

Subset method for the sign problem in one-dimensional QCD

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with Jacques Bloch and Tilo Wettig
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Outline

- introduction: random matrix model and a simple example
- subset method in random matrices – the first Bloch '11
 - why it works Bloch, FB, Kieburg, Splittorff, Verbaarschot '12
- subset method in gauge theories
 - 1d QCD – the obvious and not-so-obvious Bloch, FB, Wettig '13
 - ≥ 2 d QCD – the hard talk by J. Bloch

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similar approaches

Barbour, Davies, Sabeur '88; Hasenfratz, Toussaint '92
Aarts, Kaczmarek, Karsch, Stamatescu '02; Bringoltz '10

on clusters in Potts model

Alford, Chandrasekharan, Cox, Wiese '01

Introduction

- grandcanonical partition function of QCD (one flavor):

$$Z(\mu) = \int DA e^{-S_g[A]} \det(\not{D}[A] + m \mathbb{1} + \mu \gamma_0)$$

- and of a random matrix model:

Osborn '04

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

– 4d path integral \rightsquigarrow ordinary matrix integral

– gauge fields/lattice links \rightsquigarrow complex $N \times N$ matrices

– gauge action \rightsquigarrow Gaussian weight

both: massless Dirac operator is chiral

– chemical potential: $e^{a\mu} U_0, e^{-a\mu} U_0^\dagger$ (lattice) $\rightsquigarrow e^{\pm\mu} \Phi_{1,2}$

both: massless Dirac operator is not anti-hermitian anymore

\Rightarrow sign problem for $\mu \neq 0$

- simplest case: 1×1 matrices, $m = 0$ (problem worst)

new variables $x = \Phi_1 \Phi_2$, $y = \Phi_1 / \Phi_2$, specialize to $y = 1$:

$$Z(\mu) \sim \int_{\mathbb{C}} dx e^{-2|x|} \left(\underbrace{|x| - \text{Re } x \cosh 2\mu}_{\neq 0} - \underbrace{i \text{Im } x \sinh 2\mu}_{\text{imag.}} \right)$$

- the term causing a negative integrand (and the imag. part) is **odd** in x

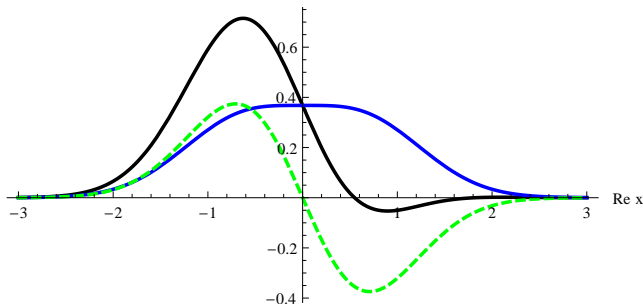
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add (average) integrand at x and $-x \Rightarrow$ positive integrand



original integrand

odd term

new integrand

$\mu = 1.8$

($\text{Im } x = 0, y = 1$)

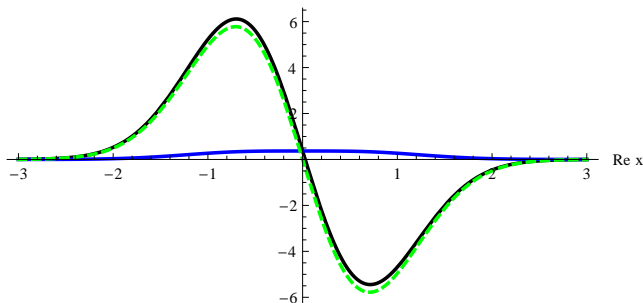
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- note that we have removed the μ -dependence altogether:

$$Z(\mu) \sim \int_{\mathbb{C}} dx e^{-2|x|} \left(|x| - \underbrace{\operatorname{Re} x \cosh 2\mu - i \operatorname{Im} x \sinh 2\mu}_{\text{gone}} \right)$$

‘Silver blaze’ forever

not so in QCD, model is of limited use

- for the generalization note that $x \rightarrow -x$ means $\Phi_{1,2} \rightarrow i \cdot \Phi_{1,2}$

- use N_s th roots of unity: $e^{i\theta_k}$ with $\theta_k = 2\pi \frac{k}{N_s}$, $k = 0, \dots, N_s - 1$

average the weights over subsets $\{e^{i\theta_k} \Phi_{1,2}\}$

- (0) integration variables $\Phi_{1,2}$ remain in the integration range
“fields remain in the configuration space”
- (1) transformation is invertible
angles yield an exact N_s -fold covering of configuration space
- (2) Gaussian weight is invariant
det's add up to positive for $N_s > 2N$ ✓
- (3) number of configurations in the subset:
linear $N_s = \mathcal{O}(N)$, not $\mathcal{O}(e^N)$ ✓

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- reinterpret phases as imaginary chem. potential:

$$e^\mu \Phi_{1,2} \rightarrow e^\mu e^{i\theta_k} \Phi_{1,2} = e^{\mu+i\theta_k} \Phi_{1,2} \quad \text{same for } e^{-\mu} \Phi_{1,2}^\dagger$$

- fugacity expansion: part. function and det.s are polynomials in e^μ

$$\det D(\mu) = \sum_{q=-2N}^{2N} e^{q\mu} D_q \quad \dots \text{canonical determinants}$$

subset weights:

$$\sigma(\mu) = \sum_{q=-2N}^{2N} e^{q\mu} \underbrace{\left(\frac{1}{N_s} \sum_k e^{2\pi i \frac{k}{N_s} q} \right)}_{\neq 0 \text{ iff } q \bmod N_s = 0} D_q = D_0 + e^{\pm N_s \mu} D_{\pm N_s} + \dots$$

$\stackrel{\text{large}}{=} D_0 \geq 0 \dots$ integrand at $\mu = 0$, 'no mu, no cry'

$\Rightarrow \mu$ -independence (Silver Blaze) at the level of the weight

D_1, D_2, \dots removed, they integrate to zero can. part. functions anyhow

- first idea:

phases on temporal links: $U_0 \longrightarrow e^{i\theta_k} U_0 \quad \theta_k = 2\pi \frac{k}{N_s}, k = 0, \dots, N_s - 1$

(0) links remain in configuration space: $e^{i\theta_k} U_0 \in SU(N_c)$?

iff restricted to **center transformations** (det must be 1), $N_s = N_c$

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NB: in $U(N_c)$ all phases are allowed, N_s is arbitrary
 μ -dependence removed \Leftrightarrow no baryons in $U(N_c)$
- (1) transformation is invertible, i.e. exact three-fold covering ✓
- (2) gauge action (plaquettes) invariant ✓
det's add up to positive??
- (3) 3 configs. in subset
effort = constant, not even $\mathcal{O}(V)$

- interpretation as imag. chemical potential $\mu/T + i\theta_k$ ✓

projects out baryon sectors: $Z(\mu) = \sum_{q \bmod 3=0} e^{q\mu/T} Z_q$ ✓

μ -dependence kept ✓

- cancellations in part. function:

$$\int dU e^{-S_g} \left(\underbrace{\det_0(U) + \det_{\pm 3}(U) e^{\pm 3\mu/T} + \dots}_{\substack{\text{give the nonvanishing } Z\text{'s} \\ \text{'essential'} \\ \text{already positive??}}} + \underbrace{\det_{\pm 1}(U) e^{\pm \mu/T} + \dots}_{\substack{\text{integrate to vanishing } Z\text{'s} \\ \text{'artificial'}^* \\ \text{removed by subsets}}} \right)$$

*: these terms contribute to Polyakov loops ('winding observables')

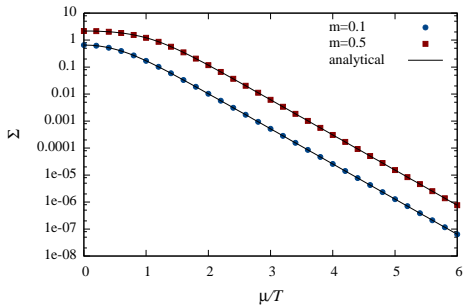
- temporal links U_0 through $\prod_{x_0} U_0 = P \dots$ Polyakov loop $\in SU(3)$
 - Dirac operator: $\det D \sim \det_{3 \times 3} (A 1_3 + e^{\mu/T} P + e^{-\mu/T} P^\dagger)$ Bilic, Demeterfi '88
- with mass parameter $A = 2 \cosh\left(\frac{\text{arsinh}(am)}{aT}\right) \geq 2$
 and chemical potential through $\prod_{x_0} e^{a\mu} = e^{\mu/T}$
- no plaquettes
 - analytically solvable Bilic, Demeterfi '88; Ravagli, Verbaarschot '07
 - subsets: $\{P, e^{2\pi i/3} P, e^{-2\pi i/3} P\}$

part. function for $N_f = 1$:

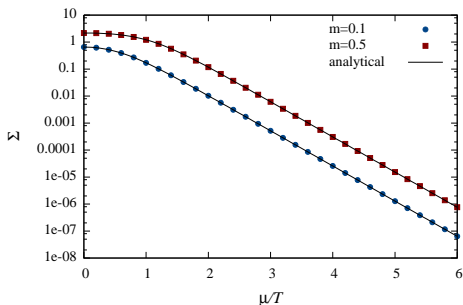
$$Z(\mu) = \int d_{\text{Haar}} P \left(\underbrace{A^3 - 3A + A|\text{tr}P|^2}_{\text{positive } \checkmark} + \underbrace{\dots e^{\pm\mu/T} + \dots e^{\pm 2\mu/T}}_{\text{removed by subsets}} + \underbrace{1 \cdot e^{\pm 3\mu/T}}_{\text{positive } \checkmark} \right)$$

\Rightarrow sign problem solved by center subsets \checkmark

- measure observables, e.g. chiral condensate:



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- computation:

$$\langle O \rangle = \frac{1}{Z(\mu)} \int dP \det(P; \mu) \cdot O(P)$$

$$= \frac{1}{Z(\mu)} \int dP \underbrace{\frac{1}{3} \sum_{k=0}^2 \det(e^{2\pi i k/3} P; \mu)}_{\sigma(\{P\}; \mu)} \cdot \sum_{l=0}^2 \underbrace{\frac{\det(e^{2\pi i l/3} P; \mu)}{\sigma(\{P\}; \mu)}}_{\text{relative weight of config. in subset}} O(e^{2\pi i l/3} P)$$

subset weight: sampling

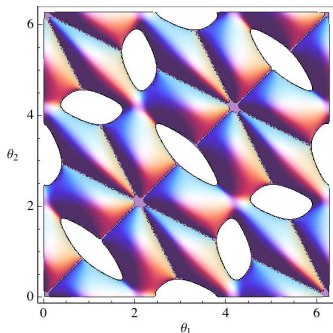
subset observable

1d QCD with many flavors

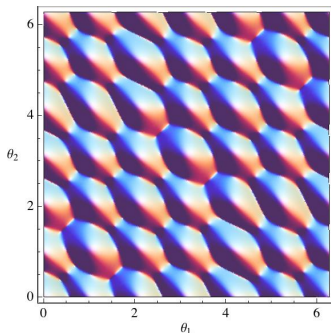
- sign problem reappears with more than 5 flavors even with subsets:

$$Z(\mu) = \int d_{\text{Haar}} P(\underbrace{\dots e^{0\mu/T} + \dots e^{3\mu/T} + \dots e^{6\mu/T} + \dots + 1 \cdot e^{3N_f\mu/T}}_{\text{not positive definite for some } (P, \mu)})$$

integrand over config. space (φ_1, φ_2) in $P \sim \text{diag}(e^{i\varphi_1}, e^{i\varphi_2}, e^{-i(\varphi_1+\varphi_2)})$ for $N_f = 24, \mu = 2.6$ ($m = 0$), logarithmically:



center subsets



center + extended subsets (see below)

Extended subsets

- beyond the center:

group multiplication: $U_0 \rightarrow G_k U_0 \quad G_k \in SU(3) \quad k = 0, \dots, N_s - 1$

- (0) links remain in $SU(3)$ ✓
translations in the (φ_1, φ_2) -diagram
- (1) invertible, N_s -fold covering ✓
- (2) plaquettes: not present in 1d
- (3) effort? which G 's??
our finding:
7 G 's solve/significantly attenuate
the sign problem with $N_f = 12, 24, 48$
(see above)

systematic? “the not-so-obvious”

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Lemma

assume:

- path integral over groups with *real* weights $w(U)$
- group multiplication subsets: $\bar{w}(U) = \frac{1}{N_s} \sum_{k=0}^{N_s-1} w(G_k U)$

subset reweighting factor larger and its relative error smaller than for conventional sign quenching

proof:

$$r_{\text{subsets}} = \frac{\int dU \sum w}{\int dU |\sum w|} \stackrel{\text{Schwarz}}{\geq} \frac{\int dU \sum w}{\int dU \sum |w|} \equiv \frac{\sum_k \int dU w(G_k U)}{\sum_k \int dU |w(G_k U)|}$$
$$\stackrel{\text{Haar}}{=} \frac{\sum_k \int dU w(U)}{\sum_k \int dU |w(U)|} = \frac{\int dU w(U)}{\int dU |w(U)|} = r_{\text{conv}}$$

$$\text{and } \left(\frac{\sigma_r}{r}\right)^2 = \frac{1}{r^2} - 1$$

also for nested subsets, but does not specify the numerical effort

Summary and outlook

explicit summation over a subset of configurations $\stackrel{!?}{\leftarrow}$ positive weight
then remaining integration left for numerics using importance sampling

- subsets with phases in $U(1)$ or center Z_3 removes sign problem
in random matrix model and QCD in 1d with $N_f \leq 5$
(and in $U(N_c)$ gauge theories)
- interpretation as imag. $\mu \Rightarrow$ projection onto particular q -sectors
only $q = 0$ $q \bmod 3 = 0$
- extended subsets remove/attenuate sign problem for QCD in 1d
with $N_f \geq 6$
- no interpretation as shift in μ , still improved weights, cf. Lemma

outlook:

- subset method for other sign problems, some thoughts below
- QCD in $\geq 2d$: see the talk by J. Bloch

More subset methods

- (ungauged) lattice Higgs model with chem. potential:

$$S(\phi) = \sum_x \left(V(|\phi|) + \text{spat. hoppings} + e^{a\mu} \phi_x^* \phi_{x+\hat{0}} + e^{-a\mu} \phi_x \phi_{x+\hat{0}}^* \right)$$

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subsets: since $\phi_x \in \mathbb{C}$ one stays in the config. space with $\phi_x \rightarrow e^{i\theta x_0} \phi_x$
interpretation as $a\mu \rightarrow a\mu + i\theta$
periodic bc.s constraint: $\theta_k = 2\pi k/N_0$

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- 2d Yang-Mills theory with theta term:

$$S(U) = \beta \sum_{\text{plaq.s } \square} \left(e^{\eta} \text{tr} U_{\square} + e^{-\eta} \text{tr} U_{\square}^{\dagger} \right) \quad \eta \sim \Theta g^2 a^2$$

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subsets: from magn. field setup one can modify: $\text{tr} U_{\square} \rightarrow e^{i\theta} \text{tr} U_{\square}$
interpretation as $\eta \rightarrow \eta + i\theta$
flux quantization constraint: $\theta_k = 2\pi k/N_x N_y$
 $SU(N_c)$: center, too