Subsets in QCD (II)

dimension=2, 3, 4

Jacques Bloch

with Falk Bruckmann and Tilo Wettig

University of Regensburg

SIGN 2014

GSI, Darmstadt, 18-21 Febrar 2014

Goal

Investigate subsets based on Z_3 center symmetry for $d \geq 2$

Note: Subsets do not yet solve the sign problem in QCD, but exhibit interesting properties. . .

Fermions in lattice simulations

Monte Carlo simulation: generate configurations U with probability $e^{-S_G - S_F}$

After integration over fermion fields:

$$Z_{\text{QCD}} = \int \mathscr{D}U \; \underbrace{e^{-S_G} \prod_{f=1}^{N_f} \det[D(U;m,\mu)]}_{\text{MCMC weight function } P[U] \text{ ?}}$$

From now on: strong coupling ($e^{-S_G} = 1$)

Subsets

- Configurations with Complex weights → what is the meaning of *relevant* configurations?
- Subset principle: if we can construct subsets with mild or no sign problem → replace sampling of relevant configurations by sampling of relevant subsets
- Subset idea: gather configurations of ensemble into subsets with real and positive weights → construct Markov chains of relevant subsets using importance sampling
- Idea for QCD: subsets based on center symmetry of SU(3).

QCD in d dimensions

- Staggered Dirac operator

$$D_{xy} = m\,\delta_{xy} + \frac{1}{2}\Big[e^{a\mu}U_0(x)\delta_{y,x+\hat{0}} - e^{-a\mu}U_0^T(x-\hat{0})\delta_{y,x-\hat{0}}\Big] + \frac{1}{2}\sum_{\mu=1}^{3}\eta_{x\mu}\Big[U_\mu(x)\delta_{y,x+\hat{\mu}} - U_\mu^T(x-\hat{\mu})\delta_{y,x-\hat{\mu}}\Big]$$

with staggered fermion phase

$$\eta_{x\mu} = (-1)^{x_0+\cdots+x_{\mu-1}} \quad (\mu = 1\cdots 3)$$

Subset method

Subset construction

- Aim of subset method: gather configurations into 'small' subsets such that sum of determinants is real and positive.
- Definition: Z_3 subset on *one SU(3) link U*
  construct subset $\Omega_U \subset \mathrm{SU}(3)$ using Z_3 rotations and c.c.:

$$\Omega_U = \{U\,,\, e^{2\pi i/3}U\,,\, e^{4\pi i/3}U\} \cup \{U \to U^*\}\,.$$

Subsets in higher dimensions

Port Z_3 subsets to higher dimension:

1. collective Z_3 rotation on all temporal links on one time slice
2. $\otimes$ of Z_3 subsets for all temporal links on one time slice, cost $\sim 3^{V_s}$
3. $\otimes$ of Z_3 subsets for temporal links on all lattice sites, cost $\sim 3^{V}$.

Construction:

- Start from 'root' configuration $\mathscr{U} = \{U_{\mu,i} \,|\, \mu = 1 \ldots d \,\&\, i = 1 \ldots V\}$
- example: full product subset:

$$\Omega = \{\mathscr{U}_k \,|\, k = 1 \ldots N_\Omega\} \equiv \{U_{\{xyz\},i}\} \bigotimes_{i=1}^{V} \{U_{t,i}, e^{2\pi i/3} U_{t,i}, e^{4\pi i/3} U_{t,i}\}$$

Subset method

Weights and observables

Subset Ω with N_Ω elements has fermionic subset weight:

$$\sigma(\Omega) = \frac{1}{N_\Omega} \sum_{\mathcal{U} \in \Omega} \det D(\mathcal{U})$$

- In simulations: subsets generated according to measure $d\mathcal{U}\, \sigma(\Omega_\mathcal{U})$ and observables computed as

$$\langle O \rangle = \frac{1}{Z} \int d\mathcal{U}\, \sigma(\Omega_\mathcal{U})\, \langle O \rangle_{\Omega_\mathcal{U}} \approx \frac{1}{N_{\mathrm{MC}}} \sum_{n=1}^{N_{\mathrm{MC}}} \langle O \rangle_{\Omega_n}$$

with subset measurements

$$\langle O \rangle_\Omega = \frac{1}{N_\Omega \sigma(\Omega)} \sum_{\mathcal{U} \in \Omega} \det D(\mathcal{U})\, O(\mathcal{U}),$$

as configurations in subset generically have different observable values.

- In contrast to 1d-QCD the direct product subsets do not correspond to a mere projection on zero triality sector → much more to it
- Z_3-based subset sum:

$$\sigma(\Omega_P) = \sum_{b=-L^3}^{L^3} C_{3b}\, e^{3b\mu/T} \,,$$

→ expansion in baryon number.

  - If subset only contains "collective Z_3" rotations → coefficients C_{3b} are canonical determinants.
  - For direct product subsets they are not.

Results – 2d QCD

Compute average reweighting factors of subsets:

$$\langle r \rangle = \frac{\int d\mathscr{U}\, |\mathrm{Re}\,\sigma(\Omega_{\mathscr{U}})|\, \mathrm{sign}\,\mathrm{Re}\,\sigma(\Omega_{\mathscr{U}})}{\int d\mathscr{U}\, |\mathrm{Re}\,\sigma(\Omega_{\mathscr{U}})|}$$

Results – 2d QCD

Some reweighting factors for 2d QCD on $N_x \times N_t$ grid
$\mu = 0.3,\ N_f = 1,\ m = 0,\ N_{\text{MC}} = 10^4 - 10^5$

grid	2×2	2×4	2×6	2×8	2×10
phase-quenched	0.8134(3)	0.4361(4)	0.233(2)	0.130(2)	0.074(2)
collective Z_3	0.9778(9)	0.777(4)	0.500(6)	0.303(8)	0.19(1)
$\otimes_x Z_3(x,0)$	1.0	0.9896(5)	0.885(2)	0.670(5)	0.446(8)
$\otimes_{\mathbf{xt}} \mathbf{Z_3(x,t)}$	**1.0**	**1.0**	**1.0**$^{N_{\text{MC}}=10^3}$	**1.0**$^{N_{\text{MC}}=10^3}$	**1.0**$^{N_{\text{MC}}=300}$

grid	4×2	4×4	4×6	4×8	4×10
phase-quenched	0.794(2)	0.292(4)	0.092(3)	0.034(2)	0.011(2)
collective Z_3	0.957(5)	0.55(2)	0.19(2)	0.10(3)	0.02(1)
$\otimes_x Z_3(x,0)$	1.0	0.9974(7)	0.81(1)	0.42(2)	0.14(3)
$\otimes_{\mathbf{xt}} \mathbf{Z_3(x,t)}$	**1.0**	**1.0**$^{N_{\text{MC}}=200}$	—	—	—

grid	6×2	6×4	6×6
phase-quenched	0.738(2)	0.189(2)	0.031(1)
collective Z_3	0.90(1)	0.36(3)	0.036(29)
$\otimes_x Z_3(x,0)$	1.0(?)	0.9992(4)	0.72(2)
$\otimes_{\mathbf{xt}} \mathbf{Z_3(x,t)}$	**1.0**$^{N_{\text{MC}}=100}$	—	—

grid	8×2	8×4	8×6
phase-quenched	0.662(7)	0.124(8)	0.014(3)
collective Z_3	0.87(2)	0.23(4)	0.04(4)
$\otimes_x Z_3(x,0)$	1.0(?)	0.994(3)	0.71(5)
$\otimes_{\mathbf{xt}} \mathbf{Z_3(x,t)}$	—	—	—

Leaving the strong coupling regime

Introduce the gauge action $e^{-S_G[\beta,\mathscr{U}]}$:

$$\text{subset weight: } \sigma_\Omega = \sum_{\mathscr{U}\in\Omega} e^{-S_G[\beta,\mathscr{U}]} \det D(\mathscr{U})$$

2×2 grid with $\mu = 0.3$

β	0	1	2	3	4	5
phase-quenched	0.8134(3)	0.848(3)	0.864(6)	0.891(6)	0.913(6)	0.932(6)
$\otimes_{xt} Z_3(x,t)$	1.0	1.0	0.9998(2)	1.0	1.0	1.0

4×4 grid with $\mu = 0.3$

β	0	1	2	3	4	5
phase-quenched	0.292(4)	0.367(6)	0.47(1)	0.56(2)	0.62(3)	0.67(3)
$\otimes_{x} Z_3(x,t)$	0.9974(7)	0.993(2)	0.981(5)	0.973(8)	0.97(1)	0.981(9)

QCD in $d = 3$ and $d = 4$

- Same procedure for subset construction as for $d = 2$
- Generate of $\mathcal{O}(100)$ subsets for 2^3, $2^2 \times 4$ and 2^4 lattices
  $\rightarrow$ all weights of $\otimes_{xyzt} Z_3(x, y, z, t)$ subsets are *positive* at huge cost 3^V
- Puzzling: *why* are these subset weights positive?

- Can we improve the speed of computation using analytical or numerical tricks? Just a little using the Hasenfratz-Toussaint reduction formula and rank-6 corrections...

Hasenfratz-Toussaint reduction formula

Temporal gauge

Dirac matrix in temporal gauge:

$$D = \begin{pmatrix} B_1 & \mathbb{1} & 0 & \cdots & \cdots & \mathscr{P}^\dagger e^{-\mu/T} \\ -\mathbb{1} & B_2 & \mathbb{1} & \cdots & \cdots & 0 \\ \cdots & & \cdots & & \cdots & \\ -\mathscr{P} e^{\mu/T} & 0 & \cdots & \cdots & -\mathbb{1} & B_{N_t} \end{pmatrix},$$

$\{B_i \,|\, i = 1 \ldots N_t\}$: spatial hops + quark mass terms on time slice i,
$\mathscr{P}$: temporal links on last time slice (= Polyakov lines).
Each block $B_i, \mathscr{P}$ is $3L^3 \times 3L^3$ matrices.

HF reduction formula for staggered fermions

$$\det D = e^{3V_s\mu/T} \det(\mathscr{B} + e^{-\mu/T})$$

with $$\mathscr{B} = \left[\prod_{j=1}^{N_t} \begin{pmatrix} B_j & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \right] \mathscr{P}$$

Hasenfratz-Toussaint reduction formula

General gauge

Generalization to *general gauge*

$$D = \begin{pmatrix} B_1 & U_1 & 0 & \cdots & \cdots & U^\dagger_{N_t} e^{-\mu/T} \\ -U^\dagger_1 & B_2 & U_2 & \cdots & \cdots & 0 \\ \cdots & & \cdots & & \cdots & \\ -U_{N_t} e^{\mu/T} & 0 & \cdots & \cdots & -U^\dagger_{N_t-1} & B_{N_t} \end{pmatrix}.$$

$\mathcal{U}_t$: temporal links on time slice t.

HF reduction formula for staggered fermions

$$\det D = e^{3V_s\mu/T} \det(\mathcal{B} + e^{-\mu/T})$$

with $$\mathcal{B} = \prod_{t=1}^{N_t} \left[\begin{pmatrix} B_t & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathcal{U}_t \right]$$

Computing subset sums

Reduction formula allows for efficient computation of subset sums

- Consider Z_3 rotation of one temporal link on time slice N_t

$$\mathscr{B} \to \mathscr{B} R$$

with $$R = \mathrm{diag}(\underbrace{z\mathbb{1}_3, \mathbb{1}_3, \ldots, \mathbb{1}_3}_{L^3}, \underbrace{z\mathbb{1}_3, \mathbb{1}_3, \ldots, \mathbb{1}_3}_{L_3}) \quad \text{and} \quad z \in Z_3$$

After rotation:

$$\begin{aligned}
\det D_R &= e^{3V_s\mu/T} \det(\mathscr{B}R + e^{-\mu/T}) = e^{3V_s\mu/T} \det(\mathscr{B} + e^{-\mu/T} R^{-1}) \\
&= e^{3V_s\mu/T} \det\left[\mathscr{B} + e^{-\mu/T} + e^{-\mu/T}\left(R^{-1} - \mathbb{1}\right)\right] \\
&= e^{3V_s\mu/T} \det\left[\mathscr{B} + e^{-\mu/T} + e^{-\mu/T}(z^* - 1)\, U U^T\right]
\end{aligned}$$

where U is $6L^3 \times 6$ matrix

$$U^T = \begin{pmatrix} \mathbb{1}_3 & \ldots & 0_3 & | & 0_3 & \ldots & 0_3 \\ 0_3 & \ldots & 0_3 & | & \mathbb{1}_3 & \ldots & 0_3 \end{pmatrix}$$

Rotation and rank-6 correction

$e^{-\mu/T}\,(z^*-1)\,UU^T$: Rank-6 correction to $6L^3 \times 6L^3$ matrix $(\mathscr{B} + e^{-\mu/T})$

- Recall matrix determinant lemma

$$\det(A + \beta U V^T) = \det A \cdot \det \Sigma$$

with *capacitance matrix*

$$\Sigma = \mathbb{1}_k + V^T A^{-1} U.$$

Here: $V = U$ and $A = \mathscr{B} + e^{-\mu}$.

If we know $\det(\mathscr{B} + e^{-\mu})$ and $Q = (\mathscr{B} + e^{-\mu})^{-1}$
Then the cost of $\det(\mathscr{B}R + e^{-\mu})$ is of O(1) because $q = U^T Q U$ just cuts out a 6×6 portion of Q.
Idea: use this procedure recursively to perform all rotations on the right most time slice in $\mathscr{B}$

Recursive rank-6 corrections

However, the rank-6 correction on A requires A^{-1} $\rightarrow$ in recursive rank-6 corrections to $\det A$ we also need the rank-6 corrections to A^{-1}. Use the Woodbury formula (extension of Sherman-Morrison formula):

$$(A+\beta UV^T)^{-1} = A^{-1} - \beta(A^{-1}U)\Sigma^{-1}(V^T A^{-1})$$

In our case QU and $U^T Q$ cut out 6 columns and 6 rows of Q. However, the ranks-6 correction is of $\mathcal{O}(n^2)$ ($n = 6L^3$).
Note that we need

$$Q_R = (BR + e^{\mu})^{-1} = R^{-1}(B + e^{\mu}R^{-1})^{-1}$$

$\rightarrow$ rotate 6 rows of $(B + e^{\mu}R^{-1})^{-1}$.

- Q_R is also necessary to compute bulk observables.

Tree algorithm

- Use matrix determinant lemma and Woodbury formula to perform and combine all Z_3 rotations of temporal links on the last time slice with recursive rank-6 corrections → compute subset weight and observables.
- Implement a depth-first tree algorithm to reach all configurations of the product subset.
- Ternary tree structure:
  Level 0: root configuration of the subset — $\det D, D^{-1}$
  Level 1: 3 Z_3-rotations of $U_{t,1}$ — $\det D_{R_1}, D_{R_1}^{-1}$
  Level 2: 3 Z_3-rotations of $U_{t,2}$ — $\det D_{R_1 R_2}, D_{R_1 R_2}^{-1}$
  $\ldots$
  Level L^3: 3 Z_3 rotations of U_{t,L^3} — $\det D_{R_1 \cdots R_{L^3}}, D_{R_1 \cdots R_{L^3}}^{-1}$
- At the bottom level the tree has 3^{L^3} 'leaves' → all configurations in the subset. The sum of all the determinants at the bottom level is subset weight. The inverse are used to compute observables.

Reaching all time slices

Above: direct product subset on a single time slice.

Now: full direct product on all time slices.

- Again HT-formula proves useful:

$$\det D = e^{3V_s\mu/T} \det(\mathscr{B} + e^{-\mu/T}) \quad \text{with} \quad \mathscr{B} = \prod_{t=1}^{N_t} \left[\begin{pmatrix} B_t & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathscr{U}_t \right]$$

- When all Z_3 rotations on the rightmost time slice have been considered we can make a cyclic permutation in $\mathscr{B}$ to allow for Z_3 rotations on the previous time slice:

$$\det(\mathscr{B} + e^{-\mu/T}) = \det(\mathscr{B}' + e^{-\mu/T})$$

where

$$\mathscr{B}' = \begin{pmatrix} B_{N_t} & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathscr{U}_{N_t} \times \prod_{t=1}^{N_t-1} \left[\begin{pmatrix} B_t & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathscr{U}_t \right]$$

Extending the tree

- After the cyclic permutation the inverse is:

$$(\mathscr{B}' + e^{-\mu/T})^{-1} = \begin{pmatrix} B_{N_t} & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \mathscr{U}_{N_t} (\mathscr{B} + e^{-\mu/T})^{-1} \mathscr{U}^{\dagger}_{N_t} \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & -B_{N_t} \end{pmatrix}$$

- The tree can now be extended from below using recursive rank-6 corrections on the new rightmost time slice → add another L^3 levels for that time slice
- When all Z_3 rotations in a time slice have been considered → make next cyclic permutation, till all N_t time slices have been treated.
- The bottom of the tree is reached after $N_t \times L^3$ levels have been constructed and the subset sum is available.
- In principle the bottom of the tree has $3^{N_t \times L^3}$ leaves. For symmetry reasons this number can be reduced to $3^{N_t \times (L^3-1)+1}$... still BIG.

Hot from the press...

Try Shalesh's idea for p-h model

$$\sigma = \sum_{R \in \otimes_i (Z_3)_i} \det D_R = e^{3V_s\mu/T} \det(\mathscr{B} R + e^{-\mu/T})$$

where R runs over all 3^{L^3} subsets on the last time slice. Rewrite as:

$$\sigma = e^{-3V_s\mu/T} \sum_R \det(\mathscr{B} e^{\mu/T} + R^{-1}), \qquad R \text{ is diagonal}, \quad z_{R,i} \in Z_3$$

$$= e^{-3V_s\mu/T} \int d\bar{\psi} d\psi \exp\left(-e^{\mu/T} \sum_{i,j=1}^{6L^3} \bar{\psi}_i \mathscr{B}_{ij} \psi_j \right) \sum_R \exp\left(-\sum_{i=1}^{6L^3} z_{R,i} \bar{\psi}_i \psi_i \right)$$

$$= e^{-3V_s\mu/T} \int d\bar{\psi} d\psi \exp\left[-e^{\mu/T} \sum_{i,j=1}^{6L^3} \bar{\psi}_i \mathscr{B}_{ij} \psi_j \right] \sum_R \prod_{i=1}^{6L^3} (1 - z_{R,i} \bar{\psi}_i \psi_i)$$

not so hot after all...?

Now:

$$\sum_R = \prod_{m=1}^{L^3} \sum_{z_m \in Z_3}, \qquad \text{every } z_m \text{ occurs 6 times in } \prod_{i=1}^{6L^3} \text{ above}$$

For one temporal link:

$$\Omega = \sum_{z\in Z_3} \prod_{i=1}^{6} (1 - z\bar\psi_i \psi_i) = 3 - \frac{1}{2} \sum_{i,j,k=1}^{6} \epsilon_{ijk} (\bar\psi_i\psi_i)(\bar\psi_j\psi_j)(\bar\psi_k\psi_k)$$
$$+ 3(\bar\psi_1\psi_1)(\bar\psi_2\psi_2)(\bar\psi_3\psi_3)(\bar\psi_4\psi_4)(\bar\psi_5\psi_5)(\bar\psi_6\psi_6)$$

NOT bilinear. Hence,

$$\sigma = e^{-3V_s\mu/T} \int d\bar\psi d\psi \exp\left[-e^{\mu/T} \sum_{i,j=1}^{6L^3} \bar\psi_i \mathscr{B}_{ij} \psi_j \right] \prod_{m=1}^{L^3} \Omega_m$$

How to proceed without falling back on the standard meson/baryon loop representation?

Conclusions & Outlook

Conclusions

Subset method in d-dimensional QCD for $d \geq 2$

- preliminary results indicate that direct product of Z_3 subsets for all temporal links have positive weights. Cost is exponential so no solution to sign problem, but puzzling observation.

Outlook

- Direct product subsets would solve sign problem if subset sums can be performed at non-exponential cost $\rightarrow$ analytical and/or numerical work
- Understanding the subset positivity could yield interesting insight
- More thinking, more discussions needed