Sign problem and subsets 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 QCD₁ as toy model to study the sign problem (Ravagli & Verbaarschot, 2007)
- Sign problem in QCD₁ 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.
- QCD₁ Dirac operator for quark of mass m at chemical potential μ:

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

where $U_t \in SU(3)$ 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 in 0+1 dimensions

Partition function

 QCD₁ 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 µ ≠ 0: 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 Ω_P ⊂ SU(3) using Z₃ rotations and c.c.:

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

- 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:

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

Computing observables

 In simulations: subsets generated according to measure dP σ(Ω_p), and observables are computed as

$$\langle O
angle = rac{1}{Z^{(N_f)}} \int dP \,\sigma(\Omega_P) \,\langle O
angle_{\Omega_P} pprox rac{1}{N_{\mathsf{MC}}} \sum_{n=1}^{N_{\mathsf{MC}}} \langle O
angle_{\Omega_n}$$

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: $\det D(e^{i\theta}P)\Big|_{\mu/T} = \det D(P)\Big|_{\mu/T+i\theta}$. Z_3 rotation of P imaginary shift of μ
- Z₃ subset: sum of determinants = projection on zero triality sector:

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

→ expansion in baryon number

Subset method for $N_f = 1$

Partition function and observables

Subset weight for $N_f = 1$

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

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

- $\rightarrow \sigma(\Omega_P)$ 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
 → Markov chains of relevant subsets,
- compute chiral condensate $\Sigma = \frac{1}{N_t} \langle \operatorname{tr} \left[D^{-1} \right] \rangle$, quark number density $n = \frac{1}{N_t} \langle \operatorname{tr} \left[D^{-1} \partial D / \partial \mu \right] \rangle$ and trace of Polyakov loop $\langle \operatorname{tr} P \rangle$ as sample means of subset measurements.

Subset method for $N_f = 1$

Numerical results



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.



Subset reweighting for $N_f \ge 6$

- IF subset weights have fluctuating sign → 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 $N_f \leq 5$: $\langle \operatorname{sign} \sigma \rangle_{|\sigma|} = 1 \rightarrow$ use subset method as is,

• for $N_f \ge 6$: $\langle \operatorname{sign} \sigma \rangle_{|\sigma|} < 1$ for some $\mu \to \text{use reweighting on subsets.}$

Compare subset reweighting factors with those in phase-quenched and sign-quenched in link formulation

→ sign problem is much milder in subset formulation.



 Z_3 subsets for large N_f

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



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

Constructing "rotated" links

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

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

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

by rotating eigenvalue matrix of P by G, such that

$$\theta_1 \rightarrow \theta_1' = \theta_1 + \alpha$$
, $\theta_2 \rightarrow \theta_2' = \theta_2 + \beta$

 to preserve symmetry under eigenvalue permutations: create 6 "rotated links" using all permutations {π₁,..., π₆} of the eigenvalues of G:

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

Constructing extended subsets

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

$$\Omega_p^{\mathsf{ext}} = \bigcup_{i=0}^6 \, \Omega_{P^{(i)}}$$

Partition function is

$$Z^{(N_f)} = \int dP \, \sigma_p^{\mathsf{ext}},$$

with Haar measure dP and extended subset weights

$$\sigma_{p}^{\mathsf{ext}} = rac{1}{7} \sum_{i=0}^{6} rac{J(P^{(i)})}{J(P)} \, \sigma_{Z_{3}}(\Omega_{P^{(i)}}),$$

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

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

Extended subset weight for $N_f = 24$

- Location of holes in Z_3 plot \rightarrow 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 QCD₁ at nonzero chemical potential.

- for $N_f \leq 5$: gather SU(3) links into Z_3 subsets \rightarrow sum of fermion determinants is real and positive .
- For N_f ≥ 6: Z₃ subset weights can become negative
 → construct extended subsets using additional SU(3) rotations.

Outlook

- Naive port to higher dimension: direct product of Z₃ 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 ($N_f = 1, m = 0$)

p 0,1.7 2, p 010								
Nt	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	$1.0 (N_{MC} = 100)$	$1.0 (N_{MC} = 60)$				

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

 $\beta = 0$

grid	2×2	4 × 4	6×6
μ	0.8	0.7	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	$1.0 (N_{MC} = 110)$	—

*(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)