The Severity of the Sign Problem in Different Regions of the QCD Phase Diagram

David Reeb

Institute of Theoretical Science, University of Oregon

Sign Problems and Complex Actions
Workshop at ECT* in Trento/Italy
March 2-6, 2009

arXiv:0808.2987 “On the sign problem in dense QCD” with Stephen Hsu (University of Oregon)
What’s the question?

Strongest evidence about severity of sign problem in the QCD phase diagram?

Quantify/define degree of severity of sign problem?

- later: focus on phase transition region
- from insights gained: suggest $Z_{\text{new}}$ method; “typicality” problems
Outline

1. Introduction
   - sign problem in dense QCD
   - split into two positive ensembles $Z_+, Z_-$

2. Free energies and analyticity
   - severity of the sign problem

3. Regions of the QCD phase diagram
   - hadronic phase, quark-gluon plasma, CSC phase
   - general considerations

4. Monte-Carlo methods
   - degrees of severity of sign problem
   - the $|\text{Re det } M(A)|$ method; typicality
   - comparision with reweighting and quenching methods

5. Conclusions & Questions
The sign problem in dense QCD

Partition function of grand canonical ensemble:

\[ Z(\beta, \mu) = \text{Tr} e^{-\beta(H-\mu N)} \]

real and positive \((\mu \in \mathbb{R})\)

\[ = \sum_{\{\Psi[\phi(x)]\}} \langle \Psi | e^{-\beta(H-\mu N)} | \Psi \rangle \text{ sum of pos. terms, typicality} \]

vastness of Hilbert space \(\{\Psi\}\)

\[ \rightarrow \text{ Euclidean functional integral over classical field configurations} \]

\[ Z = \int \mathcal{D}A \int \mathcal{D}\psi \mathcal{D}\overline{\psi} \ e^{-\int_0^\beta dx^4 \int d^3x \{ \overline{\psi}(\not{D}(A)-m-\mu \gamma_4)\psi + \frac{1}{4g^2} F^a_{\mu \nu} F^{a \mu \nu} \}} \]

\[ = \int \mathcal{D}A \ (\text{det} M(A)) \ e^{-\int_0^\beta dx^4 \int d^3x \ \frac{1}{4g^2} F^a_{\mu \nu} F^{a \mu \nu}} \]

with \( M(A) = \not{D}(A) - m - \mu \gamma_4 \) not (similar to) Hermitian
The sign problem in dense QCD

\[ Z(\beta, \mu) = \int \mathcal{D}A \ (\det M(A)) \ e^{-S_G(A)} \in \mathbb{R}^+ , \]

although \( \det M(A) \in \mathbb{C} \) for generic \( A \).

No probability interpretation for \( (\det M(A)) e^{-S_G(A)} \)
→ sign problem or phase problem: importance sampling?

Idea: lump phase into observable \( \mathcal{O} \)

\[
\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}A \ |\det M(A)| e^{-S_G(A)} \mathcal{O}(A) e^{i\theta(A)}}{\int \mathcal{D}A \ |\det M(A)| e^{-S_G(A)} e^{i\theta(A)}}
\]

and sample with measure \( |\det M(A)| e^{-S_G(A)} \)

→ phase/sign fluctuations in denominator/numerator; poor overlap?
Reality of $Z$

First: make $Z \in \mathbb{R}$ more manifest:

$$Z = \text{Re } Z = \int \mathcal{D}A \text{ Re } \left( \text{det } M(A) \ e^{-S_G(A)} \right)$$

$$= \int \mathcal{D}A \ (\text{Re } \text{det } M(A)) \ e^{-S_G(A)}$$

physical reason:

a) $\text{det } M(A') = (\text{det } M(A))^*$ for PC-conj. $A'_\mu (\vec{x}, x^4) \equiv A^*_\mu (\vec{x}, x^4)$ (and $\psi' (\vec{x}, x^4) = \gamma_5 \gamma_2 \psi^* (\vec{x}, x^4)$)

b) in lattice formulation of gauge theories:

links $U \rightarrow U^* \Rightarrow \text{det } M(U^*) = (\text{det } M(U))^*$ and $S_G(U^*) = S_G(U)$
Two positive ensembles: $Z_+$ and $Z_-$

$$Z = \int \mathcal{D}A \ (\text{Re det } M(A)) \ e^{-S_G(A)}$$

$\{+\}$: set of configurations $A^a_\mu(x)$ with $\text{Re det } M(A) > 0$

$\{-\}$: $\text{Re det } M(A) < 0$

$$Z = \sum_{\{+\}} |\text{Re det } M| e^{-S_G(A; \beta)} - \sum_{\{-\}} |\text{Re det } M| e^{-S_G(A; \beta)}$$

$$\equiv Z_+ - Z_-$$

- $Z_+ > Z_- \geq 0$

- $Z_+, Z_-$ partition functions of fictitious 4+1 dim systems?
  “potential” $V_{4+1}(A) = S_G(A) - \ln |\text{Re det } M(A)|$
Independent ensembles?

Fictitious Hamiltonian(s) (→ molecular dynamics algorithm):

\[
H_{4+1}[A, \pi; \beta] = \sum_i \frac{1}{2} \pi_i^2 + \left\{ S_G(A; \beta) - \ln |\text{Re det } M(A)| \right\}
\]

Potential barrier \( V_{4+1} = +\infty \) between \( \{+\} \) and \( \{-\} \).

- If connected & ergodic, sampling with H-equations (in principle)
Assumption – two separate ensembles

Assumption for the next part of this talk:

\( Z_+, Z_- \) are sensible ensembles on their own, i.e. each is connected and allows for ergodic sampling

- \( Z = Z_+ - Z_- \): important split for following part of talk
- useful to characterize severity of sign problem? → later
Free energy densities $F_+, F_-: \quad Z_\pm(\mu, \beta; V) \equiv \exp(-V F_\pm(\mu, \beta))$

Actually: $F_\pm$ are the intensive parts, but $\exists$ volume dependence

$Z_+(\mu, \beta; V) \equiv \exp(-V f_+(\mu, \beta; V))$

→ then define: $F_+(\mu, \beta) \equiv \lim_{V \to \infty} f_+(\mu, \beta, V)$

but finite-volume corrections: $f_+(V) = F_+ + \hat{f}_+(V)$

\[\begin{align*}
a) \quad F_+ < F_- & \implies Z_+ \text{ dominates } Z_- \text{ exponentially at large } V \\
& \implies \text{MILD sign problem: } Z_-/Z_+ \to 0 \text{ for } V \to \infty \\
b) \quad F_+ = F_- & \implies Z_+ \text{ and } Z_- \text{ generically of same size} \\
& \implies \text{SEVERE sign problem: } Z_-/Z_+ > 0 \text{ at } V \to \infty \\
& \quad (\text{if } \hat{f}_-(V) - \hat{f}_+(V) > 1/V \implies \text{MILD sign problem})
\end{align*}\]
Free energy densities

*Statistical Mechanics*: free energy densities $F_{\pm}$ are **analytic** functions of their arguments $(\mu, \beta)$, away from phase boundaries/transitions

- $F_+ = F_-$ in open set $\Rightarrow F_+ \equiv F_-$ in common domain of analyticity
- $F_+ \neq F_-$ in open set $\Rightarrow F_+ = F_-$ at most on submanifold

Severe sign problem at (potentially) $F_+(\mu) = F_-(\mu)$
Sign problem in the QCD phase diagram

Example: $\mu = 0$

$Z_- = 0, Z_+ = Z > 0$

$\rightarrow F_+ < F_- = +\infty$

Now: • examine different regions (A, B, C) of QCD phase diagram
• apply analyticity reasoning
A: hadronic phase

phase of quark matrix: \( \det M(A) = |\det M(A)| e^{i\theta(A)} \)

chiral perturbation theory at low \( \mu, T \) (Splittorff & Verbaarschot):

\( \theta \) has Gaussian distribution \( \rho(\theta) \), width \( \sqrt{\langle \theta^2 \rangle - \langle \theta \rangle^2} \sim V^{1/2} \)

So: \( Z_-/Z_+ \rightarrow 1 \) as \( V \rightarrow \infty \), i.e. in particular \( F_+ = F_- \)
(see also: \( Z_+ > Z_- \))
A: hadronic phase

\[ F_+ = F_- \] in open region of small \( \mu \), small \( T \)

analyticity \( \Rightarrow \) \( F_+ \equiv F_- \) in entire phase: SEVERE SIGN PROBLEM

at least for small \((\mu, T)\): if \( V \) large enough \( \rightarrow Z_+/Z_- \approx 1 \)

\( \rightarrow \) how can sampling at finite \( V \) give reliable results for \( V = \infty \)?

Order of limits to get ordinary QCD:

- \( V \rightarrow \infty \) first, then \( \mu \rightarrow 0 \):
  \( \lim_{\mu \rightarrow 0} F_-(\mu) < \infty \)

- \( \mu = 0 \) at any \( V \):
  \( F_-(\mu = 0, V) = +\infty \)
What’s the strongest argument for SEVERE sign problem in all of A? In all of the phase diagram?
B: quark-gluon plasma phase

- $N$ quark flavors with $\mu$:
  \[ Z_N = \int D A \det M(A) e^{-S_G(A)} \]

- $N/2$ flavors with $+\mu$, $N/2$ flavors with $-\mu$:
  \[ Z_{|N|} = \int D A \ |\det M(A)| e^{-S_G(A)} \]

\[ \Rightarrow \quad Z_N \leq Z_{|N|} \quad \text{and} \quad \frac{Z_N}{Z_{|N|}} = \frac{\exp (-VF_N)}{\exp (-VF_{|N|})} \]

a) models have different physics (pion condensation in $Z_{|N|}$)

b) $F_N$, $F_{|N|}$ perturbatively for large $T$, small $\mu/T$ (Vuorinen):
   \[ \rightarrow \text{terms linear in flavor chemical potentials} \Rightarrow \quad F_N > F_{|N|} \]
B: quark-gluon plasma phase

\[
\Rightarrow \frac{\exp(-VF_N)}{\exp(-VF_{|N|})} = \frac{Z_N}{Z_{|N|}} = \int d\theta \rho(\theta) \cos(\theta) \rightarrow 0 \quad (V \rightarrow \infty)
\]

So: 

a) \(\rho(\theta)\) peaked at \(\theta = (n + 1/2)\pi\), i.e. det \(M\) imaginary \(\rightarrow \text{NO}\)

b) \(\rho(\theta)\) smooth with large width: \(Z_{N^-}/Z_{N^+} \rightarrow 1 \quad (V \rightarrow \infty)\)

\(\rightarrow \text{SEVERE SIGN PROBLEM}\) in all of B by analyticity
if no severe sign problem: QCD inequalities apply
- rely on positive measure $d\mu = DA_\mu^a e^{-S_G(A)} \det M(A)$

Vafa & Witten: NO spontaneous breaking of vector symmetries (e.g., baryon number)

but: explicit calculations in far CSC phase show breaking (Hong & Hsu; valid in $\mu \to \infty$, $T/\mu \to 0$)

$\Rightarrow$ SEVERE SIGN PROBLEM in all of CSC phase
Possible reasonings about severity of sign problem:

- analytic (crossover) or no phase transitions/boundaries
  ⇒ analyticity suggests severe/mild sign problem

A ↔ B transition?

- QCD with $N$ flavors $\mu_1, \ldots, \mu_N$: if $F \sim \mu_i + \mu_j^3 + \mu_k^5 + \ldots$
  then $F_N > F_{|N|} \Rightarrow$ severe sign problem (via $\rho(\theta)$)
  ($F_N > F_{|N|}$ also if models have different physics)

as before in phase B
So far: sign problem at \((\mu, T)\) SEVERE if

- \(Z^-/Z^+ > 0\) for \(V \to \infty\)
- generically if \(F^+ = F^-\)

Severe only if \(Z^-/Z^+ \approx 1\) for \(V \to \infty\)? \(\rightarrow\) phases A & B

But MILD for, e.g., \(Z^-/Z^+ < 0.1\) at \(V \to \infty\) \((Z^- \ll Z^+)?\)

\(\rightarrow\) possible (only) for \(F^+ = F^-\) (subleading terms in free energy)

- around high-T phase transition line from \((T_c, \mu = 0)\) to \(\mu > 0\)?

\(\rightarrow\) NO analyticity arguments from now on, but split \(Z^+, Z^-\) useful
Good agreement at $\mu < 1.3T_c$ between:
- derivatives (Taylor) at $\mu = 0$
- Taylor exp. from imaginary $\mu$
- multi-parameter reweighting

Also: $\langle \text{sign} \rangle > 10\%$ in this region → MILD in new definition

Now: • argue: success of reweighting related to $Z_- \ll Z_+$
- suggest $Z_{\text{new}}$-method
(Multi-parameter) reweighting method

\[
\langle O \rangle(\mu, \beta) = \frac{\int DA \ e^{-S_G(\beta_0)} \det M(\mu_0) \ \frac{e^{-S_G(\beta)} \det M(\mu)}{e^{-S_G(\beta_0)} \det M(\mu_0)} \ O(A)}{\int DA \ e^{-S_G(\beta_0)} \det M(\mu_0) \ \frac{e^{-S_G(\beta)} \det M(\mu)}{e^{-S_G(\beta_0)} \det M(\mu_0)}}
\]

Difficulties for reweighting if \( Z_- / Z_+ \approx 1 \) at target point \((\mu, \beta)\):

- denominator \textit{should} be small \( \sim (Z_+ - Z_-) / (Z_+ + Z_-) \) in a \textit{true typical} ensemble for target \((\mu, \beta)\)

  \[\rightarrow \text{sign problem: numerical uncertainties (also in numerator)}\]

  - even if denominator small and uncertainties under control:
    ensemble typical for \textit{target} \((\mu, \beta)\) ???

  - if (somehow) only small uncertainties due to denominator:
    Is there good overlap between \((\mu_0, \beta_0)\) and target \((\mu, \beta)\) ?

  \[\rightarrow \text{overlap problem more generally: typicality for } C\text{-measure at all?}\]

- \( Z_- \ll Z_+ \) seems \textit{necessary} for reweighting to work, not \textit{sufficient}
\( Z_{\text{new}} \) method

MC method for whose success \( Z_- \ll Z_+ \) is also sufficient: Use

\[
Z_{\text{new}} \equiv Z_+ + Z_- = \sum_+ |\text{Re} \det M| e^{-S_G} + \sum_- |\text{Re} \det M| e^{-S_G}
\]

\[
= \int D A \, |\text{Re} \det M(A)| \, e^{-S_G(A)}
\]

for sampling.

Remember: \( Z = Z_+ - Z_- \) (so: \( Z/Z_{\text{new}} \simeq 1 \) for \( F_- > F_+ \))

Compute observable averages \textit{WITH sign of real part}:

\[
\langle O \rangle = \frac{\int D A (\text{Re} \det M(A)) \, e^{-S_G(A)} \, O(A)}{\int D A (\text{Re} \det M(A)) \, e^{-S_G(A)}}
\]
Characteristics of $Z_{\text{new}}$ method

- if $Z_- / Z_+ |_{(\mu, \beta)} \approx 1 \Rightarrow$ small denominator: sign problem
  → just as (it should be, at least) in reweighting method

- samples via $Z_{\text{new}} = Z_+ + Z_-$ likely more typical of $Z$ than
  1. reweighting: relation $Z |_{(\mu_0, \beta_0)}$ vs. $Z |_{(\mu, \beta)}$
     Configurations sampled in $(\mu_0, \beta_0)$ typical of $(\mu, \beta)$ ???
  2. phase-quenched sampling: $|\det M|$ vs. $|\Re \det M|
     - different importance for configurations on circle
     - symmetric cropping
     - modulus AND phase

- $Z_{\text{new}}$ closest to $Z = \int DA (\det M(A)) e^{-S_G(A)} \rightarrow$ biggest overlap

- smallest possible fluctuations in reweighting factor
  (de Forcrand, Kim, Takaishi: hep-lat/0209126)
Consistency check during $Z_{\text{new}}$ method

- start at some $(\mu, \beta)$ where sign problem mild (e.g., $\mu = 0$)
- slowly move in phase diagram, sampling with $Z_{\text{new}}$
- at each point, compare $\{-\}$ set to $\{+\}$ set: approximation still ok?
- thus: “good” overlap; control when sign problem becomes severe
  → tells where/how long the $Z_{\text{new}}$ method can be trusted

- seems superior to (phase-)quenched or reweighting sampling
Computational cost

- probably need full computation of $\text{Re} \det M$ at each microstep:
  - cannot update whole lattice at once, since no bosonic integral for $\text{Re} \det M \rightarrow$ no Hybrid Monte Carlo
  - $\rightarrow$ only local link updates + Metropolis tests?

- $N \times N^3$ operations for one sweep through the lattice
  (HMC for phase-quenched/reweighting sampling: $N^{9/4}$ for new *decorrelated* configuration; but *full* $(\det M) \sim N^3$ there)

- maybe for small $\mu$: approximate methods to determine phase $e^{i\theta}$
  $\Rightarrow$ $\text{Re} \det M$ (by Taylor expansion)

- method to try after numerics in conventional reweighting ok? (... and still disagreement)
Conclusions & Questions

- split into two *independent* positive ensembles $Z = Z_+ - Z_-$
- analyticity reasoning for associated free energies
- examined regions of QCD phase diagram $\rightarrow$ severe sign problem
- degrees of severity of the sign problem
- “mild” sign problem around phase transition line?
- $Z_{\text{new}}$ method with $|\text{Re det } M|$ sampling

---

- Is there meaning to “typicality” if measure $\in \mathbb{C}$? Do existing sampling methods have “good” overlap with target ensemble?
- In how far do existing simulations rely on $V \ll \infty$? Big finite-volume effects? Artificial results?
- In regions with maximally severe $Z_- / Z_+ \rightarrow 1$: can any sampling method ever be successful (for $V \rightarrow \infty$)?

Thank you!