the band of real eigenvalues and the Monte Carlo process eventually samples eigenvalues arbitrarily close to the double pole singularity in the pseudoscalar propagator. We can compare this behavior to the propagator average for the larger mass, m_q=0.10, which lies outside the band of real eigenvalues (see Fig(3)). Here the propagator appears to converge to its average value after about 400-500 sweeps and there is no obvious singular behavior.

Even if we do not directly know the eigenvalue spectrum (and this is in general the case for QCD in 4 dimensions), we can infer the singular structure of the quenched integral directly from physical quantities such as meson propagators. For example, the pseudoscalar propagator in Eq(3) is a singular function as an eigenvalue approaches the critical value $\lambda_i \to m_0$. In this singular limit, one eigenvalue will dominate the propagator sum in the form of a double pole singularity. The Monte Carlo average will sample eigenvalues in the neighborhood of this singularity so long as the mass lies within the band defined by the purely real part of the spectrum. It should be expected that eigenvalues close to the singularity will be uniformly sampled (given sufficient statistics) as neighboring gauge configurations smoothly vary the values of the real eigenvalues. (This uniform sampling is a consequence of the fact that, unlike full QCD, the distribution of quenched gauge configurations is unaffected by singularities in the quark propagator.) Hence a definitive signature of the singular structure can be obtained from the propagator by computing the value of the inverse square root of the propagator 1/rP$\equiv \frac{1}{\sqrt{P(t)}}$. Ordering the configurations according to the size of 1/rP should then reveal a linear extrapolation to a zero value at the singularity, reflecting the uniform sampling by the Monte Carlo in the neighborhood of the singularity. In Fig(4) we show these plots for the two mass

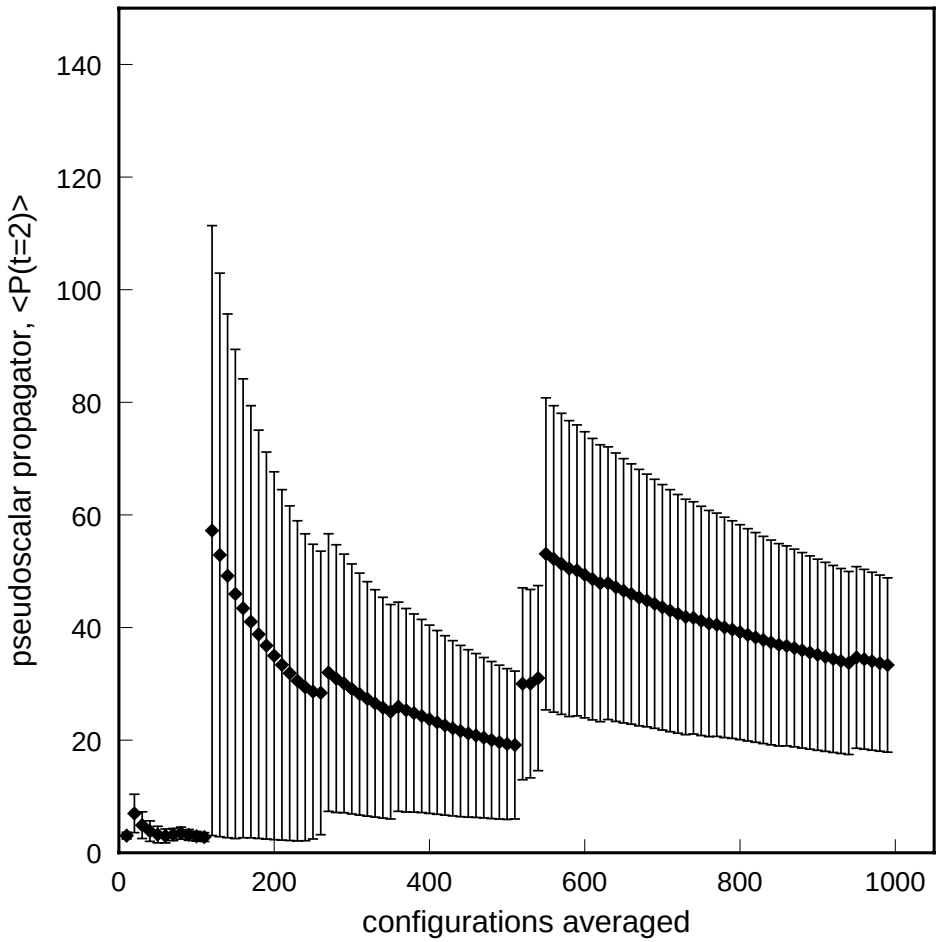

Figure 2: Convergence of pseudoscalar correlator with increasing statistics in quenched QED2. Here m_q=0.06.

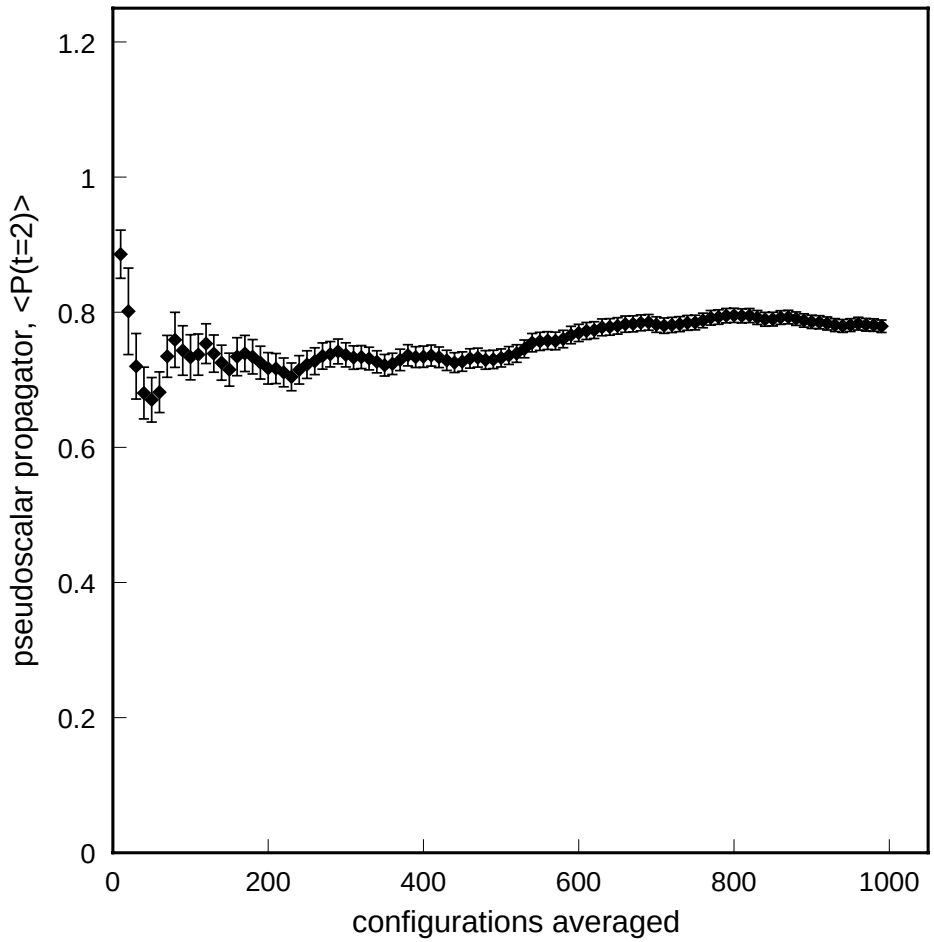

Figure 3: Convergence of pseudoscalar correlator with increasing statisitics in quenched QED2. Here m_q=0.10.

values discussed above.

It is clear that the smaller mass value, m_q=0.06, shows a smooth extrapolation of 1/rP to zero while the larger value, m_q=0.10, reveals a gap. Since the poles are expected to dominate only for configurations with eigenvalues close to the poles, only the behavior as 1/rP $\rightarrow$0 is relevant here. In Figure(5), we focus on this region for the small mass case to bring out clearly the linear behavior close to the origin.

The correlation between the singular behavior observed in the 1/rP plots and the real eigenvalues can be seen by comparing the raw data with propagators modified using the MQA procedure [5]. This procedure modifies fermion propagators by shifting the poles due to real eigenvalues to the critical value expected for the continuum theory. Only real poles to the left of the critical value, as shown in Fig(1), are shifted in this procedure. In applying the procedure to the QED2 data, it is clear that any difference observed in the behavior of the correlation functions is directly attributable to the structure of the real eigenvalues. In Fig(6) we compare the 1/rP plot for the raw propagator with that for the MQA shifted propagator. The configurations are, in each case, ordered according to the value of the raw propagator. It is apparent that all the points close to the origin in this plot were associated with the singular structure of the real modes. This correlation can be made more explicit by considering only the configurations with real poles lying within the band shown in Fig(1). We have checked that in QED2 these configurations all correspond to nonzero topological charge. In Fig(7), we plot the value of 1/rP for each configuration versus the position of the nearest real eigenvalue for that configuration. The close correlation is obvious and the position of the singular eigenvalue is clearly identified for this mass value, m_q=0.06. In many cases (especially in QCD4) it is not possible to identify all the real poles. However, we have seen that the behav-

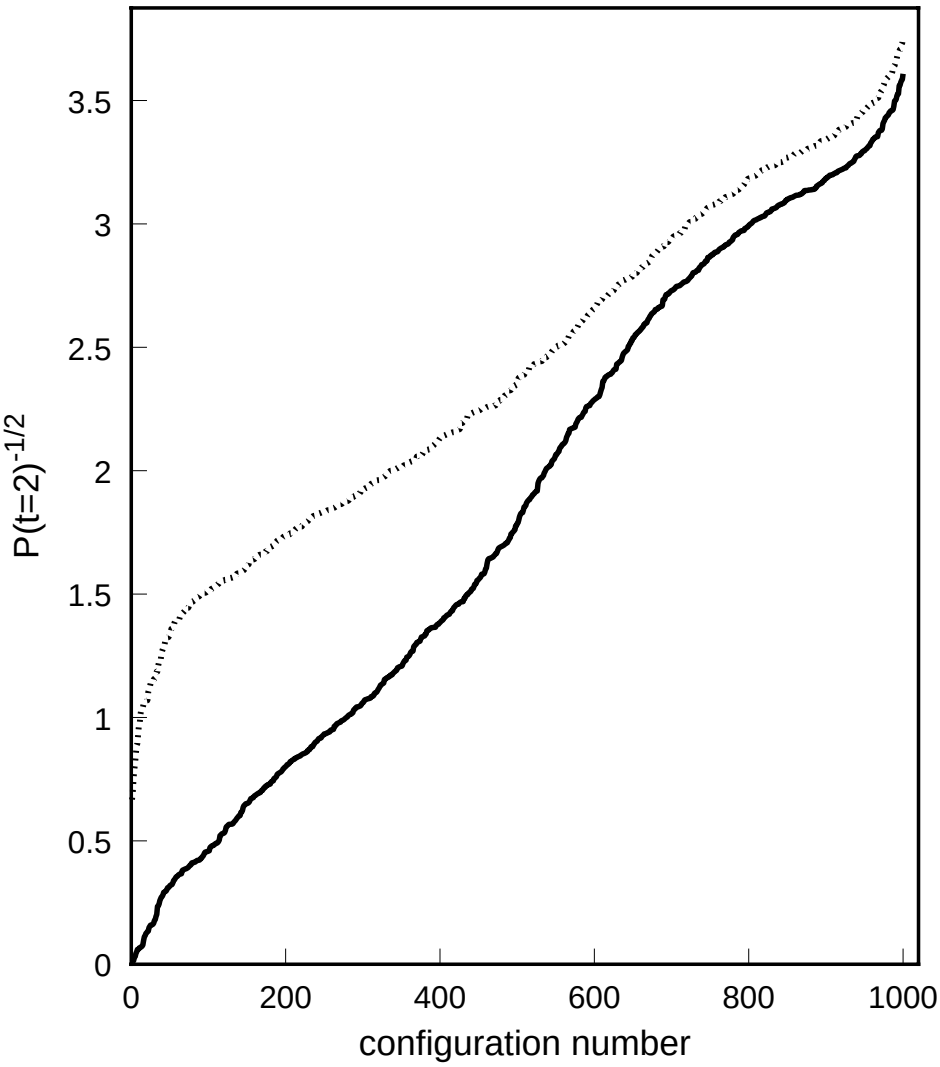

Figure 4: 1/rP plot for 1000 configurations in QED2. The configurations are ordered from lowest to highest value of 1/rP. Results for $m_q = 0.10$ (dotted curve) and $m_q = 0.06$ (solid curve) are shown.

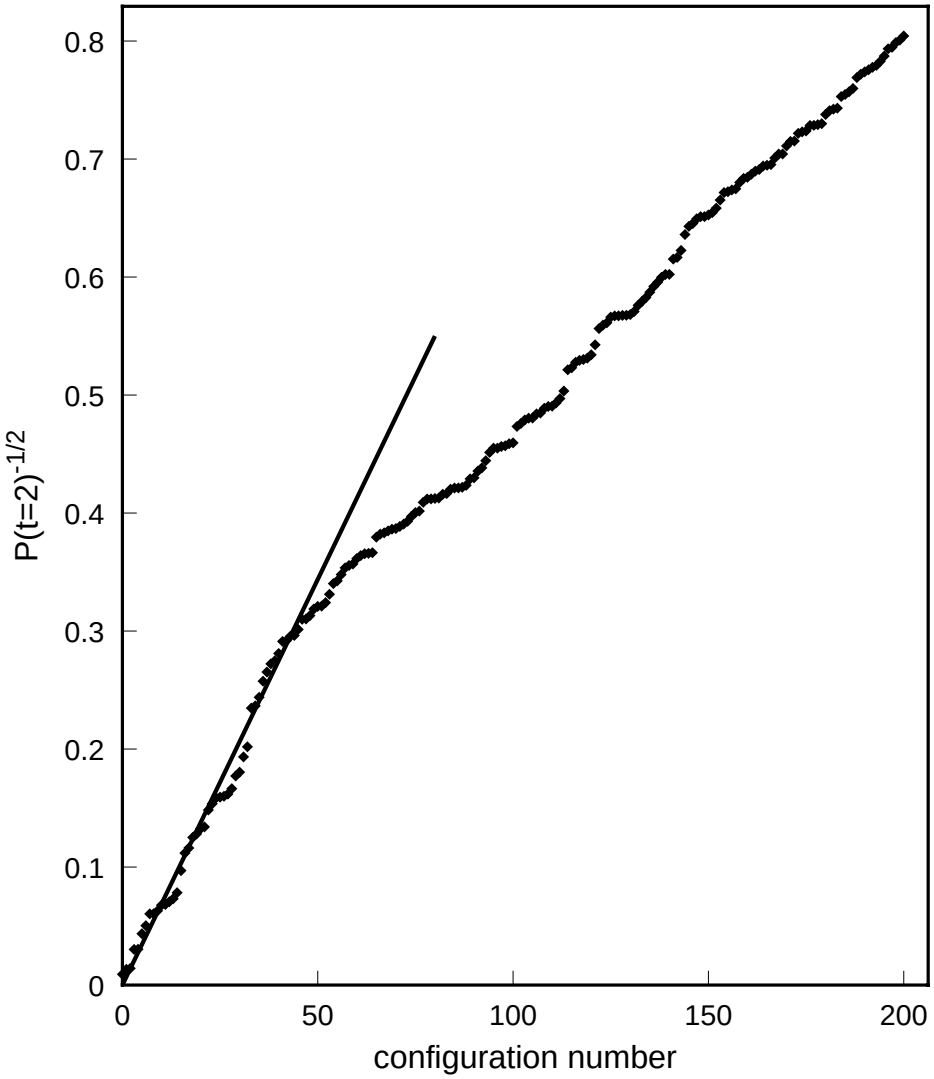

Figure 5: 1/rP plot. Results for the lowest 200 configurations with $m_q = 0.06$ in Figure 4 are shown (small diamonds). The solid line is a linear fit to the first 40 configurations.

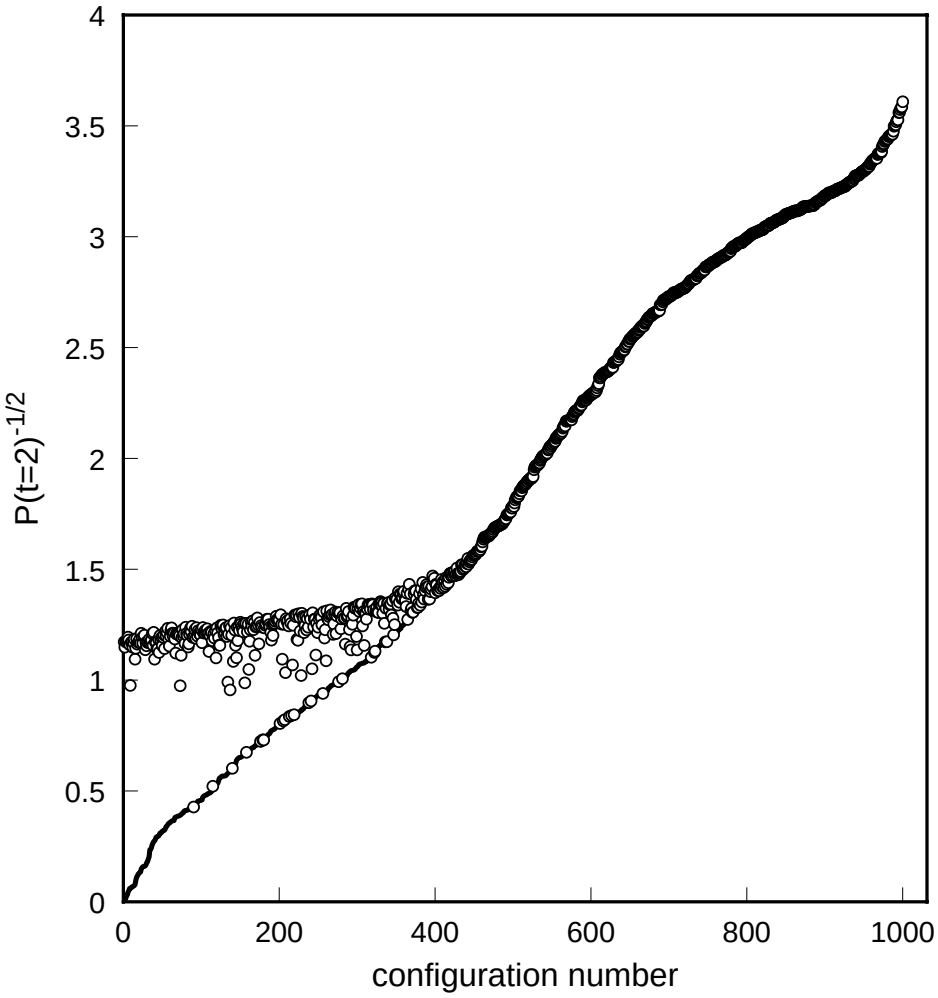

Figure 6: 1/rP plot. The pseudoscalar correlators in Figure 4 with $m_q = 0.06$ (solid line) are compared with the associated MQA correlators (open cirlces).

ior of 1/rP can clearly be used to exhibit the singularities associated with bands of real eigenvalues. The method will only be effective however when there is sufficient Monte Carlo statistics to smoothly sample the neighborhood of the propagator singularities.

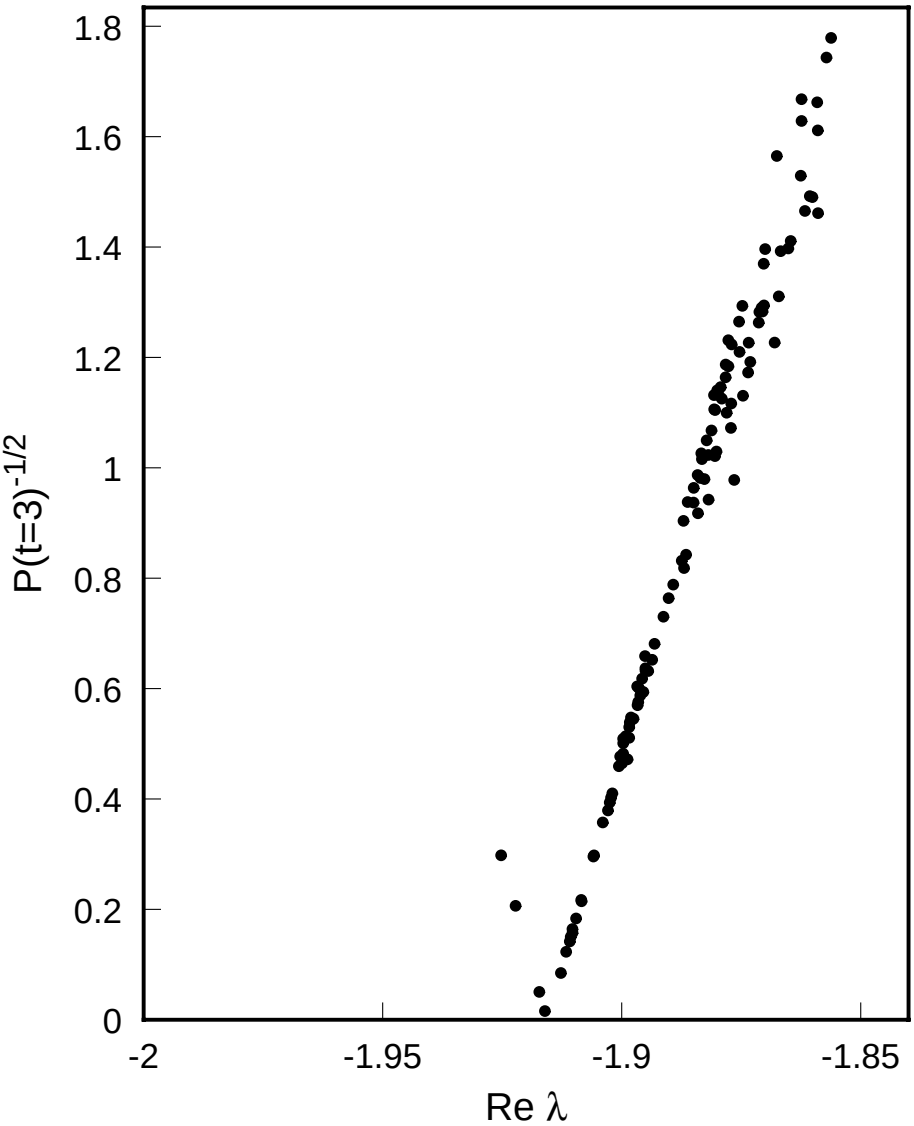

Figure 7: 1/rP versus the position of the nearest real pole eigenvalue Re λ for $m_q = 0.06$. [QED2].

3 A simple test function

We have argued that the presence of a band of real eigenvalues of the Wilson-Dirac operator implies that the unmodified quenched functional integral simply does not exist for bare fermion masses which place the propagator singularities within the real eigenvalue band. Even with unlimited Monte Carlo statistics, the real poles generate exceptional configurations at a fixed rate, with fluctuations increasing as eigenvalues appear closer to the poles of the fermion propagator. This problem can be seen in the clearest possible way by attempting to estimate a singular one dimensional integral, corresponding to the meson propagator, by Monte Carlo methods. The properties of such a simulation, where we know that the answer does not exist, can then be compared with our Monte Carlo simulations of QED2 and QCD4.

The test function we wish to examine is a simple integral of a double pole singularity with a spectral weight similar to that seen for the real eigenvalues of the QED2 analysis. We chose an integral of the form

$$I = \int_0^\infty dx 2x \frac{e^{-x^2}}{(x-a)^2 + b} \tag{4}$$

For positive values of a and b=0 the integral is divergent and we do not expect the estimate of its value by Monte Carlo methods to converge. Analogously to the case of QED2, we generate 1000 configurations according to the spectral weight $2x\exp(-x^2)$. To imitate the contributions of configurations with complex poles, we have randomly chosen the width parameter b to be either zero or a fixed nonzero value for each term in the sum. As a result we have a sample of 200 configurations to integrate a singular double pole term (with b=0) and 800 configurations with integrable complex pole contributions (the 4:1 balance chosen here was similar to that found in the QED2 simulation). In Fig(8) the cumulative averages and errors

for the integral are plotted as a function of the number of configurations included (cf Fig(2)). While there seems to be an approximate convergence with 300-400 configurations, the exceptional terms associated with Monte Carlo sampling close to the pole causes the error eventually to explode- reflecting the fact that the integral does not exist. This plot is remarkably similar to the plot for the pseudoscalar propagator for QED2 shown in Fig(2). In fact, the cause of the exceptional configurations in both cases is exactly the same - a nonintegrable dipole singularity- so the resemblance should hardly be surprising. We can also plot the analogue of the 1/rP plot of Fig(4). In Fig(9) we show the inverse square root of the individual summands placed in sequential order. The plot again shows the linear behavior near the origin due to sampling near the pole singularity. In addition, we have shown, in open circles, the effect of applying the equivalent of the MQA shift moving subcritical real eigenvalues to a=0; again, this removes the linear part of the curve as in the QED2 case and introduces a gap. We note that fluctuations in the imaginary part of the eigenvalues and in the pole residues for QED2 explain the deviations between QED2 and the simple test function. However, the approximate quantization of the pole residues (which are effectively instanton zero modes in the QED2 case) is important in generating the observed linear behavior. From the analysis we see that the 1/rP plot provides a useful and clear signal of nonintegrability in Monte Carlo simulations.

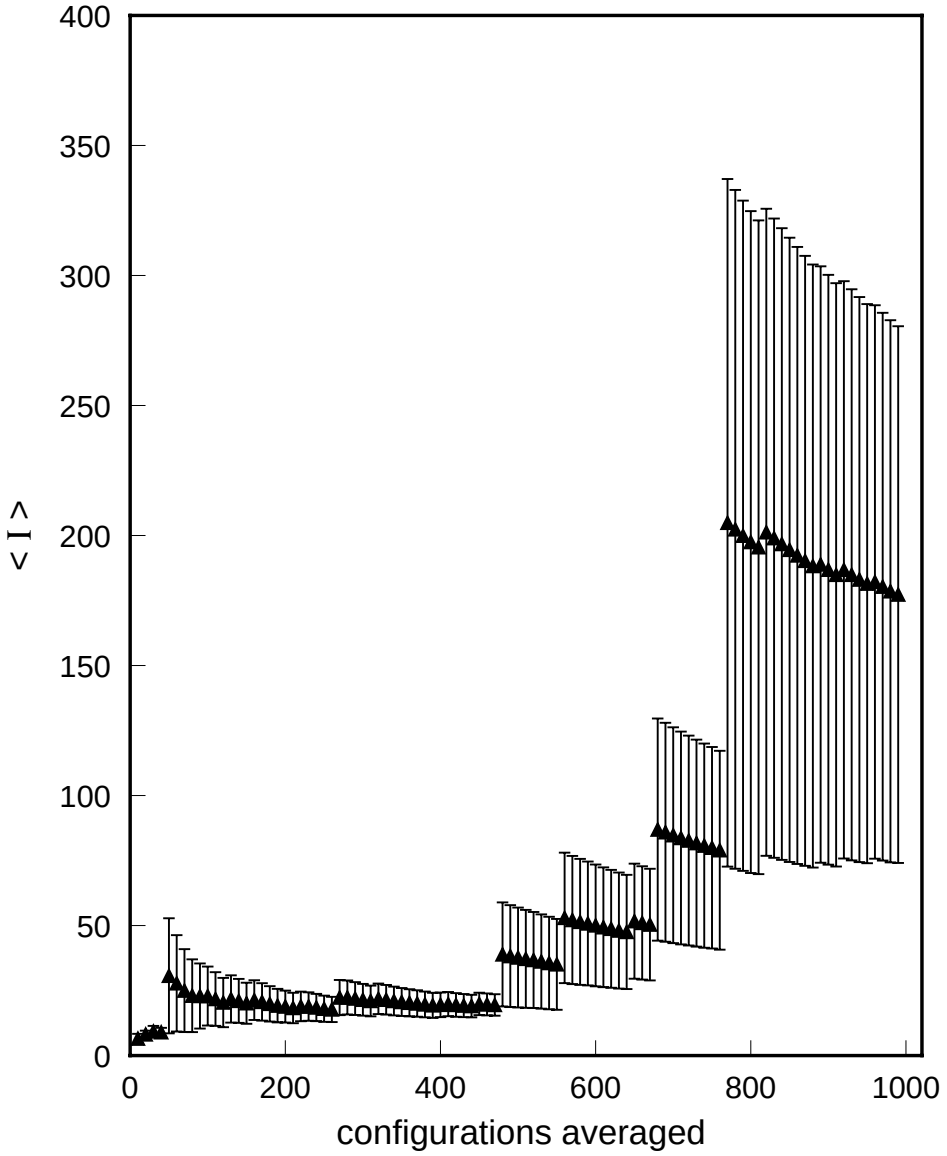

Figure 8: Cumulative average for Monte Carlo estimation of a test function I (Eq. 4) versus number of sampling points ("configurations").

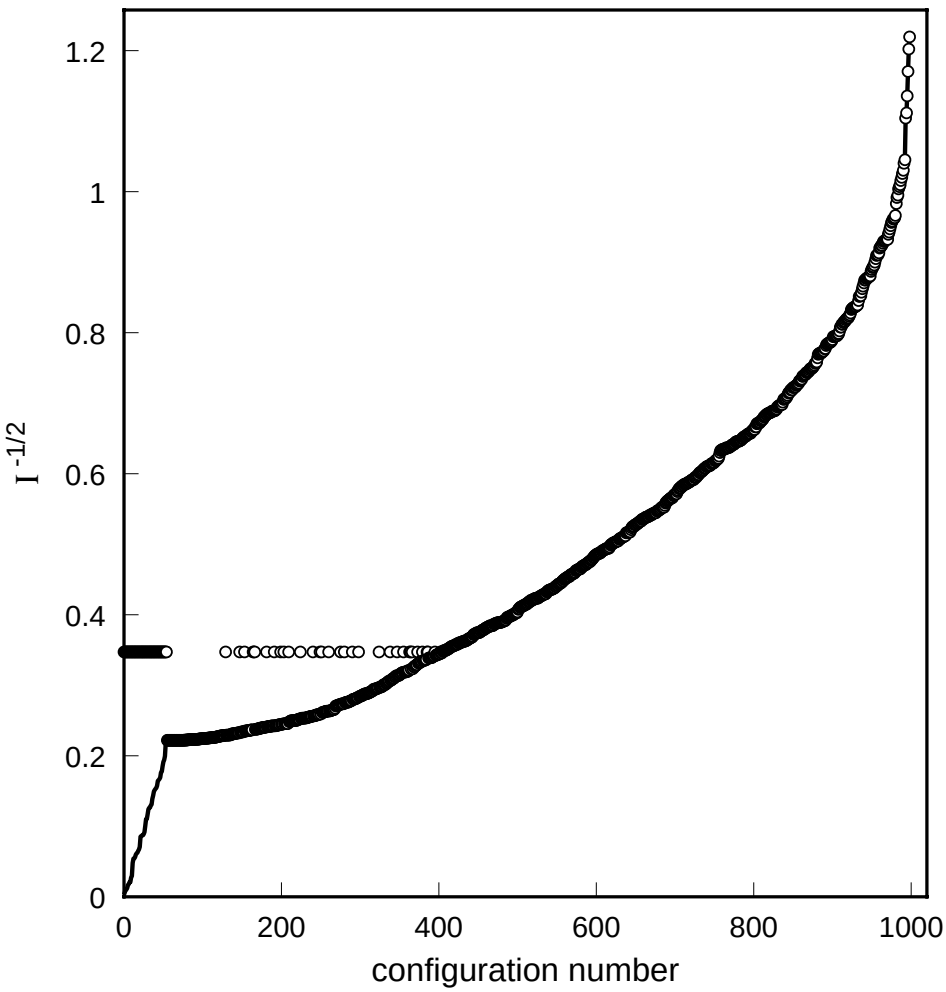

Figure 9: 1/rP for the test function I. Solid curve represents the raw "configurations" ordered by value; while the open circles show the effect of applying an MQA procedure.

4 Quenched Singularity Structure of QCD4

Quenched calculations of quantum chromodynamics in four dimensions are also known to suffer from problems associated with exceptional configurations and singularities occasioned by real eigenvalues. In a previous paper [5] we have been able to identify the spectrum of subcritical real eigenvalues using fits to the kappa dependence of observables such as the integrated pseudoscalar density. We can also study the statistical behavior of the quenched singularities using the 1/rP plots for the pion propagators discussed above. In Fig(10) we show the 1/rP plot for a 16^3x32 lattice at β=5.7 and a kappa value of 0.1685, corresponding to a quark mass within the band of real eigenvalues for this β. There is clear evidence of the linear behavior near the origin. We can see that this behavior is directly attributable to real eigenvalues by plotting (open circles) the same configurations with propagators computed using the MQA analysis where only real poles are shifted. Again, all of the contributions near the origin are removed, indicating that the real poles dominate the exceptional configurations. Here again, direct Monte Carlo simulation of the quenched functional integral will be seen to fail once sufficient statistics are accumulated. At heavier quark masses the density of real eigenvalues is smaller and a much higher level of Monte Carlo statistics may be needed to clearly identify the singular behavior, which is nevertheless still present, at least for fermion masses $m_0 < 2.0$.

The singular behavior of the Monte Carlo integrals (deriving in turn from the underlying nonintegrable singularity of the quenched functional integral) is not a unique feature of the Wilson action. Improved actions, such as the Sheikholeswami-Wohlert [9] action, also suffer from the singularities associated with real eigenvalues. Subcritical real modes can be extracted from the kappa dependence of hadron

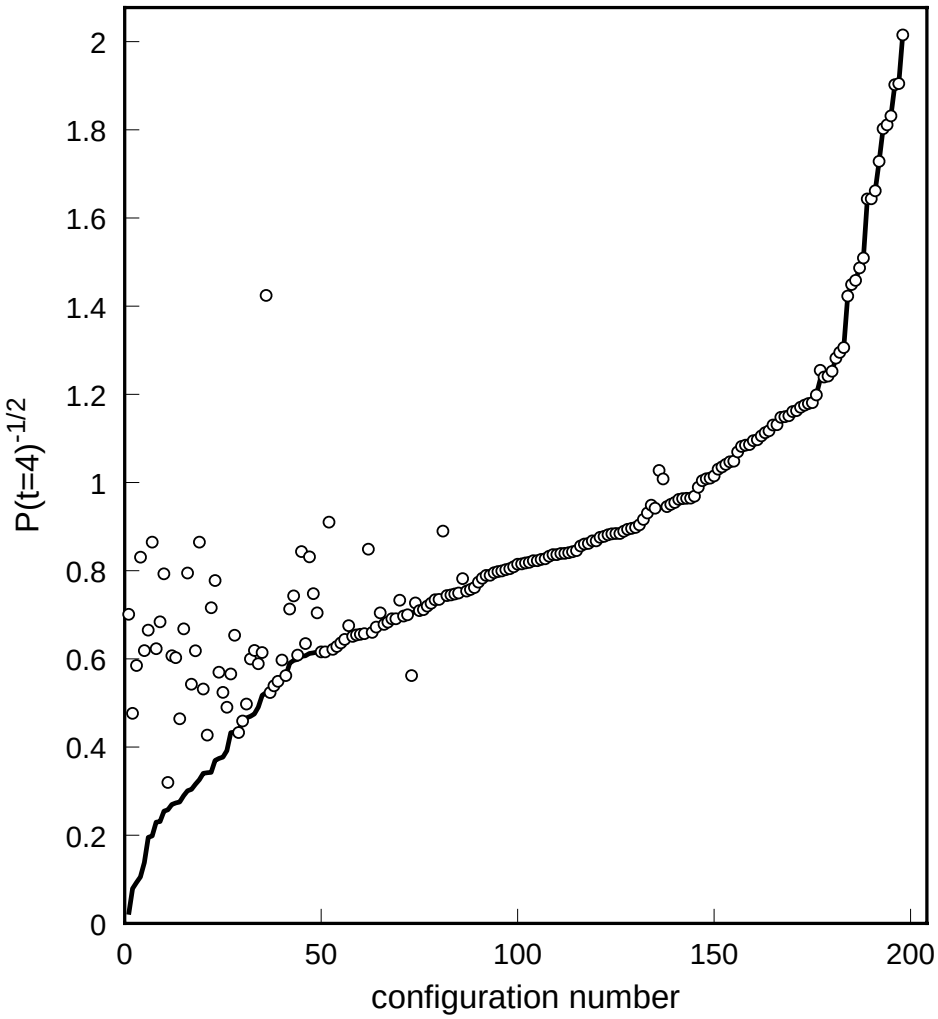

Figure 10: 1/rP plot for 200 configurations at β=5.7 on a 16^3x32 lattice [QCD4]. The Wilson quark propagators used κ=0.1685. Configurations are ordered by value of 1/rP. The naive pseudoscalar correlator results are denoted as a solid curve, while the corresponding results using the MQA proceedure are denoted by open circles.

propagators or we may use the 1/rP test to see the impact of the exceptional configurations. In Fig(11) we show the 1/rP plot for a 12^3x24 lattice at β=5.7 with clover coefficient $C_{\rm sw}$ =1.57 and κ =0.1425. Once more, the linear behavior near the origin gives a clear signal of the singular nature of the unmodified Monte Carlo integral and the comparison with the MQA analysis shows that the real eigenvalues play the essential role.

These results provide convincing evidence that real modes are responsible for generating the singular behavior of the unmodified quenched approximation. For sufficiently light quark masses, hadron propagators determined from the valence quark propagators contain nonintegrable singularities. With low statistics these singularities are manifested by the appearance of an occasional exceptional configuration. However, it is *inevitable* that the Monte Carlo average will diverge as the statistics is increased and the eigenvalues near the propagator poles are closely sampled. While we have emphasized spectral properties associated with the Wilson-Dirac operator, it is important to realize that these nonintegrable singularities are present in completely physical hadronic amplitudes in the unmodified quenched theory, such as the pseudoscalar correlation functions.

5 Exceptional configurations, gapless phases, and chiral source terms

A number of authors have preferred to use a hermitian operator $H(m)$ [10] to discuss properties of the quenched theory. This operator is simply related to the Wilson-Dirac operator

$$H(m) = \gamma_5(D - W) \tag{5}$$

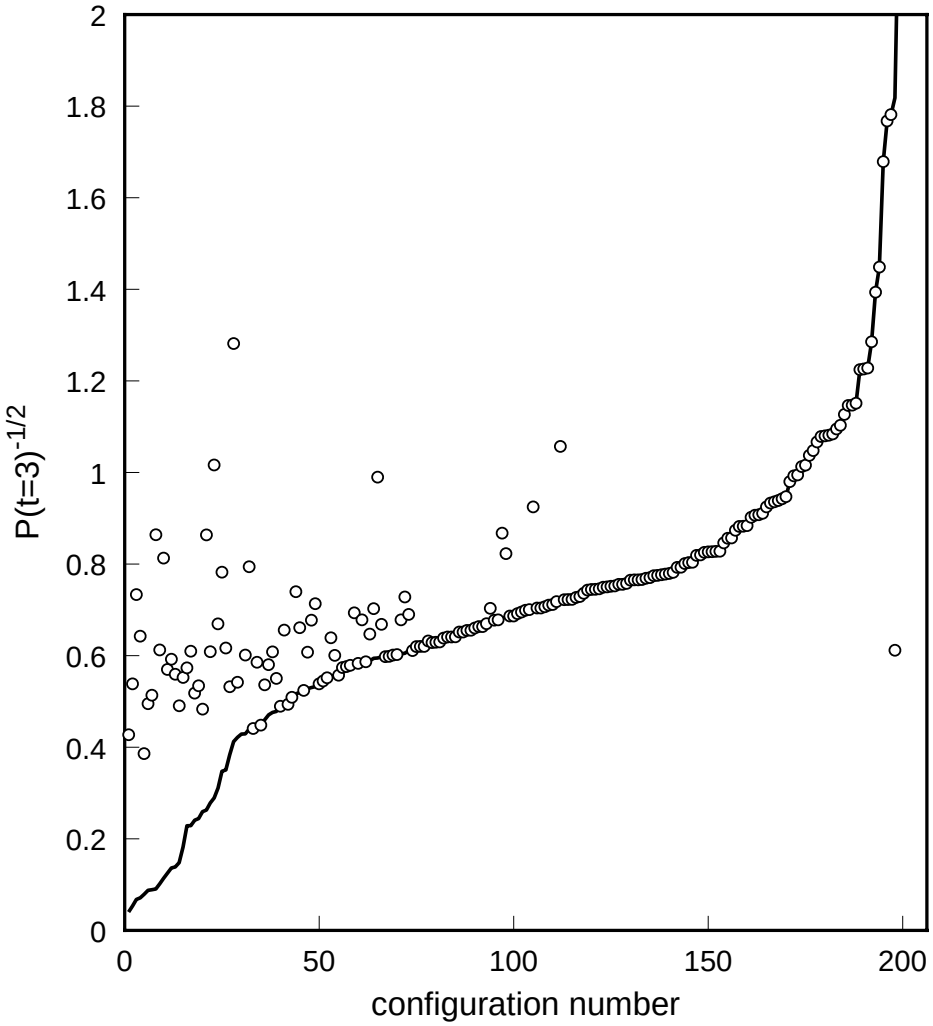

Figure 11: 1/rP plot for 200 configurations at β=5.7 on a 16^3x32 lattice [QCD4]. The SW quark propagators used κ=0.1425 and $C_{\rm sw}$ =1.57. Configurations are ordered by value of 1/rP. The naive pseudoscalar correlator results are denoted as a solid curve, while the corresponding results using the MQA proceedure are denoted by open circles.

but has a completely different eigenvalue spectrum. Since $H(m)$ is hermitian it has only real eigenvalues and (with the exception of zero eigenvalues) it is not possible to uniquely associate eigenvalues of $H(m)$ with those of the Wilson-Dirac operator in a 1-1 fashion, and therefore to identify modes which play the special role of the real eigenvalues in the Wilson-Dirac case. Nevertheless, the physical quantities of the quenched theory (meson propagators and other hadronic amplitudes) are unique and share the same singular behavior that we have established using the Wilson-Dirac approach.

The small eigenvalues of the $H(m)$ operator are usually identified with the dynamical breaking of chiral symmetry. However, we know that these eigenvalues must also reflect the nonintegrable singularities found in the Wilson-Dirac approach. Indeed, exactly zero eigenvalues arise from common eigenfunctions. By varying the fermion mass we can establish the same band of masses which correspond to singularities caused by subcritical real eigenvalues of the Wilson-Dirac operator. Thus, the closing of a gap in the spectrum of the $H(m)$ operator corresponds in part to the appearance of nonintegrable contributions in the quenched path integral. In Fig(12,13) we display the central part of the spectral region of $H(m)$ in QED2 for the bare quark value masses 0.06 and 0.10 studied earlier. The disappearance of a gap for the smaller mass exactly corresponds to the fact that the rightmost cross in Fig(1) is immersed in a band of real eigenvalues of the complex Wilson-Dirac operator.

Some authors [8] have recently suggested that this band should reflect the dynamical realization of the chiral phases of the quenched theory. They propose an identification of the entire band with a massless phase of the theory. These conclusions are based on studies with limited statistics on small lattices. We do not

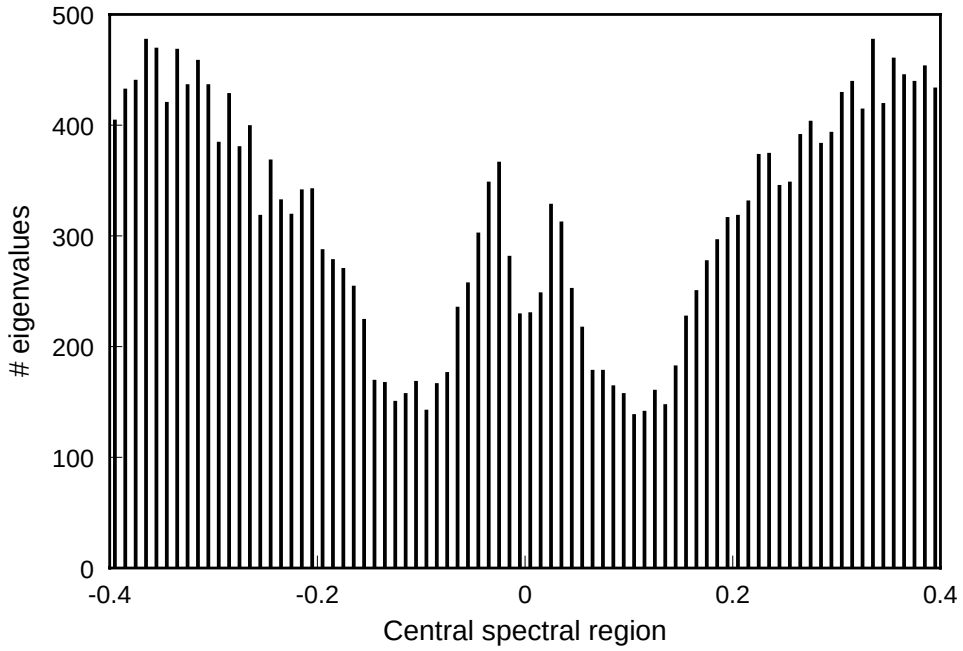

Figure 12: Spectral density of $H(m)$ for QED2 with $m_q = 0.06$. The total number of eigenvalues are shown with bin size 0.01.

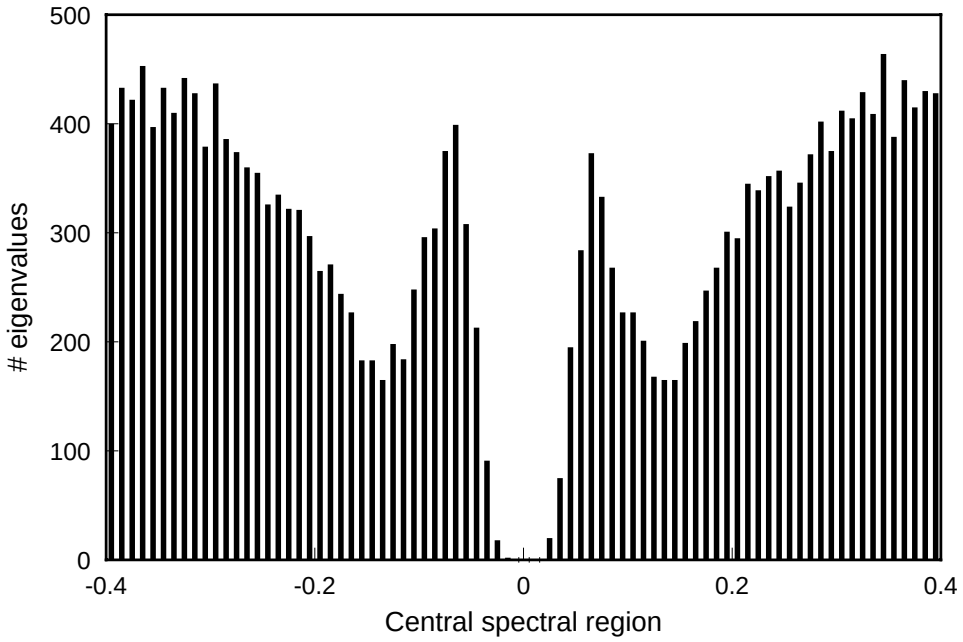

Figure 13: Spectral density of $H(m)$ for QED2 with $m_q = 0.10$. Bin size 0.01.

think that their conclusions can be sustained once larger data samples are examined. The arguments presented above show that the normal Monte Carlo integral of the quenched theory for meson propagators simply does not exist if the fermion masses lie within the band identified with the putative massless phase . Hence, any inference of a particular physical behavior of the meson propagators based on a small sample of configurations, particularly exceptional configurations where real modes are present, is unwarranted. We make no specific claims here about the possible existence, nonexistence or properties of additional massless chiral phases in the unquenched theory at infinite volume. However, for the quenched Wilson theory at finite volume, the detailed statistical analyses presented in this paper clearly demonstrate that conventional hadron correlators (and in particular, the pion correlators needed to establish the chiral spectrum in any putative new phase) *simply do not*

exist once the gapless region is entered.

The suggestion that the flavor-parity breaking Aoki phase [11, 12] of Wilson lattice QCD be studied by perturbing the system with a flavor-parity noninvariant source leads to an interesting point concerning the divergence of quenched amplitudes. The addition to the theory of any nontrivial chiral/flavor rotation of the conventional mass term as a source term (here we are dealing with two flavors of Wilson fermions, and $\vec{\sigma}$ are the corresponding isospin generators)

$$h\bar{\psi}\psi \to h\bar{\psi}e^{i\vec{\theta}\cdot\vec{\sigma}\gamma_5}\psi \tag{6}$$

modifies the hermitian Dirac operator by

$$H(m) \to H(m) + h\gamma_5\cos(\theta) + ih\sin(\theta)\hat{\theta}\cdot\vec{\sigma} \tag{7}$$

The additional antihermitian term (nonvanishing for any $\theta \neq 0, n\pi$) clearly renders the spectrum of $H(m)$ complex, introducing a gap, as all eigenvalues λ of $H(m)$ now satisfy $|\lambda| > h|\sin(\theta)|$. Consequently, pion correlators computed with quark propagators including the source term will now be perfectly well-defined even in the quenched theory, as the nonintegrable poles are moved away from the integration contour of the quenched path integral. (This corresponds to the situation in the one-dimensional test integral of Section 3 when $b \neq 0$). The properties of meson correlators in the Aoki phase can thus be studied in a well-defined way at large volume before taking the limit $h \to 0$, as is done typically in order to isolate the condensate. Of course, at finite volume, the singularity will return as the source term is set to zero, so as in the case of studies of spontaneous symmetry breaking at finite volume one has to be careful to extrapolate in an appropriate way from larger values of the source parameter. But in the absence of such a source term in the propagator inversion, or of pole shifting as in the MQA procedure, one will

necessarily encounter completely undefined statistical averages of meson propagators as more configurations are included in a quenched simulation.

6 Summary

We conclude by summarizing our basic results on the nature of the quenched chiral artifacts in the Wilson-Dirac formulation of lattice gauge theory:

(1) The appearance of exceptional configurations in quenched simulations is directly attributable to the appearance of exactly real modes of the Wilson-Dirac operator in nontrivial topological charge sectors of the theory.

(2) Even in cases where the extraction of the spectrum of the Wilson-Dirac operator is computationally prohibitive, there are a number of reliable statistical tests that can be applied to diagnose the presence of the exactly real modes. In particular, the convergence properties of cumulative averages of physical quantities (cf Figs (2,3,8)), as well as the behavior of the reordered inverse square-root of meson correlators (cf Figs(4,5,6,7,9,10,11)) can be used to signal directly the appearance of such modes.

(3) Finally, the statistical diagnostics used here clearly reveal the nature of the singularity of the quenched functional integral which corresponds to a one-dimensional integral with a nonintegrable singularity. The singularity can be removed, and a well-defined quenched theory obtained, either by the MQA pole-shifting technique introduced in our earlier papers [4,5], or by introducing a chirally rotated source at interim stages of the simulations.

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