$N_f = 1$ QCD

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$N_f \neq 1$ QCD and chiral transformations

QCD Lagrangian in continuum:

$$\mathcal{L}_{QCD} = \mathcal{L}_0 + \mathcal{L}_m - \frac{1}{4}\mathcal{G}_{\mu\nu,a}\mathcal{G}_a^{\mu\nu}$$

with,
$\mathcal{G}^i_{\mu\nu,a} = \partial_\mu \mathcal{A}_{\nu,a} - \partial_\nu \mathcal{A}_{\mu,a} + gf_{abc}\mathcal{A}_{\mu,b}\mathcal{A}_{\nu,c}$, $a = 1, ..., 8$
$\mathcal{L}_0 = \sum_f \bar{\psi}_f \{\gamma_\mu(\partial_\mu - igA_\mu)\}\psi_f$, $f = 2, ..., N_f$,
$\mathcal{L}_m = \sum_f \bar{\psi}_f m_f \psi_f$,

Chiral projections: $\psi_{R/L} = P_{R/L}\psi = \frac{1}{2}(1 \pm \gamma_5)\psi$
$\mathcal{L}_0 = \bar{\psi}_L\gamma_\mu D_\mu\psi_L + \bar{\psi}_R\gamma_\mu D_\mu\psi_R$, $D_\mu = \partial_\mu - igA_\mu$
$\mathcal{L}_m = m_q(\bar{\psi}_L\psi_R + \bar{\psi}_R\psi_L)$

Symmetries of the Lagrangian in the chiral limit

Chiral limit: $m \to 0$, $\mathcal{L}_m \to 0$
Chiral symmetry: $SU(N_f)_L \otimes SU(N_f)_R \otimes U(1)_V \otimes U(1)_A$
for $N_f = 3$:

- $SU(3)_L$: $\psi_L \mapsto \exp\left(-i \sum_{a=1}^{8} \Theta_a^L \frac{\lambda_a}{2}\right) \psi_L$
- $SU(3)_R$: $\psi_R \mapsto \exp\left(-i \sum_{a=1}^{8} \Theta_a^R \frac{\lambda_a}{2}\right) \psi_R$
- $U(1)_V$: $\psi \mapsto e^{-i\alpha}\psi$
- $U(1)_A$: $\psi \mapsto e^{-i\alpha\gamma_5}\psi$

classically conserved currents (Noether, $\partial_\mu J^\mu = 0$):
$L^{\mu,a} = \bar{q}_L \gamma^\mu \frac{\lambda^a}{2} q_L$, $R^{\mu,a} = \bar{q}_R \gamma^\mu \frac{\lambda^a}{2} q_R$,
$V^{\mu,a} = R^{\mu,a} + L^{\mu,a}$, $A^{\mu,a} = R^{\mu,a} - L^{\mu,a}$
$V^\mu = \bar{q}\gamma^\mu q$, $A^\mu = \bar{q}\gamma^\mu\gamma_5 q$

Symmetry-breaking patterns

1) **spontaneous symmetry breaking**:
consider $UH_0U^\dagger = H_0$, for $U|A\rangle = |B\rangle$,

$$E_A = \langle A| H_0 |A\rangle = \langle B| H_0 |B\rangle = E_B \tag{1}$$

consider ϕ_A, ϕ_B creations operators, $\phi_A|0\rangle = |A\rangle$, $\phi_B|0\rangle = |B\rangle$
$U\phi_A U^\dagger = \phi_B \Leftrightarrow U|0\rangle = 0$, $U|0\rangle \neq 0$ vitiates (1)

- Goldstone theorem:
  $H \subset G$ letting $|0\rangle$ invariant
  $n_G - n_H$ massless Goldstone bosons generated
- non-vanishing vacuum expectation (QCD case $<\bar{q}q> \neq 0$)
  (1D-Ising model $M =<\phi> \neq 0$)

2) **explicit symmetry breaking**:

- $\mathcal{L}_m = m\bar{\psi}\psi$
- $\mathcal{L}_{QCD} = \mathcal{L}_0 + \mathcal{L}_m$
  $m \neq 0, \quad \mathcal{L}_m = m_q(\bar{\psi}_L\psi_R + \bar{\psi}_R\psi_L) \neq 0$
  explicitly breaks the $SU(N_f)_L \otimes SU(N_f)_R$ symmetry
- expansion around the vacuum; massive bosonic states
- Goldstone bosons become massive, light pseudo-Goldstone bosons

3) **anomalous symmetry breaking**:

- L^0_{QCD} exhibits classically $SU(3)_L \otimes SU(3)_R \otimes U(1)_V \otimes U(1)_A$
  Noether Thm: $8+8+1+1=18$ conserved currents:
- $Q = \int d^3 J^0(x),\ \partial_\mu J^\mu = 0 \Rightarrow \frac{d}{dt} Q = 0$
  $[Q, H] = 0,\ Q^\dagger H Q = H \Leftrightarrow$ symmetry
- !after quantization, $\partial_\mu A^\mu = \frac{3g^2}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \mathcal{G}_a^{\mu\nu} \mathcal{G}_a^{\rho\sigma}, \quad \epsilon_{0123} = 1$
  This phenomenon is called anomaly

From the chiral limit to the "real world QCD"

Chiral limit symmetries: $SU(3)_L \otimes SU(3)_R \otimes U(1)_V \otimes U(1)_A$

- $U(1)_A$-symmetry broken by anomaly
- $Q_V^a = Q_R^a + Q_L^a$, $Q_A^a = Q_R^a - Q_L^a$, $[Q_{V,A}, H^0_{QCD}] = 0$
  parity doubling in your massless theory:
  ! not observed in nature
  assumption:
  symmetry $SU(3)_L \otimes SU(3)_R \to SU(3)$ spontaneously broken,
  $m_q = 0$: $\Rightarrow (\tilde{\pi}, \tilde{K}, \tilde{\eta})$ Goldstone bosons
- $m_q \neq 0$: $\Rightarrow$ explicit symmetry breaking
  (π, K, η) light pseudo-Goldstone bosons

Gell-Mann/Oakes/Renner relations

- **effective theory with chiral perturbative arguments**:
  mapping: $U(x) = \exp\left(\frac{i}{F_0}\sum_{i=1}^{8}\phi_a(x)\lambda_a\right) \in SU(3)$,
  $m_q \approx 0$, $U \to LUR^\dagger$, $(L,R) \in SU(N_f)_L \otimes SU(N_f)_R$,
  vacuum $U = 1$ broken under A-trafos
- leading order: $\mathcal{L}_0 = \frac{F_0^2}{4} tr(\partial_\mu U^\dagger \partial^\mu U)$,
  $\mathcal{L}_m = \frac{F_0^2}{4} tr(\chi U^\dagger + U\chi^\dagger) = -\frac{B_0}{2} tr(\phi^2 M) + \ldots$
  $\chi = 2B_0 M$, $3F_0^2 B_0 = -\langle \bar{q}q \rangle$, $M = diag(m, m, m_s)$
- **Gell-Mann/Oakes/Renner relations**:
  $M_\pi^2 = 2B_0 m$,
  $M_K^2 = B_0(m + m_s)$,
  $M_\eta^2 = \frac{2}{3} B_0(m + 2m_s)$

some generalities about $N_f \neq 1$ QCD

- $m_q \neq 0$ defined physically by explicit symmetry breaking model underlying symmetries are broken
- Mesons masses $M^2 \propto m$ (Gellmann/Oakes/Renner) gives you a "values space" (M, m_q) where the point $m_q = 0$ is well defined
- CP violation alongside explicit chiral $SU(2)_L \otimes SU(2)_R$ symmetry breaking in $N_f = 3$ QCD? (Dashen 1970)

One flavour QCD

- $SU(1)_L \otimes SU(1)_R \otimes U(1)_V \otimes U(1)_A = U(1)_V \otimes U(1)_A$
  $U(1)_A$ anomalously broken
- no spontaneous, explicit chiral symmetry breaking scenario!

Problem of **defining a mass**:

- physical meaning for $m = 0, \quad m < 0$?
  - no explicit symmetry breaking
  - no GOR-relations anymore ($M^2_{meson} \propto m_q$)
- $N_f = 1$ QCD, m_q not protected from renormalization:
  two renormalization schemes:
  $m_i = \Lambda_{QCD} H_i(M/\lambda_{QCD}) = \tilde{\Lambda}_{QCD} \tilde{H}_i(\tilde{M}/\tilde{\lambda}_{QCD})$
  - $N_f \neq 1$ QCD: $H_i(0) = \tilde{H}_i(0) = 0$, $(M = 0 \Leftrightarrow \tilde{M} = 0)$
  - $N_f = 1$ QCD: $H_i(0) \neq \tilde{H}_i(0) \neq 0$?, $(M \neq 0,\ \tilde{M} = 0)$ possible!

Science-fiction parameters

$$\mathcal{L}_{QCD} = \frac{1}{4g^2} F_{\mu\nu} F^{\mu\nu} + \bar{\psi}\gamma_\mu \partial_\mu \psi + m\bar{\psi}\psi$$

- $U(1)_A$ breaks explicitely classical $U(1)_A$ symmetry:
  $\psi \longrightarrow e^{i\gamma_5\theta/2}\psi$
  $\bar{\psi} \longrightarrow \bar{\psi}e^{i\gamma_5\theta/2}$
  $m\bar{\psi}\psi \longrightarrow m_1\bar{\psi}\psi + m_5\bar{\psi}\gamma_5\psi$
- g, m_1, m_5 parametrise the theory

Arguments for CP violation, effective Lagrangians

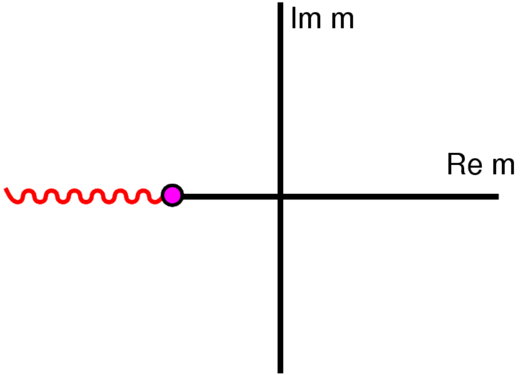
1) In analogy with $N_f = 3$ QCD

- $m^2_{\eta'} \sim m_q + c$ typical chiral perturbative argument
- build $V(\eta') = \frac{m_q+c}{2}\eta'^2 + \lambda\eta'^4$, $\eta' = \bar{\psi}\gamma_5\psi$
- after $U(1)_A$ trafo: $V(\eta'; m_1, m_5) = \frac{m_q+c}{2}\eta'^2 + \lambda\eta'^4 + m_5\eta'$,
- for $m_q < -c$
  $\langle\eta'\rangle \sim \langle\bar{\psi}\gamma_5\psi\rangle \sim \sqrt{\frac{|m_q-c|}{4\lambda}} \neq 0$,
- which is a CP odd field $\Rightarrow$ CP spontaneously broken

2)Another approach: $N_f = 3$ QCD with (m, M, M) $\quad m \ll M$

- phase transition detected at negative mass

$N_f = 1$ expected phase space?



1) Motivations for Studying $N_f = 1$ QCD

Theory

- physical meaning of $m_q = 0$
- CP breaking for $m_q < 0$?
- $m_q = 0 \rightarrow m_q \neq 0$ "dimensional transmutation"

Lattice approach: study of the phase space
vacuum expectations values around $m_q = 0$, $m_c < 0$

- other motivations:
  - (!?) relation $N_f = 1$ QCD / SYM $\mathcal{N} = 1$
  - (!?) orientifold planar equivalence ($N_c = \infty$), predictions for $\langle \bar{q}q \rangle$

QCD Path Integration with fermionic variables

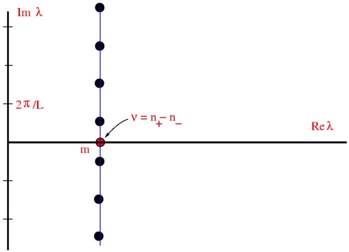
Path Integral: $Z = \int dA\, d\psi\, d\bar{\psi}\, e^{S_G(A) + \bar{\psi} D(A) \psi}$

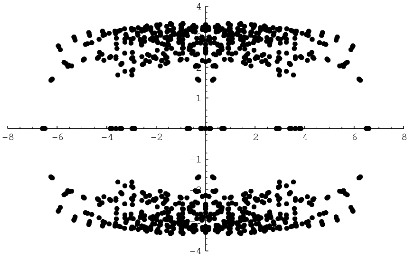
- Dirac operator: $D(A) = \gamma_\mu(\partial_\mu + igA_\mu) + m$
- $Z = \int dA\, e^{S_G(A)}\, det[D(A)]$,
  $(\int \prod_{i=1}^{N}[d\eta_i\, d\eta_i^\dagger] e^{\{-\sum_{i,j} \eta_j^\dagger Q_{ji} \eta_i\}} = \det Q)$
- "γ_5 hermiticity" $\gamma_5 D \gamma_5 = D^\dagger$, whereas $\gamma_5 = diag(1, 1, -1, -1)$
  eigenvalues occur in conjugate pairs
- $det[D(A)] = \prod_i \lambda_i = \prod_i |\lambda_i|^2 \prod_j \tilde{\lambda}_j$, $(\lambda_i \in \mathcal{C}, \tilde{\lambda}_j \in \mathcal{R})$
- !a peculiar case $det[D(A)] < 0$! consider only $\lambda_j \in \mathcal{R}$

Situation on the lattice

- D_W the Wilson fermion matrix $S_{quark} = \sum_{xy} \bar{\psi}_x (D_W)_{xy} \psi_y$
- lattice situation:
  complex eigenvalues: $\sim$ still paired
  real eigenvalues: $\sim$ isolated, clustered
  $\sim$ slightly deformed Wilson eigenvalues spectrum
- $D_W = m_q + D_W^0$,
  small m_q: !!!negative determinants($N_f > 1$)!!!

Eigenvalues spectrum: continuum vs lattice





Statistics with a negative determinant

- expectation value $< \mathcal{O} >_{e^{S_g+S_f}} = \frac{\int dU\, \mathcal{O}\, (detQ(U)e^{S_g(U)})}{\int dU\, (detQ(U)e^{S_g(U)})}$
- ?"negative statistical weight" $sgn(\ldots)|\det Q(U)e^{S_g(U)}|$!?, $sgn(\ldots) = sgn \det Q(U)$
- way out:

$$< \mathcal{O} >_{e^{S_g+S_f}} = \frac{<sgn(\ldots)\mathcal{O}>_{|e^{S_g+S_f}|}}{<sgn(\ldots)>_{|e^{S_g+S_f}|}} =$$

$$\frac{\int dU\, sgn(\ldots)\mathcal{O}\, |\det Q(U)e^{S_g(U)}|}{\int dU\, |\det Q(U)e^{S_g(U)}|} \times \frac{\int dU\, |\det Q(U)e^{S_g(U)}|}{\int dU\, sgn(\ldots)\, |\det Q(U)e^{S_g(U)}|}$$

sample point of view: $< \mathcal{O} >_{corrected} = \frac{<sgn(\ldots)\mathcal{O}>_{M.-C.}}{<sgn(\ldots)>_{M.-C.}}$, whereas $< A >_{M.-C.} = \frac{\sum_{i=1}^{N} A_i}{N}$, with A_i measurements.

2) Motivations for Studying $N_f = 1$ QCD

Lattice/algorithmic

- Determinant sign under control:
  - right statistics!
- compute lower masses
- some day: $m_u \neq m_d$?
- (?) some controversy about simulations procedure

Eigenvalues for huge sparse matrices

sparse matrices: very empty matrices...
size of the matrices: $N = 12^3 \times 24 \times 3 \times 4$, (L_x, L_t, N_c, N_D)
!storing all the elements with high precision: $\mathcal{O}(N^2) = \mathcal{O}(10^{12})$ array elements!

- optimized matrix multiplication:
  take advantage of its structure
  (needed storage/operations $\mathcal{O}(N)$)
- extract one part the eigenvalue spectrum
- methods based on **Krylov spaces**: vector v, matrix A,
  $\mathcal{K}(A,\text{v},j) = span\{v, Av, A^2v, ..., A^{j-1}v\}$
  economical definition of vector set/space (in term of storage)!

unsysmmetric eigenvalues problem

Basis

- **Schur decomposition** theorem:
  $A \in \mathcal{C}^{n\times n}$, then $\exists$ Q unitary and R uppertriangular,
  such that $AQ = Q(D+R)$,
  moreover D is diagonal, contains eigenvalues of A.

1) **Power method**: $A \in \mathcal{C}^{n\times n}$,
with $X^{-1}AX = diag(\lambda_1, ..., \lambda_n)$, $|\lambda_1| > ... > |\lambda_n|$.
applying recursively A on $q^0 = \sum_{i=1}^{n} a_i x_i$, $a_1 \neq 0$.
$q^k = A^k q^0 = \lambda_1^k \left(a_1 x_1 + \sum_{j=2}^{n} \left(\frac{\lambda_j}{\lambda_1}\right)^k x_j \right) \approx a_1 \lambda_1^k x_1$, for k big
algorithmic convergence: $dist(span\{q^k\}, span\{x_1\}) = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k \right)$

basic improvements

- **Shift idea**:
  power method convergence:
  $dist(span\{q^k\}), span\{x_1\} = \mathcal{O}\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$
  enhancement: $\tilde{A} = A - \mu I$, leading to $\mathcal{O}\left(\left|\frac{\lambda_2-\mu}{\lambda_1-\mu}\right|^k\right)$
  for exemple $\frac{0.1}{0.2} \ll \frac{3444.1}{3444.2}$!
- **spectral transformation method**:
  introduce $P_n(x) = \gamma_0 + \gamma_1 x + ... + \gamma_n x^n$,
  for eigenvectors $P_n(A)x = xP_n(\lambda_x)$
  with $\left|\frac{P_n(\lambda_2)}{P_n(\lambda_1)}\right| < \left|\frac{\lambda_2}{\lambda_1}\right|$, improved convergence rate.

QR algorithm: higher dimensional power method

p $(1 < p < n)$ eigenvalues with the power method?

- **QR algorithm**
  $A \in \mathcal{C}^{n \times n}$, $Q_0 \in \mathcal{C}^{n \times p}$ unitary with orthonormal columns,
  D, $R \in \mathcal{C}^{p \times p}$ D diagonal, R uppertriangular
  - for $k = 1, 2, \ldots$
  - $Z_k = AQ_{k-1}$
  - $Q_k(D_k + R_k) = Z_k$
- extracts automatically higher invariant subspaces
- rate of convergence $\mathcal{O}\left(\left|\frac{\lambda_{p+1}}{\lambda_p}\right|\right)$
- can be optimized with shifts, spectral transformations, …

Arnoldi

$A \in \mathcal{C}^{n\times n}$ unsymmetric

- **k-step Arnoldi factorization** of A

$$AV_k = V_k H_k + f_k e_k^T ,$$

$V_k \in \mathcal{C}^{n\times k}$ orthonormal columns, $V_k^\dagger f_k = 0$, e_k basis vector,
$H_k \in \mathcal{C}^{k\times k}$ upper-Hessenberg matrix: $H_k = D_k + R_k$.

- heuristic proof: $V_k^\dagger$ on the left to find:
  $V_k^\dagger A V_k = H_k \sim AQ = Q(D+R)$, Schur decomposition
- convergence?: Rayleigh quotient residual $r(x)$
  $\|r(x)\| = \left| \|f_k\| e_k^T y \right|, \quad x = V_k x$

Arnoldi "0"

Arnoldi factorization: $AV_k = (V_k, v_k)\begin{pmatrix} H_j \\ \beta_J e_J^T \end{pmatrix}$

$v_0 = \vec{v}/\|\vec{v}\|$, $w = A\vec{v}_0$, $\alpha_0 = v_0^\dagger w$
$f_1 \leftarrow w - v_0\alpha_0$; $V \leftarrow V_0, h_0 \leftarrow \alpha_0$
For $j = 1, 2, 3, ..., k$

- $\beta_j = \|f_j\|, \quad v_{j+1} \leftarrow f_j/\beta_j;$
- $V_{j+1} \leftarrow (V_j, v_{j+1}), \hat{H}_j \leftarrow \begin{pmatrix} H_j \\ \beta_J e_J^T \end{pmatrix};$
- $z \leftarrow Av_{j+1}$
- $h \leftarrow V_{j+1}^\dagger z, \quad f_{j+1} \leftarrow z - V_{j+1};$
- $H_{j+1} \leftarrow (\hat{H}_j, h)$

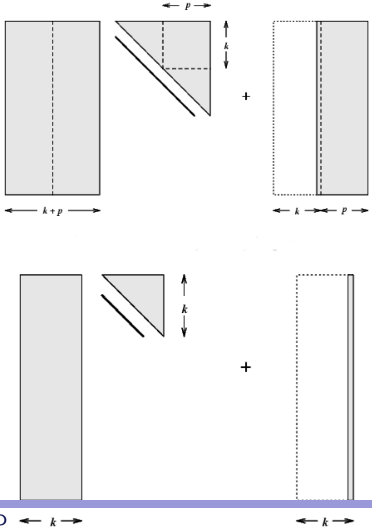
notice: entirely depends on your initial vector v_0!

"implicit restarted" Arnoldi "1"

looking for an optimal v_0:
ensure orthogonality of V elements, optimize number of iterations

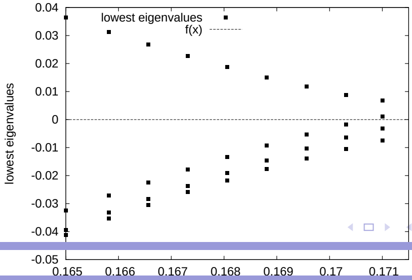
- **explicit restarting**: choose a method, test a v_0, converging? test a v'_0, converging?, repeat until convergence...
- **implicit restarting**:
  QR Arnoldi: $AV_m^+ = V_m^+ H_m^+ + f_m e_m^T Q$, $m = k + p$
  $V_m^+ = V_m Q$, $H_m^+ = Q^T H_m Q$, $Q = Q_1 ... Q_p$
  1. p QR-shifted iterations: extracts a subspace of interest
  2. k normal Arnoldi iterations:
     $AV_k = V_k H_k + f_k e_k^T$
- **further optimizations**: shifts, spectral transformations, ...

Arnoldi vs implicitly restarted Arnoldi



Conjugate flow approach

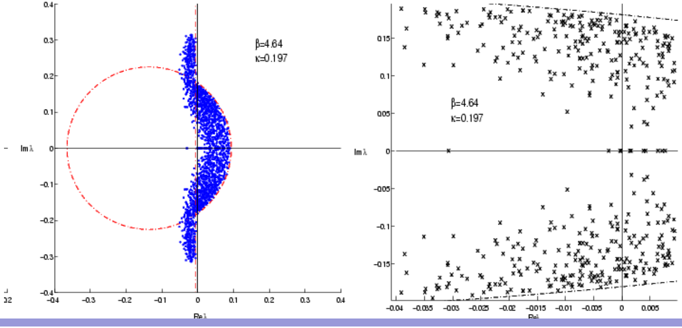
- $\tilde{D}_W = \gamma_5 D$ hermitian, real eigenvalues, $\lambda \to -\lambda$
- Ritz acceleration/ conjugate gradient algorithm
- Lattice action: $S = \sum_{xy}(\bar{\psi}_y Q_{yx} \psi_x)$,
  $Q_{yx} = \delta_{yx} - \kappa \sum_{\mu} \delta_{y,x+\hat{\mu}}[1 + \gamma_\mu]$, positive determinant $\kappa = \frac{1}{8}$ imply positive determinant
- expensive, not exact approach



Arnoldi approach

- working with D_W instead of $\tilde{D}_W$, complex eigenvalues
- direct approach, exact method!
- shape of the eigenvalues spectrum deformed

figures: numerical simulations with two degenerate m_q, $8^3 \cdot 16$



Find a way to get real eigenvalues here...

- assuming the same kind of eigenvalues spectrum for $N_f = 1$ ...