Discretization Phase Transitions and Wilson Dirac Spectra

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Relevant Papers

P.H. Damgaard, K. Splittorff and J. J. M. Verbaarschot, Microscopic Spectrum of the Wilson Dirac Operator, Phys. Rev. Lett.

G. Akemann, P.H. Damgaard, K. Splittorff and J. J. M. Verbaarschot, Spectrum of the Wilson Dirac Operator at Finite Lattice Spacing, to be published.

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M. Kieburg, J. J. M. Verbaarschot, S. Zafeiropoulos Eigenvalue Density of the Non-Hermitian Wilson Dirac Operator, Phys. Rev. Lett. **108** (2012) 022001 arXiv:1109.0656 [hep-lat].

M. Kieburg, K. Splittorff and J. J. M. Verbaarschot, The Realization of the Sharpe-Singleton Scenario, Phys. Rev. **D85**(2012) 094011 [arXiv:1202.0620 [hep-lat]].

M. Kieburg, K. Splittorff and J. J. M. Verbaarschot, to be published.

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I. Motivation

Wilson Dirac Spectra

Motivation



Distribution of the smallest eigenvalue of the Hermitian Wilson Dirac operator on a 64×32^3 lattice for two different values of the quark mass.

Del Debbio-Giusti-Lüscher-Petronzio-Tantalo-2005

Can we understand this scaling behavior?



Scaling of the width of the distribution. Del Debbio-Giusti-Lüscher-Petronzio-Tantalo-2005

First Order Behavior



Plaquette expectation value showing two first order minima.

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I. Wilson Dirac Operator

Wilson Dirac Operator

 γ_5 -Hermiticity

Chiral Lagrangian

 ϵ -Expansion

Wilson Dirac operator

Wilson introduced the Wilson term to eliminate doublers

$$D_W = \frac{1}{2}\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - \frac{1}{2}a\nabla^*_\mu\nabla_\mu \equiv D + W.$$



γ_5 -Hermiticity



- Two complex eigenvalues can collide and turn into a pair of real eigenvalues with opposite chirality. The number of real eigenvalues does not change under small deformations of the operator.
- Unpaired real eigenvalues cannot move in the complex plane, and the net chirality is equal to the index of the Dirac operator.
- What is the distribution of the real eigenvalues?
- ► Diagonalization of D_W violates γ_5 -Hermiticity. D_W can only be brought in the pseudo-diagonal form $\begin{pmatrix} x & y \\ -y & x \end{pmatrix}$.

Chiral Lagrangian

Chiral Lagrangian for Wilson Fermions

$$-\mathcal{L} = \frac{1}{2}mV\Sigma\mathrm{Tr}(U+U^{\dagger}) - \frac{F_{\pi}^{2}}{4}\mathrm{Tr}\partial_{\mu}U\partial_{\mu}U^{\dagger}$$
$$-a^{2}VW_{6}[\mathrm{Tr}(U+U^{\dagger})]^{2} - a^{2}VW_{7}[\mathrm{Tr}(U-U^{\dagger})]^{2} - a^{2}VW_{8}\mathrm{Tr}(U^{2}+U^{-2}).$$

Sharpe-Singleton-1998, Rupak-Shoresh-2002, Bär-Rupak-Shoresh-2004, Damgaard-Splittorff-JV-2011

Partition function for fixed index

$$Z_{\nu} = \int_{U \in U(N_f)} dU \det^{\nu} e^{-\int d^4 x \mathcal{L}}$$

► For twisted mass fermions the mass term is replaced by

$$\frac{i}{2}\mu V\Sigma \mathrm{Tr}\tau_3(U-U^{\dagger}).$$

The ϵ Expansion

Expansion of the chiral Lagrangian with

$$p \sim \frac{1}{L}, \qquad m \sim \frac{1}{V}, \qquad \lambda = \frac{1}{V}, \qquad a \sim \frac{1}{\sqrt{V}}.$$

To leading order the partition function factorizes into a zero momentum part and a nonzero momentum part.

The thermodynamic limit with mV, λV and a^2V fixed is known as the microscopic limit of QCD.

The zero momentum part is equivalent to a random matrix theory with the same global symmetries.

Although the physical quark mass is not in the microscopic domain, eigenvalues of the Dirac operator are in the microscopic domain.

Positivity Requirements

Collective Eigenvalue Fluctuation and Trace Squared Terms

Signs of Low Energy Constants

Positivity Requirements

► $\gamma_5(D_W + m)$ is Hermitian so that the QCD partition function is positive definite for an even number of flavors and fixed index.

The corresponding chiral partition function should have the same positivity requirements. In particular, this is the case in the ϵ domain.

This puts constraints on the parameters of the chiral Lagrangian.

Mass Dependence of Partition Function



By changing variables $U \rightarrow iU$ it follows that

$$Z_{\nu}^{\chi N_f}(0,0,W_8) = (i)^{N_f \nu} Z_{\nu}^{\chi N_f}(0,0,-W_8).$$

Positivity for all ν requires $W_8 > 0$. From the small *a* -expansion of the partition function one obtains

$$W_8 - W_6 - W_7 > 0.$$

Akemann-Damgaard-Splittorff-JV-2010

Eigenvalue Fluctuations and Low Energy Constants

- Since the QCD partition function is the average of a determinant, eigenvalue fluctuations determine the low-energy constants.
- We have seen that the broadening of the Dirac spectrum in the complex plane determines the value of W_8 .
- ▶ Which spectral fluctuations are responsible for W_6 and W_7 ?

Trace Squared Terms

- Trace squared terms can be linearized at the expense of a Gaussian integral and then can be added to the mass term.
- This random mass can interpreted in terms collective fluctuations of Dirac eigenvalues.
- Collective spectral fluctuations must be consistent with the symmetries of the QCD Dirac operator.

Collective Eigenvalue Fluctuations and W_6

For $W_6 < 0$ we have

$$e^{-a^2 V W_6 \operatorname{Tr}^2(U+U^{-1})} \sim \int dy e^{-y^2/(16V|W_6|a^2) - \frac{1}{2}y \operatorname{Tr}(U+U^{-1})}$$

The partition function can be written as

$$Z(m; W_6, W_8) = \int dy e^{-y^2/16V|W_6|a^2} Z(m - y; W_6 = 0, W_8)$$
$$= \int dy e^{-y^2/a_6V|W_6|a^2} \langle \prod_k (m - y - \lambda_k) \rangle.$$

A negative W_6 therefore corresponds to collective fluctuations of the strip of eigenvalues.

A positive W_6 would correspond to collective eigenvalues fluctuations in the imaginary direction which is not possible. This suggests that $W_6 < 0$. Kieburg-Splittorff-JV-2012

Collective Spectral Fluctuations of D_W



Collective fluctuations consistent with complex conjugation.

What is the source of these fluctuations in terms of gauge field fluctuations? Kieburg-Splittorff-JV-2013

Collective Fluctuations in Terms of D_5



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Signs of Low-Energy Constants

- ► $W_8 > 0$ independent of the value of W_6 and W_7 . Akemann-Damgaard-Splittorf-JV-2010,Hansen-Sharpe-2011
- ► Positivity of the QCD partition function requires that $W_8 W_6 W_7 > 0$.
- Interpretation in terms of eigenvalue fluctuations requires that $W_6 < 0$, $W_7 < 0$.

• Twisted mass Wilson fermions lattice simulations find $m_0^{PS} < m_+^{PS}$

$$m_0^{\text{PS}^2} - m_{\pm}^{\text{PS}^2} = \frac{16a^2(W_8 + 2W_6)}{F_{\pi}^2} \quad \begin{array}{r} \text{Iwasaki} & 0.0049(38) & -0.0119(17) \\ \text{Ilsym} & 0.0082(34) & -0.0138(22) \end{array}$$

Münster-2004, Sharpe-Wu-2004
$$\begin{array}{r} \text{Herdoiza-etal-2013} \\ \text{Extrapolation to the chiral limit} \end{array}$$

Sign of Low Energy Constants

A consistent picture emerges if

$$W_8 > 0, \quad W_6 < 0, \quad W_7 < 0,$$

 $W_8 + 2W_6 < 0.$

Kieburg-Splittorff-JV-2012, Hansen-Sharpe-2011

IV. Wilson Random Matrix Theory

Random Matrix Theory

Chiral Symmetry Breaking

Random Matrix Theory for the Wilson Dirac Operator

Since the chiral Lagrangian is determined uniquely by symmetries, in the microscopic domain it also can be obtained from a random matrix theory with the same symmetries. In the sector of index ν the random matrix partition function is given by

$$Z_{N_f}^{\nu} = \int dA dB dW \det^{N_f} (D_W + m + z\gamma_5) P(D_W),$$

with

$$D_W = \begin{pmatrix} aA & C+aD \\ -C^{\dagger}+aD^{\dagger} & aB \end{pmatrix} \quad \text{and} \quad A^{\dagger} = A, \qquad B^{\dagger} = B.$$

A is a square matrix of size $n \times n$, and B is a square matrix of size $(n + \nu) \times (n + \nu)$. The matrices C and D are complex $n \times (n + \nu)$ matrices. Damgaard-Splittorff-JV-2010

Chiral Symmetry Breaking

As a function of a this random matrix ensemble is a transition from the Chiral Unitary Ensemble to the Unitary Ensemble.

The Chiral Unitary Ensemble is equivalent to QCD in the microscopic domain with chiral symmetry breaking pattern $U(N_f) \times U(N_f) \rightarrow U(N_f)$

The Unitary Ensemble is Equivalent to QCD in 3 dimensions with symmetry breaking pattern $U(N_f) \rightarrow U(N_f/2) \times U(N_f/2)$.

For two flavors this gives two massless pions.

V. Phase Diagram

Mean Field Limit

Aoki Phase

First Order Scenario

Chiral Lagrangian

Chiral Lagrangian for Wilson Fermions in the microscopic domain

$$-\mathcal{L} = \frac{1}{2}mV\Sigma \text{Tr}(U+U^{\dagger})$$

$$-a^{2}VW_{6}[\text{Tr}(U+U^{\dagger})]^{2} - a^{2}VW_{7}[\text{Tr}(U-U^{\dagger})]^{2} - a^{2}VW_{8}\text{Tr}(U^{2}+U^{-2}).$$

This is also the Lagrangian for the mean field calculation.

Sharpe-Singleton-1998, Sharpe-Wu-2004, Golterman-Sharpe-Singleton-2005

Mean Field Limit

$$U = V \begin{pmatrix} e^{i\theta_1} & 0 \\ 0 & e^{i\theta_2} \end{pmatrix} V^{-1} \qquad \qquad Z = \int d\theta_1 d\theta_2 \sin^2 \frac{\theta_1 - \theta_2}{2} e^{-S}$$

$$-S = mV\Sigma(\cos\theta_1 + \cos\theta_2) - 4a^2W_6((\cos\theta_1 + \cos\theta_2)^2 + 4a^2W_7(\sin\theta_1 + \sin\theta_2)^2) - 4a^2W_8(\cos^2\theta_1 + \cos^2\theta_2).$$

Normal Phase: $\cos \theta_1 = \cos \theta_2 = \operatorname{sign}(m)$.

Aoki phase: $\cos \theta_1 = \cos \theta_2 = \frac{m\Sigma}{8a^2W_8}$

Because of the Haar measure: $\sin \theta_1 = -\sin \theta_2 = \left(1 - \frac{(m\Sigma)^2}{(8a^2W_8)^2}\right)^{1/2}$

Aoki Phase

$U = \cos\theta + i\sin\theta V \tau_3 V^{\dagger}.$

If $\theta \neq 0$, V contains two directions of U than remain massless. This is the Aoki phase.

The second term gives rise to an isoscalar pseudoscalar condensate.

First Order Scenario



Effetive potential for the order parameter. In the first order scenario (left) there is an effective potential potential between the two minima while in the usual case the effective potential is only slightly tilted by the quark mass.

In terms of the chiral Lagrangian a first order scenario takes place if $2W_6 + W_8 > 0$ when there is a potential barrier between the minima with $\cos \theta_1 = \cos \theta_2 = \pm 1$.

Phase Diagram



Splittorff-Lattice 2012

VI. Spectra and Phases

Chiral Condensate

First Order Scenario and Dirac Spectra

Microscopic Spectral Density of D_W

Mean Field Calculation of the spectral density

Predictions

Spectra and Phases

- A phase transition takes place when the gap closes. This happens when we enter the Aoki phase.
- For the nonhermitian Dirac operator this happens when the cloud of eigenvalues hits the quark mass.
- ► The transition to the Aoki phase is continuous.
- How can we understand the first order behavior in terms of collective fluctuations of Dirac eigenvalues?

First Order Scenario and Dirac Spectra



Mass Dependence of the Chiral Condensate in a First Order Scenario (green) and for the Aoki phase (red). Banks-Casher Relation

$$\Sigma(m) = \lim \frac{1}{V} \sum_{k} \frac{2m}{\lambda_k^2 + m^2}$$

First Order Scenario and Dirac Spectra

- Because the Wilson Dirac operator in neither Hermitian nor anti-Hermitian its eigenvalues can move.
- Because of the fermion determinant they will be repelled from the quark mass.
- The finite jump of the Dirac spectrum results in a first order phase transition.



The fuzzy string of eigenvalues is repelled from the mass, m, which results in a first order phase transition.

Spectral Density of D_W

The spectral density of the complex eigenvalues of the Wilson Dirac operator is given by Kieburg-JV-Zafeiropoulos-2011

$$\rho_c(z, z^*) = |z - z^*|^2 Z_{N_f = -2}(z, z^*; a_*) Z_{N_f = 2}(z, z^*; a_8).$$

For two dynamical quarks with mass m the spectral density is given by

$$\rho_{N_f=2}(z,z^*) = \frac{|z-z^*|^2(z-m^2)(z^*-m)^2 Z_{N_f=-2}(z,z^*;a_8) Z_{N_f=4}(m,m,z,z^*,a_8)}{Z_{N_f=2}(m,m;a_8)}$$



Kieburg-Splittorf-JV-2012

Density of Complex Eigenvalues

$$\rho_{c,N_f}^{\nu}(z,z^*,m;a_6,a_8) = \frac{\int dy e^{-\frac{y^2 V}{16|W_6|a^2}} Z_{N_f}^{\nu}(m-y;0,a_8) \rho_{c,N_f=2}^{\nu}(z-y,z^*-y,m-y;0,a_8)}{Z_{N_f}^{\nu}(m;a_6,a_8)}$$

We work this out for $mV\Sigma \gg 1$ and $a^2W_kV \gg 1$. Then we can use a mean field approximation. The Dirac spectrum is inside a strip

$$\rho_{c,N_f=2}^{\nu,\text{MFT}}(z,z^*,m;0,a_8) = \theta(8a_8^2 - x\Sigma).$$

The mean field limit of the partition function is given by

$$Z_2^{\rm MF}(m;0,a_8) = e^{2mV\Sigma - 4Va_8^2} + e^{-2mV\Sigma - 4Va_8^2} + \theta(8a_8^2 - |m\Sigma|)e^{Vm^2\Sigma^2/8a_8^2 + 4Va_8^2}.$$

Kieburg-Splittorff-JV-2012

The First Order Scenario at Work



The strip of eigenvalues is repelled from the quark mass. The distance between the quark mass and the strip of eigenvalues is given by

 $|m|V - 8(a_8 + 2a_6)V/\Sigma.$

Predictions

Pion mass

Sharpe-Singleton-2004, Münster-2004

$$m_{\pi}^2 = \frac{2|m|\Sigma - 16(W_8 + 2W_6)a^2}{F_{\pi}^2}$$

When $W_8 + 2W_6 < 0$ we have a minimum pion mass. This has been observed in lattice simulations with twisted mass fermions. Jansen-etal-2005



The minimum pion mass is O(a).

The first order scenario has only been observed for dynamical Wilson quarks, whereas the Aoki phase has been found both in the quenched case and in the case with dynamical Wilson quarks.

IV. Other Phases

Lattice simulations show the existence of a phase with

 $\langle \bar{\psi}\gamma_5\psi \rangle \neq 0.$

Azcoiti-Di Carlo-Follana-Vaquero-2013

▶ In terms of eigenvalues of $\gamma_5 D_W$ it is given by

 $\frac{1}{V} \left\langle \sum_{k} \frac{1}{\lambda_k} \right\rangle.$

- What is the source of the asymmetry in the average Dirac spectrum?
- Can we reconcile this phase with Wilson chiral perturbation theory?

VII. Determining the Low Energy Constants

Exact Results

Comparison to Lattice Data

Simple Relations for the Small *a* -Limit

Exact Results

- Low Energy Constants can be obtained by fitting analytical results to lattice data
- ► We will use exact results for Dirac spectral to do so:
 - ★ Density of complex eigenvalues: $\rho_c(z)$
 - ★ Density of the right handed modes: $\rho_r(x)$
 - ★ Density of the left handed modes: $\rho_l(x)$
 - * The chirality distribution: $\rho_{\chi}(x) \equiv \rho_r(x) \rho_l(x)$
 - ★ The eigenvalue density of $\gamma_5 D_W$: $\rho_5(x)$

Damgaard-Splittorff-JV-2010, Akemann-Nagao-2011, Larssen-2012, Kieburg-JV-Zafeiropoulos-2011, Splittorff-JV-2011, Kieburg-Splittorff-JV-2012

More Quenched Lattice Dirac Spectra at fixed ν



The spectrum of the Hermitian Wilson Dirac operator for $\nu = 0$ (top) and $\nu = 1$ (bottom). The blue curve is the WRMT result with $W_8 \neq 0$ and $W_6 = W_7 = 0$ while for the red curve they are nonzero. Deuzeman-Wenger-Wuilloud-2011

Additional Real Modes



Additional number real modes of the Wilson Dirac operator. In the left figure we show the analytical result compared to random matrix simulations (Kieburg-JV-Zafeiropoulos-2011) and in the right figure we show lattice result of (Deuzeman-Wenger-Wuilloud-2011) for two different lattice spacings. The lattice data are consistent with a logarithmic a-dependence.

Eigenvalue Density of $\gamma_5(D_W + m)$



The microscopic spectrum of $\gamma_5(D_W + m)$ for $\nu = 1$ Damgaard-Heller-Splittorff-2012.

The red and blue curves represents the analytical result for the resolvent Splittorff-JV-2011

$$G^{\nu}(m,z;a) = \frac{1}{16a^2\pi} \int \frac{dsdt}{t-is} e^{-[(s+iz)^2 + (t-z')^2]/16a^2} \frac{(m-is)^{\nu}}{(m-t)^{\nu}} \tilde{Z}_{1|1}^{\nu}(\sqrt{m^2+s^2},\sqrt{m^2-t^2};a=1)$$

where

$$\tilde{Z}_{1|1}^{\nu}(x,y;a=0) = \frac{y^{\nu}}{x^{\nu}} [yK_{\nu+1}(y)I_{\nu}(x) + xK\nu(y)I_{\nu+1}(x)]$$

The width of the topological peak behaves as $\, \sim a/\sqrt{V}$.

► The density of the projection of the eigenvalues of D_W on the imaginary axis. According to the Banks-Casher formula we have

$$\Delta = \frac{\pi}{\Sigma V}.$$

▶ The average number of the additional real modes for $\nu = 0$:

 $N_{\text{add}}^{\nu=0} \stackrel{a \ll 1}{=} 2Va^2(W_8 - 2W_7).$

► The width of the Gaussian shaped strip of complex eigenvalues:

$$\frac{\sigma^2}{(\Delta)^2} \quad \stackrel{a \leq 1}{=} \quad \frac{4}{\pi^2} a^2 V(W_8 - 2W_6).$$

Observables in the small *a* **Limit**

The variance of the distribution of chirality over the real eigenvalues:

$$\frac{\langle x^2 \rangle_{\rho_{\chi}^{\nu}}}{\Delta^2} \quad \stackrel{a \leq 1}{=} \quad \frac{8}{\pi^2} V a^2 (\nu W_8 - W_6 - W_7), \ \nu > 0.$$

There are linear dependencies between the relations. This results in the consistency condition

$$\frac{\langle x^2 \rangle_{\rho_{\chi}}^{\nu=1}}{\Delta^2} = \frac{\sigma^2}{\Delta^2} + \frac{2}{\pi^2} N_{\text{add}}^{\nu=0}.$$

Kieburg-JV-Zafeiropoulos-2013

VIII. Overlap Dirac Operator

Random Matrix Overlap Dirac Operator

Aoki Phase for the Overlap Dirac Operator

Overlap Dirac Operator at a = 0

The overlap Dirac operator

$$D_{\rm ov} = 1 + \gamma_5 U {\rm sign}(D_5) U^{-1}, \qquad D_5 = D_W + m \gamma_5$$

- Looks drastic to replace the eigenvalues by their sign, but at zero lattice spacing this is actually exact.
- ► The eigenvectors contain the information on the eigenvalues.

$$D_5 = \begin{pmatrix} u & 0 \\ 0 & v \end{pmatrix} \begin{pmatrix} m & \lambda \\ \lambda & -m \end{pmatrix} \begin{pmatrix} u^{-1} & 0 \\ 0 & v^{-1} \end{pmatrix}$$

► Complete diagonalization by addition rotation with $tan 2\phi_k = \lambda_k/m$

Overlap Dirac Operator at a = 0

- ▶ The projected eigenvalues are given by λ_k/m .
- At nonzero lattice spacing overlap eigenvalues are expected to have correlations that different by O(a) or O(a²) terms
- What happens to eigenvalue correlation of when the Wilson Dirac operator is in the Aoki phase?



The spectral density of the projected overlap Dirac operator for a = 0.3, m = 100 and index $\nu = 0$ and $\nu = 1$. The black curve shows the analytical result and the red and blue curve the result from the computed eigenvalues.



The spectral density of the projected overlap Dirac spectra for m =0.2 and a = 0.05, a = 0.15, a = 0.24, a = 0.35, a = 0.45, a = 0.55 (from top to bottom). The critical value for the transition to the Aoki phase is a = 0.35 (green curve). The curves have been rescaled to have the same small x behavior, separately for the normal phase and the Aoki phase.



Comparison of the spectral density of the overlap Dirac operator for a = 0.15and m = 0.2 and the analytical chiral random matrix theory result. The unfolded eigenvalues are shown right.



Global behavior of the spectral density of the projected overlap Dirac operator for same set of parameters as in Fig. 1.

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- Collective spectral fluctuations drive the first order scenario.
- In the quenched case a transition to the Aoki phase takes place in the approach to the chiral limit at fixed a. A first order scenario is not possible.
- For dynamical quarks both a transition to the Aoki phase and a first order scenario are possible in the approach to the chiral limit. A first order scenario is consistent with the constraints of the the low energy constants and is favored by current lattice simulations.

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- Lattice simulations that show a phase with an isoscalar pseudoscalar condensate should be understood.
- ► The overlap operator is in a different phase when the Wilson Dirac operator is in the Aoki phase, but is very robust outside this phase.