Positivity of center subsets for QCD

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SIGN 2015, Atomki/Debrecen, Oct. 2015

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1508.03522

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Introduction

QCD at high density/with chemical potential μ has a sign problem:

- path integral weight det $\not{D} \ngeq 0 \Rightarrow$ no importance sampling

‘subsets’: add up configurations until the weight is positive

works in:

- random matrix model with μ — Bloch 11
  fugacity expansion — Bloch, FB, Kieburg, Splittorff, Verbaarschot 12
- lattice QCD in 0+1 dimensions — Bloch, FB, Wettig 13
  no gauge action, solvable — (Bilic, Demeterfi 88, Ravagli, Verbaarschot 07)

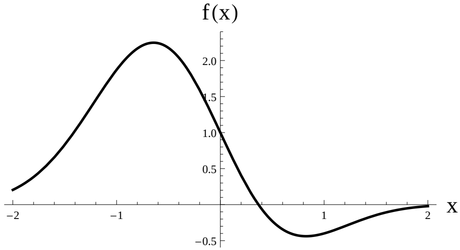
here:

- higher-dimensional lattices
  analytical & numerical evidence for positivity of subsets

Subset idea: an example

- 'partition function': (from the random matrix model)

$$Z = \int_{-\infty}^{\infty} dx\, f(x)\,, \qquad f(x) = e^{-x^2}\left(1 + x^2 - \cosh(\mu)\, x\right) \lessgtr 0$$



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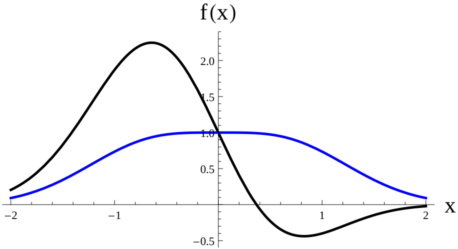

- subsets: add values at x and $-x$ = integrate over even part

$$Z = \int_{-\infty}^{\infty} dx\, \underbrace{\frac{1}{2}\left[f(x) + f(-x)\right]}_{e^{-x^2}(1+x^2) > 0}$$

Subsets in a random matrix model

- partition function for $\Phi_{1,2}$ complex $N \times N$ matrices Osborn '04

$$Z(\mu) = \int d\Phi_{1,2}\, e^{-N\,\mathrm{Tr}\,(\Phi_1\Phi_1^\dagger + \Phi_2\Phi_2^\dagger)} \det \begin{pmatrix} m & e^{\mu}\Phi_1 - e^{-\mu}\Phi_2^\dagger \\ -e^{-\mu}\Phi_1^\dagger + e^{\mu}\Phi_2 & m \end{pmatrix}$$

- subsets: measure and Gaussian invariant under $\Phi_{1,2} \to e^{i\theta}\,\Phi_{1,2}$

  determinant changes (not a kind of gauge trafo!)

  add up the weight of those rotated matrices

- but before that: interpret the rotation as an imag. μ

$$Z(\mu) = \int d\Phi_{1,2}\, ..\det \begin{pmatrix} m & e^{\mu}e^{i\theta}\Phi_1 - e^{-\mu}e^{-i\theta}\Phi_2^\dagger \\ -e^{-\mu}e^{-i\theta}\Phi_1^\dagger + e^{\mu}e^{i\theta}\Phi_2 & m \end{pmatrix}$$

$$= Z(\mu + i\theta) \qquad \forall\theta$$

$$= \frac{1}{n}\sum_{k=0}^{n-1} Z(\mu + ik/n)$$

- fugacity expansion:

$$Z(\mu) = \sum_{q=-2N}^{2N} e^{q\mu} Z_q$$

Z_q: canonical partition functions

range of q from det being a polynomial in $e^{\pm\mu}$ of order $2N$

- put together:

$$Z(\mu) = \sum_{q=-2N}^{2N} e^{q\mu} \underbrace{\frac{1}{n}\sum_{k=0}^{n-1} e^{2\pi i k/n \cdot q}}_{\delta_{q \bmod n, 0}} Z_q$$

sum of nth roots (and most of their powers) vanish

- choose $n > 2N$:

$$Z(\mu) = e^0 Z_0 = Z(\mu = 0) \quad \text{“no mu, no cry”}$$

- actually, the μ-dep. disappears on the level of the integrand

$\Rightarrow$ the integrand is that at $\mu = 0$ and thus is positive

Subset definition in lattice QCD

add up configurations $\leftarrow$ multiplication of links with group elements (not gauge trafos!)

- formally using the invariance of the group measure [Haar]

$$Z = \int DU\, w[U] = \int_{SU(3)} \prod_{\mu,x} d\big(U_\mu(x)\big)\, w[U]$$

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- cf. group U(1):

$$\int_{U(1)} dU \overset{U=e^{i\phi}}{=} \frac{1}{2\pi}\int_0^{2\pi} d\phi = \frac{1}{2\pi}\int_0^{2\pi} d(-\phi_V + \phi) = \int_{U(1)} d(V^{-1}U)$$

(translation invariance on the circle)

Center subsets in lattice QCD

add up configurations $\leftarrow$ multiplication of links with center elements

- center Z_3: $g = e^{2\pi ik/3}\,1_3$ with $k = 0, 1, 2$
  commutes with all $SU(3)$ group elements
- center subsets:

$$Z = \int DU\, w[gU] \qquad g \in Z_3 \otimes Z_3 \otimes \dots$$

$$= \int DU\, \underbrace{\frac{1}{\#_g}\sum_g w[gU]}_{\equiv\, \sigma(U) \overset{?}{>} 0}$$

if the subset weight σ is positive one can use importance sampling even if the original weight w was not positive

- observables can be measured, too

alternative view:

- part of the integral = center sum performed deterministically, while remaining part = integral over the coset subject to sampling

why center?

- gauge theories w/o center ($SU(N)_{\text{adj}}$, G_2) have no sign problem
- confinement criterion on Polyakov loop:
  $\text{tr}P \to g\,\text{tr}P$ (approx.) preserved/broken at low/high T (and μ?)
- technically easy
- seemingly sufficient
- below: connected to imag. μ and diagrammatics
- similarity to clusters in Pott model   Alford, Chandrasekharan, Cox, Wiese 01

Center subsets in 0+1 dimensions

- no plaquette $\Rightarrow w = \det \not{D}$
- temporal links can be gauged to a single link $\leftarrow$ Polyakov loop P
- original weight, $m = 0$, one flavor:

$$
\begin{aligned}
w(P) &= \det_{3\times 3}(1 + e^{\mu/T} P)(1 + e^{-\mu/T} P^\dagger) \\
&= e^{-3\mu/T} + e^{-2\mu/T}\, 2\,\mathrm{tr}\, P + e^{-\mu/T}\left[2\,\mathrm{tr}\, P^\dagger + (\mathrm{tr}\, P)^2\right] \\
&\quad + e^{3\mu/T} + e^{2\mu/T}\, 2\,\mathrm{tr}\, P^\dagger + e^{\mu/T}\left[2\,\mathrm{tr}\, P + (\mathrm{tr}\, P^\dagger)^2\right] \\
&\quad + 2 + 2\,|\mathrm{tr}\, P|^2 \not> 0 \quad (\mathrm{Re}\, w \text{ matters, still } \not> 0)
\end{aligned}
$$

- center subsets:

$$
\frac{1}{3}\left(w(P) + w(e^{2\pi i/3}P) + w(e^{-2\pi i/3}P)\right) = e^{-3\mu/T} + e^{3\mu/T} + 2 + 2\,|\mathrm{tr}\, P|^2 > 0
$$

positive, used for importance sampling ✓

only baryon chemical potential $\mu_B = 3\mu$ enters (see below)

Collective subsets and imag. μ

- lattice implementation of μ on one (say last) time slice:

$$e^{\mu/T} U_0, \quad e^{-\mu/T} U_0^\dagger$$

- 'collective subsets': same center element, only on that time slice:

$$e^{\mu/T} U_0 \to e^{\mu/T} \cdot \frac{1}{3} \sum_{k=0}^{2} e^{2\pi i k/3} U_0 = \frac{1}{3} \sum_{k=0}^{2} e^{\mu/T + 2\pi i k/3} \cdot U_0$$

& analogously for $U_0^\dagger$

$$\det \not{D}_{\mu/T} \to \frac{1}{3} \sum_{k=0}^{2} \det \not{D}_{\mu/T + 2\pi i k/3}$$

& plaquette unchanged

= adding/averaging 3 complex μ's

= Roberge-Weiss symmetry (on integrals) utilized on integrands

- fugacity expansion:

$$\det \not{D}_{\mu/T} = \sum_q e^{q\mu/T} \not{D}_q \to \sum_q e^{q\mu/T} \underbrace{\frac{1}{3}\sum_{k=0}^{2} e^{2\pi i k/3\cdot q}}_{\delta_{q \text{ mod } 3,0}} \not{D}_q$$

nonzero triality terms removed

from the path integrand; the corresponding integrals = canonical partition functions vanish anyhow

expansion in $3\mu = \mu_B$

- these collective subsets attenuate the sign problem, but in general do not solve it

$\Rightarrow$ independent center multiplications on all temporal links

Positivity of center subsets: numerical evidence

- 1+1 dimensional QCD

  one (unrooted) staggered quark

  $\mu = 0.3$, $m = 0$ (sign problem worst)

  no plaquette = strong coupling approx.

  reweighting factors on 100,000 configurations (* means 1,000):

$N_t \times N_x$	2×2	4×2	6×2	8×2	10×2
phase-quenched	0.8134(3)	0.4361(4)	0.233(2)	0.130(2)	0.071(1)
sign-quenched	0.9271(2)	0.6150(5)	0.355(3)	0.203(2)	0.109(2)
collective subsets	0.9778(9)	0.777(4)	0.500(6)	0.303(8)	0.178(3)
full subsets	1.0	1.0	1.0*	1.0*	1.0*

$N_t \times N_x$	2×4	4×4	6×4	2×6	2×8
pq	0.7934(5)	0.295(1)	0.0961(9)	0.7364(6)	0.6725(7)
sq	0.9197(3)	0.442(2)	0.149(1)	0.8917(4)	0.8523(5)
collective	0.959(1)	0.557(6)	0.214(8)	0.912(3)	0.867(2)
full	1.0*	1.0*	1.0*	1.0*	1.0*

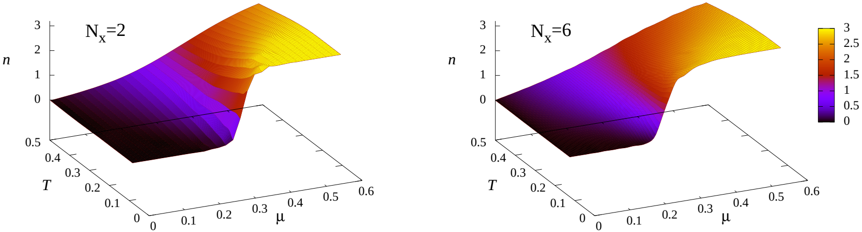
- higher dimensions
  on 200 random configurations:
  full subsets give reweighting factors 1.0 for 2^3, $2^2 \times 4$ and 2^4

- with gauge action
  $\beta = 1, 2, 3, 4, 5$ on 2×6
  reweighting factors 1.0, 1.0, 0.984(7), 0.964(13), 0.972(17)
  = mild sign problem

- subsets can always be used to attenuate the sign problem
  reweighting factor has to increase (Cauchy-Schwarz)
  or combined with other methods

A first physics result

- quark number density as a function of μ and T (in lattice units)



$(N_t = 2, \ldots, 12$ and $N_t = 2, \ldots, 8)$

- Silver-Blaze property visible

Positivity of center subsets: analytical proof for $N_t = 2$

massless staggered determinant at $\mu = 0$

- the usual argument:

  $\not{D}$ is antihermitian and chiral*

  $\Rightarrow$ eigenvalues in pairs $\pm i\cdot$ real $\Rightarrow \det \not{D}_{\mu=0} \geq 0$

  chiral*: anticommutes with η_5, $\eta_5(x_{\text{ev,od}}) = \pm 1$

- argument using quarks as Grassmannians:

$$\det \not{D}_{\mu=0} = \int D\bar{\psi} D\psi \exp(\bar{\psi} \not{D}_{\mu=0} \psi)$$

  and even-odd decomposition

$$\int D\bar\psi D\psi \exp(\bar\psi \not{D}_{\mu=0}\psi)$$
$$= \int D\bar\psi_{\text{ev}} D\psi_{\text{od}} \cdot D\psi_{\text{ev}} D\bar\psi_{\text{od}}$$
$$\times \prod_{x,\nu} \exp\left(\bar\psi(x)_a \eta_\nu U_\nu(x)_{ab} \psi(x+\hat\nu)_b\right) \cdot \exp\left(\psi(x)_a \eta_\nu U^*_\nu(x)_{ab} \bar\psi(x+\hat\nu)_b\right)$$

- of the two hoppings, one is even-odd and the other odd-even

  separate the hoppings to the integrals accordingly

  integration variable change $\psi \rightleftharpoons \bar\psi$: same integral up to $U \leftrightharpoons U^*$

  $$p[U_{\text{ev}}, U^*_{\text{od}}] \cdot p[U^*_{\text{ev}}, U_{\text{od}}] = p[U_{\text{ev}}, U^*_{\text{od}}] \cdot p[U_{\text{ev}}, U^*_{\text{od}}]^* \geq 0 \quad \checkmark$$

  since p is a polynomial in the links with real coefficients

  actually, $p = \det \not{D}_{\text{even-odd}}$

massless determinant is positive at $\mu = 0$ ✓

- antiperiodic boundary conditions do not interfere
- similar argument with mass

  (mass terms just saturate some Grassmann integrals)
- violated by real μ's, on $\nu = 0$

  $\Rightarrow$ need subsets

  antiperiodic bc.s are actually essential [not discussed here] subsets on $N_t = 2$:

- take the two points in the temporal direction together
  pecularity: $U_0(x)$ and $U_0^\dagger(x+\hat{0})$ connect the same sites
  = contain the same Grassmannians, but with inverse μ-factors
- subset weight of the form:

$$\sigma = \int D\bar{\psi}_{\text{even}} D\psi_{\text{odd}} \cdot D\psi_{\text{even}} D\bar{\psi}_{\text{odd}}$$
$$\times \prod_{x,i} \exp\left(\bar{\psi}(x)\eta_i U_i(x)\psi(x+\hat{\nu})\right) \cdot \exp\left(\psi(x)\eta_i U_i^*(x)\bar{\psi}(x+\hat{\nu})\right)$$
$$\times \prod_{\vec{x}} \sum_{\alpha} h_\alpha\big(\bar{\psi}(1,\vec{x}), \psi(2,\vec{x}); U_0\big) \cdot h_\alpha\big(\psi(1,\vec{x}), \bar{\psi}(2,\vec{x}); U_0^*\big)$$

- again: in all terms, one factor is even-odd and the other odd-even

$\Rightarrow$ even-odd structure with $U_\nu \leftrightharpoons U_\nu^*$ $\Rightarrow$ subset weight positive ✓

- μ tamed in $h_{\alpha=0}$:
  $\left(1 - 2\cosh(\mu_B)\bar{\psi}(1,\vec{x})^3\psi(2,\vec{x})^3\right) \cdot \left(1 - 2\cosh(\mu_B)\psi(1,\vec{x})^3\bar{\psi}(2,\vec{x})^3\right)$

Center subsets and diagrammatics

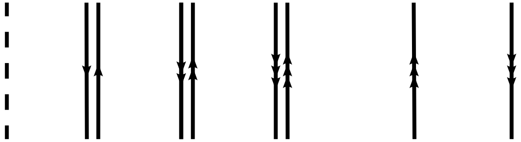
- fermion action and Grassmann character:

$$\exp(S_F) \sim \exp\left(e^{\mu}\,\underbrace{\bar\psi(x)U_0(x)\psi(x+\hat 0)}_{u}\right)\exp\left(e^{-\mu}\,\underbrace{\psi(x)U_0^*(x)\bar\psi(x+\hat 0)}_{\bar u}\right)$$

$$= \sum_{m,n=0}^{3}\frac{1}{m!n!}\left(e^{\mu}u\right)^m\left(e^{-\mu}\bar u\right)^n \qquad (\mu \equiv a\,\mu)$$

$$\sigma \sim \underbrace{1 + u\bar u + \frac{(u\bar u)^2}{2!^2} + \frac{(u\bar u)^3}{3!^2}}_{\text{mesonic}} + \underbrace{\frac{e^{3\mu}u^3}{3!} + \frac{e^{-3\mu}\bar u^3}{3!}}_{\text{baryonic}} + \text{~~nonzero triality~~}$$

- from 16 down to 6 hoppings = ‘building blocks’ per bond:



(anti)baryons carry $\pm 3\mu = \pm\mu_B$

- same diagrams as if U integrated out completely

  Rossi, Wolff 84, Karsch, Mütter 89

  because center sums already remove the same nonzero triality hoppings as whole link integrals

  zero triality terms contain a singlet, e.g. $u\bar{u} \sim 3 \times \bar{3}$, $u^3 \sim 3 \times 3 \times 3$

- some weights simplify:

$$u^3 \sim (\bar{\psi} U \psi)^3 \sim \underbrace{\bar{\psi}^3}_{\epsilon_{\dots}} U_{.\circ} U_{.\circ} U_{.\circ} \underbrace{\psi^3}_{\epsilon_{\circ\circ\circ}} \sim \det U = 1$$

  $\Rightarrow$ (anti)baryons and 3-mesons are link-independent (again as if U integrated out)

  used in the proof above

- 1- and 2-mesons remain U-independent

  (U's enter traces of closed Wilson loops $\rightleftharpoons$ gauge invariance)

  $\Rightarrow$ can measure e.g. Polyakov loops

Future plan: hybrid approach

subsets on all temporal links contain 3^V summands $\leftarrow$ exp. expensive

$\Rightarrow$ combine with diagrammatics

- in $N_t = 2$ proof the subset weights consists of many positive terms
  $\Rightarrow$ which subset diagrams to add up to achieve positivity
  configurations: those diagrams

- constraint: at every site 3 arrows have to go in and out
  (representing mass terms $\bar{\psi}(x)\psi(x)$ as arrows returning to the same site)
  simulation: worm algorithm — see also Fromm, de Forcrand 09

- use U-dependence to reweight gauge action back in

Summary and Outlook

adding up configurations obtained by center rotating the temporal links give a positive weight and thus solve the sign problem in

- 0+1d QCD
- $N_t = 2 \times \langle \text{any} \rangle$ lattices in strong coupling $\leftarrow$ analytical proof
- various lattices in strong coupling $\leftarrow$ numerical evidence
  always positive? proof?

subset diagrams: mesonic and baryonic hoppings in temporal direction
(spatial subsets: same hoppings in spatial directions)

- hybrid approach

beyond strong coupling = including the gauge action:

- numerical evidence: the sign problem might be mild, such that reweighting could be used

  check volume dependence!