

# Anomalies, gauge field topology, and the lattice

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Three sources of chiral symmetry breaking in QCD

- spontaneous breaking  $\langle \bar{\psi}\psi \rangle \neq 0$ 
  - explains lightness of pions
- implicit breaking of  $U(1)$  by the anomaly
  - explains why  $\eta'$  is not so light
- explicit breaking from quark masses
  - pions are not exactly massless

Rich physics from the interplay of these three effects

Based on very old ideas

- Dashen, 1971: possible spontaneous strong CP violation
  - before QCD!
- 't Hooft, 1976: ties between anomaly and gauge field topology
- Fujikawa, 1979: fermion measure and the anomaly
- Witten, 1980: connections with effective Lagrangians
  - many extensions shortly after
  - I won't use the large N aspects here
- MC 1995: Why is chiral symmetry so hard on the lattice
  - $Z_n$  symmetry and transition at  $\Theta = \pi$

Why rehash old ideas?

- consequences have raised bitter recent controversies

## Axial anomaly in $N_f$ flavor massless QCD

- leaves behind a residual  $Z_{N_f}$  flavor-singlet chiral symmetry
- tied to gauge field topology and the QCD theta parameter

## Consequences

- degenerate quarks with  $m \neq 0$ :
    - first order transition at  $\Theta = \pi$
  - sign of mass relevant for odd  $N_f$ :
    - perturbation theory incomplete
  - $N_f = 1$ : no symmetry for mass protection
  - nontrivial  $N_f$  dependence: invalidates rooting
- } controversial

Consider QCD with  $N_f$  light quarks and assume

- the field theory exists and confines
- spontaneous chiral symmetry breaking  $\langle \bar{\psi}\psi \rangle \neq 0$
- $SU(N_f) \times SU(N_f)$  chiral perturbation theory makes sense
- anomaly gives  $\eta'$  a mass
- $N_f$  small enough to avoid any conformal phase

Use continuum language

- imagine some non-perturbative regulator in place (lattice?)
  - momentum space cutoff much larger than  $\Lambda_{QCD}$
  - lattice spacing  $a$  much smaller than  $1/\Lambda_{QCD}$

Construct effective potential  $V$  for meson fields

- $V$  represents vacuum energy density for a given field expectation
- formally via a Legendre transformation

For simplicity initially consider

- degenerate quarks with small mass  $m$
- $N_f$  even
  - interesting subtleties for odd  $N_f$

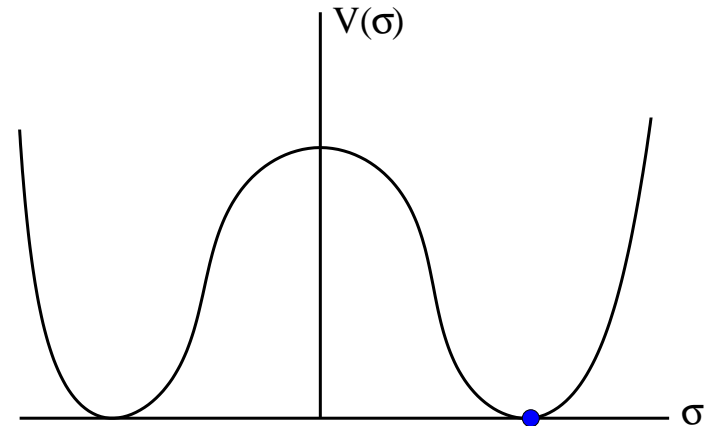
## Work with composite fields

- $\sigma \sim \bar{\psi}\psi$
- $\pi_\alpha \sim i\bar{\psi}\lambda_\alpha\gamma_5\psi$
- $\eta' \sim i\bar{\psi}\gamma_5\psi$

$\lambda_\alpha$ : Gell-Mann matrices for  $SU(N_f)$

## Spontaneous symmetry breaking at $m = 0$

- $V(\sigma)$  has a double well structure
  - vacuum has  $\langle\sigma\rangle = v \neq 0$
  - minimum of  $V(\sigma) = \pm v$



## Ignore convexity issues

- phase separation occurs when a field is in a concave region

## Nonsinglet pseudoscalars are Goldstone bosons

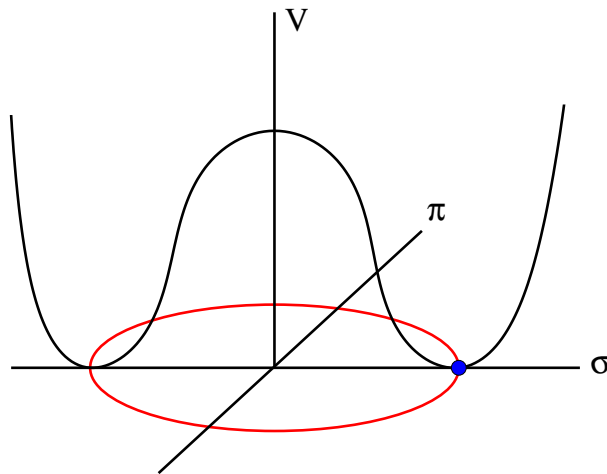
- symmetry under flavored rotations

- $\sigma \rightarrow \cos(\phi)\sigma + \sin(\phi)\pi^\alpha$
- $\pi^\alpha \rightarrow \cos(\phi)\pi^\alpha - \sin(\phi)\sigma$   $(N_f = 2)$

- $\psi \rightarrow e^{i\phi\gamma_5\lambda^\alpha}\psi$

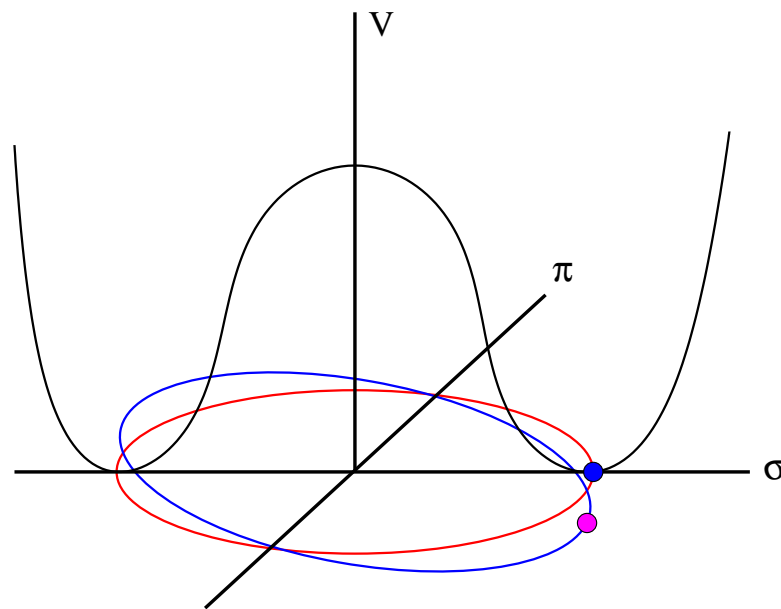
- potential has  $N_f^2 - 1$  “flat” directions

- one for each generator of  $SU(N_f)$



## Small mass selects vacuum

- $V \rightarrow V - m\sigma$
- $\langle \sigma \rangle \sim +v \quad \langle \pi \rangle = 0$
- Goldstones acquire mass  $\sim \sqrt{m}$



Anomaly gives the  $\eta'$  a mass even if  $m_q = 0$

- $m_{\eta'} = O(\Lambda_{QCD})$
- $V(\sigma, \eta')$  **not** symmetric under
  - $\psi \rightarrow e^{i\phi\gamma_5}\psi$
  - $\sigma \rightarrow \sigma \cos(\phi) + \eta' \sin(\phi)$
  - $\eta' \rightarrow -\sigma \sin(\phi) + \eta' \cos(\phi)$

Expand the effective potential near the vacuum state  $\sigma \sim v$  and  $\eta' \sim 0$

- $V(\sigma, \eta') = m_\sigma^2(\sigma - v)^2 + m_{\eta'}^2\eta'^2 + O((\sigma - v)^3, \eta'^4)$ 
  - both masses of order  $\Lambda_{QCD}$

## In quark language

### Classical symmetry

- $\psi \rightarrow e^{i\phi\gamma_5/2}\psi$
- $\bar{\psi} \rightarrow \bar{\psi}e^{i\phi\gamma_5/2}$
- mixes  $\sigma$  and  $\eta'$ 
  - $\sigma \rightarrow \sigma \cos(\phi) + \eta' \sin(\phi)$
  - $\eta' \rightarrow -\sigma \sin(\phi) + \eta' \cos(\phi)$

This symmetry is “anomalous”

- any valid regulator must break chiral symmetry
  - remnant of the breaking survives in the continuum

Variable change alters fermion measure

- $d\psi \rightarrow |e^{-i\phi\gamma_5/2}|d\psi = e^{-i\phi\text{Tr}\gamma_5/2}d\psi$

But doesn't  $\text{Tr}\gamma_5 = 0$  ???

Fujikawa: **Not in the regulated theory!!!**

- i.e.  $\lim_{\Lambda \rightarrow \infty} \text{Tr} \left( \gamma_5 e^{D^2/\Lambda^2} \right) \neq 0$

Dirac action  $\bar{\psi}(D + m)\psi$

- $D^\dagger = -D$
- $[D, \gamma_5]_+ = 0$

Use eigenstates of  $D$  to define  $\text{Tr}\gamma_5$

- $D|\psi_i\rangle = \lambda_i|\psi_i\rangle$
- $\text{Tr}\gamma_5 = \sum_i \langle \psi_i | \gamma_5 | \psi_i \rangle$

## Index theorem

- with gauge winding  $\nu$ ,  $D$  has  $\nu$  zero modes  $D|\psi_i\rangle = 0$ 
  - modes are chiral:  $\gamma_5|\psi_i\rangle = \pm|\psi_i\rangle$
  - $\nu = n_+ - n_-$

## Non-zero eigenstates in chiral pairs

- $D|\psi\rangle = \lambda|\psi\rangle$
- $D\gamma_5|\psi\rangle = -\lambda\gamma_5|\psi\rangle = \lambda^*\gamma_5|\psi\rangle$

Space spanned by  $|\psi\rangle$  and  $|\gamma_5\psi\rangle$  gives no contribution to  $\text{Tr}\gamma_5$

- $\langle\psi|\gamma_5|\psi\rangle = 0$  when  $\lambda \neq 0$
- only the zero modes count!

$$\text{Tr}\gamma_5 = \sum_i \langle\psi_i|\gamma_5|\psi_i\rangle = \nu$$

Where did the opposite chirality go?

- continuum: lost at “infinity”
  - opposite chirality states “above the cutoff”
- overlap: modes on opposite side of unitarity circle
  - $D\gamma_5 = -\hat{\gamma}_5 D$        $\text{Tr } \hat{\gamma}_5 = 2\nu$
- Wilson: real eigenvalues in doubler region

This phenomenon involves both short and long distances

- zero modes compensated by modes lost at the cutoff
- cannot ignore instanton physics at short distances

Cannot uniquely separate perturbative and non-perturbative effects

- small instantons can “fall through the lattice”
- scheme and scale dependent

Under the transformation

- $\psi \rightarrow e^{i\phi\gamma_5/2}\psi$
- $\bar{\psi} \rightarrow \bar{\psi}e^{i\phi\gamma_5/2}$

Regulated fermion measure changes by  $e^{-i\phi\text{Tr}\gamma_5} = e^{-i\phi\nu}$

- changes weighting of gauge configurations with winding
  - non-zero  $\phi$  introduces a sign problem for Monte Carlo

Note: here  $\phi$  is the conventional  $\Theta/N_f$

- each flavor contributes equally
- $\text{Tr}\gamma_5 = N_f\nu$

## Expanding in smooth gauge fields

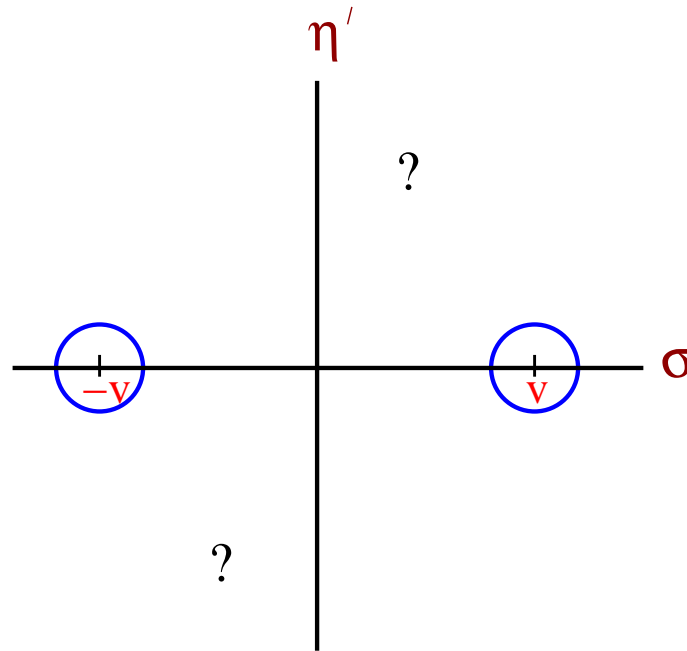
- $\nu = \text{Tr} \gamma_5 e^{D^2/\Lambda^2} = \text{Tr} e^{-\partial^2/\Lambda^2} \left( \frac{g^2}{\Lambda^4} F_{\mu\nu} \tilde{F}_{\mu\nu} + O(\Lambda^{-5}) \right)$
- trace over space, spinor, and color indices
- $e^{-\partial^2/\Lambda^2}$  “heat kernel regulator” for space
  - $\text{Tr}_x(e^{-\partial^2/\Lambda^2} f(x)) = \frac{\Lambda^4}{16\pi^2} \int d^4x f(x)$

$$\nu = \frac{g^2}{16\pi^2} \int d^4x \text{Tr}_c F_{\mu\nu} \tilde{F}_{\mu\nu}$$

- If  $F = \tilde{F}$  then  $S = \int d^4x \frac{1}{2} F^2 = \frac{8\pi^2}{g^2} \nu$ 
  - classical “instanton” action

## Back to effective field language

At least two minima in the  $\sigma, \eta'$  plane



Question: do we know anything about the potential elsewhere in the  $\sigma, \eta'$  plane?

Yes!

- there are actually  $N_f$  equivalent minima

Define  $\psi_L = \frac{1+\gamma_5}{2}\psi$

Singlet rotation  $\psi_L \rightarrow e^{i\phi}\psi_L$

- not a good symmetry for generic  $\phi$

Flavored rotation  $\psi_L \rightarrow g_L\psi_L = e^{i\phi_\alpha\lambda_\alpha}\psi_L$

- is a symmetry for  $g_L \in SU(N_f)$

For special discrete values of  $\phi$  these rotations can cross

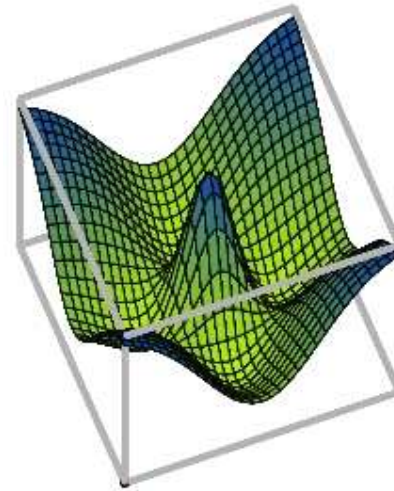
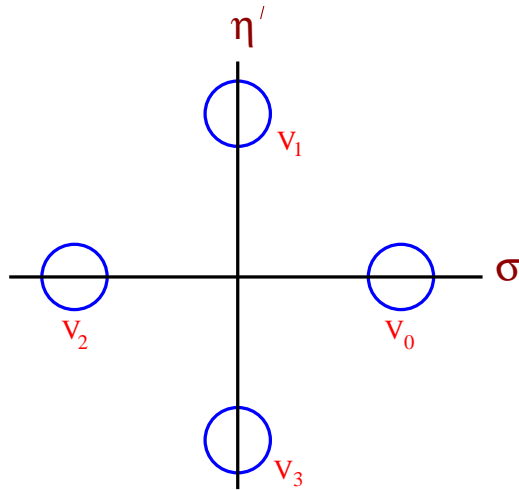
- $g = e^{2\pi i/N_f} \in Z_{N_f} \subset SU(N_f)$

A valid discrete singlet symmetry:

$$\begin{aligned}\sigma &\rightarrow \sigma \cos(2\pi/N_f) + \eta' \sin(2\pi/N_f) \\ \eta' &\rightarrow -\sigma \sin(2\pi/N_f) + \eta' \cos(2\pi/N_f)\end{aligned}$$

$V(\sigma, \eta')$  has a  $Z_{N_f}$  symmetry

- $N_f$  equivalent minima in the  $(\sigma, \eta')$  plane
- $N_f = 4$ :

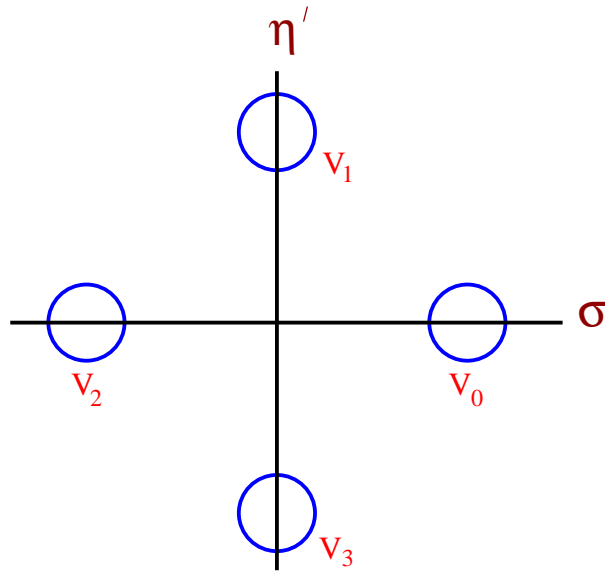


At the chiral lagrangian level

- $Z_N$  is a subgroup of both  $SU(N)$  and  $U(1)$

At the quark level

- measure gets a contribution from each flavor ('t Hooft vertex)
- $\psi_L \rightarrow e^{2\pi i/N_f} \psi_L$  is a symmetry



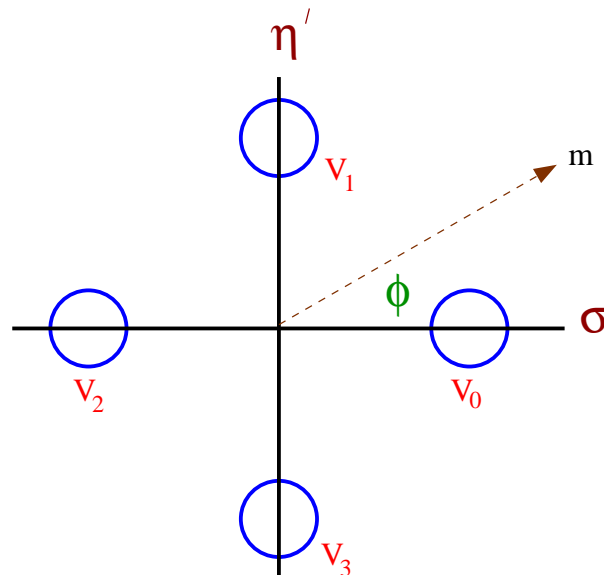
Mass term  $m\bar{\psi}\psi$  tilts effective potential

- picks one vacuum as the lowest
- in  $n$ 'th minimum  $m_\pi^2 \sim m \cos(2\pi n/N_f)$ 
  - highest minima are unstable in the  $\pi_\alpha$  direction
  - multiple meta-stable minima when  $N_f > 4$

## Anomalous rotation of the mass term

- $m\bar{\psi}\psi \rightarrow m \cos(\phi)\bar{\psi}\psi + im \sin(\phi)\bar{\psi}\gamma_5\psi$
- twists tilt away from the  $\sigma$  direction

An inequivalent theory!

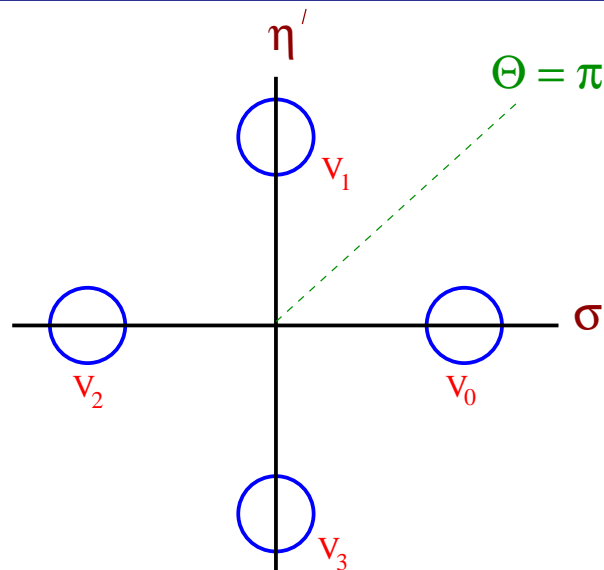


- as  $\phi$  increases, vacuum jumps from one minimum to the next

Here each flavor has been given the same phase

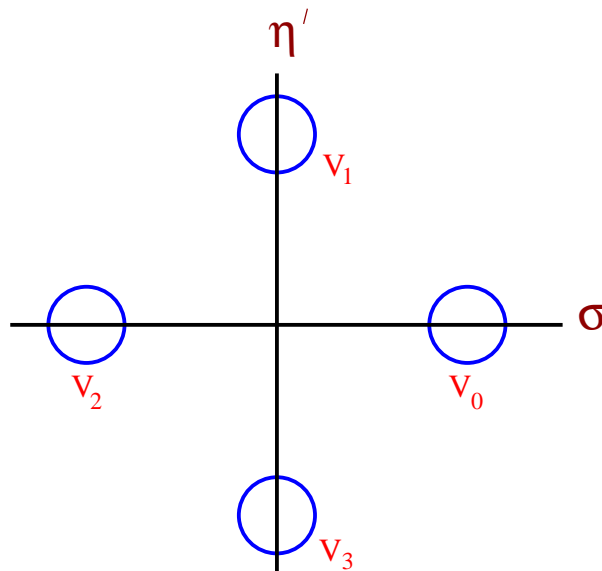
- Conventional notation uses  $\Theta = N_f \phi$
- $Z_{N_f}$  symmetry implies  $2\pi$  periodicity in  $\Theta$

Degenerate light quarks  $\Rightarrow$  first order transition at  $\Theta = \pi$



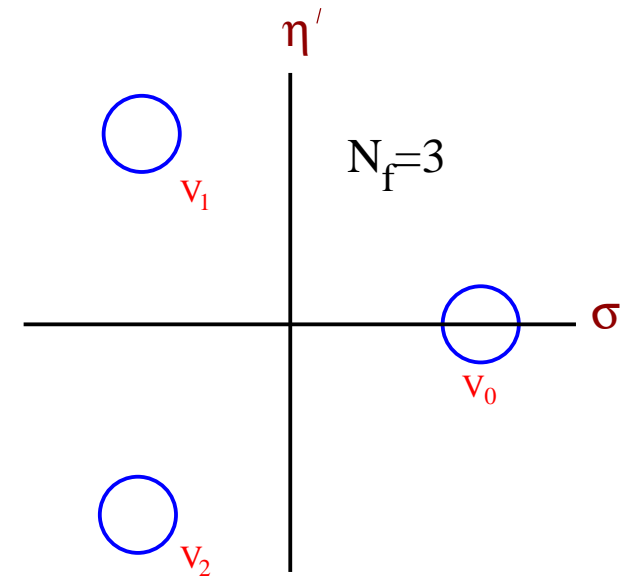
Discrete symmetry in mass parameter space  $m \rightarrow m \exp\left(\frac{2\pi i \gamma_5}{N_f}\right)$

- for  $N_f = 4$ :
  - $m\bar{\psi}\psi$  and  $im\bar{\psi}\gamma_5\psi$  mass terms give **equivalent** theories
  - true **if and only if**  $N_f$  is a multiple of 4



Odd number of flavors,  $N_f = 2N + 1$

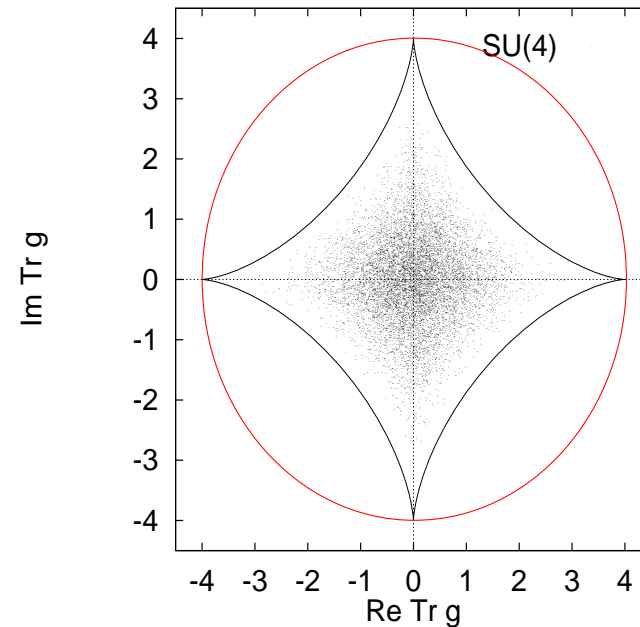
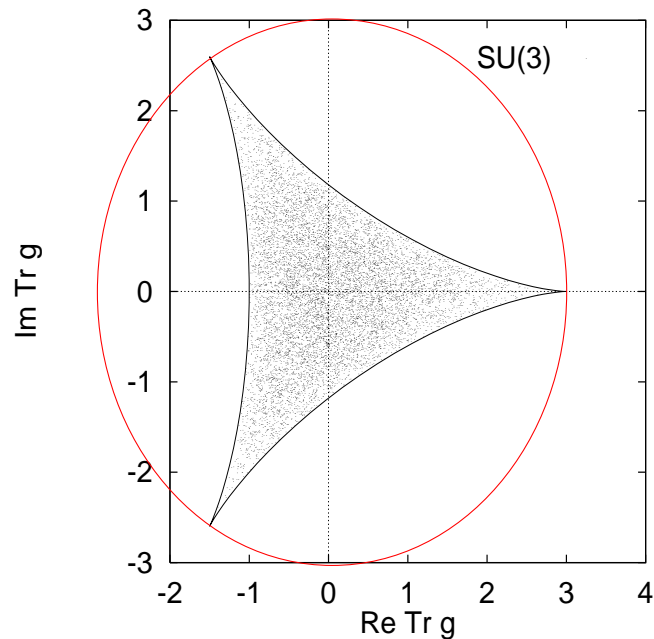
- $-1$  is not in  $SU(2N + 1)$
- $m > 0$  and  $m < 0$  not equivalent!
- $m < 0$  represents  $\Theta = \pi$ 
  - an inequivalent theory
  - spontaneous CP violation:  $\langle \eta' \rangle \neq 0$



Inequivalent theories can have identical perturbative expansions!

Center of  $SU(N_f)$  is a subgroup of  $U(1)$

- 10,000 random  $SU(3)$  and  $SU(4)$  matrices:



- region for  $SU(3)$  bounded by  $\exp(i\phi\lambda_8)$
- all  $SU(N)$  points enclosed by the  $U(1)$  circle  $e^{i\phi}$ 
  - boundary reached at center elements

$N_f = 1$ : No chiral symmetry at all!

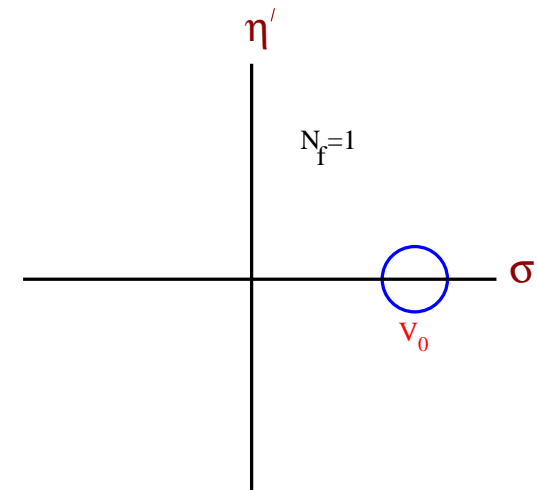
- unique vacuum
- $\langle \bar{\psi}\psi \rangle \sim \langle \sigma \rangle \neq 0$  from 't Hooft vertex
- not a spontaneous symmetry breaking

No singularity at  $m = 0$

- $m = 0$  not protected

For small mass

- no first order transition at  $\Theta = \pi$ 
  - larger masses?



Instanton effects scheme dependent (“renormalon” ambiguity)

- $(\Theta, m)$  singular coordinates when  $N_f = 1$ 
  - $(\text{Re } m, \text{Im } m)$  better
- rough gauge configurations: ambiguous winding number
  - overlap operator not unique: depends on “domain wall height”

$m = 0$  for a non-degenerate quark is an ambiguous concept

$N_f = 0$ : pure gauge theory

- $\Theta = \pi$  behavior unknown

## When is rooting OK?

Starting with four flavors

- can we adjust  $N_f$  using

$$\left| \begin{array}{cccc} D + m & 0 & 0 & 0 \\ 0 & D + m & 0 & 0 \\ 0 & 0 & D + m & 0 \\ 0 & 0 & 0 & D + m \end{array} \right|^{\frac{1}{4}} = |D + m|?$$

A vacuous question outside the context of a regulator!

Rooting before removing regulator **OK** if

- regulator **breaks** anomalous symmetries on each factor
  - i.e. four copies of the overlap operator:  $D\gamma_5 = -\hat{\gamma}_5 D$
  - winding  $\nu$  from  $\text{Tr}\hat{\gamma}_5 = 2\nu$

Forcing  $Z_{N_f}$  symmetry with regulator in place

$$\begin{vmatrix} D + me^{\frac{i\pi\gamma_5}{4}} & 0 & 0 & 0 \\ 0 & D + me^{\frac{-i\pi\gamma_5}{4}} & 0 & 0 \\ 0 & 0 & D + me^{\frac{3i\pi\gamma_5}{4}} & 0 \\ 0 & 0 & 0 & D + me^{\frac{-3i\pi\gamma_5}{4}} \end{vmatrix}$$

- maintains  $m \rightarrow me^{i\pi\gamma_5/2}$  symmetry
  - permutes flavors

Four one-flavor theories with different values of  $\Theta$

- theta cancels out for the full four flavor theory

Rooting averages four inequivalent theories: **NOT OK**

- $(|D + M_1||D + M_2|)^{1/2} \neq |D + \sqrt{M_1 M_2}|$

## Staggered fermions

- regulator maintains one **exact** chiral symmetry

- $|D_s + m| = |D_s + me^{i\gamma_5\phi}|$

- OK since actually a flavored symmetry

- separate into four “effective tastes”  $D_i$

- two tastes of each chirality

$$|D_s + me^{i\gamma_5\phi}| \sim \begin{vmatrix} D_1 + me^{i\phi\gamma_5} & 0 & 0 & 0 \\ 0 & D_2 + me^{-i\phi\gamma_5} & 0 & 0 \\ 0 & 0 & D_3 + me^{i\phi\gamma_5} & 0 \\ 0 & 0 & 0 & D_4 + me^{-i\phi\gamma_5} \end{vmatrix}$$

- plus “taste mixing” (not the crucial issue)

Rooting to get to one flavor **NOT OK**

- rooting does not remove the  $Z_4$
- tastes are not equivalent
  - rooting averages **inequivalent** theories

**Rooted staggered fermions are not QCD!**

Extra minima from  $Z_{N_f}$

- expected to drive  $\eta'$  mass down
  - **testable but difficult**

## Summary

QCD with  $N_f$  massless flavors has a discrete  $Z_{N_f}$  chiral symmetry

- flavor singlet

Associated with a first order transition at  $\Theta = \pi$  when  $m \neq 0$

Sign of mass significant for  $N_f$  odd

- not seen in perturbation theory

No symmetry for  $N_f = 1$

- $m = 0$  unprotected

Structure inconsistent with rooted staggered quarks

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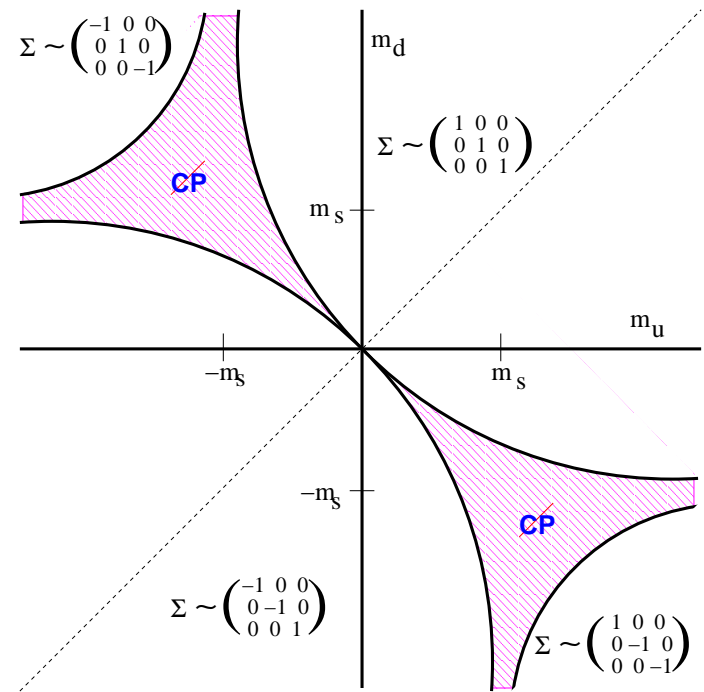
References:

- Ann. Phys. 324 (2009), 1573: arXiv:0901.0150
- arXiv:0909.5101

## Extra slides: generalized quark masses

# General masses can give intricate phase diagrams:

- three flavors
- fixed  $m_s$
- vary  $m_u, m_d$
- transition along  $m_u = -\frac{m_d m_s}{m_d + m_s}$



## Generalized mass term

- Renormalizable: look at fermion bilinears
- Lorentz invariant

## Two flavors:

- $m_s \bar{\psi}\psi + m_v \bar{\psi}\tau_3\psi + im_3 \bar{\psi}\gamma_5\psi + im_4 \bar{\psi}\gamma_5\tau_3\psi$ 
  - $m_s$  average quark mass, isoscalar
  - $m_v$  quark mass difference, isovector
  - $m_3$  CP violating
  - $m_4$  “twisted mass” (useful with Wilson fermions)

## These are not independent

- Fermion kinetic term symmetric under  $\psi \rightarrow e^{i\phi\gamma_5\tau_3}\psi$
- mixes  $m_s$  with  $m_4$  and  $m_v$  with  $m_3$

Can set any single  $m_i = 0$  and another  $m_j > 0$

- Choose convention  $m_4 = 0$  and  $m_s > 0$ 
  - $m_s \bar{\psi}\psi + m_v \bar{\psi}\tau_3\psi + im_3 \bar{\psi}\gamma_5\psi$

2 flavor QCD depends on three independent quark mass parameters

- $m_{\pi_{\pm}}^2 \sim m_s$
- $m_{\pi_{\pm}}^2 - m_{\pi_0}^2 \sim m_v^2$  (+EM effects)
- neutron electric dipole moment  $\sim m_3$

Strong CP problem: why is  $m_3$  experimentally extremely small?

- unification with CP violating weak interactions?

Symmetries make each term multiplicatively renormalizable

- CP symmetry protects  $m_3$
- Isospin protects  $m_v$
- Flavored chiral symmetry protects  $m_s$

$m_s$  and  $m_v$  transform differently under isospin

- $m_v/m_s$  renormalization can depend on scheme
  - $m_p, m_{\pi_{\pm}}$  and  $m_{\pi_0}$  constant
  - $m_p, m_{\pi_{\pm}}$  and  $m_v/m_s$  constant
- not equivalent non-perturbatively (“renormalon ambiguity”)

## Renormalization group interpretation

$$a \frac{dm}{da} = m\gamma(g) = m(\gamma_0 g^2 + \gamma_1 g^4 + \dots) + \text{non-perturbative}$$

- non-perturbative part vanishes faster in  $g$  than any power

Bare quark masses run to zero logarithmically with the cutoff

- $m = m_r g^{\gamma_0/\beta_0} (1 + O(g^2)) \rightarrow_{a \rightarrow 0} 0$

Renormalized quark mass  $m_r = \lim_{a \rightarrow 0} m g^{-\gamma_0/\beta_0}$

- “integration constant” of RG equation

Numerical value of  $m_r$  depends on scheme

- 't Hooft vertex contributes a non-perturbative part  $\sim m^{N_f-1}$ 
  - not proportional to  $m$  for  $N_f = 1$
  - $m_{\eta'} \propto \frac{1}{a} e^{-1/2\beta_0 g^2} g^{-\beta_1/\beta_0^2}$
  - similar form can appear in RG equation

Example new scheme:

- $\tilde{a} = a$
- $\tilde{g} = g$
- $\tilde{m} = m - m_r g^{\gamma_0/\beta_0} \times \frac{e^{-1/2\beta_0 g^2} g^{-\beta_1/\beta_0^2}}{\Lambda a}$
- on RG trajectory the last factor approaches unity

Non-perturbative redefinition of parameters makes

- $\tilde{m}_r \equiv \lim_{a \rightarrow 0} \tilde{m} \tilde{g}^{-\gamma_0/\beta_0} = m_r - m_r = 0$
- $m_u = 0$  is not a solution to the strong CP problem

With degenerate quarks  $m_\pi = 0$  defines  $m = 0$