

issues around $N_f = 1$ QCD

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Summary

from $N_f > 1$ QCD to meson masses

$$\mathcal{L}_{QCD} = \sum_f^{N_f} \bar{\psi}_f [\gamma_\mu (\partial_\mu - igA_\mu) - m_f] \psi_f + L_g(A_\nu, \partial_\mu A_\nu)$$

chiral symm.: $SU(N_f)_L \otimes SU(N_f)_R \otimes U(1)_A \otimes U(1)_V$

- $U(1)_A$ **broken** by quantum effects (anomaly $\partial_\mu A^\mu \neq 0$)
- **spontaneous SB**: $SU(N_f)_L \otimes SU(N_f)_R \rightarrow SU(N_f)_V$
→ massless Goldstone bosons
- $m_q > 0 \leftrightarrow$ **explicit SB**: $SU(N_f)_L \otimes SU(N_f)_R$
Goldstone bosons → pseudo Goldstone bosons (pions)

effective theory ($N_f = 3$, $m_u = m_d = m_q$)

- **GMOR** $m_\pi^2 \propto m_q$ (Gell-Mann, Oakes, Renner)
imposes $m_q \geq 0!$

$N_f = 1$ case

$$\mathcal{L}_{QCD} = \bar{\Psi}[\gamma_\mu(\partial_\mu - igA_\mu) - m_q]\Psi + L_g(A_\nu, \partial_\mu A_\nu)$$

no Chiral symmetry: $U(1)_A \otimes U(1)_V$

- $U_A(1)$ **broken** by quantum effects (anomaly)
- no explicit SB for $m_q \neq 0$
- let M_q be the physical quark mass,
 $M_q > 0$ vs $M_q = 0$ ill defined (RGT on m_q ambiguous)

some puzzles in QCD

- mechanisms spontaneous symmetry breaking?
- mechanism generating quark masses?
(responsible for the explicit symmetry breaking...)
- strong CP problem (why is $\theta \simeq 0$?), $m_u \rightarrow 0$ way out?
- role of instantons effects for the chiral symmetry breaking?

Answers, indications from the lattice?

a closer look to the anomalous symmetry $U(1)_A$

consider fermion gauge invariant theory:

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu \mathcal{D}_\mu - m)\psi + \left(\frac{1}{2g^2}\right)\text{Tr} F_{\mu\nu} F^{\mu\nu}, \quad \mathcal{D}_\mu = \partial_\mu + A_\mu$$

anomalous axial symmetry $U(1)_A$: $\psi \rightarrow e^{i\frac{\theta}{2}\gamma_5}\psi$

- functional integral measure: $d\mu \equiv \prod_x [DA_\mu] \mathcal{D}\bar{\psi} \mathcal{D}\psi$
 $U(1)_A$: $d\mu \rightarrow d\mu e^{-i\theta Q[A]}$
 $Q[A] = \int d^4x q(x), \quad q(x) = -\frac{e^2}{16\pi^2} \epsilon^{\mu\nu\lambda\sigma} \text{Tr}(F_{\mu\nu} F_{\lambda\sigma})$
- $U(1)_A$: $m\bar{\Psi}\Psi \rightarrow m \cos(\theta)\bar{\Psi}\Psi + im \sin(\theta)\bar{\Psi}\gamma_5\Psi$
 $U(1)_A$: $m \rightarrow me^{i\gamma_5\theta}$ (rotated into the complex plane)

notice:

- for $\theta = \pi$, $U(1)_A$: $m \rightarrow -m$!
- $\bar{\Psi}\gamma_5\Psi$ and $\{q(x), Q\}$ break CP!

strong CP problem

we noticed for $U(1)_A : \psi \rightarrow e^{i\frac{\theta}{2}\gamma_5}\psi$

- $U(1)_A : \omega \frac{g^2}{16\pi^2} \epsilon^{\mu\nu\lambda\sigma} \text{Tr}(F_{\mu\nu} F_{\lambda\sigma}) \rightarrow (\omega - \theta) \frac{g^2}{16\pi^2} \epsilon^{\mu\nu\lambda\sigma} \text{Tr}(F_{\mu\nu} F_{\lambda\sigma})$
- $U(1)_A : m e^{i\gamma_5\phi} \rightarrow m e^{i(\phi+\theta)\gamma_5}$

$\Rightarrow \bar{\theta} = \theta + \phi$ is unique invariant CP-violating parameter!

experimentally: $\bar{\theta} < 10^{-11}$ (neutron dipole moment)

Strong CP problem: why is $\bar{\theta}$ set to zero?

($\bar{\theta} = 0 \Leftrightarrow$ CP conservation in strong interactions)

- a possible way out? $m_u \rightarrow 0$

CP breaking in effective $N_f = 3$ QCD [Creutz 2003]

eff. theory: $L_{\text{eff}} = \frac{f_\pi^2}{4} \text{Tr}(\partial_\mu \Sigma^\dagger \partial_\mu \Sigma) - \nu \text{ReTr}(\Sigma M)$,

$\Sigma = \exp(i\pi_\alpha \lambda_\alpha / f_\pi) \in SU(3)$

where $M = \text{diag}(m, m_d, m_s) = \frac{m_u + m_d + m_s}{3} 1 - \frac{m_d - m_u}{2} \lambda_3 - 2 \frac{2m_s - m_d - m_u}{2\sqrt{3}} \lambda_8$,

$$\Sigma_{\text{min}} = \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} e^{i\phi_1} & 0 & 0 \\ 0 & e^{i\phi_2} & 0 \\ 0 & 0 & e^{i(\phi_1 + \phi_2)} \end{pmatrix} \right\},$$

with $m_u \sin(\phi_1) = m_d \sin(\phi_2) = -m_s \sin(\phi_1 + \phi_2)$,

degeneracy: $\{\phi_1, \phi_2\} \leftrightarrow \{-\phi_1, -\phi_2\}$ is a symmetry

now recall the following mass relations:

$$m_{\pi_0}^2 \propto \frac{2}{3} \left(m_u + m_d + m_s - \sqrt{m_u^2 + m_d^2 + m_s^2 - m_u m_d - m_u m_s - m_d m_s} \right)$$

$$m_\eta^2 \propto \frac{2}{3} \left(m_u + m_d + m_s + \sqrt{m_u^2 + m_d^2 + m_s^2 - m_u m_d - m_u m_s - m_d m_s} \right)$$

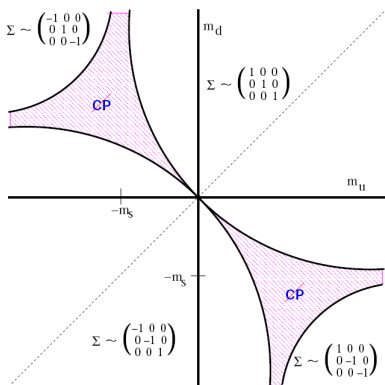
$$\Rightarrow m_{\pi_0}^2 m_\eta^2 \propto m_u m_d + m_u m_s + m_d m_s = 0$$

$$m_{\pi_0} = 0 \Leftrightarrow m_u = -\frac{m_s m_d}{m_s + m_d} \equiv m_c$$

CP breaking in effective $N_f = 3$ QCD [Creutz 2003]

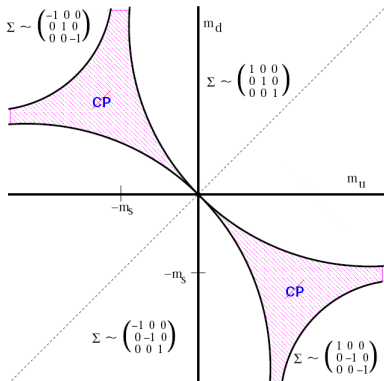
$$m_C = -\frac{m_s m_d}{m_s + m_d}$$

- $m_u \geq m_C$: $\Sigma_{min} = 1$ (unique vacuum)
 - $m_u < m_C$: $\Sigma_{min} = \Sigma_{min}$ (degenerate vacuum)
- pseudoscalar $\langle \pi_0 \rangle \neq 0$: \Rightarrow CP broken



CP breaking in effective $N_f = 3$ QCD [Creutz 2003]

In $N_f = 3$ QCD, after chiral symmetry breaking ($m_u \neq m_d \neq m_s$, no GMOR relation), CP should be spontaneously broken for $m_u < 0$!



toy model toward $N_f = 1$ QCD [Creutz]

consider effective $N_f = 3$ QCD with quark masses $\{m, M, M\}$

$$\Sigma = \exp(i\pi_\alpha \lambda_\alpha / f_\pi) \in SU(3),$$

$$V_{\text{eff}}(\Sigma) \propto -\text{Re Tr}(\mathcal{M}\Sigma) = -\frac{M+m}{2} \text{Re Tr}(\Sigma) + \frac{M-m}{2} \text{Re Tr}(\Sigma h),$$

$$\text{where } \mathcal{M} = \begin{pmatrix} m & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & M \end{pmatrix}, \quad h = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

1. 1 is minimum of $-\frac{M+m}{2} \text{Re Tr}(\Sigma)$
2. $e^{\pm 2\pi i/3} h$ degenerated minima of $\frac{M-m}{2} \text{Re Tr}(\Sigma h)$
 - $m \geq M$: one unique vacuum
 - $m = -M$: two degenerated vacua
 - $\Rightarrow \exists m_c, \text{ s.t. } -M \leq m_c \leq M$ where the symmetry breaks spontaneously

CP violating phase diagram in $N_f = 1$ QCD

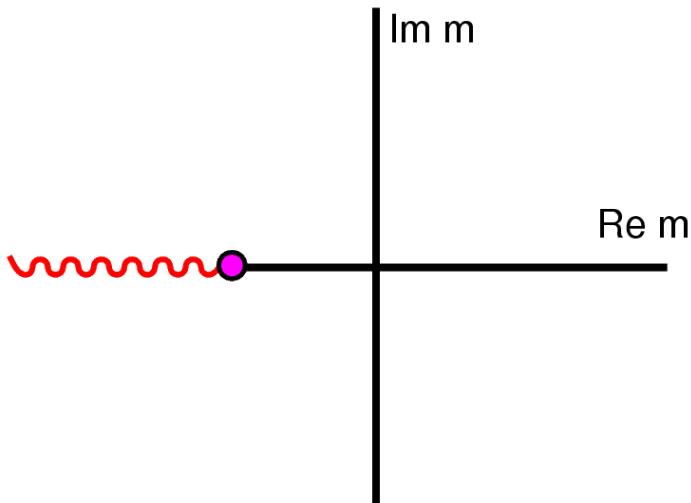
rough argument for CP breaking [Creutz]

$$V_{\text{eff}}(\eta', m_1, m_5) = \frac{m_1 + c}{2} \eta'^2 + \lambda \eta'^4 + im_5 \eta'$$

- $\eta' \equiv \eta_q = \bar{\Psi}_s \gamma_5 \Psi_s$ (pseudoscalar meson state, CP odd)
- $m_{\eta'}^2 = m_1 + c$ effective-theory like
- $U(1)_A : \Psi_s \rightarrow e^{i\gamma_5 \theta/2} \Psi_s, m \bar{\Psi}_s \Psi_s \rightarrow m_1 \bar{\Psi}_s \Psi_s + im_5 \bar{\Psi}_s \gamma_5 \Psi_s$

spontaneous SB of CP expected $\langle \eta' \rangle \neq 0$ for $m_1 < -c$

CP violating phase diagram in $N_f = 1$ QCD



our $N_f = 1$ QCD on the lattice

Partial Quenching: add valence, ghost quarks (graded Lie algebra)

$$\mathcal{L} = \bar{\Psi} D_{PQ} \Psi + L_g, \quad D_{PQ} \equiv \left(\begin{array}{cc|c} \gamma_\mu D_\mu + m_V & 0 & 0 \\ 0 & \gamma_\mu D_\mu + m_S & 0 \\ \hline 0 & 0 & \gamma_\mu D_\mu + \tilde{m} \end{array} \right)$$

Chiral Symm.: $SU(3|2)_L \otimes SU(3|2)_R \otimes U(1)_A \otimes U(1)_V$

- spontaneous SB $SU(3|2)_L \otimes SU(3|2)_R \rightarrow SU(3|2)$

$m_S = m_V = \tilde{m} \rightarrow$ same fermionic determinant as $N_f = 1$ QCD!

Quantities and analytic evaluations

particle spectrum

- "physical states" $\eta_s = \bar{s}\gamma_5 s$, $\sigma = \bar{s}s$
- "unphysical states" degenerate pions octet π^a (s, \bar{s}, v, \bar{v})

PCAC hypothesis

- PCAC quark mass: $am_{PCAC} \equiv \frac{\langle \partial^* A_{x\mu}^+ P_y^- \rangle}{2\langle P_x^+ P_y^- \rangle}$,
 $m_{PCAC}^R = \frac{Z_A}{Z_P} m_{PCAC}$, $\chi_{PCAC} = 2B_0 m_{PCAC}^R$

PQ χ PT

- pion masses $m_\pi^2 = \chi_{PCAC} + \frac{\chi_{PCAC}^2}{16\pi^2 F_0^2} \ln \frac{\chi_{PCAC}}{\Lambda^2} + \dots$ (\sim GMOR)
- decay constant $F_\pi = F_0 \cdot \{1 - \frac{\chi_{PCAC}}{32\pi^2 F_0^2} \ln \frac{\chi_{PCAC}}{\Lambda^2} + \dots\}$

PQ effective theory

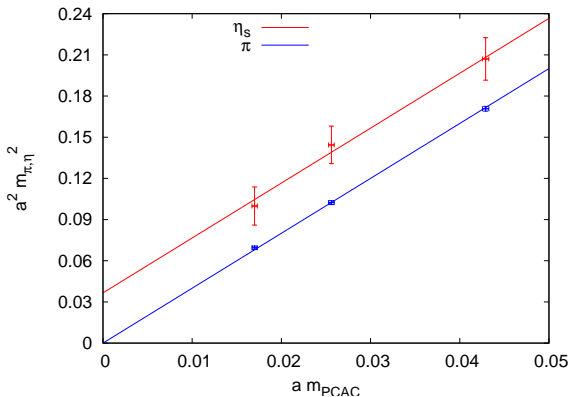
- η_s mass $m_\eta^2 = \frac{m_\phi^2 + \chi_{PCAC}}{1 + \alpha}$

simulation and results

simulation:

tl-improved Symanzik action, PHMC algorithm, stout smearing

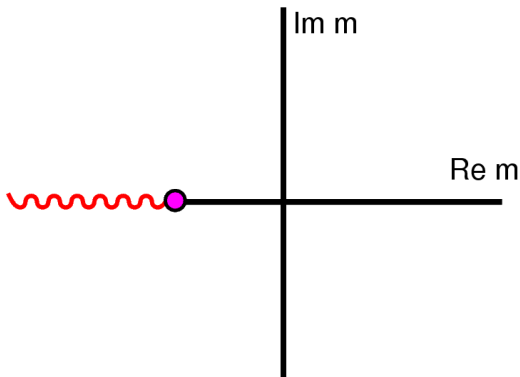
main results: PQ χ PT fits:





work in progress

- refine the statistics on large lattice
- detect CP violation with $\langle \bar{\psi} \gamma_5 \psi \rangle \neq 0$,
decrease m_q controlled by $\kappa = \frac{1}{2am_q + 8}$ for simulations



the fermionic determinant sign is an issue

Vafa-Witten theorem:

- No CP violation if fermionic measure is positive

As our goal is precisely to construct a CP-breaking model

⇒ the sign problem has to be an issue!

statistics with negative determinant

$$Z = \int dA d\bar{\psi} d\psi e^{S_g(A) + \bar{\psi} \mathcal{D}(A) \psi} = \int dA e^{S_g(A)} \det \mathcal{D}(A),$$

Dirac operator $\mathcal{D}(A) = \gamma_\mu (\partial_\mu + igA_\mu) + m$

- $\sigma \equiv \text{sign}(\det \mathcal{D}(A)),$

$$\langle \mathcal{O} \rangle_{e^{S_g+S_f}} = \frac{\int dA \{ \mathcal{O} \sigma \} |\det \mathcal{D}(A) e^{S_g(A)}|}{\int dA \{ \sigma \} |\det \mathcal{D}(A) e^{S_g(A)}|} = \frac{\langle \mathcal{O} \sigma \rangle_{|e^{S_g+S_f}|}}{\langle \sigma \rangle_{|e^{S_g+S_f}|}}$$

- statistical sample: $\langle \mathcal{O} \rangle_{st.} = \frac{\sum_{i=1}^N \mathcal{O}_i}{N}$

$$\Rightarrow \langle \mathcal{O} \rangle_{st.} = \langle \sigma \mathcal{O} \rangle_{st.} / \langle \sigma \rangle_{st.}$$

knowledge of σ 's \Rightarrow statistical corrections (reweighting)

- σ depends on the eigenvalues of $D(A)$

the sign problem...

let us rewrite $\langle \mathcal{O} \rangle_{st.} = \frac{\sum_i^{N^+} \mathcal{O}_i - \sum_j^{N^-} \mathcal{O}_j}{N^+ - N^-}$

(recall $\langle \mathcal{O} \rangle_{st.} = \langle \sigma \mathcal{O} \rangle_{st.} / \langle \sigma \rangle_{st.}$, with $\langle \mathcal{O} \rangle_{st.} = \frac{\sum_{i=1}^N \mathcal{O}_i}{N}$)

- !the sign problem could "destroy" your statistics!

properties, symmetries and boundaries

- $D_W = 1 - \kappa Q$ **Dirac-Wilson operator**
- Q **Hopping matrix** ($Q = \sum_{\mu=1}^4 [1 - \gamma_{\mu} U_{\mu} \delta(x + a_{\mu} - y) + (1 + \gamma_{\mu}) U_{\mu}^{\dagger}(y) \delta(x - a_{\mu} - y)]$)
 1. pairing $\{\lambda, \lambda^*\} / \{\lambda, \lambda^*\}$
(γ_5 hermicity) $Q^{\dagger} = \gamma_5 Q \gamma_5$
 2. pairing $\{\lambda, -\lambda\} / \{1 + \kappa\lambda, 1 - \kappa\lambda\}$
 $\Xi Q \Xi = -Q$, $\Xi(x, y) = (-1)^{x_1 + \dots + x_D} \delta(x - y)$
 3. **bounded** $|\lambda| < 2D$, $D = 4$ / **also bounded**

$Q \equiv \gamma_5 D$ is the **hermitian Dirac operator**

$Q^{\dagger} = Q$ (from $\gamma_5 D \gamma_5 = D^{\dagger}$)

- **real eigenvalues**
 - no known relations between λ_Q 's and λ_D 's in general
 - $D|\psi\rangle = 0 \leftrightarrow Q|\psi\rangle = 0$ (λ_Q small $\leftrightarrow \lambda_D$ small)

sign computation:

available Krilov space methods

$$\mathcal{K}(D_W, v, j) = \text{span}\{v, D_W v, D_W^2 v, \dots, D_W^j v\}$$

- conjugate gradient method on $\gamma_5 D_W$ (expensive, not exact)
- Arnoldi algorithm on D_W
algo. efficiency \propto
 1. matrix size
 2. computed eigenvalues number
 3. eigenvalues separation/density

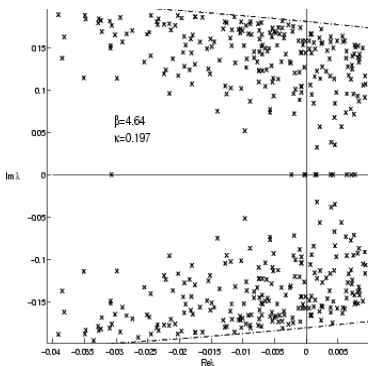
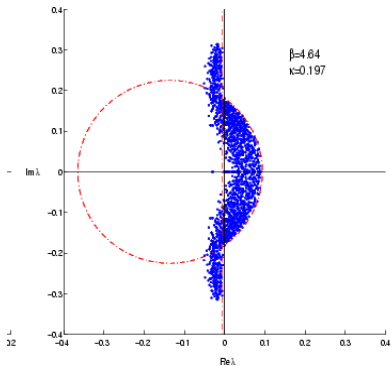
Improvement for 2., 3. (acceleration):

Preconditioning $D \rightarrow P_n(D)$, $P_n(D)$ polynomial:

- which polynomial?

Find a way to get real eigenvalues here...(a year ago)

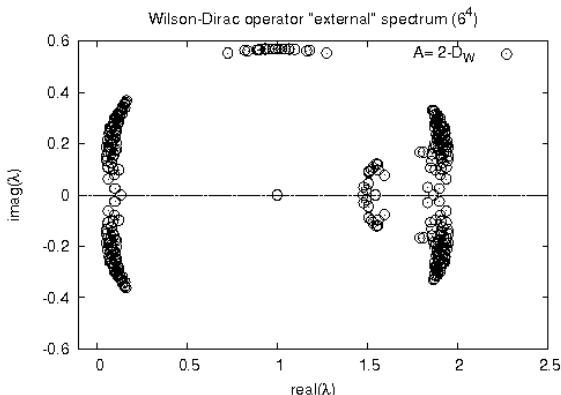
- the outer spectrum for $N_f = 1$ was observed to be similar to the ones for $N_f > 1$
- only the real negative eigenvalues matters! $\lambda \in \mathcal{C}, \lambda\lambda^* = |\lambda|^2$





preconditioning techniques

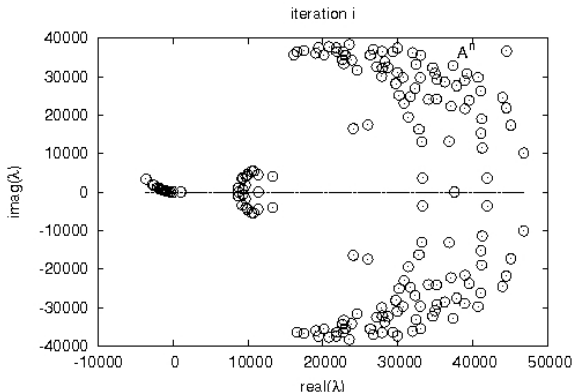
- **basic preconditioning** $D_W \rightarrow P_n(D_W) = (\sigma \mathbf{1} - D_W)^n$:
rotates away complex eigenvalues
($\lambda = \rho e^{i\theta} \rightarrow \lambda^n = \rho^n e^{in\theta}$)





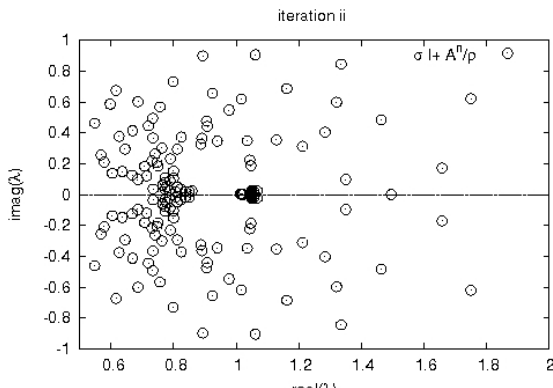
preconditioning techniques

- basic preconditioning $D_W \rightarrow P_n(D_W) = (\sigma \mathbf{1} - D_W)^n$:
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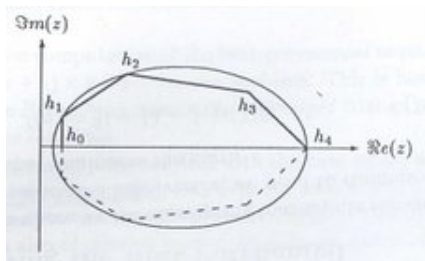


preconditioning techniques

- **basic preconditioning** $D_W \rightarrow P_n(D_W) = (\sigma \mathbf{1} - D_W)^n$:
rotates away complex eigenvalues
($\lambda = \rho e^{i\theta} \rightarrow \lambda^n = \rho^n e^{in\theta}$)
- **iterated version** $P(D_W) \rightarrow (\rho \mathbf{1} - P(D_W)/C_{Ren.})^n$:
"peels" complex eigenvalues away (partially)



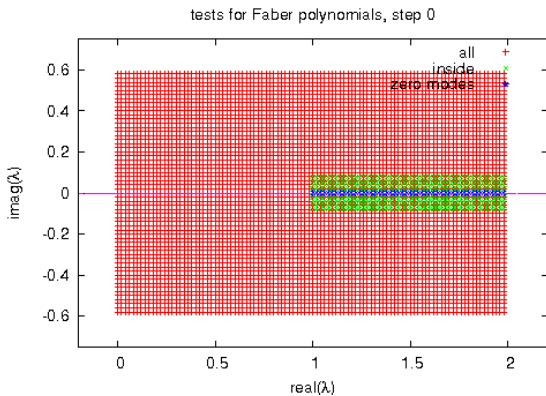
methods with Faber polynomials



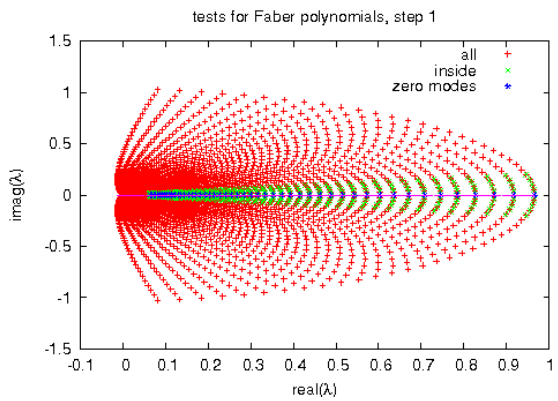
- polygonal hull
- **min max problem**: $\{ \min_{p \in \mathbf{P}_n} \max_{\lambda \in P} |p(\lambda)|, s.t. |p(\lambda_1)| = 1 \}$
- solve it with Faber polynomials



example

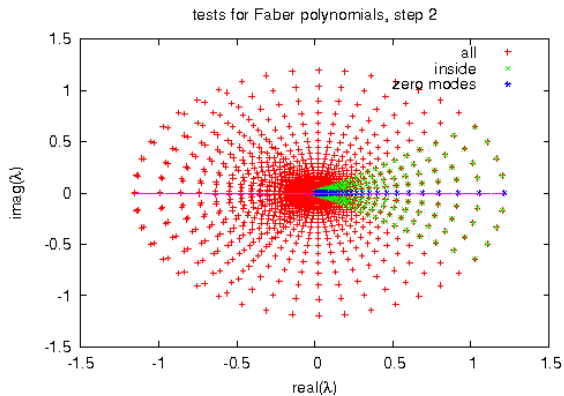


example

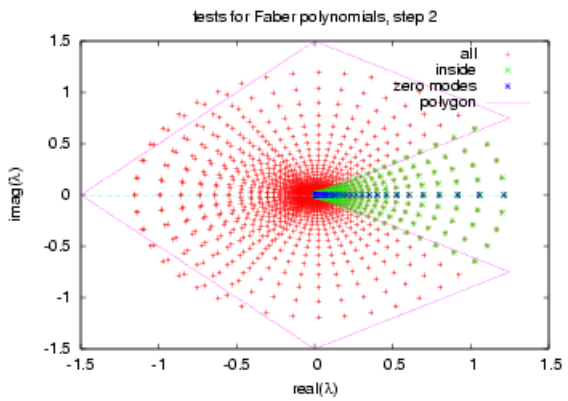




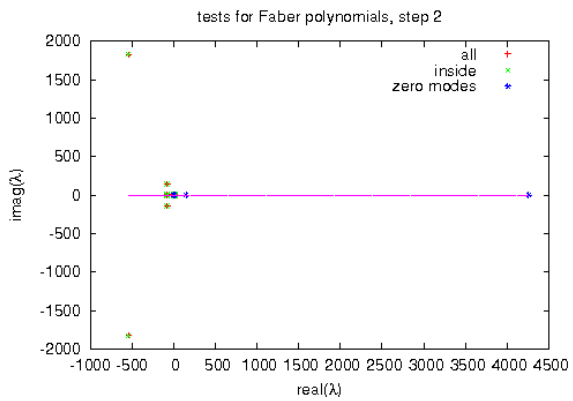
example



example

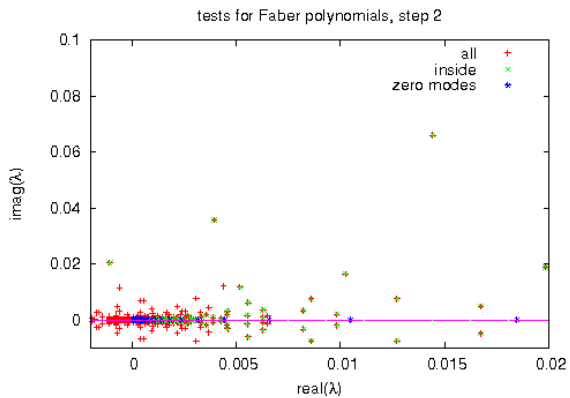


example





example





limitations, issues for optimisation?

- optimal shape for the polygon?
 - mix the methods?
 - polynomial order for the transformation?
 - number of eigenvalues to look for?
 - cpu, memory limitations?
 - inner spectrum eigenvalues density?
1. is there an optimal fairly systematic approach?
(\neq cooking)?
 2. challenge: get all the real eigenvalues!

eigenvalues spectrum, what is interesting there?

configurations generated through a Monte-Carlo algorithm:

"Path integral realisation on the lattice"

eigenvalues spectrum as "fingerprint" of the "lattice" situation
which information is available?

- det. sign

ok

- ...?

some understanding of how the Dirac-Wilson spectrum in
continuum is "translated" onto the lattice is needed

zero modes in continuum

we have $\{\mathcal{D}, \gamma_5\} = 0$

the eigenvalues/eigenvectors are paired $\{\psi, (+iE)\}, \{\gamma_5\psi, (-iE)\}$

($\mathcal{D}\psi = iE\psi \Leftrightarrow \mathcal{D}(\gamma_5\psi) = -iE(\gamma_5\psi)$)

chirality of a state $\chi = (\psi, \gamma_5\psi)$,

$\chi = (\psi, \gamma_5\psi) \neq 0 \Leftrightarrow E = 0$

- only **zero modes** can have non vanishing chirality.
- **Atiyah-Singer/index Theorem** $\nu[A] = n_+ - n_-$
(connects topological charge to the zero modes chirality)

situation on the lattice with the non-hermitian Dirac-Wilson operator

Here we have $D^\dagger = \Gamma_5 D \Gamma_5$,

$$D v_i = \lambda_i v_i \Leftrightarrow (v_i^\dagger \Gamma_5) D = (v_i^\dagger \Gamma_5) \lambda_i^*$$

$$\text{Therefore } v_i^\dagger \Gamma_5 D v_j = \lambda_i^* (v_i^\dagger \Gamma_5 v_j) = \lambda_j (v_i^\dagger \Gamma_5 v_j)$$

we find $v_i^\dagger \Gamma_5 v_j \neq 0 \Leftrightarrow \lambda_i = \lambda_j^*$

- only the real eigenvalues have non-vanishing chiralities

the topological charge on the lattice

the condensate density on the lattice $q(x) \simeq \frac{1}{2} \text{tr}(\gamma_5 D(x, x))$
(from the Casher Banks relation)

$$\text{now } \sum_x q(x) = \frac{1}{2} \text{tr}(\gamma_5 D) = -\frac{1}{2} \text{tr}(2 - \gamma_5 D) =$$

$$-\frac{1}{2} \sum_{\lambda_Q} (2 - \lambda_Q) (\phi_{\lambda_Q}, \gamma_5 \phi_{\lambda_Q})$$

This leads to

- Index theorem on the lattice: $\nu[A] = n_+ - n_-$

the Dirac-Wilson spectrum real eigenvalues

- real eigenvalues can reasonably be interpreted as remnants of continuum zero modes!

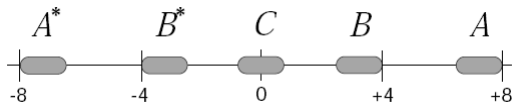
Which informations can be extracted from the zero-modes!?

(dominance of the low eigenmodes (low vs high energy physics)?, spectral decomposition method, topological issues with the fields configurations, consistency checks with random matrix theory,...)

localisation of real eigenvalues: theory vs lattice

16 zeros doublers in the brillouin zone, at $(0, 0, 0, 0)$, ..., (π, π, π, π)
 their global contributions to the topological charge cancel

[Bell, Jackiw]



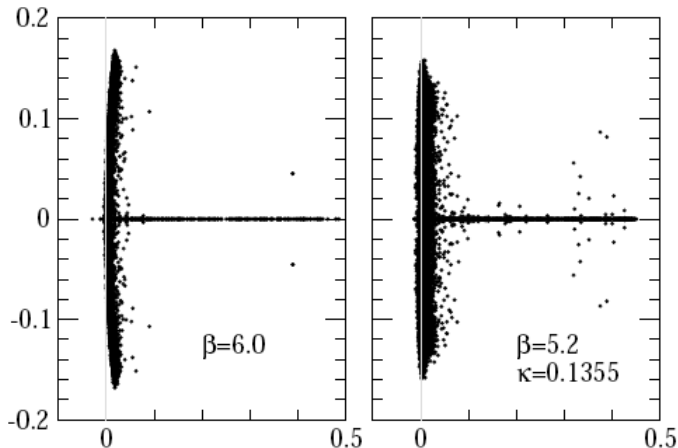
branch	A^*	B^*	C	B	A
$R_- - R_+$	ν	-4ν	6ν	-4ν	ν
corners of B.Z.	(π, π, π, π)	$(\pi, \pi, \pi, 0)$ + 3 perm.	$(\pi, \pi, 0, 0)$ + 5 perm.	$(\pi, 0, 0, 0)$ + 3 perm.	$(0, 0, 0, 0)$



localisation of real eigenvalues: theory vs lattice

!real daily life on the lattice!

[Schierholz 2001]



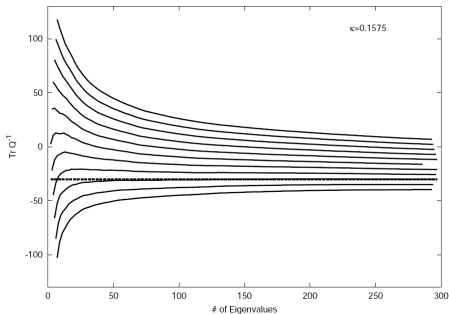
the spectral decomposition approach

idea: reconstruct the Dirac operator from the eigenvectors

- $D^{-1} = \sum_i \frac{1}{\lambda_i^D} \frac{|\psi_i\rangle\langle\psi_i|\gamma_5}{\langle\psi_i|\gamma_5|\psi_i\rangle}$
- $Q^{-1} = \gamma_5 \sum_i \frac{1}{\lambda_i^Q} \frac{|\psi_i\rangle\langle\psi_i|\gamma_5}{\langle\psi_i|\gamma_5|\psi_i\rangle}$

in continuum limit $\nu[A] = \text{tr} Q^{-1}$

Does this connection still hold on the lattice (Q, no level crossing)?



Conclusion

After a theoretical introduction, I discussed/introduced:

- the possibility of CP breaking for negative quark masses in $N_f = 1$ QCD!
- a strategy to test this model with a partially quenched extension of the $N_f = 1$ theory
- the sign problem
- practical techniques to evaluate it with the computation of Dirac-Wilson operator real eigenvalues
- the physical meaning of the real eigenvalues as remnants of the zero modes and the fact that low energy physics is contained in the small eigenvalues