Solving the sign problem in one-dimensional QCD

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Introduction

- Sign problem in QCD is particularly serious in d=4, but already exists in (0+1)-dimensions (Bilic & Demeterfi, 1988) → use QCD_1 as toy model to study the sign problem (Ravagli & Verbaarschot, 2007)
- Sign problem in QCD_1 is mild → reweighting methods can be used, but solution to sign problem could help for higher dimensions.
- Subset idea originates from solution to sign problem for random matrix model of QCD (JB, PRL 107 (2011) 132002, PRD 86 (2012) 074505): gather configurations in subsets with real and positive weights → construct Markov chains of relevant subsets using importance sampling.
- RMT subsets: related to projection on the $q = 0$ canonical determinant (JB, Bruckmann, Kieburg, Splittorff, Verbaarschot, PRD 87 (2013) 034510).
- Same subsets solve sign problem in U(N_c) theory but are NOT allowed in QCD because configurations would *leave* SU(3).
- Idea for QCD: subsets based on center symmetry of SU(3).

QCD in 0+1 dimensions

Dirac operator & determinant

- Consider QCD_1: SU(3) on one spatial point and $N_t = 1/aT$ time slices.
- QCD_1 Dirac operator for quark of mass m at chemical potential μ:

$$D_{tt'} = m\,\delta_{tt'} + \frac{1}{2a}\left[e^{a\mu} U_t \delta_{t',t+1} - e^{-a\mu} U^\dagger_{t-1} \delta_{t',t-1}\right],$$

  where $U_t \in \mathrm{SU}(3)$ and $\delta_{tt'}$ is anti-periodic Kronecker delta.
- Dirac determinant can be reduced to determinant of a 3×3 matrix:

$$\det(aD) = \frac{1}{2^{3N_t}} \det\left[e^{\mu/T} P + e^{-\mu/T} P^\dagger + 2\cosh\left(\mu_c/T\right)\, \mathbb{1}_3\right]$$

  with Polyakov loop $P = \prod_t U_t$ and *effective mass* $a\mu_c = \operatorname{arsinh}(am)$.
- Determinant depends on P and μ through the combination $e^{\mu/T} P$ only:
  (i) all gauge links can be shifted into Polyakov loop: $U_1 \cdots U_{N_t} \equiv P$,
  (ii) μ-dependence through closed temporal loops only $\rightarrow (e^{a\mu})^{N_t} = e^{\mu/T}$.

- QCD_1 has no gauge action → partition function is one-link integral of Dirac determinant for N_f quark flavors:

$$Z^{(N_f)} = \int dP \, \det{}^{N_f} D(P) \,,$$

with SU(3) Haar measure dP.

- Imaginary part of $\det^{N_f} D(P)$ could be canceled by pairing P with P^*, because $\det D(P^*) = [\det D(P)]^*$.
- However, for $\mu \neq 0$: $\text{Re} \det^{N_f} D$ has fluctuating sign → sign problem in MC simulations.

Subset method

Subset construction

- Aim of subset method: gather configurations into small subsets such that sum of determinants is real and positive.
- Recipe: starting from configuration P, construct subset $\Omega_P \subset \mathrm{SU}(3)$ using Z_3 rotations and c.c.:

$$\Omega_P = \{P\,,\, e^{2\pi i/3} P\,,\, e^{4\pi i/3} P\} \cup \{P \rightarrow P^*\}\,.$$

- Set of all subsets forms six-fold covering of original SU(3) ensemble.
- Subset weights:

$$\sigma(\Omega_P) = \frac{1}{6} \sum_{k=0}^{2} \det^{N_f} D(P_k) + \text{c.c.}\,, \quad P_k = e^{2\pi i k/3} P\,.$$

- Partition function can be rewritten as an integral over subsets:

$$Z^{(N_f)} = \int dP\, \sigma(\Omega_P)\,.$$

- In simulations: subsets generated according to measure $dP\,\sigma(\Omega_P)$, and observables are computed as

$$\langle O\rangle = \frac{1}{Z^{(N_f)}}\int dP\,\sigma(\Omega_P)\,\langle O\rangle_{\Omega_P} \approx \frac{1}{N_{\mathrm{MC}}}\sum_{n=1}^{N_{\mathrm{MC}}}\langle O\rangle_{\Omega_n}$$

with subset measurements

$$\langle O\rangle_{\Omega_P} = \frac{1}{6\sigma(\Omega_P)}\sum_{k=0}^{2}\left[\det^{N_f} D(P_k)\,O(P_k) + (P_k \to P_k^*)\right],$$

as configurations in subset generically have different observable values.

Subset method

Subset properties

- N_f-flavor determinant can be decomposed into powers of $e^{\mu/T}$ as

$$\det^{N_f} D(P) = \sum_{q=-3N_f}^{3N_f} D_q \, e^{q\mu/T} .$$

- Determinant satisfies: $$\det D(\underbrace{e^{i\theta}P}_{Z_3 \text{ rotation of } P})\Big|_{\mu/T} = \det D(P)\Big|_{\underbrace{\mu/T+i\theta}_{\text{imaginary shift of } \mu}} .$$

- Z_3 subset: sum of determinants = projection on zero triality sector:

$$\sigma(\Omega_P) = \frac{1}{3} \sum_{q=-3N_f}^{3N_f} \operatorname{Re} D_q \, e^{q\mu/T} \underbrace{\sum_{k=0}^{2} e^{2\pi i q k/3}}_{3\delta_{q \bmod 3, 0}} = \sum_{b=-N_f}^{N_f} \operatorname{Re} D_{3b} \, e^{3b\mu/T} ,$$

$\rightarrow$ expansion in baryon number

Subset method for $N_f = 1$

Partition function and observables

Subset weight for $N_f = 1$

$$\sigma(\Omega_P) = 2\cosh(3\mu/T) + A^3 - 3A + A|\operatorname{tr} P|^2 \quad > 0$$

with $A = 2\cosh\left(\mu_c/T\right)$

$\rightarrow$ $\sigma(\Omega_P)$ is real and positive for any μ, m, and P
$\rightarrow$ use to generate subsets with importance sampling.

Analytical results:

- group integration of $\sigma(\Omega_P) \rightarrow$ partition function,
- derivatives of free energy $\rightarrow$ chiral condensate Σ and quark number density n ,
- trace of Polyakov loop: computed with one-link integral, satisfies $\langle \operatorname{tr} P^\dagger \rangle = \langle \operatorname{tr} P \rangle\Big|_{\mu\to-\mu}$.

Subset method for $N_f = 1$

Simulations

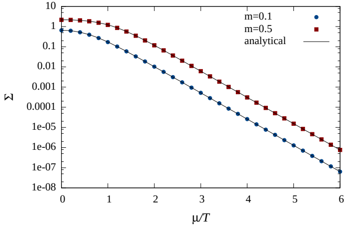
Implement subset method and verify with analytical predictions:

- generate SU(3) links according to Haar measure,
- construct Z_3 subsets and explicitly compute determinants and subset weights ,
- perform Metropolis accept-reject on the real and positive subset weights $\rightarrow$ Markov chains of relevant subsets,
- compute chiral condensate $\Sigma = \frac{1}{N_t}\langle \mathrm{tr}\left[D^{-1}\right]\rangle$, quark number density $n = \frac{1}{N_t}\langle \mathrm{tr}\left[D^{-1}\partial D/\partial \mu\right]\rangle$ and trace of Polyakov loop $\langle \mathrm{tr}\, P\rangle$ as sample means of subset measurements.

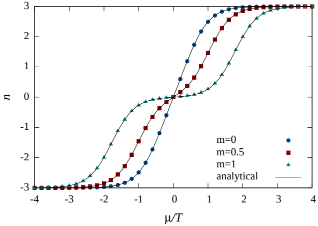
Numerical results

$N_{\text{MC}} = 100,000$ subsets

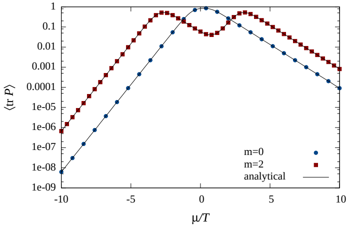
Chiral condensate



Quark number density



Trace of the Polyakov loop



Observe the $\mu \longleftrightarrow -\mu$ asymmetry (or $\operatorname{tr} P \longleftrightarrow \operatorname{tr} P^\dagger$ asymmetry), which is clearly illustrated by the different exponential decays for large positive and negative μ.

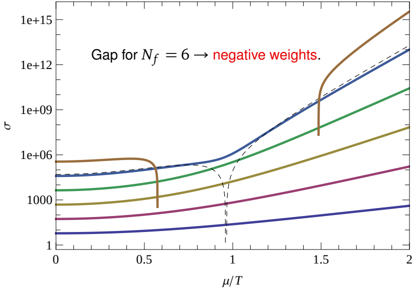
N_f larger than one

Subset properties

- Subset weights are real, but there is no general argument for their positivity for arbitrary N_f.
- Subset weights are strictly positive for all μ and P for $N_f < 5.11$
- For $N_f > 5.11$: regions in P and μ with negative weights.

$\sigma(\Omega_P)$ with $P = \mathrm{diag}(1, -1, -1)$

$N_f = 1, \ldots, 6$ and $N_f = 5.11$ ($m = 0$)



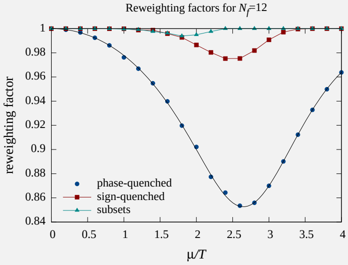
Subset reweighting for $N_f \geq 6$

- IF subset weights have fluctuating sign $\longrightarrow$ no importance sampling.
- Instead: use subsets as auxiliary system for reweighting method.
- Generate subsets according to $|\sigma|$ and absorb sign in observable:

$$\langle O \rangle = \frac{\langle \operatorname{sign} \sigma \times \langle O \rangle_\Omega \rangle_{|\sigma|}}{\langle \operatorname{sign} \sigma \rangle_{|\sigma|}} .$$

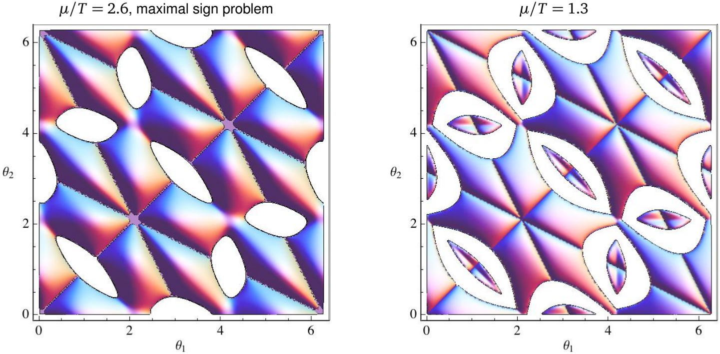
  - for $N_f \leq 5$: $\langle \operatorname{sign} \sigma \rangle_{|\sigma|} = 1 \longrightarrow$ use subset method as is,
  - for $N_f \geq 6$: $\langle \operatorname{sign} \sigma \rangle_{|\sigma|} < 1$ for some $\mu \longrightarrow$ use reweighting on subsets.

Compare subset reweighting factors with those in phase-quenched and sign-quenched in link formulation
$\longrightarrow$ sign problem is much milder in subset formulation.



- For Z_3 subsets: analyse subset weights $\times$ Haar measure
- diagonalize SU(3) link: $P = U\,\mathrm{diag}(e^{i\theta_1}, e^{i\theta_2}, e^{-i\theta_1 - i\theta_2})\,U^\dagger$

$\log[J(P)\,\sigma(\Omega_P)]$ for $N_f = 24$ $(m = 0)$



- Holes in surface $\longrightarrow$ negative weights on the logarithmic scale.
- permutation symmetries of $\theta_1, \theta_2, \theta_3$ $\longrightarrow$ mosaic of six replicated regions

Extended subsets

Constructing "rotated" links

Extend subset construction beyond Z_3 to solve sign problem for $N_f \geq 6$

- consider constant diagonal SU(3) matrix $G = \mathrm{diag}(e^{i\alpha}, e^{i\beta}, e^{-i\alpha-i\beta})$
- for any link $P = U\,\mathrm{diag}(e^{i\theta_1}, e^{i\theta_2}, e^{-i\theta_1-i\theta_2})\,U^\dagger$ define "rotated" link

$$R(P,G) = U\mathrm{diag}(e^{i\theta_1'}, e^{i\theta_2'}, e^{-i\theta_1'-i\theta_2'})\,U^\dagger \quad \in \mathrm{SU}(3)$$

by rotating eigenvalue matrix of P by G, such that

$$\theta_1 \to \theta_1' = \theta_1 + \alpha\,, \qquad \theta_2 \to \theta_2' = \theta_2 + \beta$$

- to preserve symmetry under eigenvalue permutations: create 6 "rotated links" using all permutations $\{\pi_1, \ldots, \pi_6\}$ of the eigenvalues of G:

$$P^{(i)} = R(P, \pi_i(G))$$

- Extended subsets: union of Z_3 subsets for $P^{(0)} = P$ and $P^{(1)}, \ldots, P^{(6)}$:

$$\Omega_P^{\text{ext}} = \bigcup_{i=0}^{6} \Omega_{P^{(i)}}$$

- Partition function is

$$Z^{(N_f)} = \int dP \, \sigma_P^{\text{ext}},$$

with Haar measure dP if extended subset weights are defined as

$$\sigma_P^{\text{ext}} = \frac{1}{7} \sum_{i=0}^{6} \frac{J(P^{(i)})}{J(P)} \, \sigma_{Z_3}(\Omega_{P^{(i)}}),$$

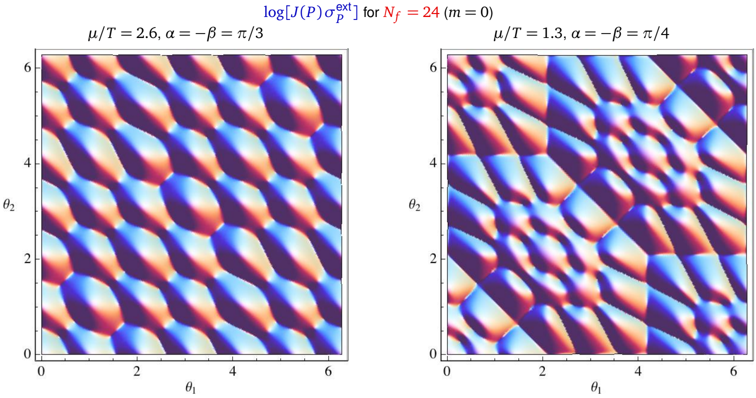
with $\sigma_{Z_3}(\Omega_{P^{(i)}})$ the Z_3 subset weight of $\Omega_{P^{(i)}}$ and Jacobian

$$J(\theta_1, \theta_2) = \frac{8}{3\pi^2} \sin^2 \frac{\theta_1 - \theta_2}{2} \sin^2 \frac{2\theta_1 + \theta_2}{2} \sin^2 \frac{\theta_1 + 2\theta_2}{2} \, .$$

Extended subsets

Extended subset weight for $N_f = 24$

- Location of holes in Z_3 plot → guess values for shifts α and β in G
- Extended subsets solve the sign problem for suitable G



Conclusions & Outlook

Conclusions

Subset method to eliminate the sign problem in simulations of QCD_1 at nonzero chemical potential.

- for $N_f \leq 5$: gather SU(3) links into Z_3 subsets → sum of fermion determinants is real and positive .
- For $N_f \geq 6$: Z_3 subset weights can become negative
  → construct extended subsets using additional SU(3) rotations.

Outlook

- Naive port to higher dimension: direct product of Z_3 subsets for each temporal link on lattice → computing cost grows exponentially as 3^{L^d}.
- To solve exponential growth: subsets should have a *collective* nature.
- A first look at $d = 2$?

2d QCD

Some reweighting factors for 2d QCD on $N_x \times N_t$ grid ($N_f = 1$, $m = 0$)

$\beta = 0, N_x = 2, \mu = 0.8$

N_t	2	4	6	8
phase-quenched	0.384(2)	0.134(2)	0.0471(1)	0.0187(8)
sign-quenched	0.551(3)	0.207(3)	0.078(2)	0.0283(11)
collective Z_3	0.703(4)	0.329(7)	0.141(8)	0.055(9)
$\otimes_x Z_3(x,0)$	0.99914(13)	0.927(2)	0.660(7)	0.402(14)
$\otimes_{xt} Z_3(x,t)$	1.0	1.0	1.0 ($N_{\text{MC}} = 100$)	1.0 ($N_{\text{MC}} = 100$)

$\beta = 0$

grid μ	2×2 0.8	4×4 0.7	6×6 0.6
phase-quenched	0.384(2)	0.088(2)	0.0126(12)
sign-quenched	0.551(3)	0.134(6)	0.015(2)*
collective Z_3	0.703(4)	0.197(8)	0.025(8)*
$\otimes_x Z_3(x,0)$	0.99914(13)	0.883(8)*	0.307(27)*
$\otimes_{xt} Z_3(x,t)$	1.0	1.0 ($N_{\text{MC}} = 190$)	—

*(N_{MC}=10,000)

2×2 grid with $\mu = 0.8$

β	0	1	2	3
phase-quenched	0.384(2)	0.426(13)	0.437(12)	0.499(14)
sign-quenched	0.551(3)	0.576(20)	0.623(22)	0.731(20)
collective Z_3	0.703(4)	0.77(3)	0.78(4)	0.856(37)
$\otimes_x Z_3(x,0)$	0.99914(13)	0.978(7)	0.914(18)	0.948(15)
$\otimes_{xt} Z_3(x,t)$	1.0	1.0	0.992(3)	0.966(10)