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Effects of dynamical quarks on the spectrum of the Wilson Dirac operator

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Effects of dynamical quarks on the microscopic spectrum of the Wilson Dirac operator are analyzed by means of effective field theory. We consider the distributions of the real modes of the Wilson Dirac operator as well as the spectrum of the Hermitian Wilson Dirac operator, and work out the case of one flavor in all detail. In contrast to the quenched case, the theory has a mild sign problem that manifests itself by giving a spectral density that is not positive definite as the spectral gap closes.

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1. Introduction

The low-lying spectrum of the Dirac operator is a fascinating subject, which also contains important physics. Recently, three of the present authors presented an analysis of the quenched spectrum of the Wilson Dirac operator D_W [1]. Focus was on the low-lying real modes of D_W and the Hermitian counterpart $D_5 = \gamma_5(D_W + m)$. Effects of the lattice spacing a were taken into account to leading order. A chiral Random Matrix Theory that encapsulates these leading order terms was then established. As the size N of the random matrices goes to infinity, a scaling regime is reached where this chiral Random Matrix Theory coincides with what one obtains from the Wilson chiral Lagrangian to leading order in a. This extends in a precise manner the universal Random Matrix Theory results of continuum fermions [2, 3] to Wilson fermions in the microscopic scaling regime. In particular, the appropriate definition of an ε-regime [4] for the low-lying eigenvalues of the Wilson Dirac operator is identified [1]. The corresponding spectrum away from the microscopic limit was first analyzed at the mean field level by Sharpe in ref. [5]. The Letter [1] was very much motivated by that work and a wish to understand in detail and at an analytical level some of the results of the lattice simulations in ref. [6].

Here we report on a study of the effect of dynamical quarks on these results. Because the case of two light flavors is significantly more difficult in terms of computational complexity, we take here the first step of unquenching by considering $N_f = 1$. This case is of interest in its own right because there are no Goldstone bosons and hence no chiral Lagrangian at our disposal. Nevertheless, effective field theory can be used to describe in a precise way the leading-order effects of Wilson terms in lattice gauge theory also in this case. By projecting onto sectors of a fixed number ν of real modes (counted with the sign of their chiralities, see below), we can also establish a chiral Random Matrix Theory with exactly the same properties as the effective field theory in the scaling limit. As for continuum fermions, the effective field theory in each fixed sector looks just like the leading term in an ε-regime counting of a chiral Lagrangian. Yet there are no Goldstone bosons and hence no way to systematically introduce a full-fledged space-time dependent chiral Lagrangian which could incorporate sub-leading effects of an associated ε-expansion.

2. The effective field theory

Chiral symmetry for QCD with just one flavor is broken explicitly due to the $U(1)$ anomaly, and there are no Goldstone bosons. As a consequence, we do not have the toolbox of chiral Perturbation Theory available. Leutwyler and Smilga [4] faced a similar situation when dealing with the spectrum of the continuum Dirac operator, and we will here follow the same line of reasoning. In the continuum, the leading effect of a quark mass m is proportional to the four-volume V. Because the logarithmic derivative yields the chiral condensate Σ, it follows that the partition function must read $Z \sim \exp[m\Sigma V]$. This term corresponds to $m\bar{\psi}\psi$ in the QCD Lagrangian. For Wilson fermions, the Symanzik effective action has additional operators $\sim a^2(\bar{\psi}\psi)^2$. Such terms give an additional contribution to the free energy of order a^2 so that now

$$Z \;=\; \exp\left[m\Sigma V - 2W_8 V a^2\right] \tag{2.1}$$

where W_8 is a so far unknown constant. We have chosen the parametrization so that this constant is naturally positive (the factor of 2 is for later convenience). As argued in ref. [1] a positive sign of W_8 is follows from from the Hermiticity properties of D_W. We define the appropriate ε-regime here by requiring that

$$\hat{m} \equiv m\Sigma V \qquad \text{and} \qquad \hat{a}^2 \equiv a^2 W_8 V$$

remain fixed as $V \to \infty$. This is the regime where there is competition between m and a^2 effects and one can imagine that a phase transition may occur. This turns out to be a transition to the Aoki phase [7] (see also [8]). Other countings can also be considered [9], but they are not of direct interest to us here.

In the continuum, a chiral rotation α shifts the vacuum angle $\theta \to \theta + \alpha$. Noting that the a^2-term in the effective action comes from operators $a^2(\bar{\psi}\psi)^2$, we define

$$Z(\theta) = \exp\left[m\cos(\theta)\Sigma V - 2W_8 V a^2 \cos(2\theta)\right], \tag{2.2}$$

and its Fourier components read:

$$Z_\nu \equiv \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{i\nu\theta} \exp\left[m\cos(\theta)\Sigma V - 2W_8 V a^2 \cos(2\theta)\right] \tag{2.3}$$

Inverting this, we recover the original partition function as a sum over each Z_ν after setting $\theta = 0$:

$$Z(\theta = 0) = \sum_{\nu=-\infty}^{\infty} Z_\nu. \tag{2.4}$$

Let us now look at each Z_ν separately. Interestingly,

$$Z_\nu \equiv \int_{U(1)} dU \ \det(U)^\nu \exp\left[\frac{1}{2} m\Sigma V \mathrm{Tr}[U + U^{-1}] - W_8 V a^2 \mathrm{Tr}[U^2 + U^{-2}]\right]. \tag{2.5}$$

This looks exactly like the zero-momentum piece of the leading terms of a $U(1)$ chiral Lagrangian for Wilson fermions [10]. However, there are no Goldstone bosons, and the $U(1)$ 'degree of freedom' results from the angular integration variable of the Fourier transform.

For general N_f there would also be double-trace terms like $(\mathrm{Tr}[U + U^{-1}])^2$ and $(\mathrm{Tr}[U - U^{-1}])^2$, but in this $U(1)$ case such terms just change the normalization of W_8 after use of elementary trigonometric identities.

3. Low-lying modes of the Wilson Dirac Operator

To get spectral information for the Wilson Dirac operator we need either

* Pairs of extra species with opposite statistics (the graded method [12]) or
* Replicas [11, 2].

Here we use the graded method. We thus add a bosonic quark and a corresponding additional fermionic quark, both with appropriate sources. When these sources are set equal to each other, the two additional determinants exactly cancel each other. In this limit, the partition function of this graded theory therefore equals the partition function of QCD with the original one flavor.

The graded method can be used in the effective field theory as well. Additional Grassmann integrations truncate and trivially converge, but care must be taken to ensure convergence of the *bosonic* integrations. This problem has been solved in the context of continuum fermions in ref. [12]. The graded partition function is

$$Z_{2|1}(\hat{\mathscr{M}}, \hat{\mathscr{Z}}) = \int_{Gl(2|1)} dU \, \mathrm{Sdet}(U)^{\nu} e^{i\frac{1}{2}\mathrm{STr}(\hat{\mathscr{M}}[U-U^{-1}])+i\frac{1}{2}\mathrm{STr}(\hat{\mathscr{Z}}[U+U^{-1}])+\hat{a}^2\mathrm{STr}(U^2+U^{-2})}. \tag{3.1}$$

The source terms are

$$\hat{\mathscr{M}} = \begin{pmatrix} \hat{m}_f & 0 & 0 \\ 0 & \hat{m} & 0 \\ 0 & 0 & \hat{m}' \end{pmatrix} \qquad \hat{\mathscr{Z}} = \begin{pmatrix} \hat{z}_f & 0 & 0 \\ 0 & \hat{z} & 0 \\ 0 & 0 & \hat{z}' \end{pmatrix}$$

and when $\hat{m} = \hat{m}'$ and $\hat{z} = \hat{z}'$ a little miracle occurs: the graded partition function becomes equal to the original partition function of $N_f = 1$. This follows from general principles, but it arises in a highly non-trivial manner from the actual integrations of eq. (3.1). An explicit parametrization of the graded matrix U has been provided in ref. [12]:

$$U = \begin{pmatrix} e^{it+iu}\cos(\theta) & ie^{it+i\phi}\sin(\theta) & 0 \\ ie^{it-i\phi}\sin(\theta) & e^{it-iu}\cos(\theta) & 0 \\ 0 & 0 & e^{s} \end{pmatrix} \exp \begin{pmatrix} 0 & 0 & \alpha_1 \\ 0 & 0 & \alpha_2 \\ \beta_1 & \beta_2 & 0 \end{pmatrix}$$

where $\theta, t, u \in [-\pi, \pi]$ and $\phi \in [0, \pi]$. The bosonic degree of freedom s is integrated over the real line, and the α's and β's are Grassmann variables.

A careful reader will have noticed the unusual form of (3.1). Before extending the theory to the graded case, a rotation $U \to iU$ has been performed. In the original $U(1)$-integral this simply shifts the angular variable by $\pi/2$, while still integrating it over the full circle. Doing such a rotation prior to extending the action to the graded case corresponds to a particular path of integration for the bosonic variable s. It is the integration path used in eq. (3.1) which corresponds to a non-Hermitian (but γ_5-Hermitian) Wilson Dirac operator D_W.

The integrals in eq. (3.1) are tedious but doable. We have performed the Grassmann integrations and one of the angular integrations explicitly. The resulting expressions will be published elsewhere. Here we choose to present our results in a graphical manner.

While the Wilson Dirac Operator is not Hermitian, it is important that it nevertheless retains γ_5-Hermiticity: $D_W^\dagger = \gamma_5 D_W \gamma_5$. Indeed, it is this property that ensures Hermiticity of D_5. The spectrum of D_W thus lies in the complex plane, each non-real eigenvalue being matched by its complex conjugate partner. To compute the spectrum of the (non-Hermitian) Wilson Dirac operator by analytical means is slightly cumbersome because of this. However, D_W also has a certain number of eigenvalues sitting on the real line. The distribution of the chiralities of the corresponding states over the Dirac spectrum is much easier to compute. To this end, let us define a resolvent (and put $\hat{z} = \hat{z}' = 0$)

$$\Sigma^{\nu}(\hat{m}_f, \hat{m}) \equiv \lim_{\hat{m}' \to \hat{m}} \frac{\partial}{\partial \hat{m}} \ln Z_{2|1}^{\nu}(\hat{m}_f, \hat{m}, \hat{m}'). \tag{3.2}$$

The discontinuity across the real line gives us the distribution of the chiralities over the Dirac spectrum

$$\rho_\chi^\nu(\hat{\zeta}) \equiv \sum_{k, \zeta_k \in \mathscr{R}} \delta(\hat{\zeta} - \hat{\zeta}_k)\, \chi_k = \frac{1}{\pi} \mathrm{Im}[\Sigma^\nu(\hat{m}_f, \hat{\zeta})] \tag{3.3}$$

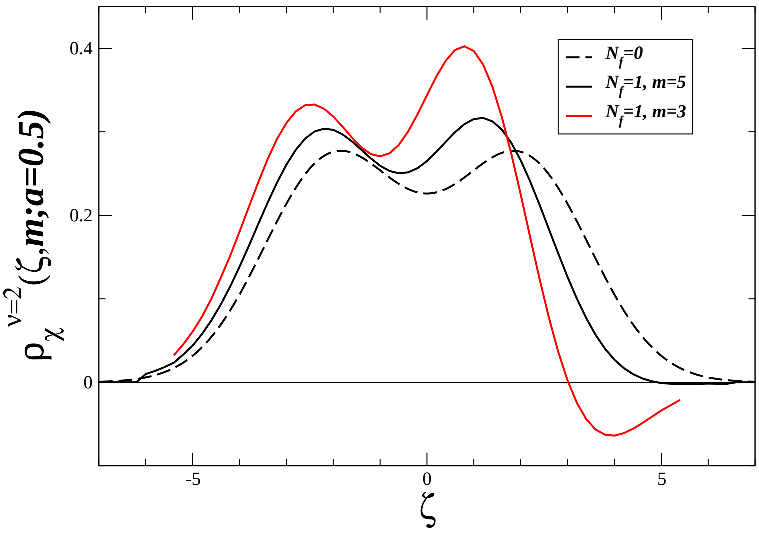

Figure 1: The density of chiralities of the Wilson Dirac operator.

with the chirality $\chi_k = \mathrm{sign}(\langle k|\gamma_5|k\rangle)$.

The integral over this distribution is normalized to ν,

$$\int_{-\infty}^{\infty} d\hat{\zeta}\ \rho_\chi^\nu(\hat{\zeta}) \ = \ \nu. \tag{3.4}$$

The index ν counts chiralities of the real modes of D_W in Z_ν: $\nu = \sum_n \chi_n$ where n runs over all real modes. In the limit of small a the probability of finding configurations with real modes that have chiralities of different signs vanishes. In that limit ν is simply the number of real modes. The non-positivity of the density of real modes is unrelated to this: a change of sign occurs at $\hat{\zeta} = \hat{m}$. Only when $\hat{m}$ is on the order of or less than $8\hat{a}^2$ does this have significance in the density since otherwise the density is very small anyway. We show an example of the distribution of the chiralities over the real modes in fig. 1.

We now wish to compute the spectrum of the Hermitian Wilson Dirac operator $D_5 = \gamma_5(D_W + m)$. To that end, introduce the new resolvent

$$G^\nu(\hat{z},\hat{m}) \ \equiv \ \lim_{\hat{z}'\to\hat{z}} \frac{\partial}{\partial\hat{z}} \ln Z^\nu_{2|1}(\hat{m},\hat{m},\hat{m},0,\hat{z},\hat{z}') \ = \ \left\langle \mathrm{Tr}\left(\frac{1}{D_5+\hat{z}}\right)\right\rangle \tag{3.5}$$

and take the discontinuity across the real line. This gives us the spectral density of D_5:

$$\rho_5^\nu(\hat{x}) \ = \ \frac{1}{\pi}\mathrm{Im}[G^\nu(\hat{x},\hat{m})]. \tag{3.6}$$

Let us first consider the spectrum corresponding to $\nu = 0$. In fig. 2 we show the density for fixed $\hat{m} = 5$ and various values of $\hat{a}^2$. When $\hat{a}$ is small, a gap clearly opens up around $\pm\hat{m}$, as it should. The spectrum of D_5 then approaches the standard spectrum of the continuum Dirac operator with one massive fermion [13], up to a trivial change of variables. In contrast to the

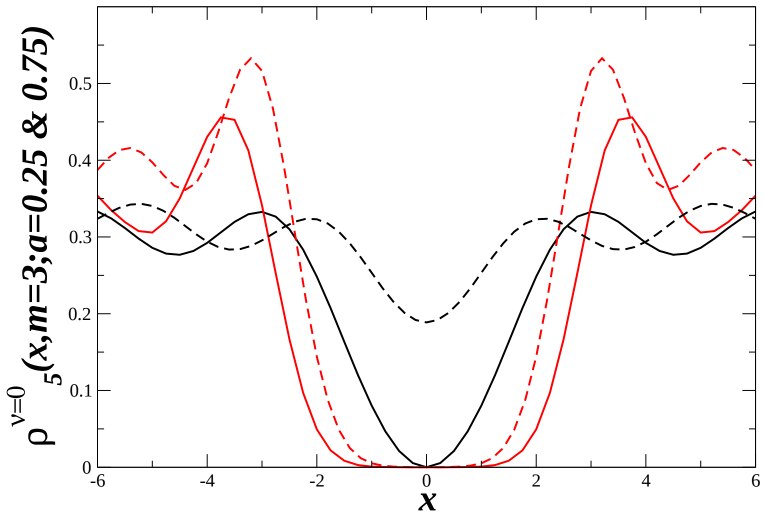

Figure 2: Spectral density of the Hermitian Wilson Dirac operator for $\nu = 0$. (Dashed lines $N_f = 0$.)

quenched spectrum, the microscopic spectrum of D_5 in this $N_f = 1$ theory always has a zero at the origin. This is clearly visible in fig. 2.

There are other differences with the quenched spectrum. Because of the real modes, the spectrum of D_5 can change sign in the $N_f = 1$ theory. A negative density simply corrersponds to a theory with a sign problem: the Boltzmann weight in the path integral is not positive definite. The existence of a negative density is thus a potential problem for numerical simulations. Fortunately the sign problem in this theory is mild: it is only signifact in the small-m limit, and it can be postponed by going to smaller lattice spacings a. We illustrate this phenomenon in fig. 3, where we consider a case with $\nu = 1$. The analytical understanding we can provide here should be valuable for numerical simulations.

4. Conclusions

We have presented an explicit computation of the microscopic eigenvalue distributions of the Wilson Dirac operator, the real modes of this operator, and the eigenvalues of the Hermitian Wilson Dirac operator. We have focused on effects that most clearly distinguish a theory with dynamical quarks from the quenched counterpart [1]. A sum over the index ν can be done straightforwardly. This will be presented elsewhere.

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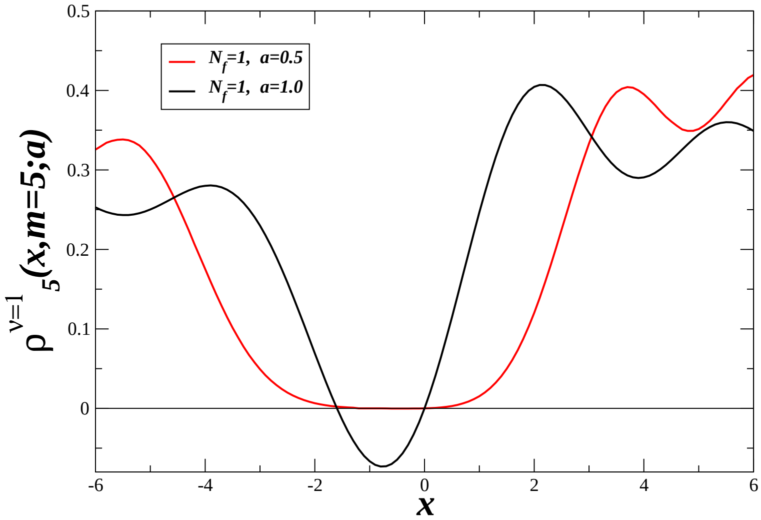

Figure 3: Same as fig.2, but now for $\nu = 1$. The spectral density is no longer positive.

References

[1] P. H. Damgaard, K. Splittorff and J. J. M. Verbaarschot, Phys. Rev. Lett. **105** (2010) 162002.

[2] E. V. Shuryak and J. J. M. Verbaarschot, Nucl. Phys. A **560**, 306 (1993) J. J. M. Verbaarschot and I. Zahed, Phys. Rev. Lett. **70**, 3852 (1993) J. J. M. Verbaarschot, Phys. Rev. Lett. **72**, 2531 (1994).

[3] G. Akemann, P. H. Damgaard, U. Magnea and S. Nishigaki, Nucl. Phys. B **487**, 721 (1997)

[4] H. Leutwyler and A. V. Smilga, Phys. Rev. D **46**, 5607 (1992).

[5] S. R. Sharpe, Phys. Rev. D **74**, 014512 (2006).

[6] L. Del Debbio, L. Giusti, M. Luscher, R. Petronzio and N. Tantalo, JHEP **0602**, 011 (2006).

[7] S. Aoki, Phys. Rev. D **30** (1984) 2653.

[8] K. M. Bitar, U. M. Heller and R. Narayanan, Phys. Lett. B **418**, 167 (1998).

[9] O. Bar, S. Necco and S. Schaefer, JHEP **0903** (2009) 006;
O. Bar, S. Necco and A. Shindler, JHEP **1004** (2010) 053.

[10] S. R. Sharpe and R. L. Singleton, Phys. Rev. D **58**, 074501 (1998);
G. Rupak and N. Shoresh, Phys. Rev. **66**, 054503 (2002);
O. Bar, G. Rupak and N. Shoresh, Phys. Rev. D **70**, 034508 (2004).

[11] P. H. Damgaard and K. Splittorff, Phys. Rev. D **62** (2000) 054509.

[12] P. H. Damgaard, J. C. Osborn, D. Toublan and J. J. M. Verbaarschot, Nucl. Phys. B **547**, 305 (1999).

[13] P. H. Damgaard and S. M. Nishigaki, Nucl. Phys. B **518** (1998) 495.