$N_f = 1$ QCD

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- Eur. Phys. J. C52, 305-314, 2007 (arXiv:0706.1131)
- PoS (LATTICE 2008) (arxiv:0810.0161)

$N_f = 1$ QCD!?

QCD in absence of chiral symmetry:

- CP breaking for negative quark masses?

  R.F.Dashen [1971], M.Creutz [1995]

  $m_u \rightarrow 0$ solution of the strong CP problem?
- quark mass definition?

other aspects:

- relics of SUSY from an orientifold large N_C equivalence

  A.Armoni, M.Shifman, G.Veneziano [2003, 2004]
- test for the sign problem in QCD ($T = 0$)

from $N_f > 1$ QCD to meson masses

$$\mathcal{L}_{QCD} = \sum_{f=1}^{N_f} \bar{\psi}_f[\gamma_\mu(\partial_\mu - igA_\mu) - m_f]\psi_f + L_g(A_\nu, \partial_\mu A_\nu)$$

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: $SU(N_f)_L \otimes SU(N_f)_R \to SU(N_f)_V$
  $\longrightarrow$ massless Goldstone bosons
- $m_q > 0 \leftrightarrow$ explicit SB: $SU(N_f)_L \otimes SU(N_f)_R$
  Goldstone bosons $\longrightarrow$ pseudo Goldstone bosons (pions)

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

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

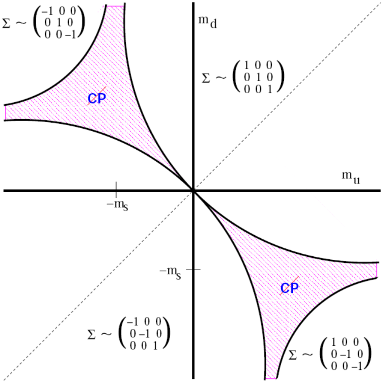
CP symmetry breaking in $N_f = 3$ effective theory

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

$\Sigma = \exp(i\pi_\alpha \lambda_\alpha / f_\pi) \in SU(3)$, $M = \mathrm{diag}(m_u, m_d, m_s)$

quark masses tuning and vacuum Σ_{min} structure study:

M.Creutz [1995]

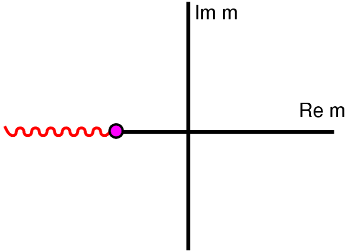


situation in $N_f = 1$ QCD

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

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

breaking of CP symmetry? M.Creutz [2006]



sign problem I

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

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

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

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

- 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)

sign problem II

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

  sign problem spoils your statistics

- no CP violation possible if fermionic measure is positive

  C.Vafa, E.Witten [1984]

  the sign problem has to be an issue!

realisation with partial quenching

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

C.W.Bernard, M.F.L.Golterman [1994], S.R.Sharpe [1997]

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

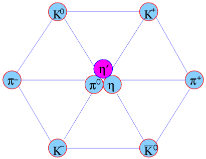
Chiral Symmetry: $SU(3|2)_L \otimes SU(3|2)_R \otimes U(1)_A \otimes U(1)_V$

- spontaneous Symmetry Breaking:
  $SU(3|2)_L \otimes SU(3|2)_R \to SU(3|2)$

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

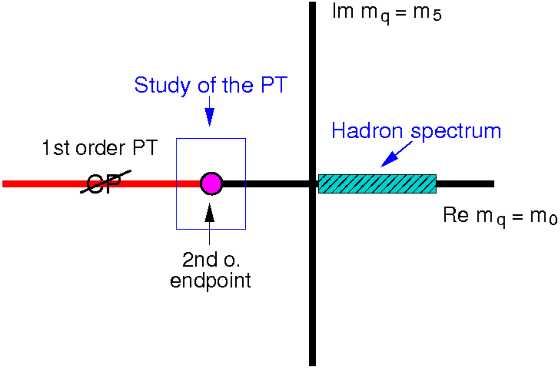
realisation with partial quenching

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



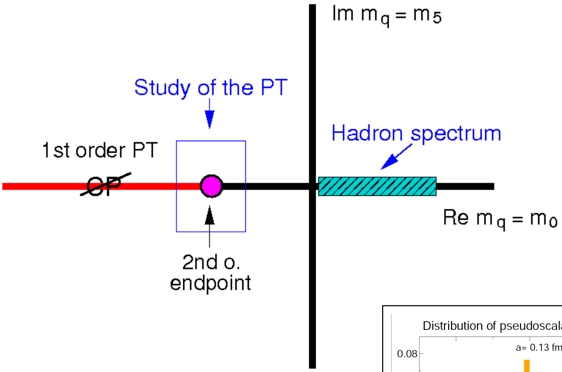
- quark mass definition with intermediary quantities?
  m_{PCAC}, $m_{\eta'}$ versus pion masses (GMOR type relations)
- PQχPT partially quenched chiral perturbation theory

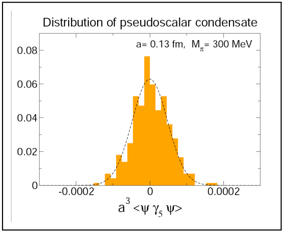
strategy



- Mass term:
  $m_q\,\bar{\psi}_L\psi_R + m_q^*\,\bar{\psi}_R\psi_L =$
  $m_0\,\bar{\psi}\psi + im_5\,\bar{\psi}\gamma_5\psi$

strategy

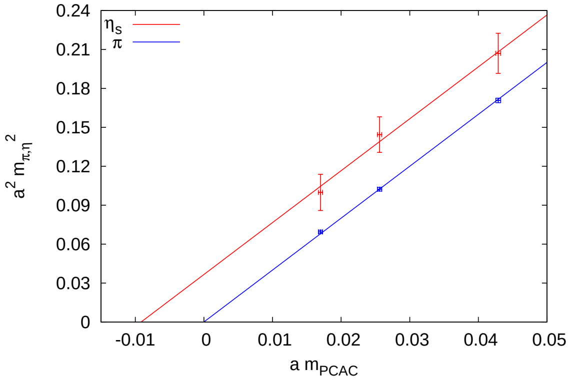




- Mass term:
  $m_q \bar{\psi}_L \psi_R + m_q^* \bar{\psi}_R \psi_L =$
  $m_0 \bar{\psi}\psi + i m_5 \bar{\psi}\gamma_5\psi$

some results

PQχPT fit: $m_\eta^2 = \frac{m_\Phi^2 + \chi_{PCAC}}{1+\alpha}$

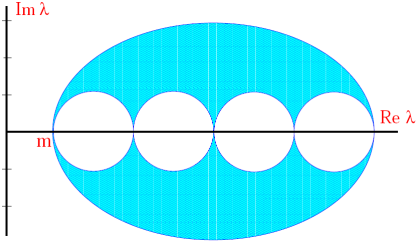


lattice formulation

Wilson action:

tree-level improved (tlSym), stout smeared fermion action

- Wilson-Dirac operator
  $D_W = m + \frac{1}{a}\sum_\mu(i\sin(p_\mu a)\gamma_\mu) + \frac{r}{a}\sum_\mu(1-\cos(p_\mu a))$



lattice formulation

Wilson action:

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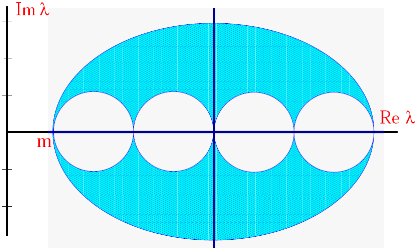
- Wilson-Dirac operator D_W on the lattice
  symmetries $\{\lambda, \lambda^*\}$, $\{1 - \kappa\lambda, 1 + \kappa\lambda\}$,
  $\kappa = \frac{1}{2am+8r}$ Hopping parameter
  bounded



Wilson-Dirac operator real eigenvalues

- determinant sign depends on $\{\lambda\} \in \mathbb{R}^-$
  $det[D(A)] = det[S^{-1}D(A)S] = \prod_i |\lambda_i|^2 \prod_j \bar{\lambda}_j$, $\lambda_j \in \mathbb{C}$, $\bar{\lambda}_j \in \mathbb{R}$

- corresponding eigenvectors role in CP breaking detection
  $v_i^+ \gamma_5 v_j \neq 0 \Leftrightarrow \lambda_i = \lambda_i^*$,
  real eigenmodes as pseudo zero modes on the lattice

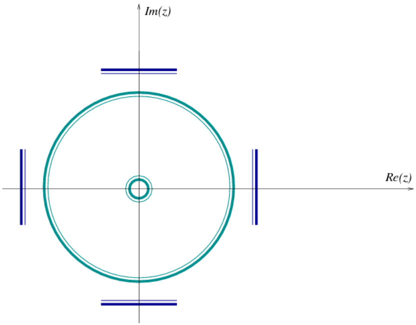
Arnoldi algorithm, features

returns set of k eigenvalues/eigenvectors

iteratively realising a Schur decomposition

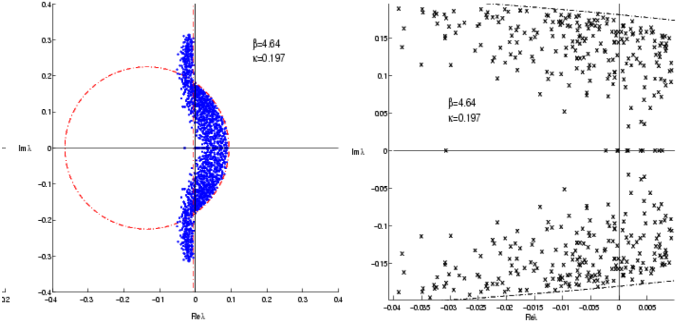
computational modes:

- largest/smallest real/complex part
- largest/smallest absolute value



the computational problem

very large sparse matrices ($\mathcal{O}(10^{14})$ size, $\mathcal{O}(10^7)$ entries)



bottlenecks:

- Wilson-Dirac operator size
- number of eigenvalues computed memory
- eigenvalues separation/density algorithm convergence

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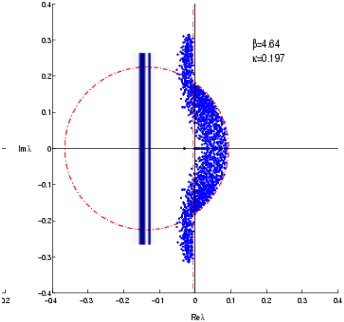

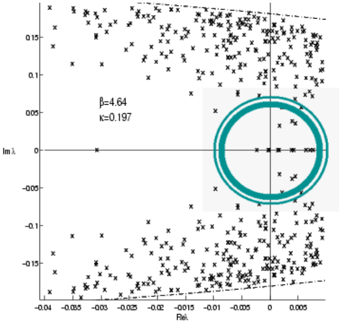

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enhancements

algorithmic optimizations:

matrix multiplication, SSE, MPI, ...

efficient eigensolvers (implicit restarting, ARPACK's Arnoldi for nonsymmetric matrix)

acceleration strategies:

explicit preconditionings $D_W \to \mathcal{P}_n(D_W)$

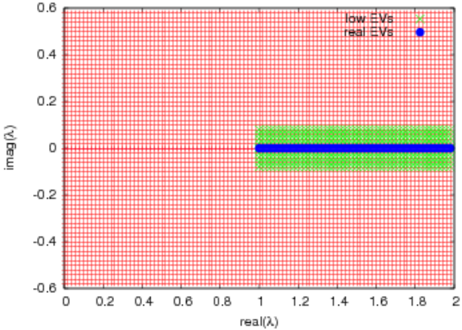
$\mathcal{P}_n$ polynomial transformation

- more operations with the Wilson-Dirac operator
- extract out one particular part of the eigenvalue spectrum
  less eigenvalues computed
- lower the eigenvalues density
  better convergence properties

acceleration strategies I

- power transformations with shift: H.Neff [2001]
  $D_W \to \mathcal{P}_n(D_W, \sigma) = (\sigma \mathbf{1} - D_W)^n$, $\lambda e^{i\theta} \to (\sigma - \lambda)^n e^{in\theta_{\sigma-\lambda}}$

improvement with even-odd preconditioning



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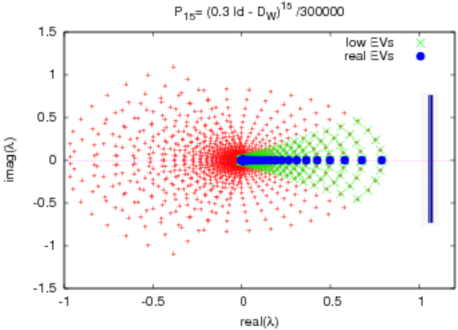

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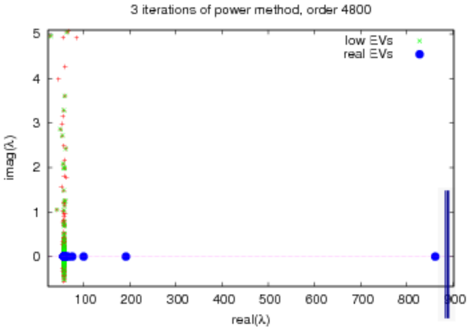
- Iterated version:
  $\mathcal{P}_m(D_W, \sigma_1) \to (\sigma_2 \mathbf{1} - P_m(D_W, \sigma_1))^n / C_{renorm}$.

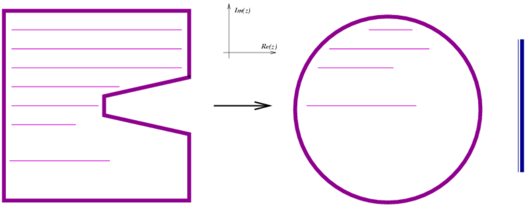


acceleration strategies II

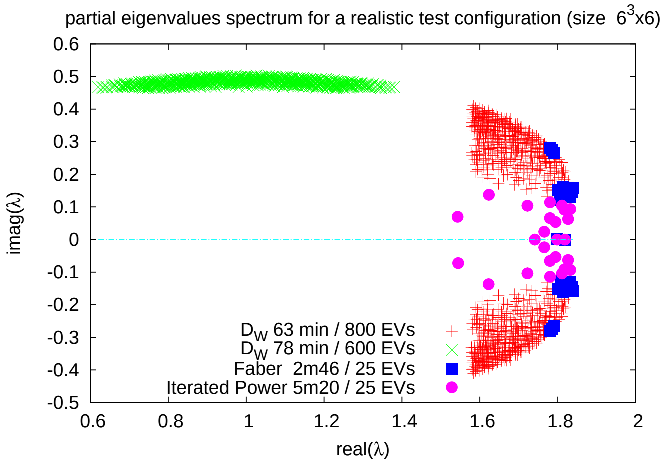
- min max problem for a polygonal, convex hull

  Chebyshev polynomials Y.Saad, numerical method for large eigenvalue problem [1992]

- Faber polynomial V.Heuveline, M.Sadkane [1997]



example



H.Neff [2001] for other examples

conclusion

$N_f = 1$ QCD phase structure study

computation of the real eigenvalues/eigenvectors becomes essential

- for the determinant sign problem

  up to 20% of negative determinant signs!

- for the study of CP breaking

Wilson-Dirac operator eigenvalues extraction

- acceleration through polynomial transformations

  Factor 10 to 100 improvements for memory requirements/computation time!

- best polynomial? problem dependent

  velocity performances versus eigenvalues number, κ dependent, tunings